



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 07:27 AM EDT

PDB ID : 5KAI / pdb_00005kai
Title : NH3-bound RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 2.8 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 : 2.80 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

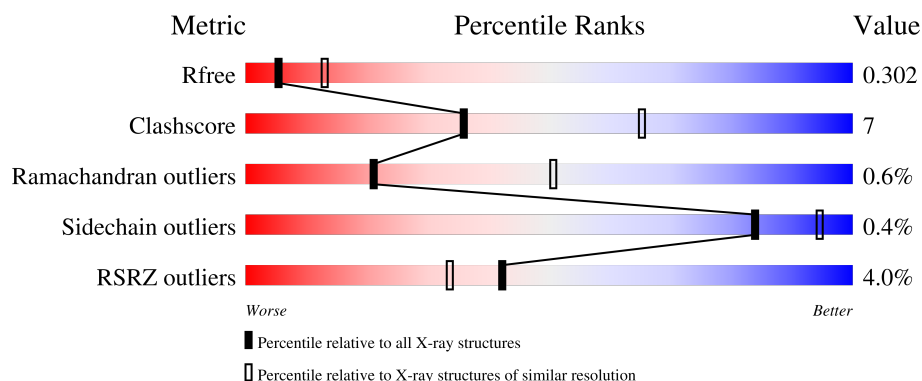
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	 85% 11% ..

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Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
1	a	344	
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	63	
7	h	63	
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	

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Mol	Chain	Length	Quality of chain
14	T	32	
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
31	BCT	A	615	-	X	-	-
31	BCT	a	706	-	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 50284 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
			2622	1717	431	459	15			
1	a	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	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
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	1	0
			3968	2605	661	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
			2716	1800	444	460	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
			661	432	107	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
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	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	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- 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
			260	173	38	48	1			
12	m	33	Total	C	N	O	S	0	0	0
			260	173	38	48	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
			1874	1170	317	383	4			
13	o	244	Total	C	N	O	S	0	0	0
			1874	1170	317	383	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	27	Total	C	N	O	S	0	0	0
			200	131	35	31	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
			281	188	45	48				
18	x	38	Total	C	N	O		0	0	0
			279	187	45	47				

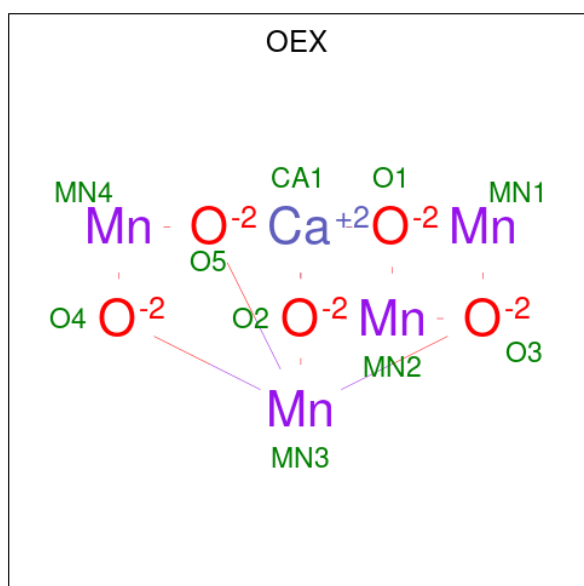
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			478	328	72	76	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
			270	183	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).

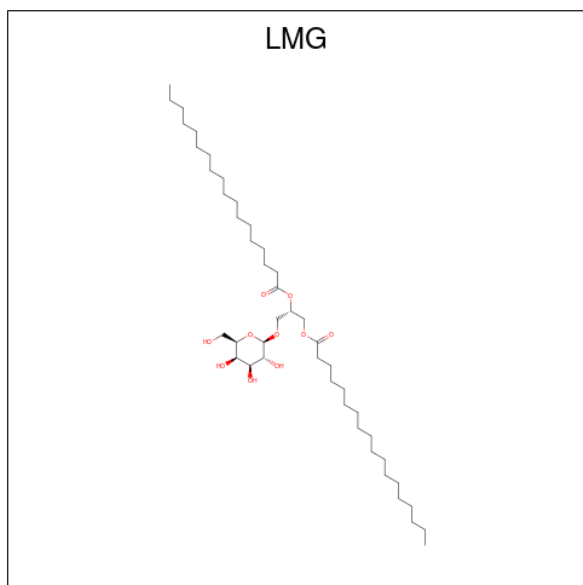
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

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

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	D	1	Total	C	O	0	0
			51	41	10		
23	M	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C	O	0	0
			51	41	10		

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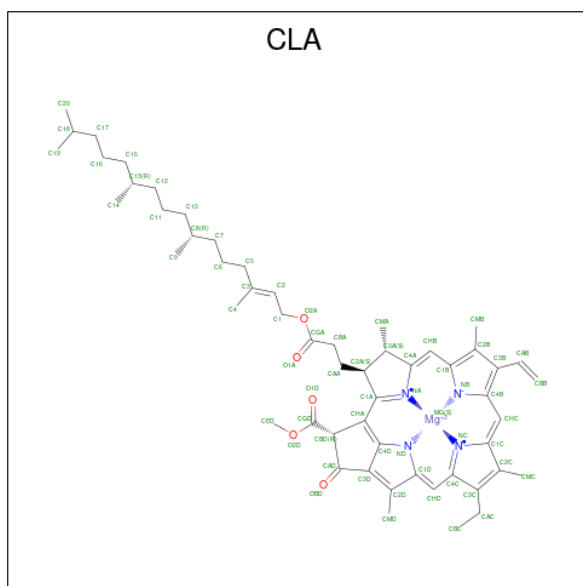
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	b	1	Total C O 51 41 10	0	0
23	b	1	Total C 9 9	0	0
23	c	1	Total C O 51 41 10	0	0
23	c	1	Total C O 51 41 10	0	0
23	d	1	Total C O 40 35 5	0	0
23	f	1	Total C O 51 41 10	0	0

- 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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	A	1	Total 54	C 44	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
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

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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	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	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	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 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 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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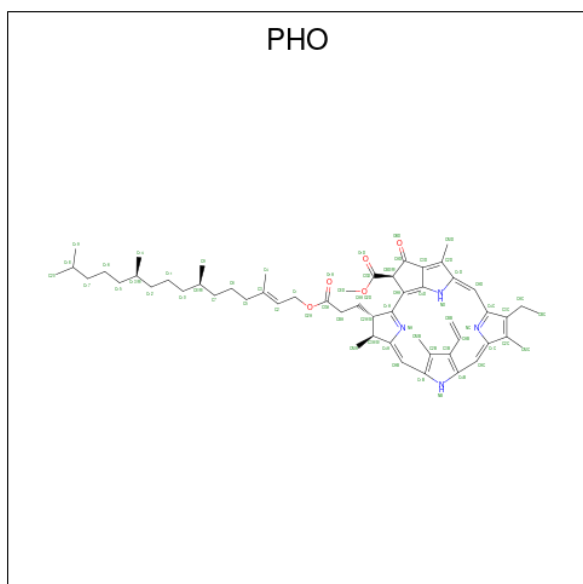
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 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 47	C 37	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 58	C 48	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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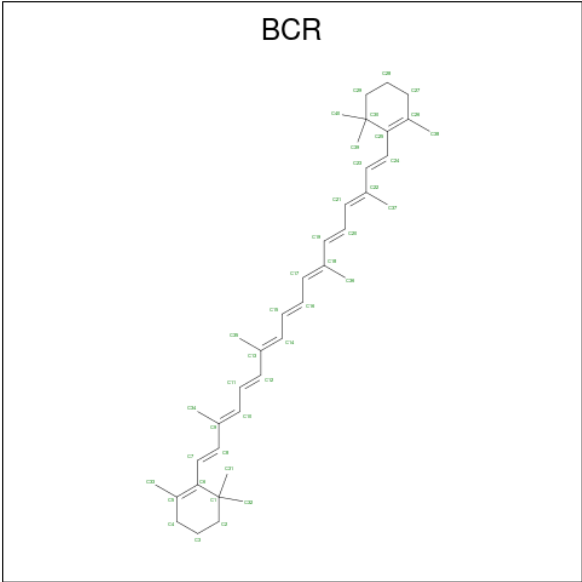
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



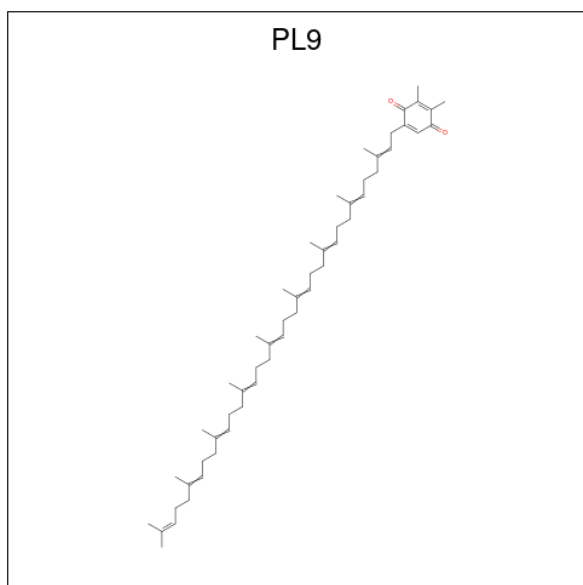
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	k	1	Total C 40 40	0	0
27	t	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: C₅₃H₈₀O₂).



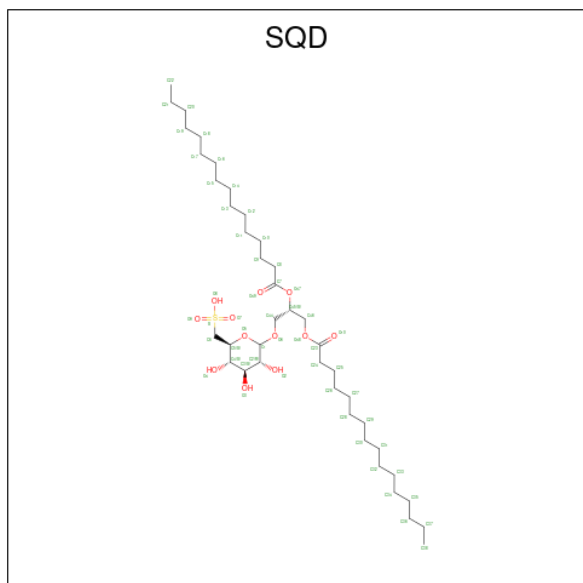
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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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		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).

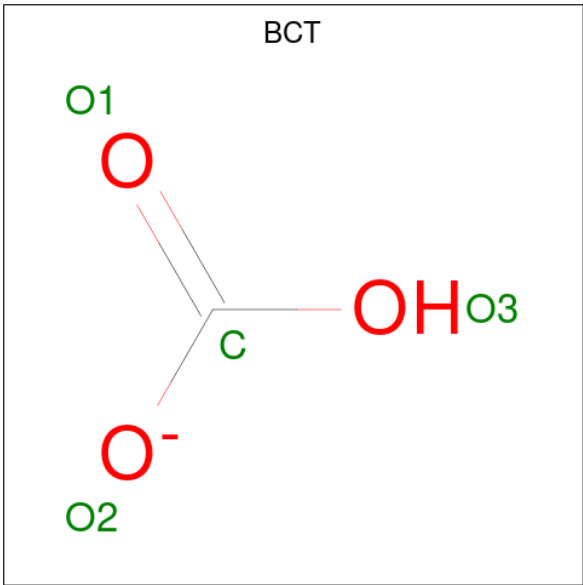


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O		0	0
			40	35	5			
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			43	30	12	1		
29	I	1	Total	C	O		0	0
			40	35	5			
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O	S	0	0
			54	41	12	1		
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

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

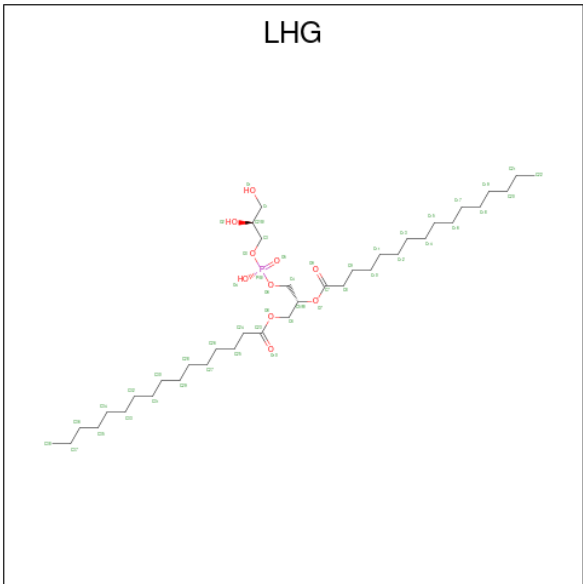
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C 7 7	0	0
30	B	3	Total C 29 29	0	0
30	H	1	Total C 8 8	0	0
30	I	1	Total C 9 9	0	0
30	M	2	Total C 22 22	0	0
30	a	3	Total C 24 24	0	0
30	b	4	Total C 48 48	0	0
30	d	1	Total C 22 22	0	0
30	i	1	Total C 22 22	0	0
30	j	1	Total C 9 9	0	0
30	m	2	Total C 17 17	0	0
30	t	2	Total C 15 15	0	0
30	z	1	Total C 11 11	0	0

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



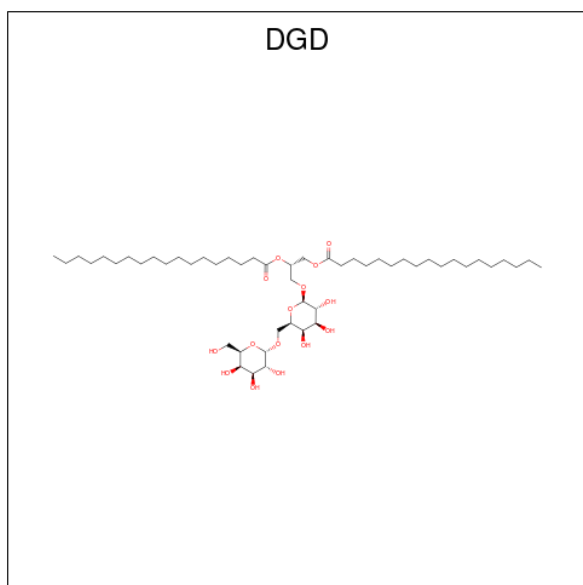
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	P	0	0
			49	38	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			49	38	10	1		
32	L	1	Total	C	O	P	0	0
			49	38	10	1		
32	a	1	Total	C	O	P	0	0
			39	28	10	1		
32	b	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		

- 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		
33	C	1	Total	C	O	0	0
			62	47	15		

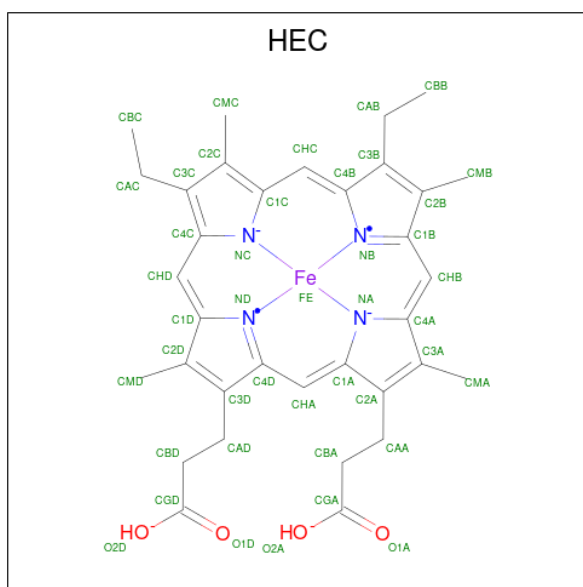
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total 62	C 47	O 15	0	0
33	H	1	Total 62	C 47	O 15	0	0
33	c	1	Total 62	C 47	O 15	0	0
33	c	1	Total 62	C 47	O 15	0	0
33	c	1	Total 62	C 47	O 15	0	0
33	h	1	Total 62	C 47	O 15	0	0

- # HEM

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

- 



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	14	Total	O		
			14	14	0	0
36	B	5	Total	O		
			5	5	0	0
36	C	2	Total	O		
			2	2	0	0
36	D	5	Total	O		
			5	5	0	0
36	H	1	Total	O		
			1	1	0	0
36	K	1	Total	O		
			1	1	0	0
36	L	1	Total	O		
			1	1	0	0
36	M	1	Total	O		
			1	1	0	0
36	O	9	Total	O		
			9	9	0	0
36	U	1	Total	O		
			1	1	0	0

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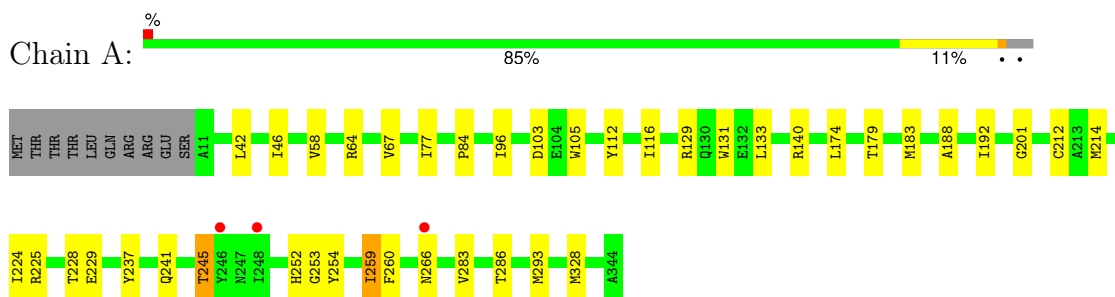
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	V	6	Total 6	O 6	0	0
36	a	13	Total 13	O 13	0	0
36	b	12	Total 12	O 12	0	0
36	c	8	Total 8	O 8	0	0
36	d	11	Total 11	O 11	0	0
36	e	1	Total 1	O 1	0	0
36	h	1	Total 1	O 1	0	0
36	l	1	Total 1	O 1	0	0
36	o	5	Total 5	O 5	0	0
36	u	5	Total 5	O 5	0	0
36	v	3	Total 3	O 3	0	0
36	z	1	Total 1	O 1	0	0

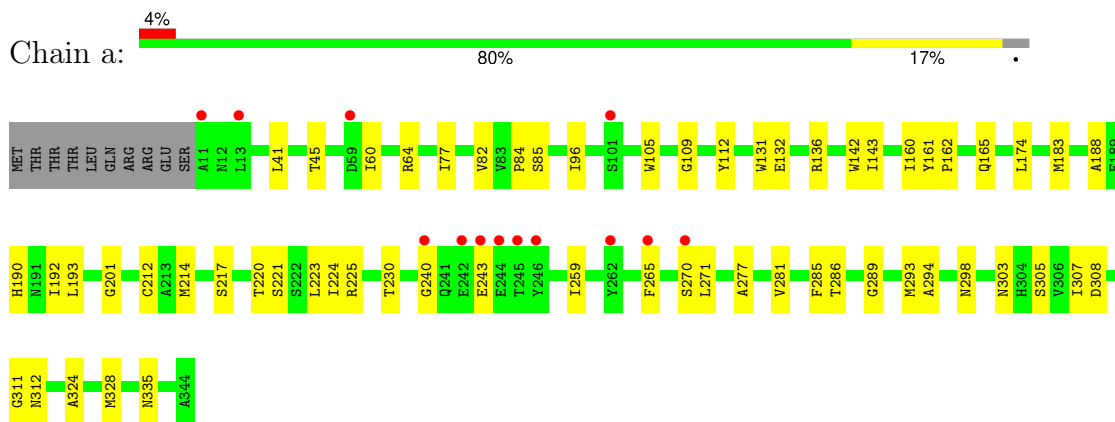
3 Residue-property plots [i](#)

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

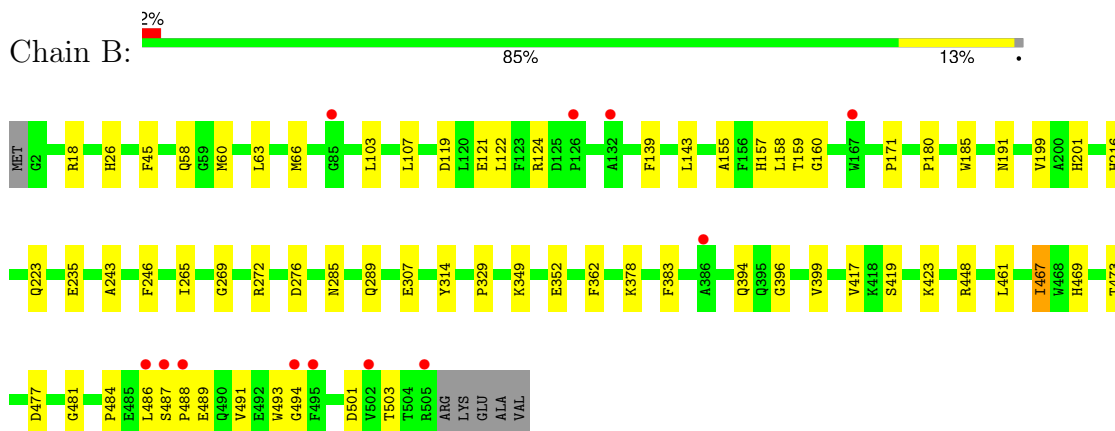
• Molecule 1: Photosystem II protein D1 1



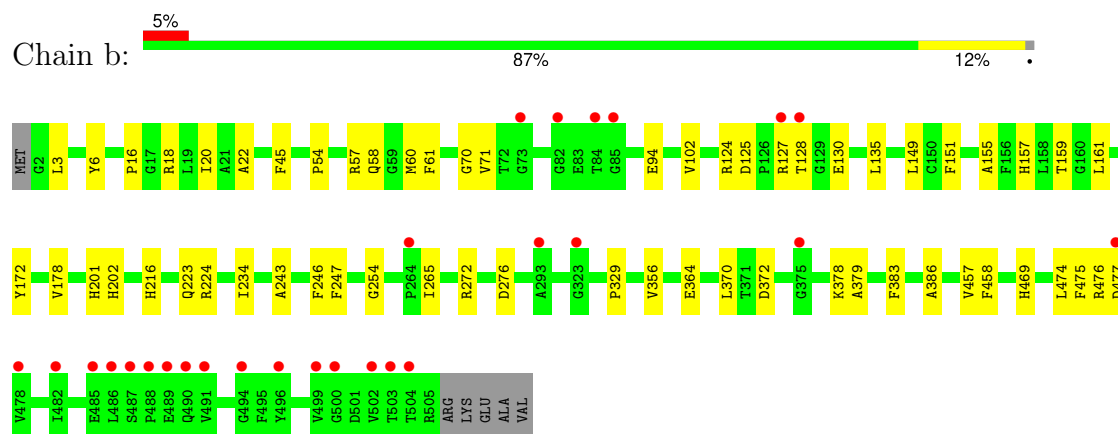
• Molecule 1: Photosystem II protein D1 1



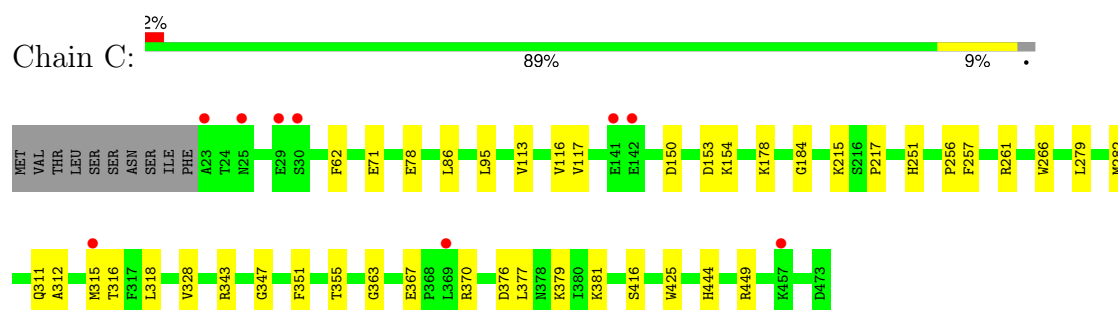
• Molecule 2: Photosystem II CP47 reaction center protein



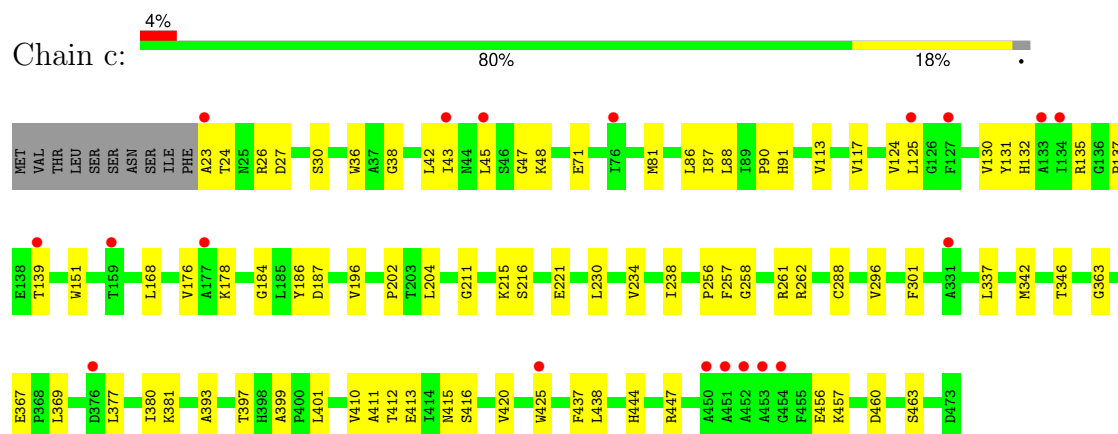
- Molecule 2: Photosystem II CP47 reaction center protein



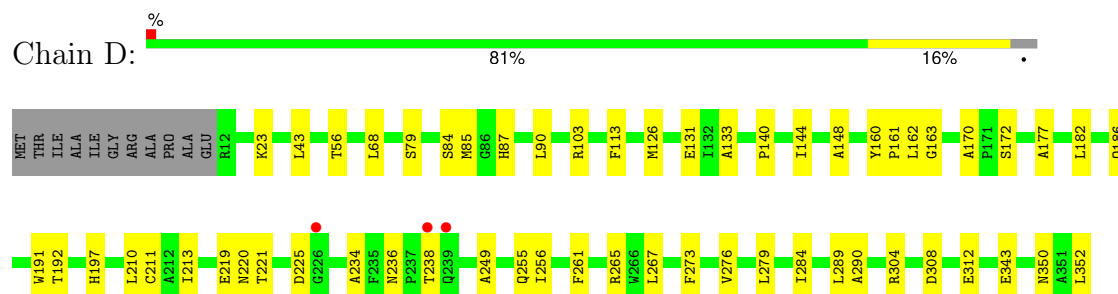
- Molecule 3: Photosystem II CP43 reaction center protein



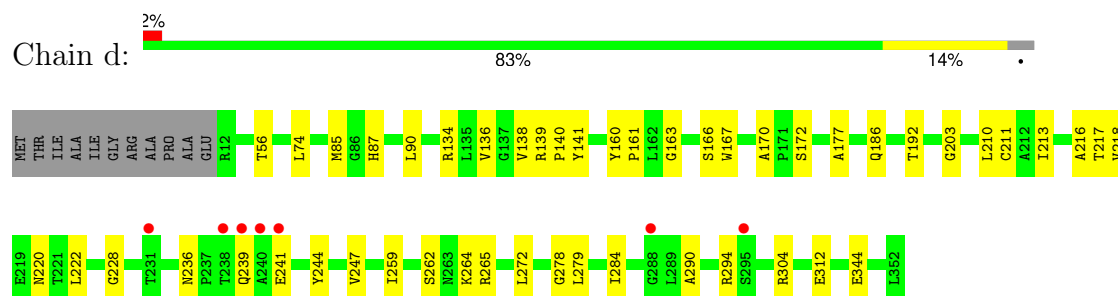
- Molecule 3: Photosystem II CP43 reaction center protein



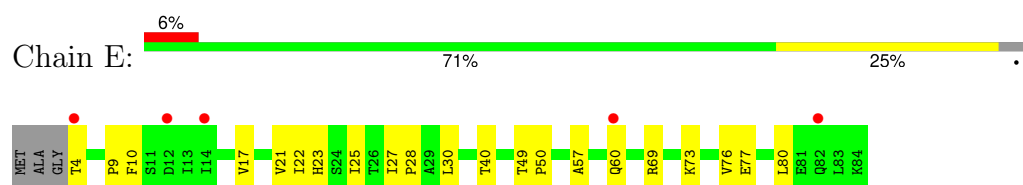
- Molecule 4: Photosystem II D2 protein



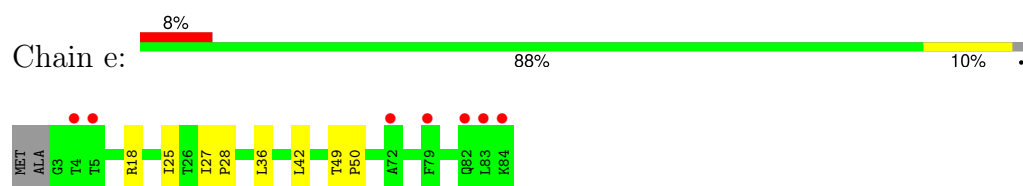
- Molecule 4: Photosystem II D2 protein



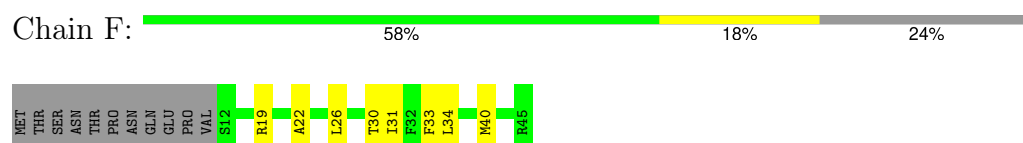
- Molecule 5: Cytochrome b559 subunit alpha



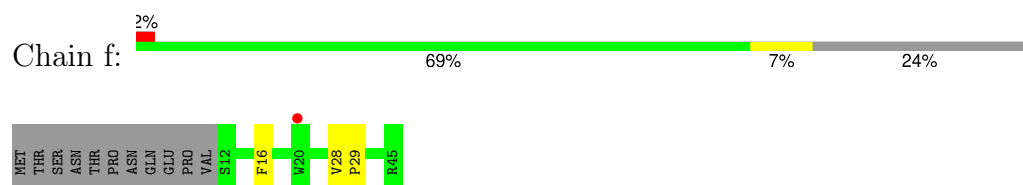
- Molecule 5: Cytochrome b559 subunit alpha



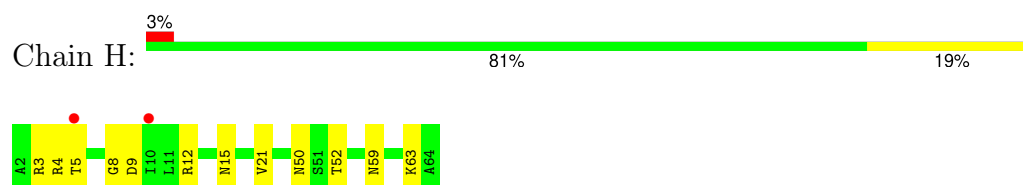
- Molecule 6: Cytochrome b559 subunit beta



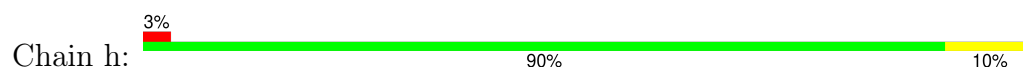
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H

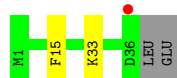
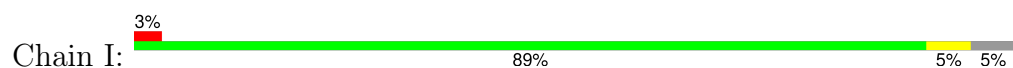


- Molecule 7: Photosystem II reaction center protein H

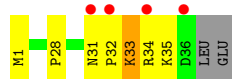
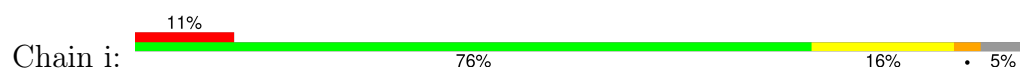




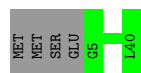
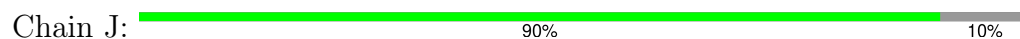
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



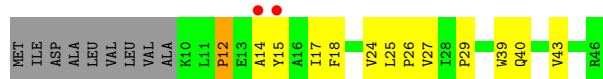
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L

Chain L:  86% 11% 3%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  92% 8% 3%



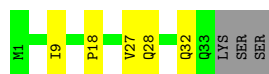
- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 14% 8% 3%



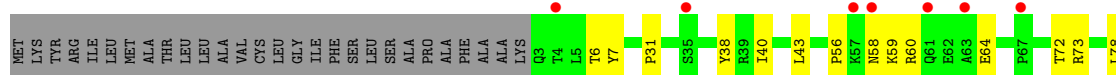
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 14% 8%



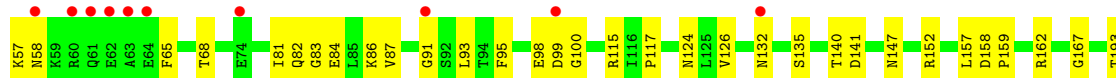
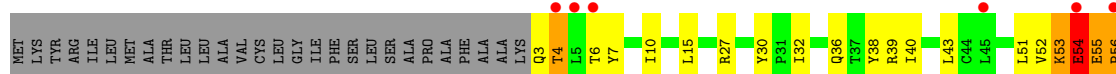
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  77% 12% 10% 4%



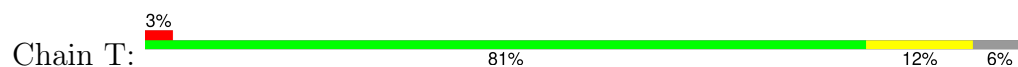
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  67% 21% 10% 6%

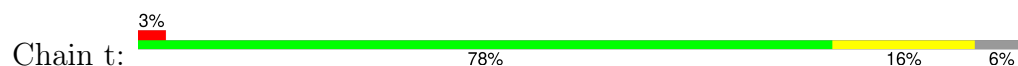




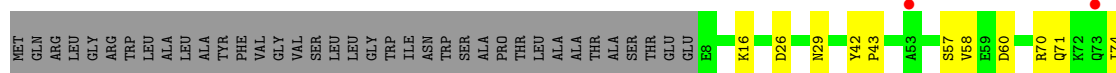
- Molecule 14: Photosystem II reaction center protein T



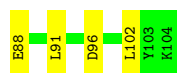
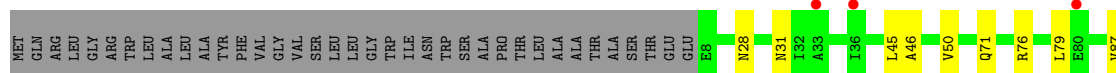
- Molecule 14: Photosystem II reaction center protein T



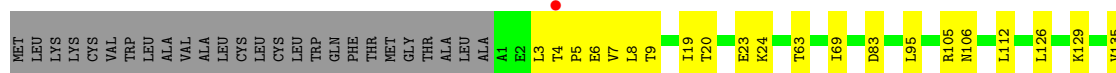
- Molecule 15: Photosystem II 12 kDa extrinsic protein



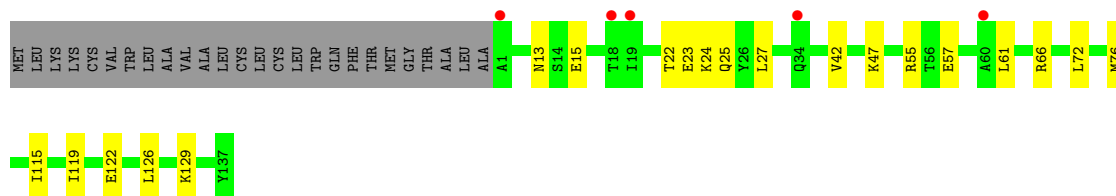
- Molecule 15: Photosystem II 12 kDa extrinsic protein



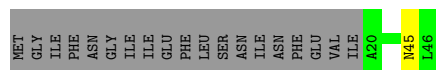
- Molecule 16: Cytochrome c-550



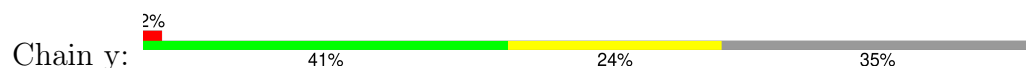
- Molecule 16: Cytochrome c-550



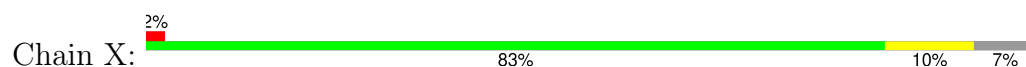
• Molecule 17: Photosystem II reaction center protein Ycf12



• Molecule 17: Photosystem II reaction center protein Ycf12



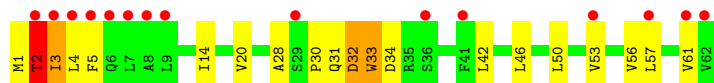
• Molecule 18: Photosystem II reaction center X protein



• Molecule 18: Photosystem II reaction center X protein

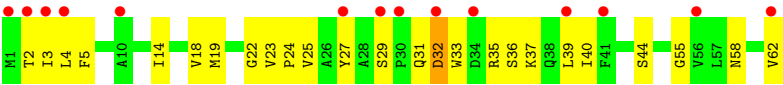


• Molecule 19: Photosystem II reaction center protein Z



• 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	117.91Å 224.27Å 331.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.57 – 2.80 43.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.57-2.80) 87.6 (43.57-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.81Å)	Xtriage
Refinement program	PHENIX dev_2411	Depositor
R, R_{free}	0.250 , 0.300 0.253 , 0.302	Depositor DCC
R_{free} test set	1792 reflections (0.83%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50284	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.13	0/2707	0.30	0/3692
1	a	0.09	0/2707	0.28	0/3692
2	B	0.11	0/4109	0.29	0/5600
2	b	0.11	0/4111	0.27	0/5603
3	C	0.09	0/3599	0.25	0/4900
3	c	0.15	0/3599	0.32	0/4900
4	D	0.10	0/2811	0.27	0/3830
4	d	0.09	0/2811	0.27	0/3830
5	E	0.18	0/680	0.34	0/928
5	e	0.21	0/684	0.29	0/933
6	F	0.11	0/284	0.28	0/387
6	f	0.08	0/284	0.24	0/387
7	H	0.18	0/511	0.34	0/697
7	h	0.11	0/511	0.25	0/697
8	I	0.16	0/293	0.34	0/396
8	i	0.51	1/293 (0.3%)	0.47	0/396
9	J	0.08	0/263	0.23	0/356
9	j	0.10	0/263	0.25	0/356
10	K	0.18	0/303	0.52	0/416
10	k	0.34	0/303	0.38	0/416
11	L	0.17	0/311	0.38	0/422
11	l	0.09	0/311	0.26	0/422
12	M	0.09	0/253	0.25	0/346
12	m	0.14	0/253	0.29	0/346
13	O	0.12	0/1905	0.30	0/2583
13	o	0.18	0/1905	0.46	2/2583 (0.1%)
14	T	0.10	0/257	0.27	0/349
14	t	0.09	0/257	0.24	0/349
15	U	0.11	0/785	0.31	0/1064
15	u	0.22	0/785	0.35	0/1064
16	V	0.13	0/1085	0.27	0/1473
16	v	0.12	0/1085	0.28	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.11	0/201	0.35	0/268
17	y	0.20	0/225	0.40	0/301
18	X	0.11	0/284	0.26	0/384
18	x	0.10	0/282	0.28	0/381
19	Z	0.28	0/490	0.57	2/669 (0.3%)
19	z	0.24	0/489	0.46	0/669
20	R	0.17	0/279	0.44	0/383
20	r	0.19	0/276	0.44	0/379
All	All	0.14	1/42844 (0.0%)	0.31	4/58320 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	33	LYS	CB-CG	-5.42	1.36	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	54	GLU	CA-C-N	7.99	136.08	121.70
13	o	54	GLU	C-N-CA	7.99	136.08	121.70
19	Z	2	THR	CA-C-N	5.79	132.12	121.70
19	Z	2	THR	C-N-CA	5.79	132.12	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	4	THR	Peptide

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	2622	0	2519	39	0
1	a	2622	0	2519	48	0
2	B	3969	0	3828	53	0
2	b	3968	0	3829	50	0
3	C	3486	0	3407	31	0
3	c	3486	0	3407	59	0
4	D	2716	0	2621	44	0
4	d	2716	0	2621	43	0
5	E	661	0	648	23	0
5	e	665	0	651	7	0
6	F	275	0	282	9	0
6	f	275	0	282	2	0
7	H	498	0	518	13	0
7	h	498	0	518	6	0
8	I	296	0	311	2	0
8	i	296	0	311	5	0
9	J	257	0	268	0	0
9	j	257	0	268	4	0
10	K	293	0	305	5	0
10	k	293	0	305	9	0
11	L	304	0	316	5	0
11	l	304	0	316	3	0
12	M	260	0	275	4	0
12	m	260	0	275	4	0
13	O	1874	0	1846	25	0
13	o	1874	0	1846	46	0
14	T	258	0	261	3	0
14	t	258	0	261	5	0
15	U	774	0	773	10	0
15	u	774	0	773	9	0
16	V	1064	0	1073	16	0
16	v	1064	0	1073	18	0
17	Y	200	0	226	1	0
17	y	224	0	252	8	0
18	X	281	0	312	4	0
18	x	279	0	307	7	0
19	Z	479	0	516	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	478	0	516	28	0
20	R	273	0	305	13	0
20	r	270	0	296	12	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	51	0	72	3	0
23	B	51	0	72	1	0
23	C	153	0	216	1	0
23	D	51	0	72	3	0
23	M	51	0	72	3	0
23	a	102	0	144	3	0
23	b	111	0	158	3	0
23	c	102	0	144	2	0
23	d	40	0	61	2	0
23	f	51	0	72	2	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	184	0	192	4	0
25	B	1040	0	1152	32	0
25	C	845	0	936	23	0
25	D	195	0	216	6	0
25	a	260	0	288	13	0
25	b	1022	0	1115	31	0
25	c	838	0	919	25	0
25	d	130	0	144	8	0
26	A	64	0	74	1	0
26	D	64	0	74	2	0
26	a	128	0	148	8	0
27	A	40	0	56	4	0
27	B	120	0	168	5	0
27	C	80	0	112	5	0
27	D	40	0	56	4	0
27	H	40	0	56	3	0
27	K	40	0	56	0	0
27	Y	40	0	56	0	0
27	a	40	0	56	2	0
27	b	160	0	224	11	0
27	c	80	0	112	1	0
27	d	40	0	56	0	0
27	h	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	k	80	0	112	6	0
27	t	40	0	56	6	0
28	A	55	0	80	5	0
28	D	55	0	80	2	0
28	a	55	0	80	4	0
28	d	55	0	80	0	0
29	A	92	0	138	3	0
29	B	101	0	135	7	0
29	D	43	0	53	4	0
29	I	40	0	67	3	0
29	a	54	0	78	1	0
29	b	54	0	77	3	0
29	f	41	0	49	1	0
30	A	7	0	0	0	0
30	B	29	0	0	0	0
30	H	8	0	0	0	0
30	I	9	0	0	0	0
30	M	22	0	0	0	0
30	a	24	0	0	0	0
30	b	48	0	0	0	0
30	d	22	0	0	0	0
30	i	22	0	0	0	0
30	j	9	0	0	0	0
30	m	17	0	0	0	0
30	t	15	0	0	0	0
30	z	11	0	0	0	0
31	A	4	0	0	0	0
31	a	4	0	0	1	0
32	B	49	0	74	2	0
32	D	98	0	148	7	0
32	E	49	0	74	3	0
32	L	49	0	74	4	0
32	a	39	0	51	1	0
32	b	49	0	74	1	0
32	d	98	0	148	6	0
32	e	42	0	57	2	0
33	C	186	0	246	5	0
33	H	62	0	82	0	0
33	c	186	0	246	4	0
33	h	62	0	82	3	0
34	E	43	0	30	3	0
34	e	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	V	43	0	30	1	0
35	v	43	0	30	0	0
36	A	14	0	0	0	0
36	B	5	0	0	0	0
36	C	2	0	0	0	0
36	D	5	0	0	0	0
36	H	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	O	9	0	0	2	0
36	U	1	0	0	0	0
36	V	6	0	0	1	0
36	a	13	0	0	2	0
36	b	12	0	0	0	0
36	c	8	0	0	0	0
36	d	11	0	0	1	0
36	e	1	0	0	0	0
36	h	1	0	0	0	0
36	l	1	0	0	0	0
36	o	5	0	0	0	0
36	u	5	0	0	0	0
36	v	3	0	0	0	0
36	z	1	0	0	0	0
All	All	50284	0	51202	742	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 7.

The worst 5 of 742 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)
7:H:4:ARG:NH2	7:H:9:ASP:OD2	1.66	1.23
13:o:54:GLU:HA	13:o:55:GLU:HB2	1.42	1.02
3:c:38:GLY:HA3	25:c:511:CLA:HMD2	1.52	0.91
1:A:225:ARG:HD3	2:B:484:PRO:HD3	1.58	0.83
13:o:55:GLU:OE1	13:o:56:PRO:HD3	1.79	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	324 (98%)	7 (2%)	1 (0%)	36	66
1	a	332/344 (96%)	325 (98%)	6 (2%)	1 (0%)	36	66
2	B	502/510 (98%)	482 (96%)	19 (4%)	1 (0%)	43	72
2	b	503/510 (99%)	484 (96%)	19 (4%)	0	100	100
3	C	449/461 (97%)	431 (96%)	17 (4%)	1 (0%)	43	72
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	30	60
4	D	339/352 (96%)	325 (96%)	14 (4%)	0	100	100
4	d	339/352 (96%)	323 (95%)	16 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
7	h	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
8	I	34/38 (90%)	29 (85%)	5 (15%)	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%)	32 (94%)	1 (3%)	1 (3%)	3	13
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	3	13
10	k	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	3	13
11	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	3	11
12	m	31/36 (86%)	29 (94%)	1 (3%)	1 (3%)	3	11
13	O	242/272 (89%)	230 (95%)	10 (4%)	2 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	223 (92%)	15 (6%)	4 (2%)	7	25
14	T	28/32 (88%)	28 (100%)	0	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%)	88 (93%)	7 (7%)	0	100	100
16	V	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	36/41 (88%)	32 (89%)	3 (8%)	1 (3%)	4	14
19	Z	60/62 (97%)	51 (85%)	1 (2%)	8 (13%)	0	0
19	z	60/62 (97%)	53 (88%)	4 (7%)	3 (5%)	1	5
20	R	32/41 (78%)	29 (91%)	3 (9%)	0	100	100
20	r	32/41 (78%)	30 (94%)	1 (3%)	1 (3%)	3	12
All	All	5237/5694 (92%)	4987 (95%)	220 (4%)	30 (1%)	21	51

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	Z	30	PRO
19	Z	31	GLN
19	Z	33	TRP
19	Z	61	VAL
3	c	24	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	268 (99%)	2 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	270/280 (96%)	269 (100%)	1 (0%)	84	94
2	B	402/407 (99%)	398 (99%)	4 (1%)	68	88
2	b	402/407 (99%)	402 (100%)	0	100	100
3	C	352/362 (97%)	352 (100%)	0	100	100
3	c	352/362 (97%)	350 (99%)	2 (1%)	78	92
4	D	276/283 (98%)	276 (100%)	0	100	100
4	d	276/283 (98%)	275 (100%)	1 (0%)	84	94
5	E	72/73 (99%)	72 (100%)	0	100	100
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	53/53 (100%)	53 (100%)	0	100	100
7	h	53/53 (100%)	53 (100%)	0	100	100
8	I	32/34 (94%)	32 (100%)	0	100	100
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	35/35 (100%)	34 (97%)	1 (3%)	37	73
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	207/228 (91%)	207 (100%)	0	100	100
13	o	207/228 (91%)	205 (99%)	2 (1%)	68	88
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%)	116 (99%)	1 (1%)	70	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	20/37 (54%)	20 (100%)	0	100	100
17	y	23/37 (62%)	22 (96%)	1 (4%)	26	60
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	30/34 (88%)	30 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	50	81
19	z	52/52 (100%)	52 (100%)	0	100	100
20	R	29/33 (88%)	29 (100%)	0	100	100
20	r	28/33 (85%)	27 (96%)	1 (4%)	31	66
All	All	4339/4650 (93%)	4322 (100%)	17 (0%)	84	94

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	v	66	ARG
20	r	9	LEU
19	Z	1	MET
1	a	270	SER
3	c	346	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	335	ASN
3	c	322	GLN
2	b	216	HIS
2	b	331	ASN
4	d	239	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.98	0	8,9,11	1.15	1 (12%)
8	FME	i	1	8	8,9,10	0.97	0	8,9,11	1.10	1 (12%)
8	FME	I	1	8	8,9,10	0.99	0	8,9,11	1.19	0
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	1.03	0
14	FME	t	1	14	8,9,10	0.97	0	8,9,11	1.03	0
12	FME	M	1	12	8,9,10	0.94	0	8,9,11	1.00	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
14	FME	T	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	M	1	12	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	CB-CA-N	2.25	114.62	110.52
8	i	1	FME	CB-CA-N	2.06	114.27	110.52

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	CB-CA-N-CN
14	T	1	FME	O-C-CA-CB
8	i	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
12	M	1	FME	N-CA-CB-CG
14	T	1	FME	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	t	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 180 ligands modelled in this entry, 6 are monoatomic and 23 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	$\# Z > 2$
25	CLA	b	614	2	69,73,73	1.12	6 (8%)	82,113,113	1.17	6 (7%)
25	CLA	C	504	3	69,73,73	1.14	6 (8%)	82,113,113	1.24	5 (6%)
25	CLA	d	403	4	69,73,73	1.12	5 (7%)	82,113,113	1.19	8 (9%)
25	CLA	C	512	3	69,73,73	1.14	5 (7%)	82,113,113	1.24	6 (7%)
26	PHO	D	401	-	58,69,69	2.17	9 (15%)	55,99,99	1.45	7 (12%)
29	SQD	D	410	-	41,43,54	1.07	3 (7%)	51,54,65	1.57	10 (19%)
25	CLA	c	513	3	69,73,73	1.12	5 (7%)	82,113,113	1.23	9 (10%)
27	BCR	b	602	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	7 (12%)
25	CLA	B	613	2	69,73,73	1.13	7 (10%)	82,113,113	1.23	7 (8%)
33	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.41	9 (11%)
23	LMG	b	627	-	51,51,55	0.77	0	59,59,63	1.27	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCT	a	706	22	3,3,3	3.22	1 (33%)	2,3,3	2.78	2 (100%)
27	BCR	k	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.14	2 (3%)
33	DGD	c	517	-	63,63,67	0.95	4 (6%)	77,77,81	1.40	9 (11%)
28	PL9	a	713	-	55,55,55	0.96	4 (7%)	68,69,69	1.49	12 (17%)
34	HEM	e	102	5,6	50,50,50	1.51	8 (16%)	67,82,82	1.24	5 (7%)
25	CLA	c	504	36	62,66,73	1.19	8 (12%)	73,104,113	1.25	7 (9%)
23	LMG	b	626	-	51,51,55	0.80	3 (5%)	59,59,63	1.54	9 (15%)
25	CLA	C	513	3	69,73,73	1.13	6 (8%)	82,113,113	1.28	5 (6%)
25	CLA	C	503	3	69,73,73	1.13	6 (8%)	82,113,113	1.20	6 (7%)
29	SQD	A	612	-	50,52,54	0.97	3 (6%)	60,63,65	1.61	12 (20%)
32	LHG	E	101	-	48,48,48	0.68	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	D	404	4	69,73,73	1.13	6 (8%)	82,113,113	1.18	5 (6%)
25	CLA	B	603	2	69,73,73	1.13	6 (8%)	82,113,113	1.16	6 (7%)
27	BCR	a	712	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	6 (10%)
25	CLA	B	602	36	69,73,73	1.13	7 (10%)	82,113,113	1.21	5 (6%)
25	CLA	b	621	2	69,73,73	1.13	6 (8%)	82,113,113	1.24	6 (7%)
25	CLA	c	506	3	69,73,73	1.12	5 (7%)	82,113,113	1.15	5 (6%)
25	CLA	c	508	3	69,73,73	1.13	5 (7%)	82,113,113	1.19	6 (7%)
25	CLA	b	619	2	69,73,73	1.13	6 (8%)	82,113,113	1.25	7 (8%)
25	CLA	b	615	2	69,73,73	1.13	7 (10%)	82,113,113	1.20	6 (7%)
27	BCR	B	620	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	5 (8%)
25	CLA	c	511	3	69,73,73	1.14	7 (10%)	82,113,113	1.22	5 (6%)
25	CLA	b	609	2	69,73,73	1.13	6 (8%)	82,113,113	1.10	5 (6%)
27	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	8 (14%)
25	CLA	a	708	36	69,73,73	1.13	7 (10%)	82,113,113	1.17	6 (7%)
21	OEX	a	702	3,1,36	0,14,14	-	-	-	-	-
25	CLA	B	608	36	69,73,73	1.13	6 (8%)	82,113,113	1.13	5 (6%)
32	LHG	b	629	-	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
33	DGD	H	103	-	63,63,67	0.87	1 (1%)	77,77,81	1.34	7 (9%)
25	CLA	a	711	1	69,73,73	1.13	6 (8%)	82,113,113	1.17	6 (7%)
28	PL9	d	405	-	55,55,55	0.94	4 (7%)	68,69,69	1.49	13 (19%)
25	CLA	B	610	2	69,73,73	1.15	6 (8%)	82,113,113	1.19	6 (7%)
27	BCR	H	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	7 (12%)
23	LMG	a	701	-	51,51,55	0.79	0	59,59,63	1.33	7 (11%)
25	CLA	b	611	2	69,73,73	1.13	6 (8%)	82,113,113	1.17	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
27	BCR	C	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	8 (14%)
28	PL9	D	406	-	55,55,55	0.97	4 (7%)	68,69,69	1.50	12 (17%)
23	LMG	B	621	-	51,51,55	0.73	0	59,59,63	1.37	8 (13%)
23	LMG	b	628	-	8,8,55	0.14	0	7,7,63	0.93	0
23	LMG	A	603	-	51,51,55	0.94	3 (5%)	59,59,63	1.41	8 (13%)
26	PHO	A	608	-	58,69,69	2.19	9 (15%)	55,99,99	1.44	7 (12%)
32	LHG	L	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
23	LMG	C	520	-	51,51,55	0.74	1 (1%)	59,59,63	1.31	5 (8%)
27	BCR	k	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	6 (10%)
25	CLA	B	611	36	69,73,73	1.13	6 (8%)	82,113,113	1.19	6 (7%)
25	CLA	B	612	2	69,73,73	1.13	6 (8%)	82,113,113	1.23	7 (8%)
27	BCR	C	516	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
25	CLA	B	609	2	69,73,73	1.12	6 (8%)	82,113,113	1.12	6 (7%)
23	LMG	C	501	-	51,51,55	0.73	1 (1%)	59,59,63	1.32	5 (8%)
27	BCR	b	623	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	7 (12%)
25	CLA	B	614	2	69,73,73	1.14	6 (8%)	82,113,113	1.21	5 (6%)
29	SQD	f	102	-	39,41,54	1.09	3 (7%)	49,52,65	1.50	9 (18%)
25	CLA	a	707	1	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
31	BCT	A	615	22	3,3,3	3.24	1 (33%)	2,3,3	2.73	2 (100%)
23	LMG	f	101	-	51,51,55	0.71	1 (1%)	59,59,63	1.36	7 (11%)
35	HEC	v	201	16	50,50,50	1.56	8 (16%)	68,82,82	1.48	9 (13%)
25	CLA	C	509	3	69,73,73	1.12	6 (8%)	82,113,113	1.22	7 (8%)
25	CLA	A	607	36	69,73,73	1.14	6 (8%)	82,113,113	1.19	7 (8%)
23	LMG	D	409	-	51,51,55	0.72	1 (1%)	59,59,63	1.30	5 (8%)
27	BCR	t	103	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	5 (8%)
28	PL9	A	611	-	55,55,55	1.01	4 (7%)	68,69,69	1.49	13 (19%)
27	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)
25	CLA	C	508	36	69,73,73	1.14	6 (8%)	82,113,113	1.26	4 (4%)
25	CLA	b	616	36	69,73,73	1.14	7 (10%)	82,113,113	1.15	4 (4%)
25	CLA	b	618	2	69,73,73	1.13	6 (8%)	82,113,113	1.22	5 (6%)
25	CLA	c	505	3	69,73,73	1.13	7 (10%)	82,113,113	1.12	4 (4%)
26	PHO	a	710	-	58,69,69	2.17	9 (15%)	55,99,99	1.43	6 (10%)
27	BCR	D	405	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	7 (12%)
25	CLA	B	604	2	69,73,73	1.12	6 (8%)	82,113,113	1.16	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	b	625	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	8 (14%)
29	SQD	A	614	-	39,39,54	0.89	2 (5%)	41,41,65	1.21	3 (7%)
25	CLA	C	510	3	69,73,73	1.14	6 (8%)	82,113,113	1.20	4 (4%)
25	CLA	b	622	2	51,55,73	1.29	7 (13%)	60,91,113	1.33	6 (10%)
33	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.40	11 (14%)
33	DGD	h	102	-	63,63,67	0.88	1 (1%)	77,77,81	1.29	7 (9%)
23	LMG	a	715	-	51,51,55	0.75	0	59,59,63	1.32	6 (10%)
25	CLA	C	514	3	69,73,73	1.12	5 (7%)	82,113,113	1.22	8 (9%)
21	OEX	A	601	3,1,36	0,14,14	-	-	-		
25	CLA	B	607	2	69,73,73	1.14	7 (10%)	82,113,113	1.19	4 (4%)
25	CLA	c	503	3	69,73,73	1.14	6 (8%)	82,113,113	1.24	6 (7%)
23	LMG	c	520	-	51,51,55	0.82	1 (1%)	59,59,63	1.36	5 (8%)
23	LMG	M	101	-	51,51,55	0.74	0	59,59,63	1.33	5 (8%)
27	BCR	Y	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.17	5 (8%)
32	LHG	d	406	-	48,48,48	0.62	2 (4%)	51,54,54	1.30	7 (13%)
25	CLA	c	501	3	69,73,73	1.13	7 (10%)	82,113,113	1.19	6 (7%)
27	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	6 (10%)
25	CLA	b	608	2	69,73,73	1.13	6 (8%)	82,113,113	1.10	5 (6%)
27	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	7 (12%)
25	CLA	c	509	3	69,73,73	1.14	5 (7%)	82,113,113	1.24	6 (7%)
29	SQD	I	102	-	39,39,54	0.87	2 (5%)	41,41,65	1.23	2 (4%)
25	CLA	c	502	3	69,73,73	1.12	7 (10%)	82,113,113	1.21	5 (6%)
33	DGD	C	518	-	63,63,67	0.92	4 (6%)	77,77,81	1.43	10 (12%)
25	CLA	C	505	36	69,73,73	1.12	5 (7%)	82,113,113	1.16	7 (8%)
27	BCR	b	624	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
32	LHG	D	407	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
34	HEM	E	102	5,6	50,50,50	1.50	8 (16%)	67,82,82	1.14	6 (8%)
27	BCR	d	404	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	8 (14%)
25	CLA	C	502	3	69,73,73	1.13	7 (10%)	82,113,113	1.20	6 (7%)
25	CLA	A	609	1	58,62,73	1.23	6 (10%)	68,99,113	1.25	6 (8%)
25	CLA	C	507	3	69,73,73	1.14	7 (10%)	82,113,113	1.14	5 (6%)
25	CLA	c	510	3	69,73,73	1.13	6 (8%)	82,113,113	1.20	6 (7%)
27	BCR	A	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
27	BCR	h	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	7 (12%)
32	LHG	D	408	-	48,48,48	0.61	0	51,54,54	1.27	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	1.41	9 (11%)
33	DGD	c	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	10 (12%)
25	CLA	B	606	2	69,73,73	1.13	7 (10%)	82,113,113	1.14	4 (4%)
23	LMG	d	408	-	39,39,55	0.54	1 (2%)	41,41,63	1.30	4 (9%)
25	CLA	b	610	2	69,73,73	1.14	5 (7%)	82,113,113	1.31	7 (8%)
25	CLA	b	620	2	69,73,73	1.13	5 (7%)	82,113,113	1.13	6 (7%)
29	SQD	B	626	-	52,54,54	0.95	3 (5%)	62,65,65	1.64	9 (14%)
25	CLA	a	719	36	69,73,73	1.13	7 (10%)	82,113,113	1.15	7 (8%)
35	HEC	V	201	16	50,50,50	1.56	8 (16%)	68,82,82	1.46	10 (14%)
25	CLA	B	605	2	69,73,73	1.14	7 (10%)	82,113,113	1.33	7 (8%)
29	SQD	b	601	-	52,54,54	0.94	3 (5%)	62,65,65	1.63	10 (16%)
25	CLA	c	507	36	69,73,73	1.14	5 (7%)	82,113,113	1.24	4 (4%)
26	PHO	a	709	-	58,69,69	2.18	9 (15%)	55,99,99	1.41	7 (12%)
25	CLA	b	617	2	69,73,73	1.12	7 (10%)	82,113,113	1.24	7 (8%)
25	CLA	C	511	3	69,73,73	1.13	6 (8%)	82,113,113	1.21	6 (7%)
25	CLA	A	606	1	69,73,73	1.13	6 (8%)	82,113,113	1.11	6 (7%)
25	CLA	b	612	2	69,73,73	1.13	6 (8%)	82,113,113	1.17	7 (8%)
32	LHG	d	407	-	48,48,48	0.63	1 (2%)	51,54,54	1.27	7 (13%)
23	LMG	c	519	-	51,51,55	0.71	0	59,59,63	1.32	5 (8%)
25	CLA	C	506	3	69,73,73	1.13	7 (10%)	82,113,113	1.18	5 (6%)
25	CLA	c	512	3	69,73,73	1.12	6 (8%)	82,113,113	1.23	6 (7%)
32	LHG	B	625	-	48,48,48	0.64	2 (4%)	51,54,54	1.30	6 (11%)
32	LHG	a	720	-	38,38,48	0.69	0	41,44,54	1.20	3 (7%)
25	CLA	B	617	2	69,73,73	1.13	7 (10%)	82,113,113	1.21	7 (8%)
29	SQD	B	623	-	45,47,54	1.01	2 (4%)	55,58,65	1.77	13 (23%)
25	CLA	D	402	36	69,73,73	1.12	6 (8%)	82,113,113	1.17	6 (7%)
25	CLA	B	615	2	69,73,73	1.13	6 (8%)	82,113,113	1.18	6 (7%)
25	CLA	D	403	4	69,73,73	1.14	6 (8%)	82,113,113	1.13	5 (6%)
32	LHG	e	101	-	41,41,48	0.69	2 (4%)	44,47,54	1.34	7 (15%)
25	CLA	d	402	4	69,73,73	1.13	6 (8%)	82,113,113	1.14	5 (6%)
25	CLA	b	607	36	69,73,73	1.13	7 (10%)	82,113,113	1.24	6 (7%)
25	CLA	B	616	2	69,73,73	1.15	6 (8%)	82,113,113	1.23	4 (4%)
25	CLA	b	613	36	69,73,73	1.13	6 (8%)	82,113,113	1.11	7 (8%)
29	SQD	a	714	-	52,54,54	0.95	3 (5%)	62,65,65	1.57	12 (19%)
23	LMG	C	521	-	51,51,55	0.79	1 (1%)	59,59,63	1.36	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	614	2	-	3/39/115/115	-
25	CLA	C	504	3	-	11/39/115/115	-
25	CLA	d	403	4	-	8/39/115/115	-
25	CLA	C	512	3	-	14/39/115/115	-
26	PHO	D	401	-	-	6/37/103/103	0/5/6/6
29	SQD	D	410	-	-	16/38/58/69	0/1/1/1
25	CLA	c	513	3	-	17/39/115/115	-
27	BCR	b	602	-	-	6/29/63/63	0/2/2/2
25	CLA	B	613	2	-	8/39/115/115	-
33	DGD	C	517	-	-	18/51/91/95	0/2/2/2
23	LMG	b	627	-	-	19/46/66/70	0/1/1/1
27	BCR	k	101	-	-	6/29/63/63	0/2/2/2
33	DGD	c	517	-	-	19/51/91/95	0/2/2/2
28	PL9	a	713	-	-	13/53/73/73	0/1/1/1
34	HEM	e	102	5,6	-	7/14/54/54	-
25	CLA	c	504	36	-	4/31/107/115	-
23	LMG	b	626	-	-	16/46/66/70	0/1/1/1
25	CLA	C	513	3	-	10/39/115/115	-
25	CLA	C	503	3	-	18/39/115/115	-
29	SQD	A	612	-	-	17/47/67/69	0/1/1/1
32	LHG	E	101	-	-	26/53/53/53	-
25	CLA	D	404	4	-	16/39/115/115	-
25	CLA	B	603	2	-	8/39/115/115	-
27	BCR	a	712	-	-	4/29/63/63	0/2/2/2
25	CLA	B	602	36	-	14/39/115/115	-
25	CLA	b	621	2	-	9/39/115/115	-
25	CLA	c	506	3	-	12/39/115/115	-
25	CLA	c	508	3	-	10/39/115/115	-
25	CLA	b	619	2	-	10/39/115/115	-
25	CLA	b	615	2	-	12/39/115/115	-
27	BCR	B	620	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	511	3	-	7/39/115/115	-
25	CLA	b	609	2	-	14/39/115/115	-
27	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	CLA	a	708	36	-	7/39/115/115	-
25	CLA	B	608	36	-	8/39/115/115	-
32	LHG	b	629	-	-	18/53/53/53	-
33	DGD	H	103	-	-	10/51/91/95	0/2/2/2
25	CLA	a	711	1	-	13/39/115/115	-
28	PL9	d	405	-	-	7/53/73/73	0/1/1/1
25	CLA	B	610	2	-	12/39/115/115	-
27	BCR	H	102	-	-	5/29/63/63	0/2/2/2
23	LMG	a	701	-	-	25/46/66/70	0/1/1/1
25	CLA	b	611	2	-	12/39/115/115	-
27	BCR	K	101	-	-	3/29/63/63	0/2/2/2
27	BCR	C	515	-	-	1/29/63/63	0/2/2/2
28	PL9	D	406	-	-	9/53/73/73	0/1/1/1
23	LMG	B	621	-	-	19/46/66/70	0/1/1/1
23	LMG	b	628	-	-	3/6/6/70	-
23	LMG	A	603	-	-	24/46/66/70	0/1/1/1
26	PHO	A	608	-	-	9/37/103/103	0/5/6/6
32	LHG	L	101	-	-	17/53/53/53	-
23	LMG	C	520	-	-	25/46/66/70	0/1/1/1
27	BCR	k	102	-	-	3/29/63/63	0/2/2/2
25	CLA	B	611	36	-	12/39/115/115	-
25	CLA	B	612	2	-	5/39/115/115	-
27	BCR	C	516	-	-	4/29/63/63	0/2/2/2
25	CLA	B	609	2	-	11/39/115/115	-
23	LMG	C	501	-	-	22/46/66/70	0/1/1/1
27	BCR	b	623	-	-	3/29/63/63	0/2/2/2
25	CLA	B	614	2	-	8/39/115/115	-
29	SQD	f	102	-	-	13/36/56/69	0/1/1/1
25	CLA	a	707	1	-	6/39/115/115	-
35	HEC	v	201	16	1/1/3/7	4/14/54/54	-
23	LMG	f	101	-	-	16/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	509	3	-	5/39/115/115	-
25	CLA	A	607	36	-	8/39/115/115	-
23	LMG	D	409	-	-	19/46/66/70	0/1/1/1
27	BCR	t	103	-	-	8/29/63/63	0/2/2/2
28	PL9	A	611	-	-	8/53/73/73	0/1/1/1
27	BCR	c	515	-	-	5/29/63/63	0/2/2/2
25	CLA	C	508	36	-	11/39/115/115	-
25	CLA	b	616	36	-	6/39/115/115	-
25	CLA	b	618	2	-	11/39/115/115	-
25	CLA	c	505	3	-	8/39/115/115	-
26	PHO	a	710	-	-	7/37/103/103	0/5/6/6
27	BCR	D	405	-	-	8/29/63/63	0/2/2/2
25	CLA	B	604	2	-	17/39/115/115	-
27	BCR	b	625	-	-	7/29/63/63	0/2/2/2
29	SQD	A	614	-	-	21/41/41/69	-
25	CLA	C	510	3	-	17/39/115/115	-
25	CLA	b	622	2	-	2/18/94/115	-
33	DGD	c	518	-	-	11/51/91/95	0/2/2/2
33	DGD	h	102	-	-	16/51/91/95	0/2/2/2
23	LMG	a	715	-	-	25/46/66/70	0/1/1/1
25	CLA	C	514	3	-	5/39/115/115	-
25	CLA	B	607	2	-	16/39/115/115	-
25	CLA	c	503	3	-	8/39/115/115	-
23	LMG	c	520	-	-	16/46/66/70	0/1/1/1
23	LMG	M	101	-	-	13/46/66/70	0/1/1/1
27	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
32	LHG	d	406	-	-	17/53/53/53	-
25	CLA	c	501	3	-	9/39/115/115	-
27	BCR	B	619	-	-	5/29/63/63	0/2/2/2
25	CLA	b	608	2	-	6/39/115/115	-
27	BCR	c	514	-	-	5/29/63/63	0/2/2/2
25	CLA	c	509	3	-	4/39/115/115	-
29	SQD	I	102	-	-	25/41/41/69	-
25	CLA	c	502	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	C	518	-	-	23/51/91/95	0/2/2/2
25	CLA	C	505	36	-	12/39/115/115	-
27	BCR	b	624	-	-	7/29/63/63	0/2/2/2
32	LHG	D	407	-	-	17/53/53/53	-
34	HEM	E	102	5,6	-	4/14/54/54	-
27	BCR	d	404	-	-	7/29/63/63	0/2/2/2
25	CLA	C	502	3	-	12/39/115/115	-
25	CLA	A	609	1	-	2/26/102/115	-
25	CLA	C	507	3	-	14/39/115/115	-
25	CLA	c	510	3	-	16/39/115/115	-
27	BCR	A	610	-	-	3/29/63/63	0/2/2/2
27	BCR	h	101	-	-	6/29/63/63	0/2/2/2
32	LHG	D	408	-	-	23/53/53/53	-
33	DGD	C	519	-	-	16/51/91/95	0/2/2/2
33	DGD	c	516	-	-	16/51/91/95	0/2/2/2
25	CLA	B	606	2	-	16/39/115/115	-
23	LMG	d	408	-	-	19/41/41/70	-
25	CLA	b	610	2	-	9/39/115/115	-
25	CLA	b	620	2	-	11/39/115/115	-
29	SQD	B	626	-	-	23/49/69/69	0/1/1/1
35	HEC	V	201	16	1/1/3/7	6/14/54/54	-
25	CLA	a	719	36	-	8/39/115/115	-
25	CLA	B	605	2	-	12/39/115/115	-
29	SQD	b	601	-	-	25/49/69/69	0/1/1/1
25	CLA	c	507	36	-	9/39/115/115	-
26	PHO	a	709	-	-	5/37/103/103	0/5/6/6
25	CLA	b	617	2	-	11/39/115/115	-
25	CLA	C	511	3	-	11/39/115/115	-
25	CLA	A	606	1	-	1/39/115/115	-
25	CLA	b	612	2	-	8/39/115/115	-
32	LHG	d	407	-	-	13/53/53/53	-
23	LMG	c	519	-	-	22/46/66/70	0/1/1/1
25	CLA	C	506	3	-	7/39/115/115	-
25	CLA	c	512	3	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	B	625	-	-	19/53/53/53	-
32	LHG	a	720	-	-	18/43/43/53	-
25	CLA	B	617	2	-	12/39/115/115	-
29	SQD	B	623	-	-	25/42/62/69	0/1/1/1
25	CLA	D	402	36	-	4/39/115/115	-
25	CLA	B	615	2	-	16/39/115/115	-
25	CLA	D	403	4	-	12/39/115/115	-
32	LHG	e	101	-	-	22/46/46/53	-
25	CLA	d	402	4	-	10/39/115/115	-
25	CLA	b	607	36	-	15/39/115/115	-
25	CLA	B	616	2	-	13/39/115/115	-
25	CLA	b	613	36	-	8/39/115/115	-
29	SQD	a	714	-	-	17/49/69/69	0/1/1/1
23	LMG	C	521	-	-	18/46/66/70	0/1/1/1

The worst 5 of 630 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	C1B-C2B	9.71	1.50	1.39
26	a	709	PHO	C1B-C2B	9.68	1.50	1.39
26	a	710	PHO	C1B-C2B	9.68	1.50	1.39
26	D	401	PHO	C1B-C2B	9.65	1.50	1.39
26	A	608	PHO	C3B-C4B	8.73	1.50	1.41

The worst 5 of 957 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	605	CLA	C4A-NA-C1A	6.58	109.68	106.68
25	b	610	CLA	C4A-NA-C1A	6.37	109.58	106.68
25	C	508	CLA	C4A-NA-C1A	6.33	109.57	106.68
25	C	513	CLA	C4A-NA-C1A	6.26	109.53	106.68
25	b	619	CLA	C4A-NA-C1A	6.18	109.50	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 1703 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	621	LMG	C2-C1-O1-C7
23	B	621	LMG	O6-C1-O1-C7
23	C	521	LMG	O6-C1-O1-C7
23	c	520	LMG	O6-C1-O1-C7
23	d	408	LMG	C11-C10-O7-C8

There are no ring outliers.

129 monomers are involved in 262 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	614	CLA	2	0
25	C	504	CLA	2	0
25	d	403	CLA	2	0
25	C	512	CLA	2	0
26	D	401	PHO	2	0
29	D	410	SQD	4	0
25	c	513	CLA	3	0
27	b	602	BCR	4	0
25	B	613	CLA	2	0
33	C	517	DGD	2	0
23	b	627	LMG	3	0
31	a	706	BCT	1	0
27	k	101	BCR	3	0
28	a	713	PL9	4	0
34	e	102	HEM	3	0
25	c	504	CLA	1	0
29	A	612	SQD	2	0
32	E	101	LHG	3	0
25	D	404	CLA	1	0
25	B	603	CLA	1	0
27	a	712	BCR	2	0
25	B	602	CLA	2	0
25	b	621	CLA	1	0
25	c	506	CLA	3	0
25	c	508	CLA	3	0
25	b	619	CLA	1	0
25	b	615	CLA	3	0
27	B	620	BCR	1	0
25	c	511	CLA	4	0
25	b	609	CLA	2	0
27	B	618	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	708	CLA	1	0
25	B	608	CLA	1	0
32	b	629	LHG	1	0
25	a	711	CLA	6	0
25	B	610	CLA	4	0
27	H	102	BCR	3	0
23	a	701	LMG	1	0
25	b	611	CLA	1	0
27	C	515	BCR	2	0
28	D	406	PL9	2	0
23	B	621	LMG	1	0
23	A	603	LMG	3	0
26	A	608	PHO	1	0
32	L	101	LHG	4	0
23	C	520	LMG	1	0
27	k	102	BCR	3	0
25	B	611	CLA	1	0
25	B	612	CLA	3	0
27	C	516	BCR	3	0
25	B	609	CLA	1	0
27	b	623	BCR	1	0
25	B	614	CLA	1	0
29	f	102	SQD	1	0
25	a	707	CLA	4	0
23	f	101	LMG	2	0
25	C	509	CLA	6	0
25	A	607	CLA	2	0
23	D	409	LMG	3	0
27	t	103	BCR	6	0
28	A	611	PL9	5	0
27	c	515	BCR	1	0
25	b	616	CLA	1	0
25	b	618	CLA	1	0
25	c	505	CLA	3	0
26	a	710	PHO	6	0
27	D	405	BCR	4	0
25	B	604	CLA	3	0
27	b	625	BCR	4	0
29	A	614	SQD	1	0
33	c	518	DGD	1	0
33	h	102	DGD	3	0
23	a	715	LMG	2	0

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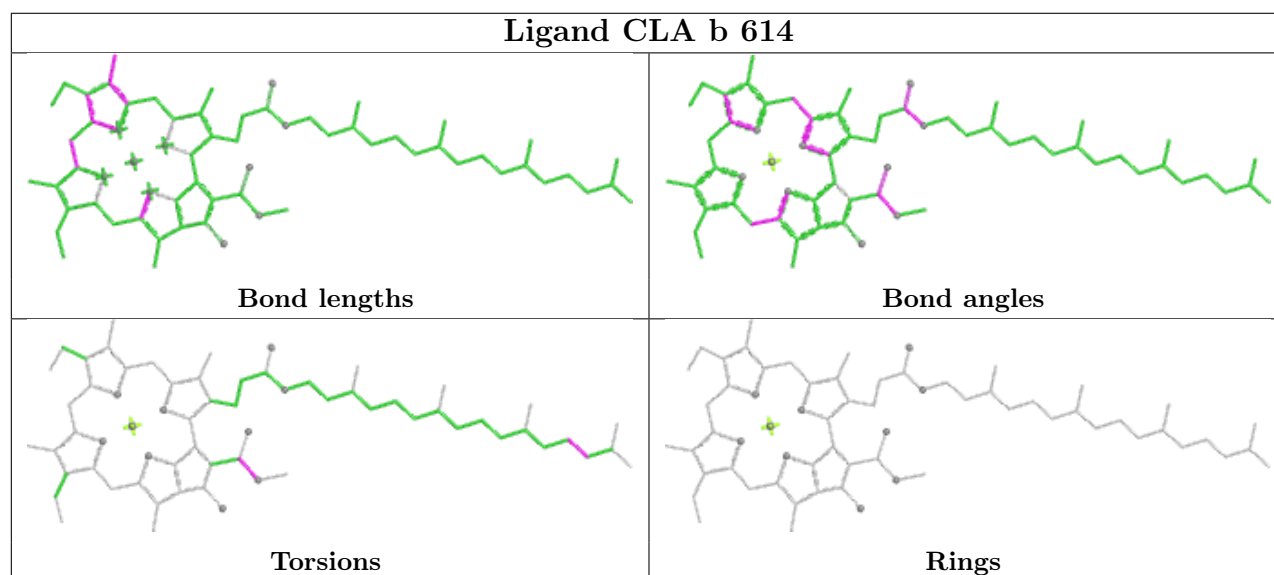
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	514	CLA	1	0
25	B	607	CLA	3	0
25	c	503	CLA	2	0
23	c	520	LMG	1	0
23	M	101	LMG	3	0
32	d	406	LHG	2	0
25	c	501	CLA	2	0
27	B	619	BCR	2	0
25	b	608	CLA	2	0
25	c	509	CLA	3	0
29	I	102	SQD	3	0
33	C	518	DGD	2	0
25	C	505	CLA	5	0
27	b	624	BCR	2	0
32	D	407	LHG	1	0
34	E	102	HEM	3	0
25	C	502	CLA	2	0
25	A	609	CLA	1	0
25	C	507	CLA	3	0
25	c	510	CLA	1	0
27	A	610	BCR	4	0
27	h	101	BCR	3	0
32	D	408	LHG	6	0
33	C	519	DGD	2	0
33	c	516	DGD	3	0
25	B	606	CLA	1	0
23	d	408	LMG	2	0
25	b	610	CLA	3	0
25	b	620	CLA	2	0
29	B	626	SQD	6	0
25	a	719	CLA	2	0
35	V	201	HEC	1	0
25	B	605	CLA	3	0
29	b	601	SQD	3	0
25	c	507	CLA	1	0
26	a	709	PHO	2	0
25	b	617	CLA	1	0
25	C	511	CLA	1	0
25	A	606	CLA	1	0
25	b	612	CLA	6	0
32	d	407	LHG	4	0
23	c	519	LMG	1	0

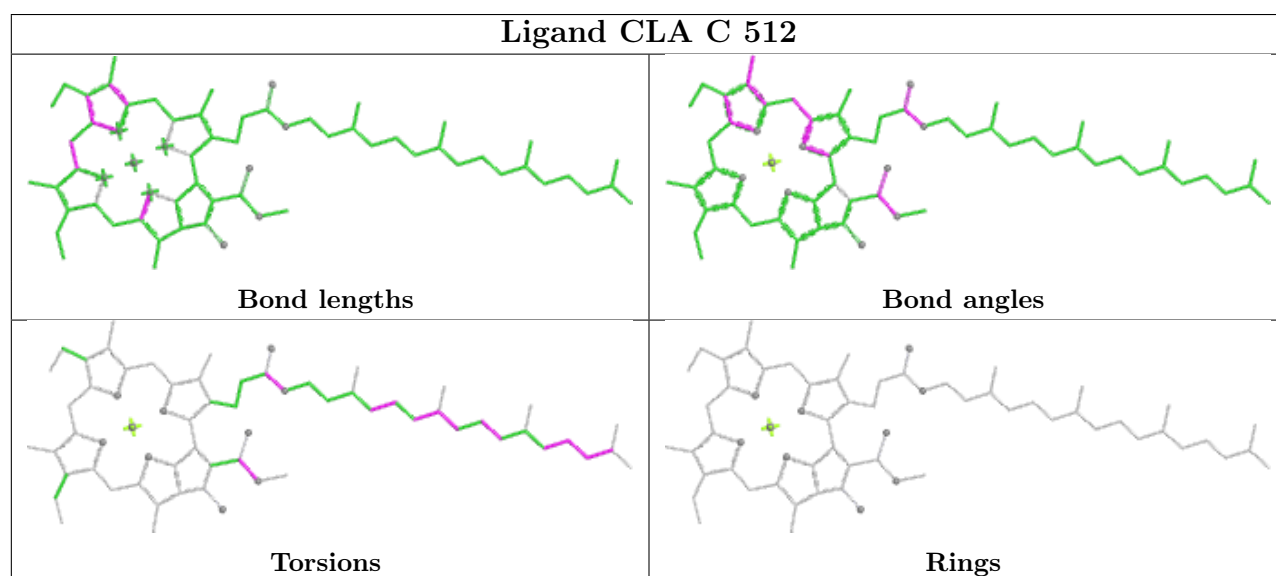
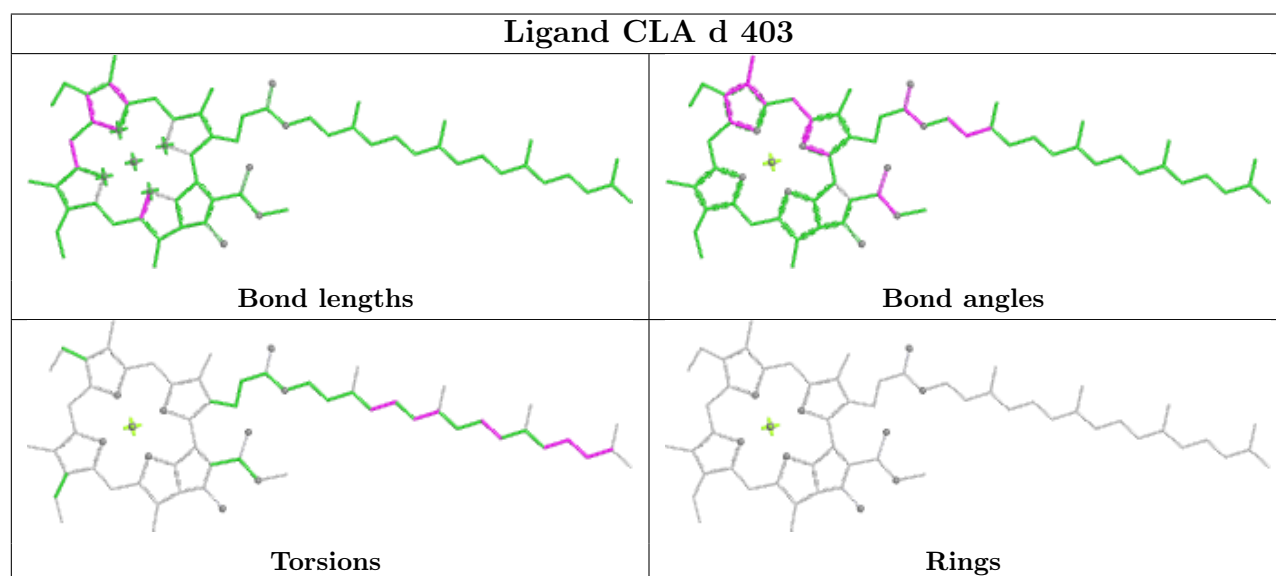
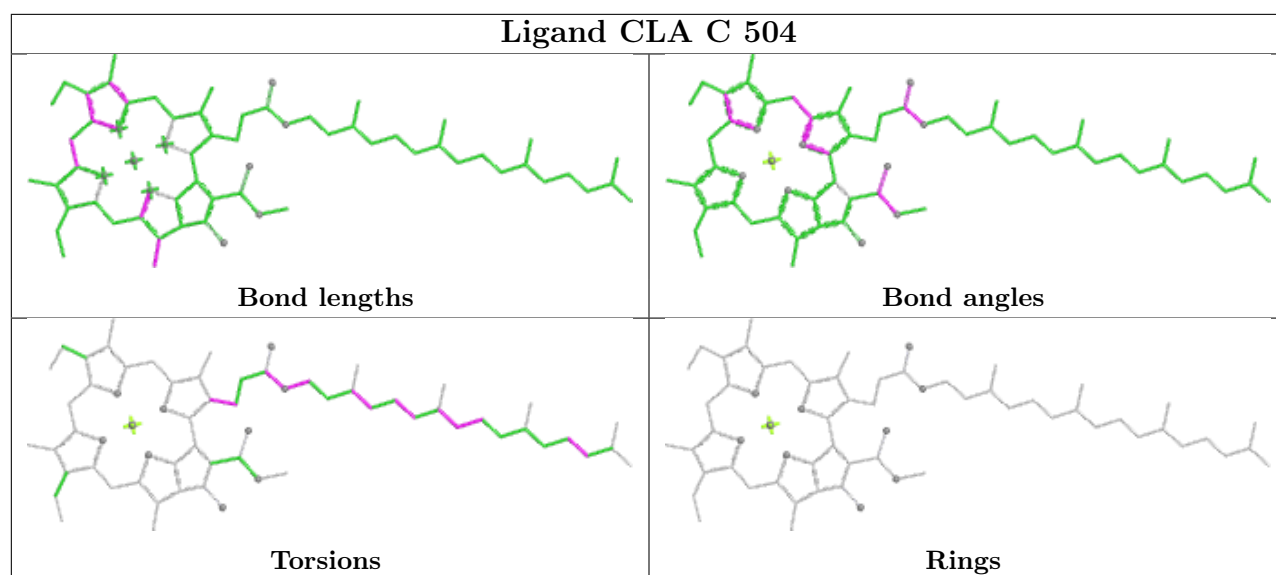
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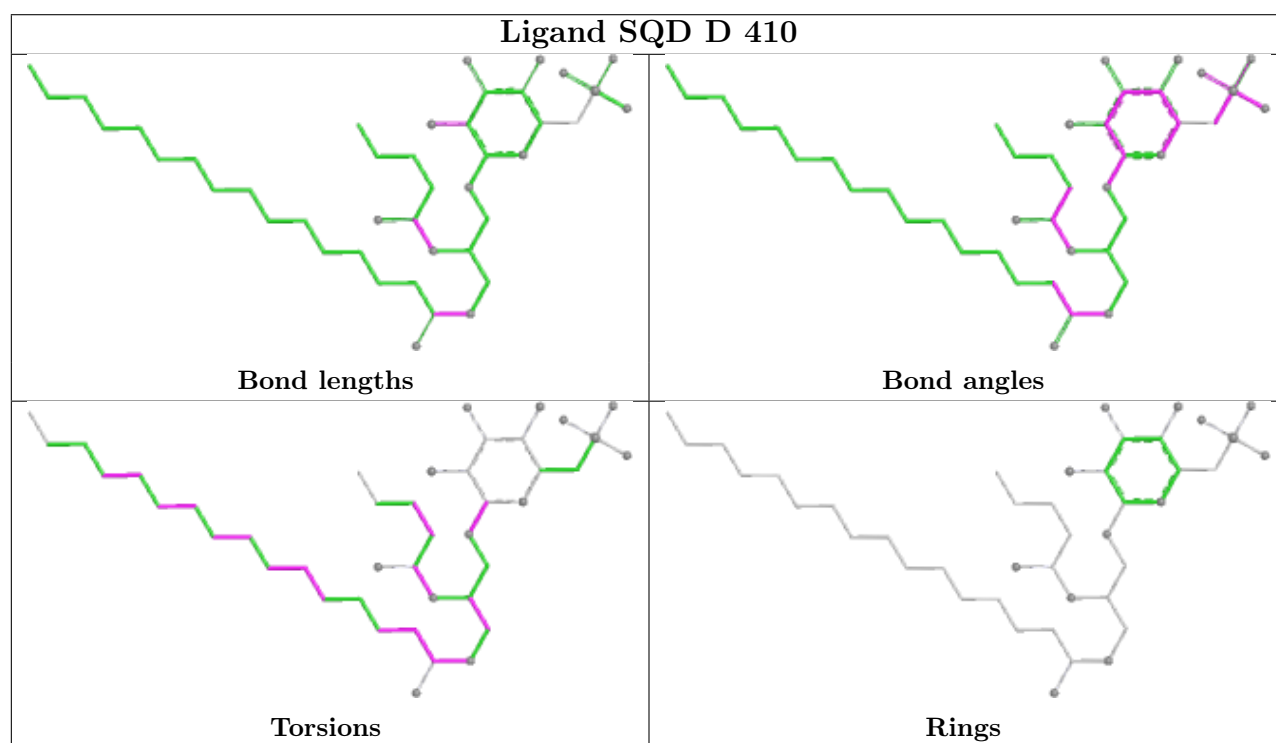
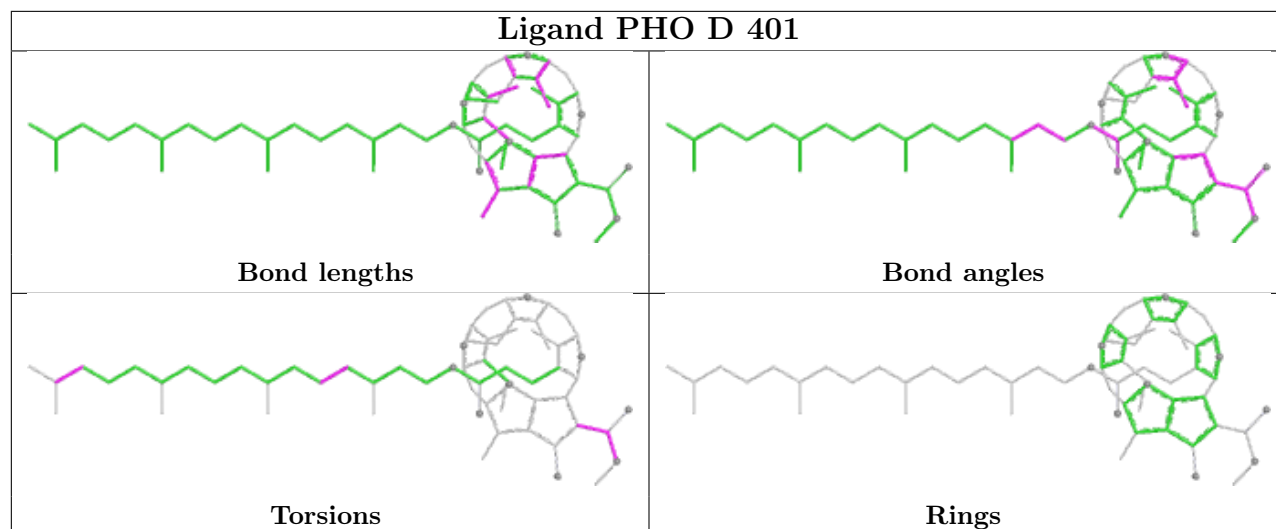
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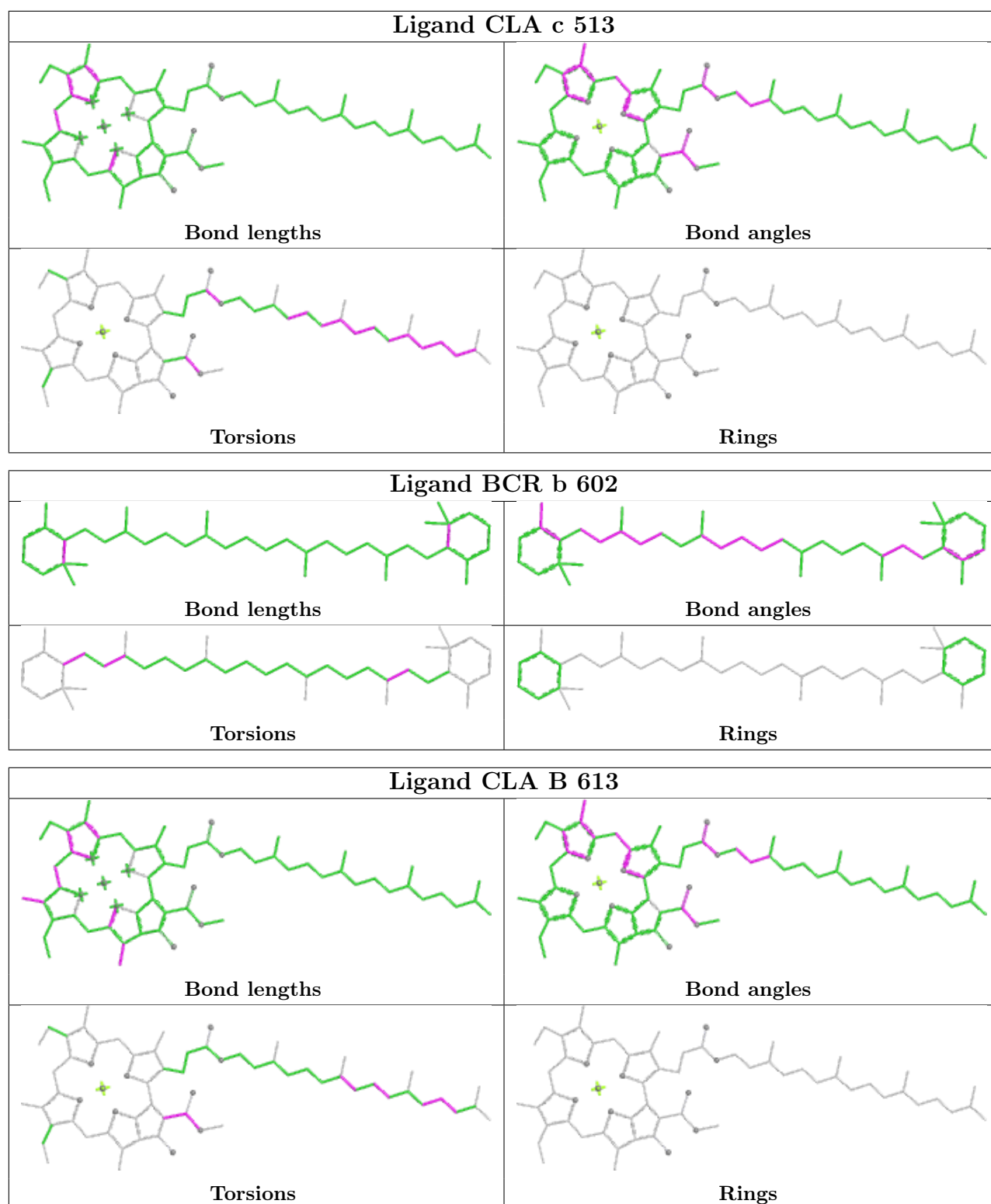
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	506	CLA	2	0
25	c	512	CLA	2	0
32	B	625	LHG	2	0
32	a	720	LHG	1	0
25	B	617	CLA	5	0
29	B	623	SQD	1	0
25	D	402	CLA	3	0
25	B	615	CLA	2	0
25	D	403	CLA	2	0
32	e	101	LHG	2	0
25	d	402	CLA	6	0
25	b	607	CLA	6	0
25	B	616	CLA	3	0
29	a	714	SQD	1	0

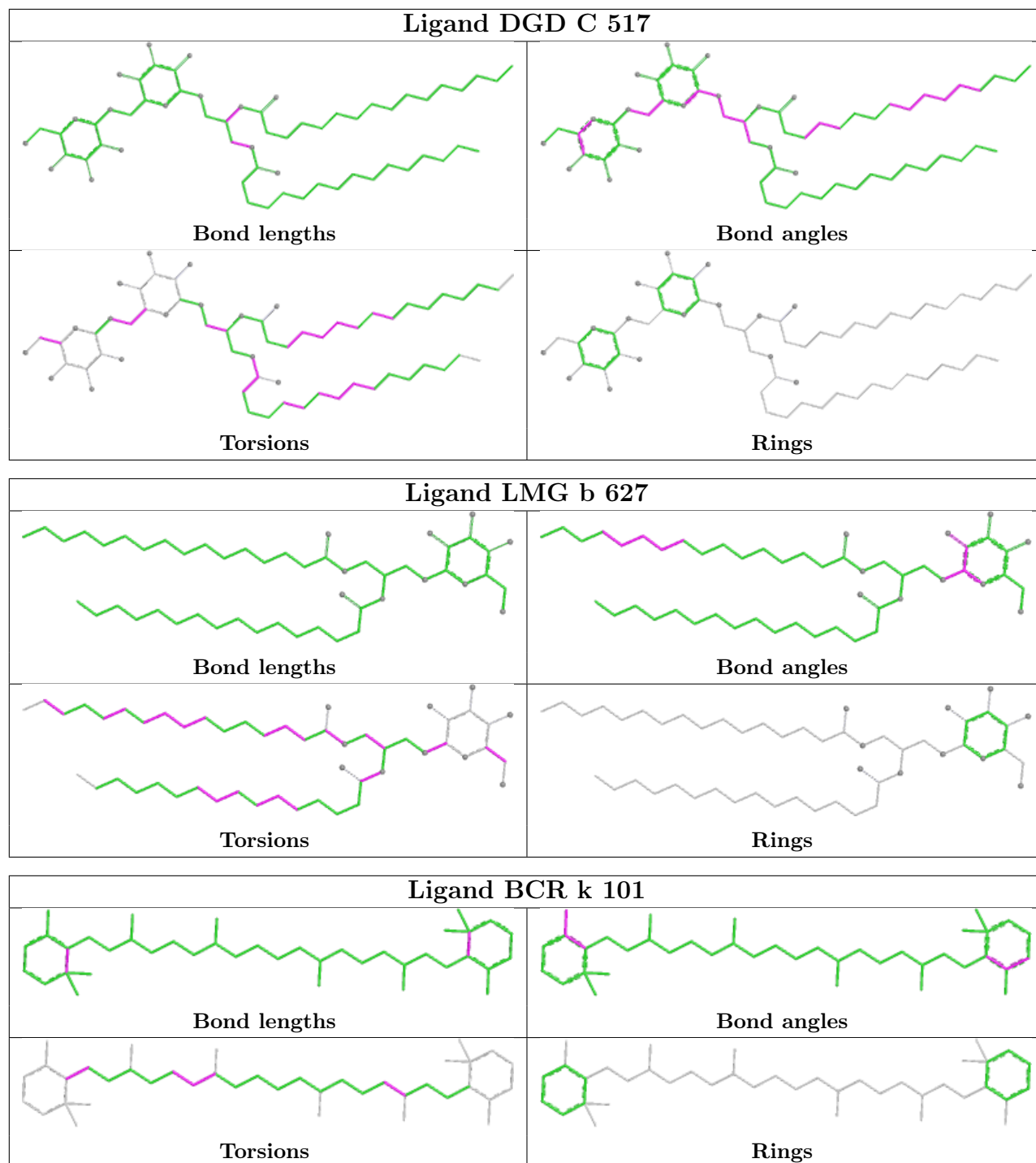
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

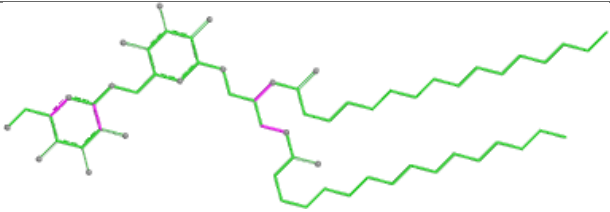
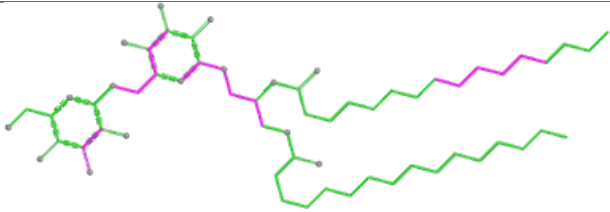
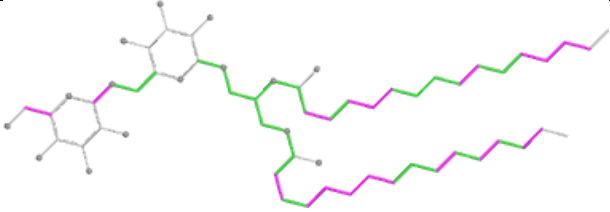
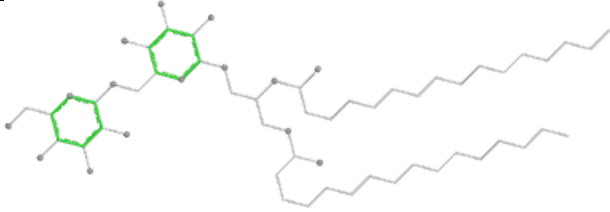
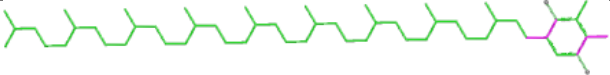
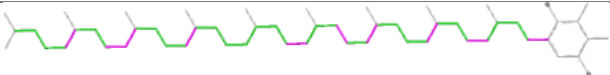
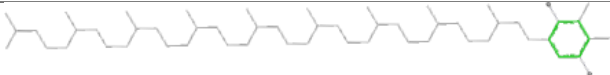




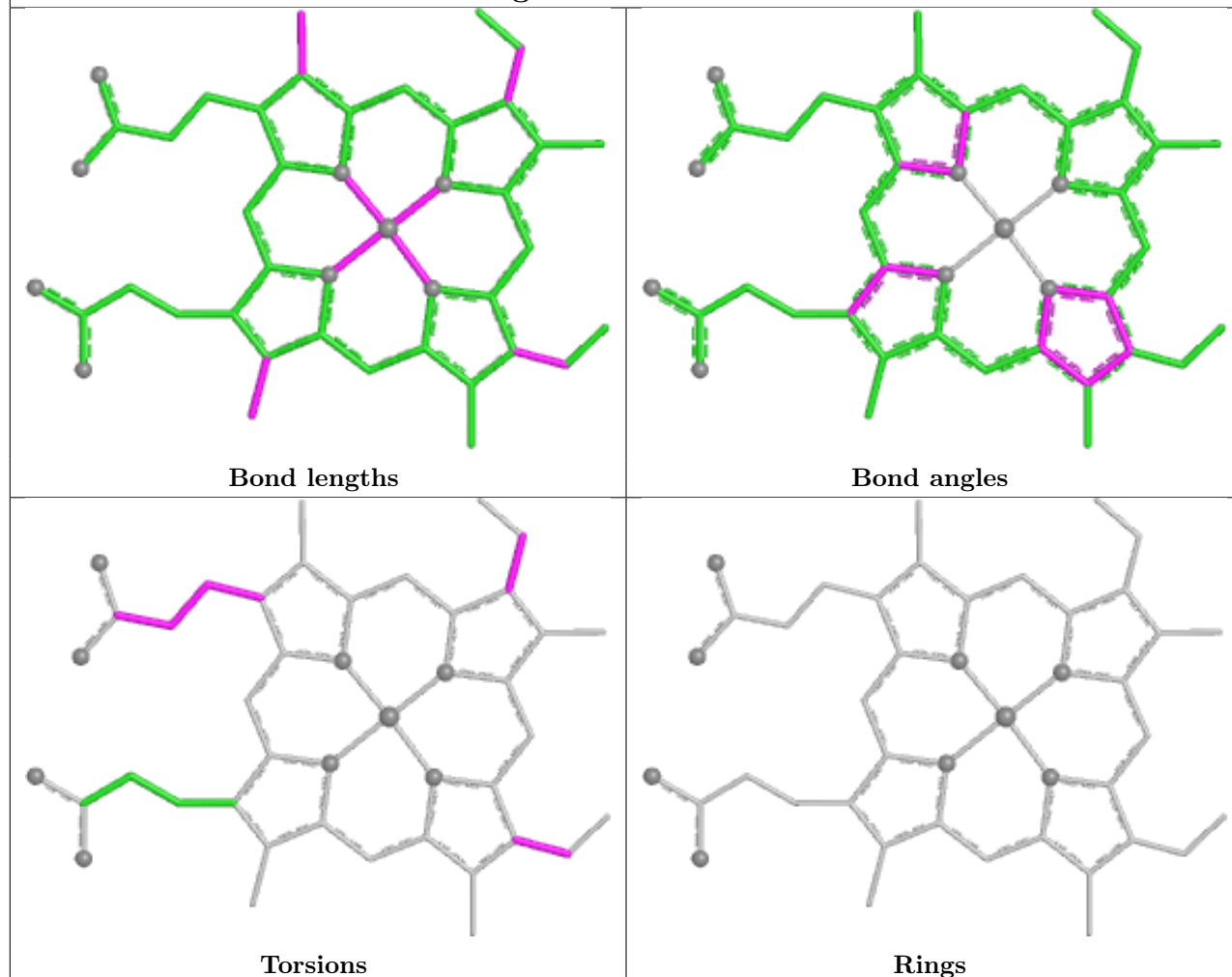




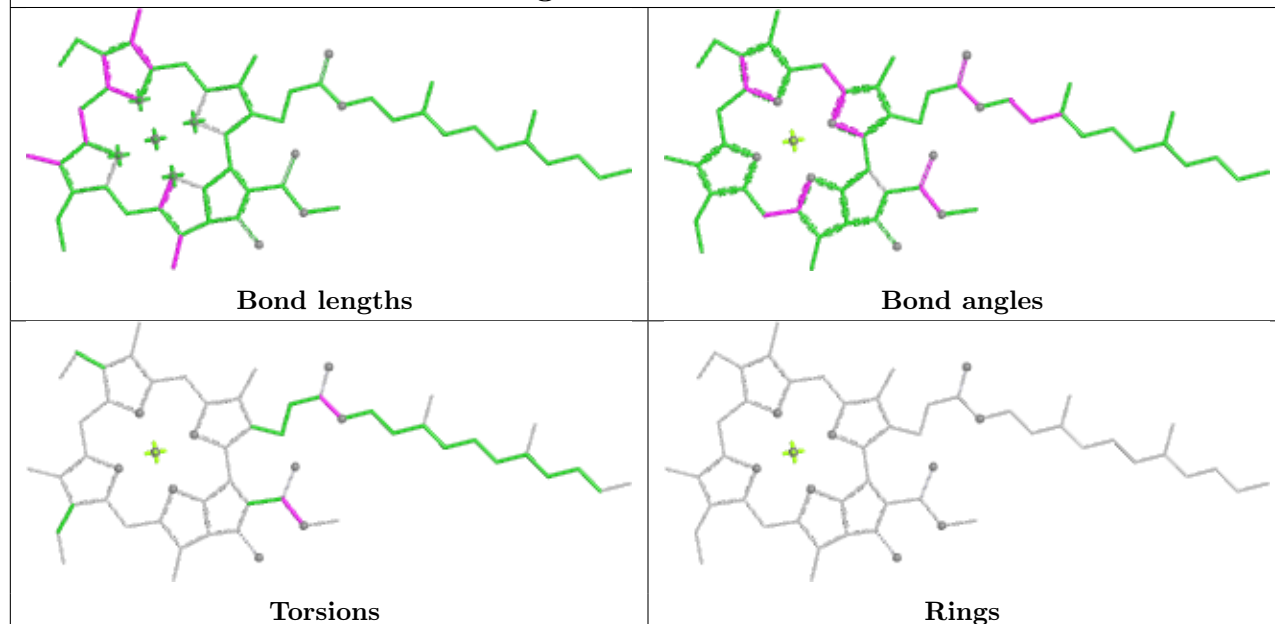


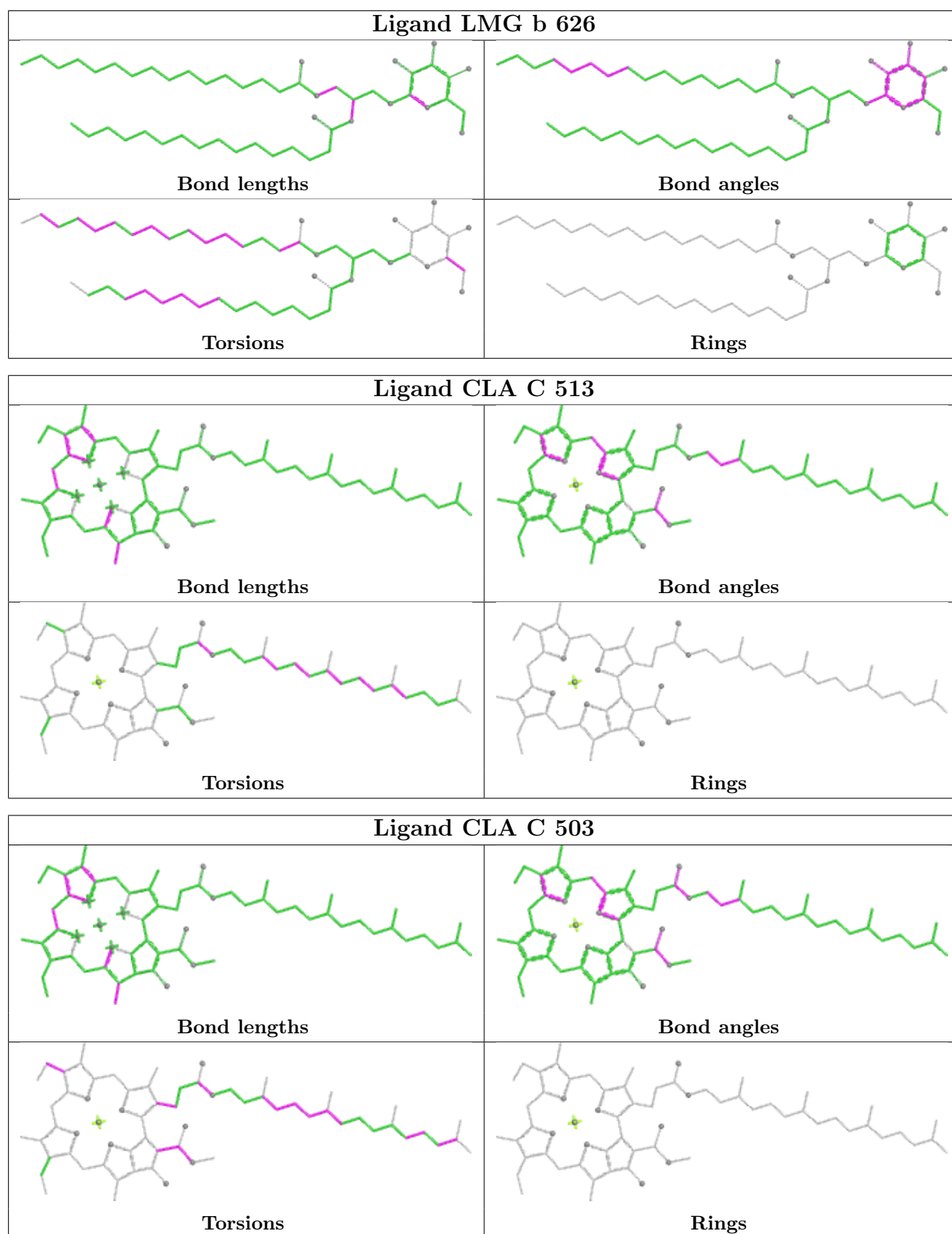
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 a 713	
 Bond lengths	 Bond angles
 Torsions	 Rings

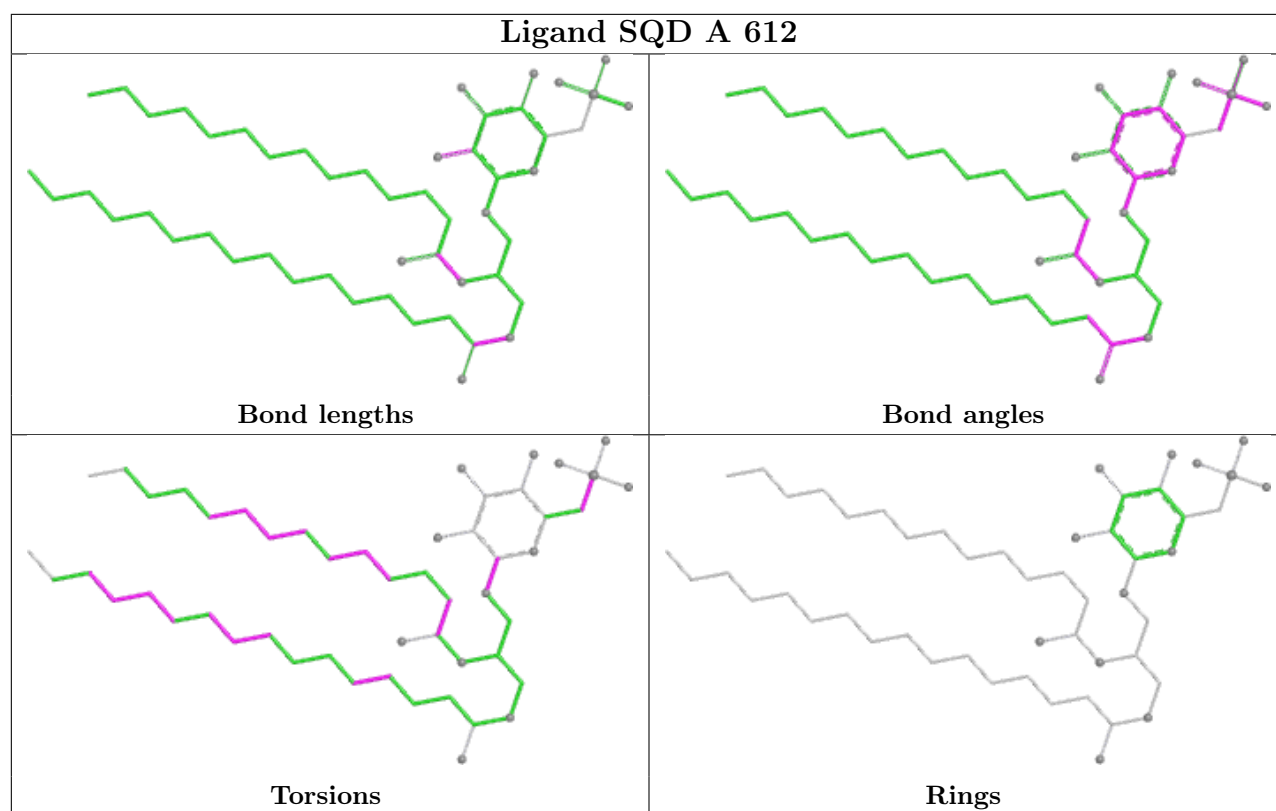
Ligand HEM e 102

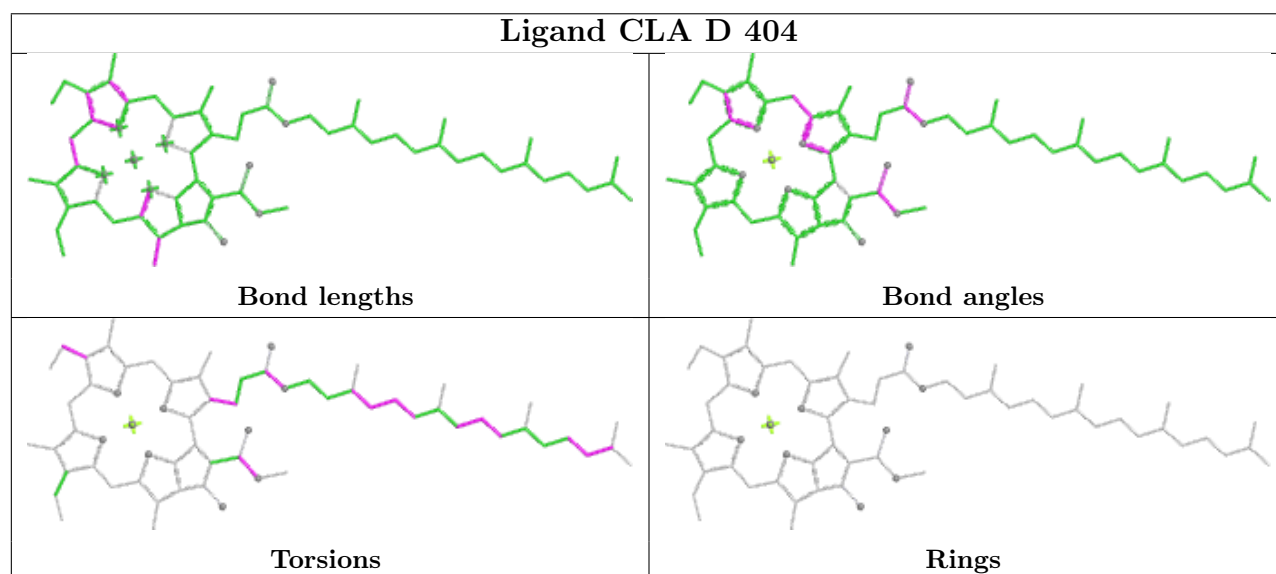
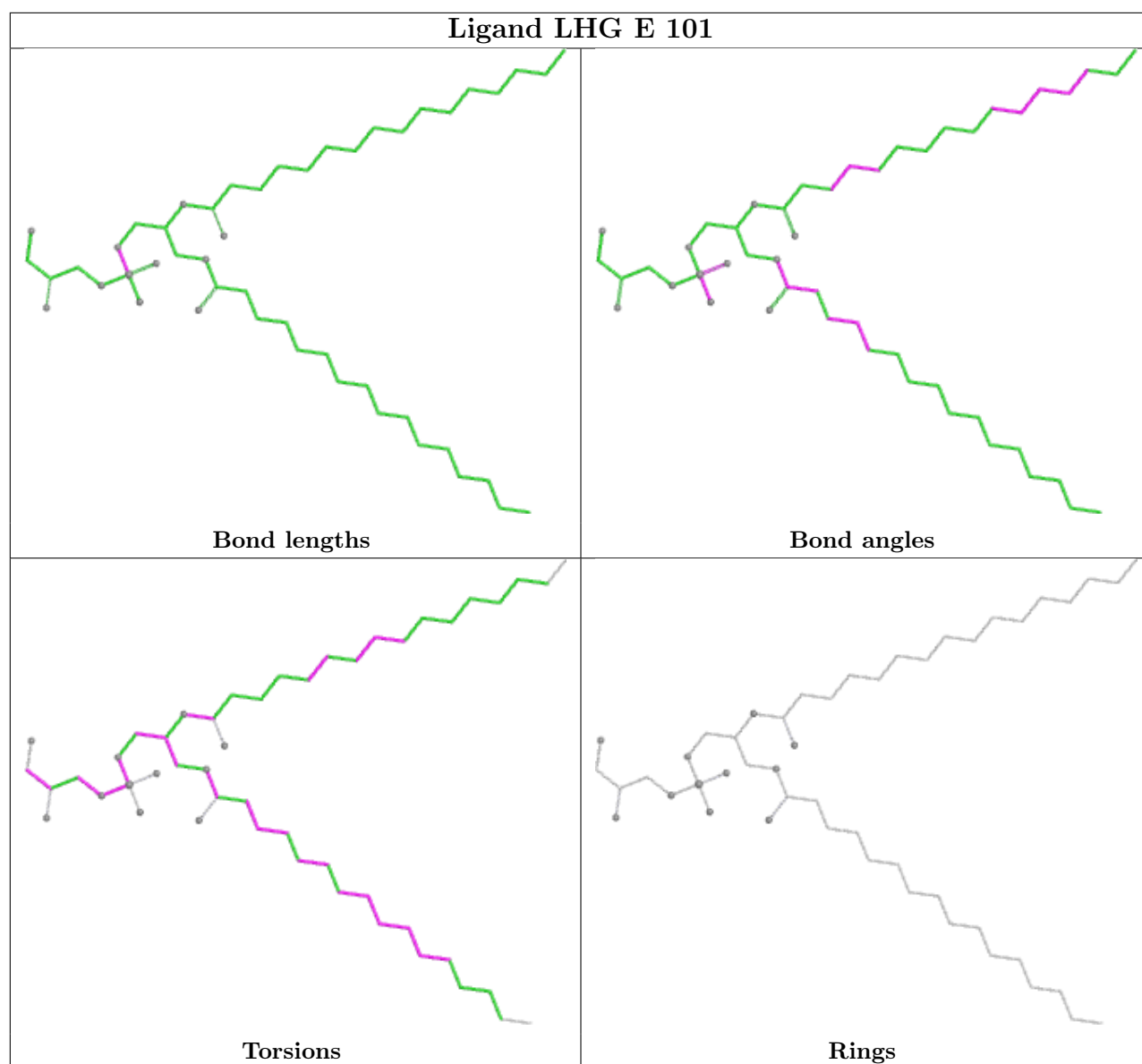


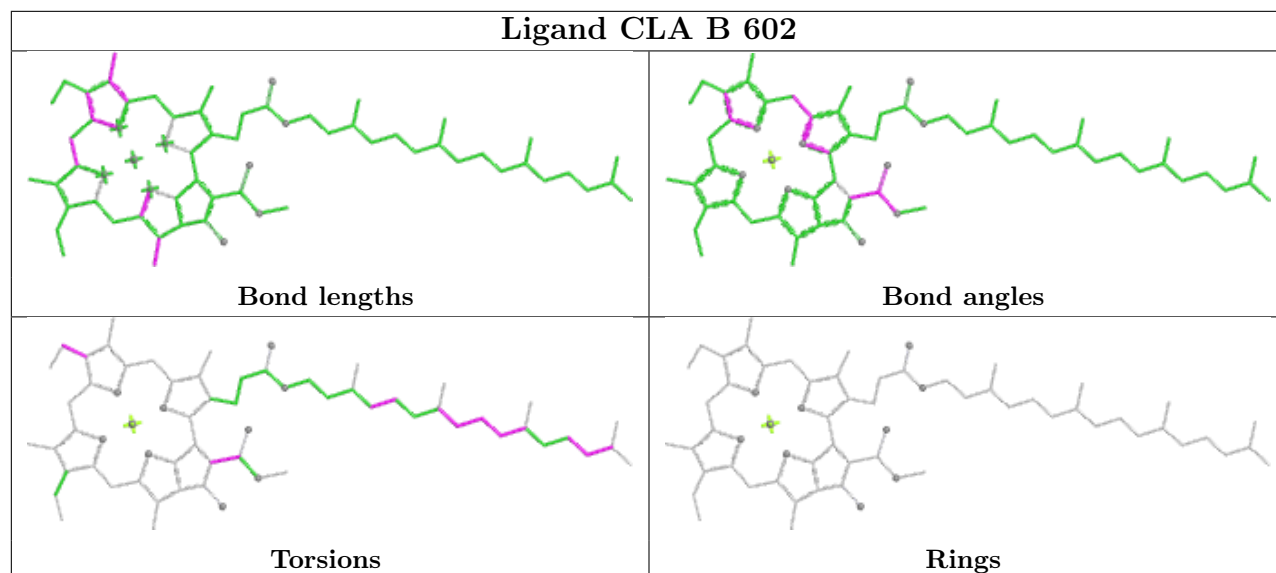
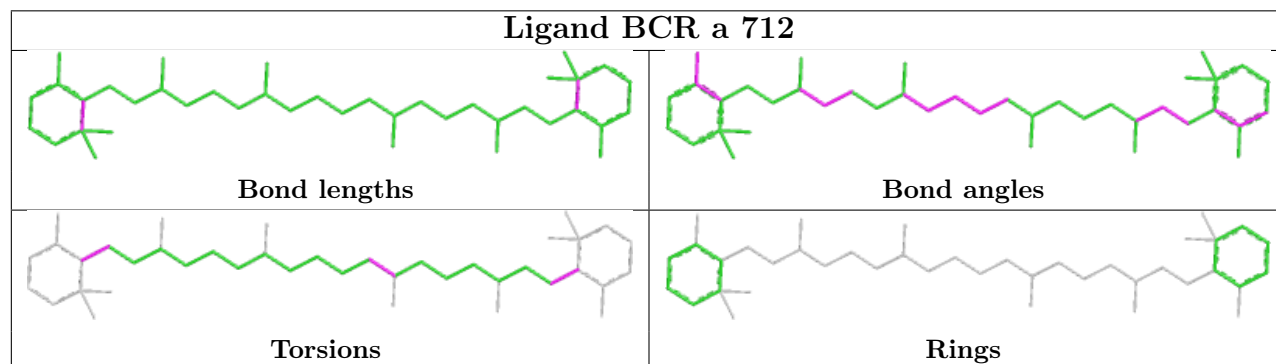
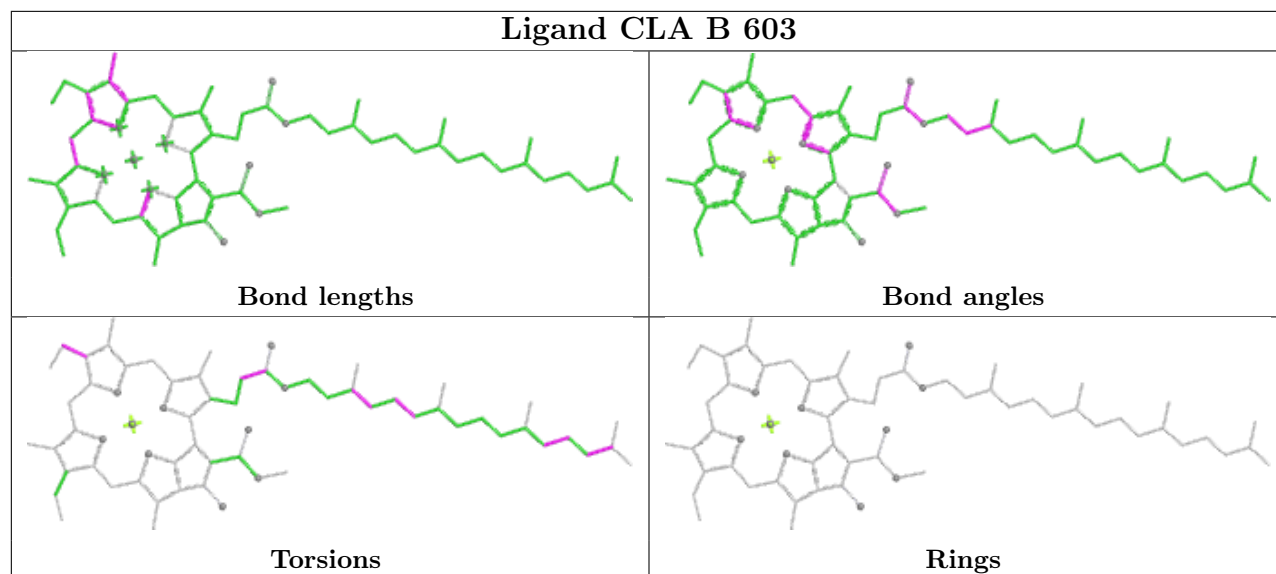
Ligand CLA c 504

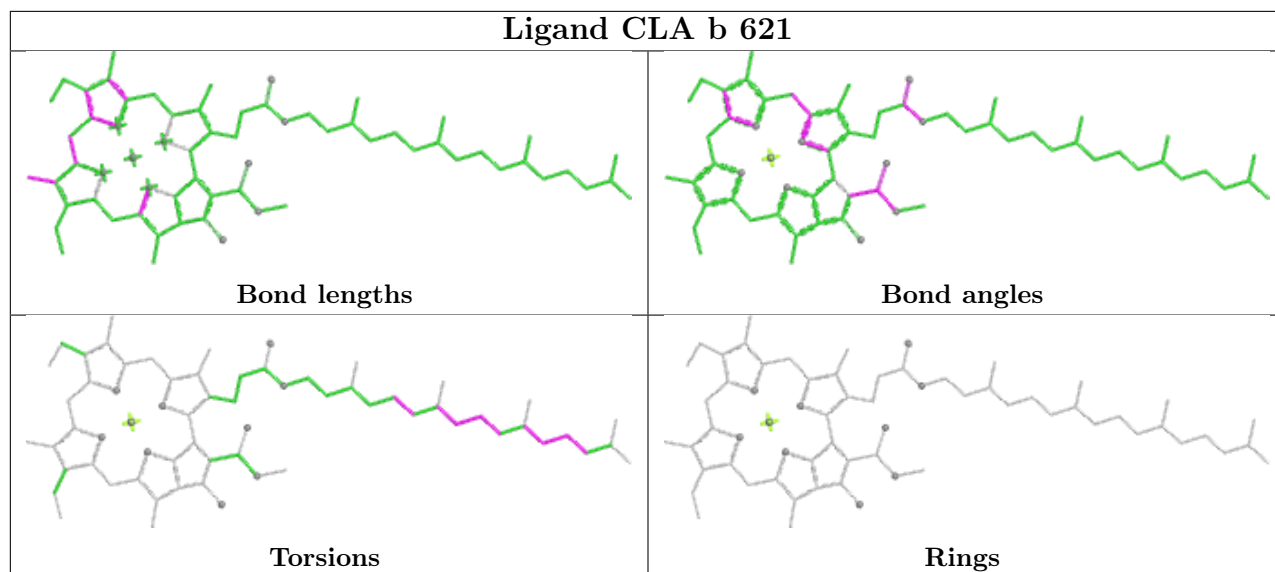
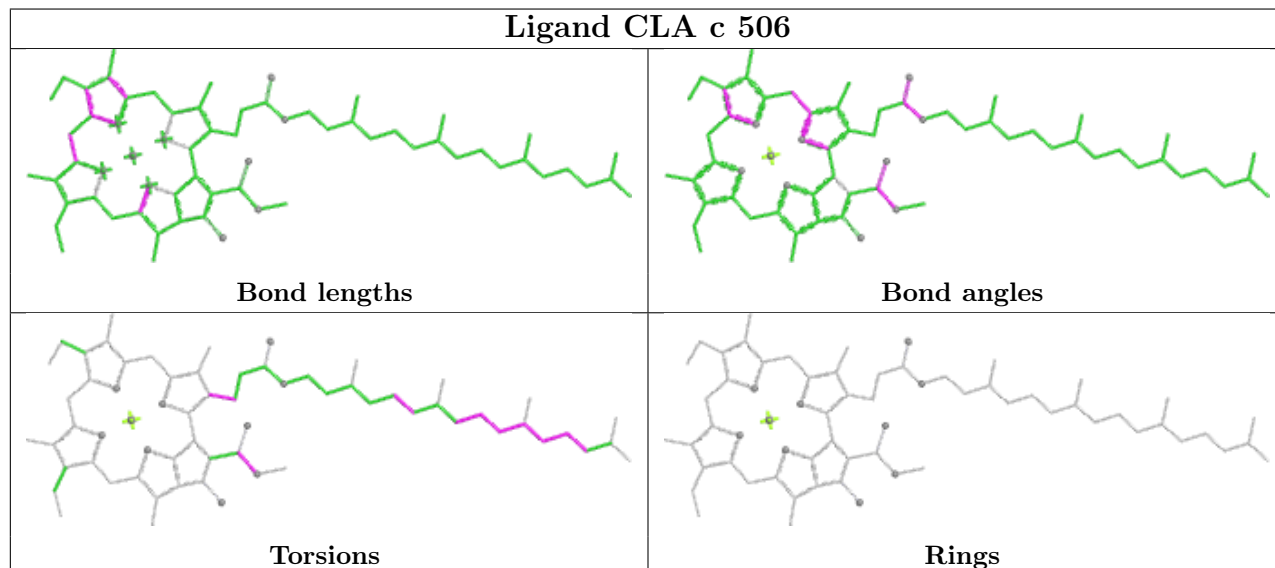
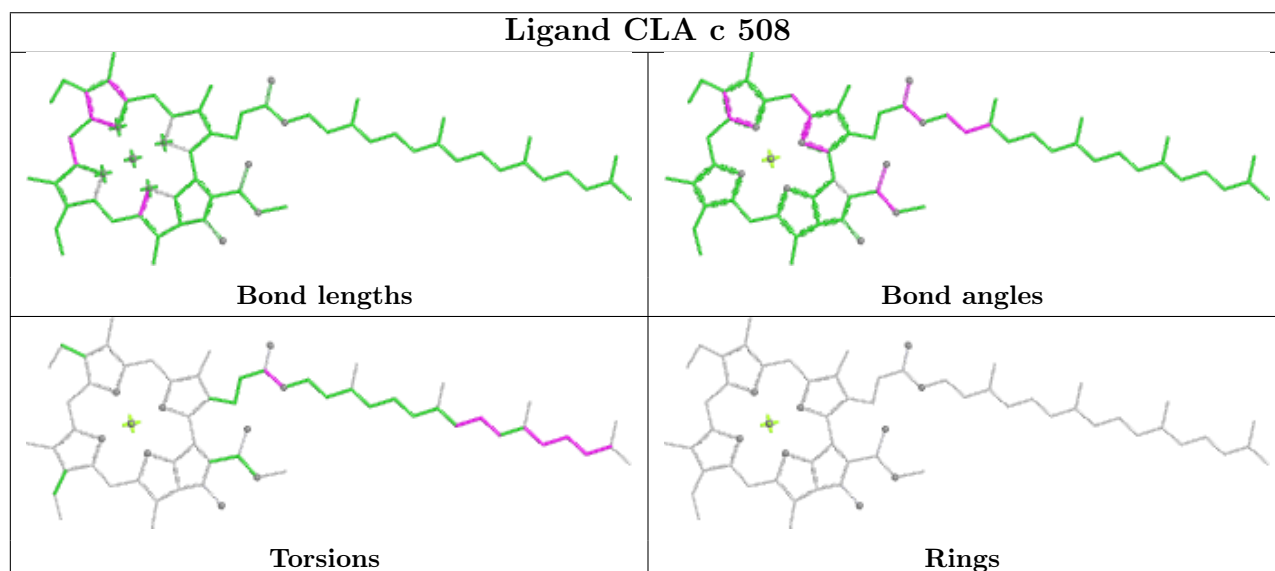




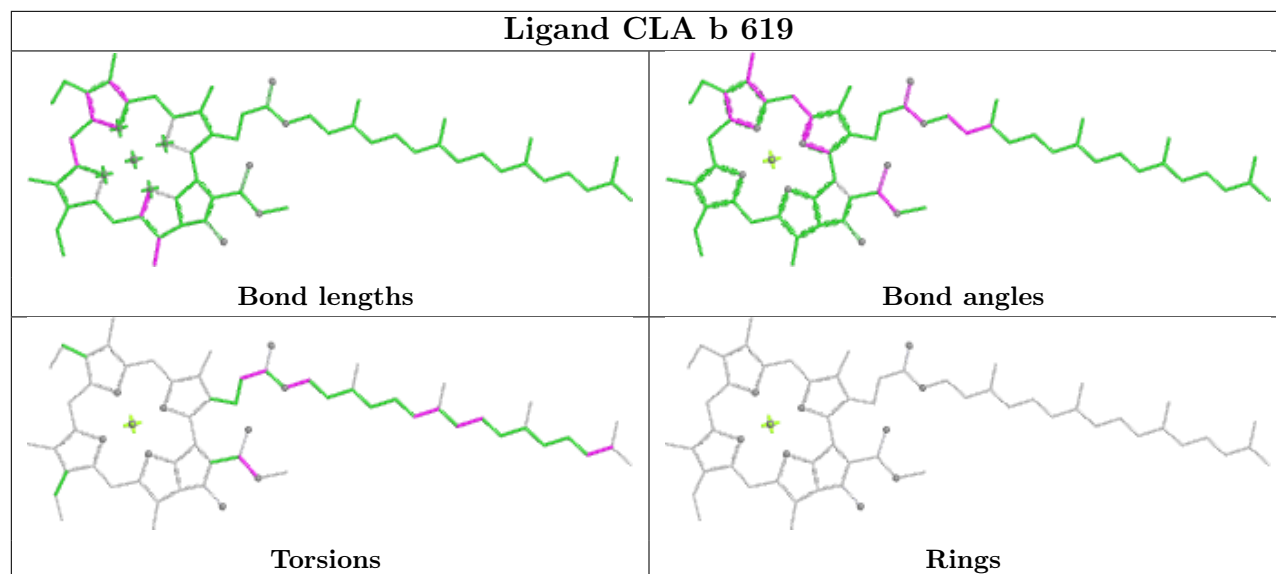




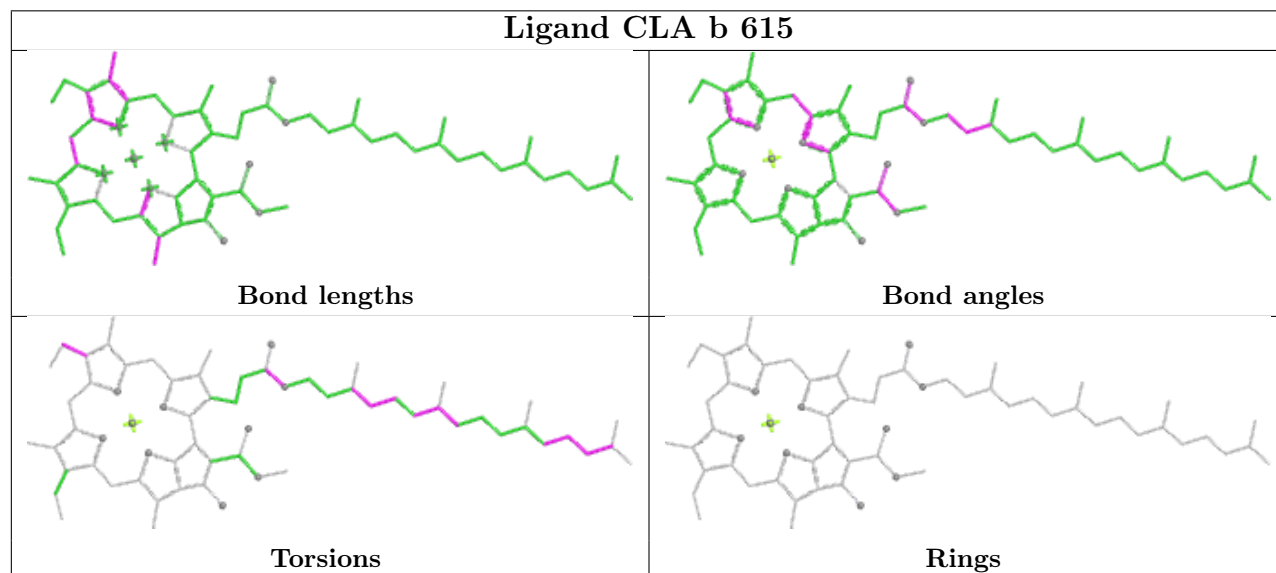


Ligand CLA b 621**Ligand CLA c 506****Ligand CLA c 508**

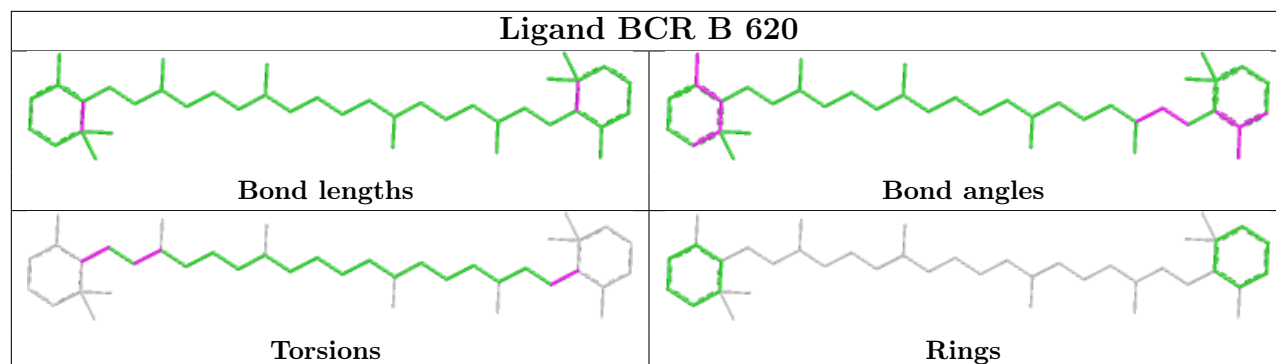
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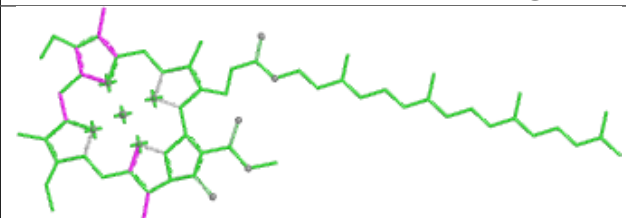
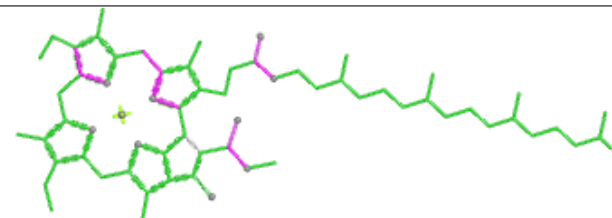
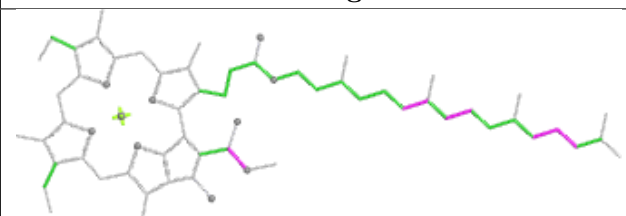
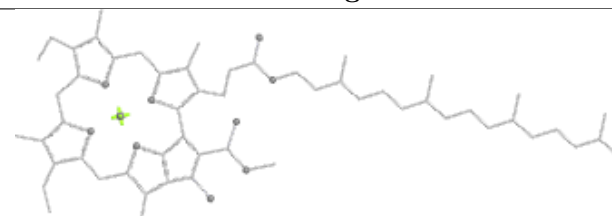


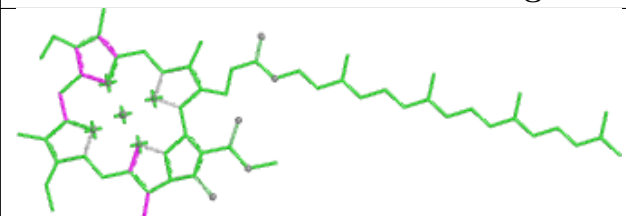
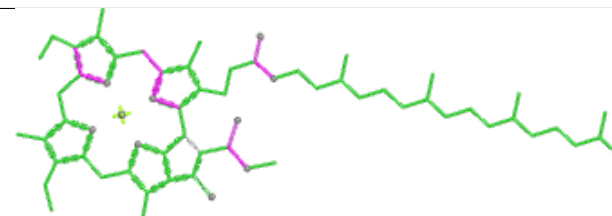
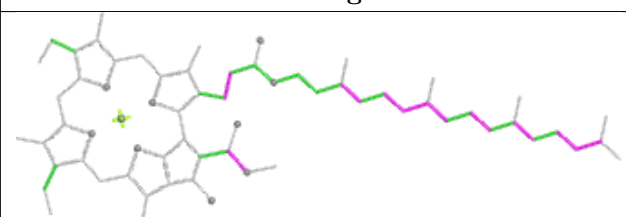
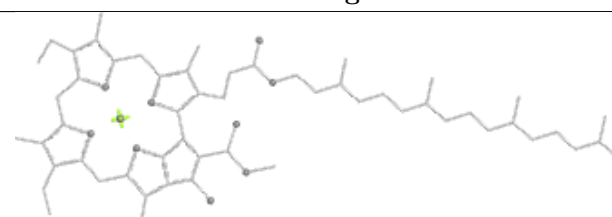
Ligand CLA b 615

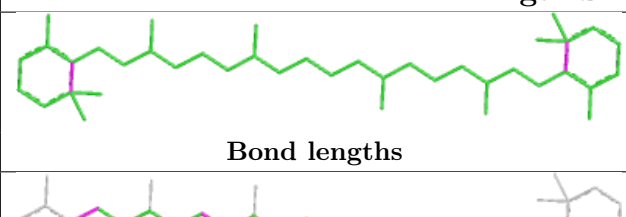
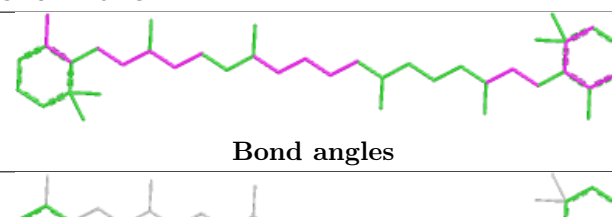


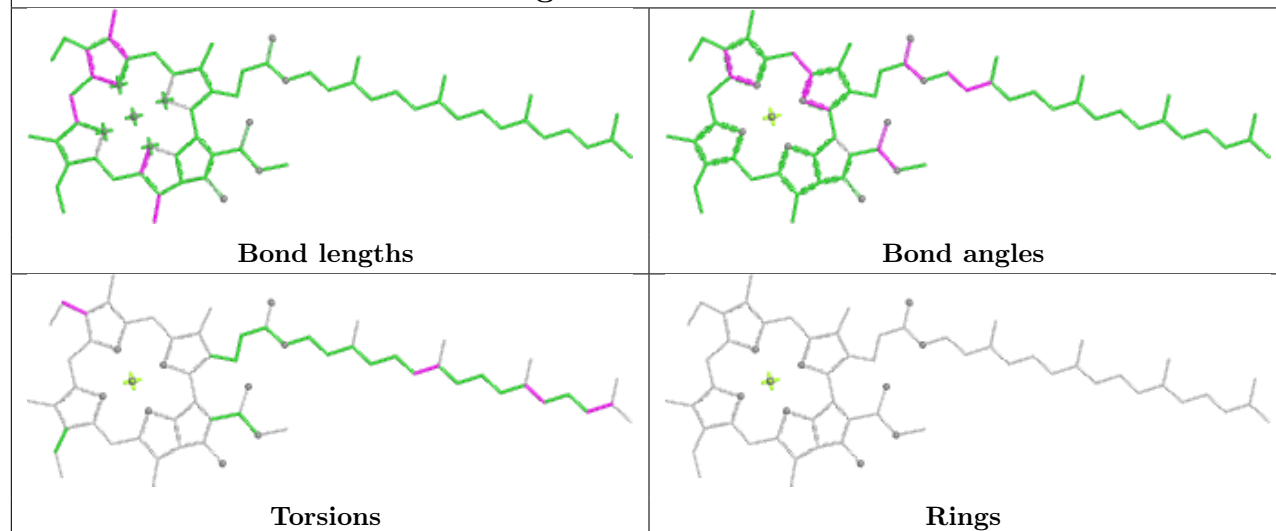
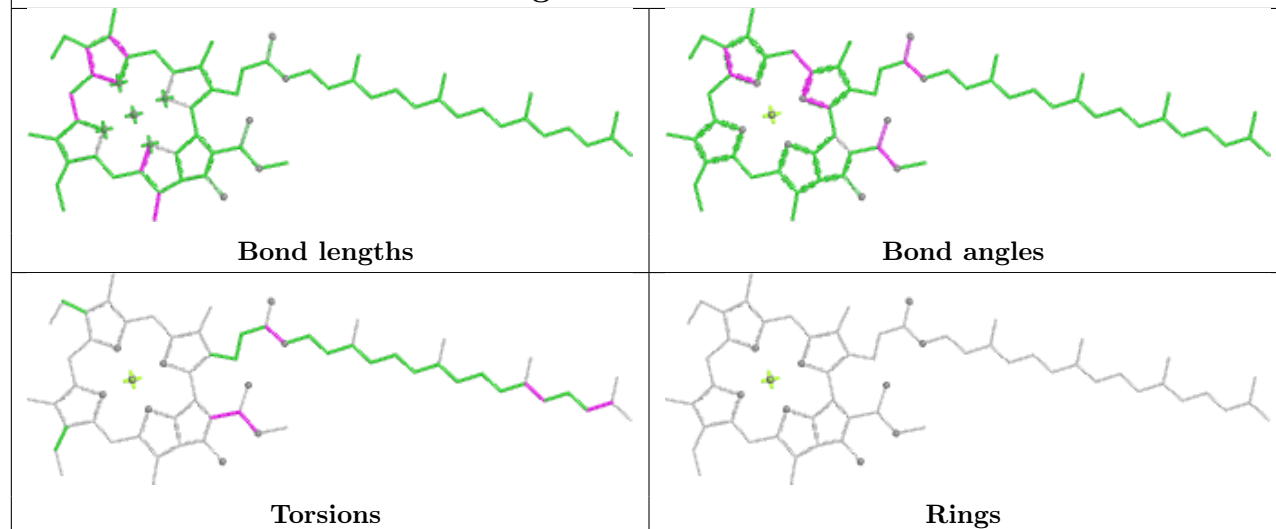
Ligand BCR B 620

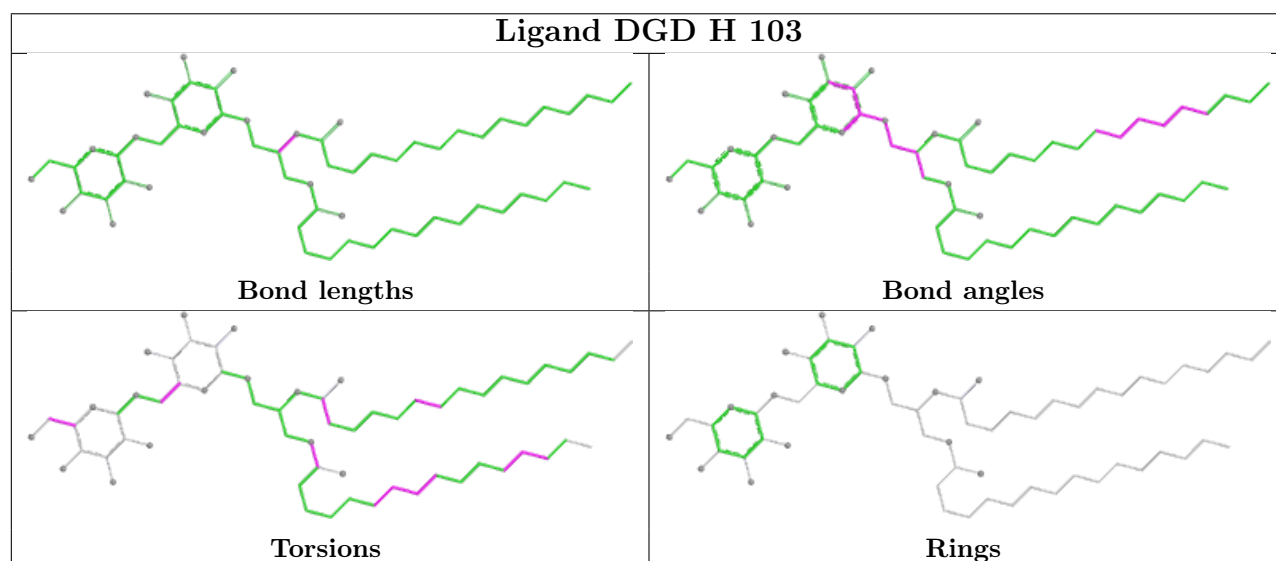
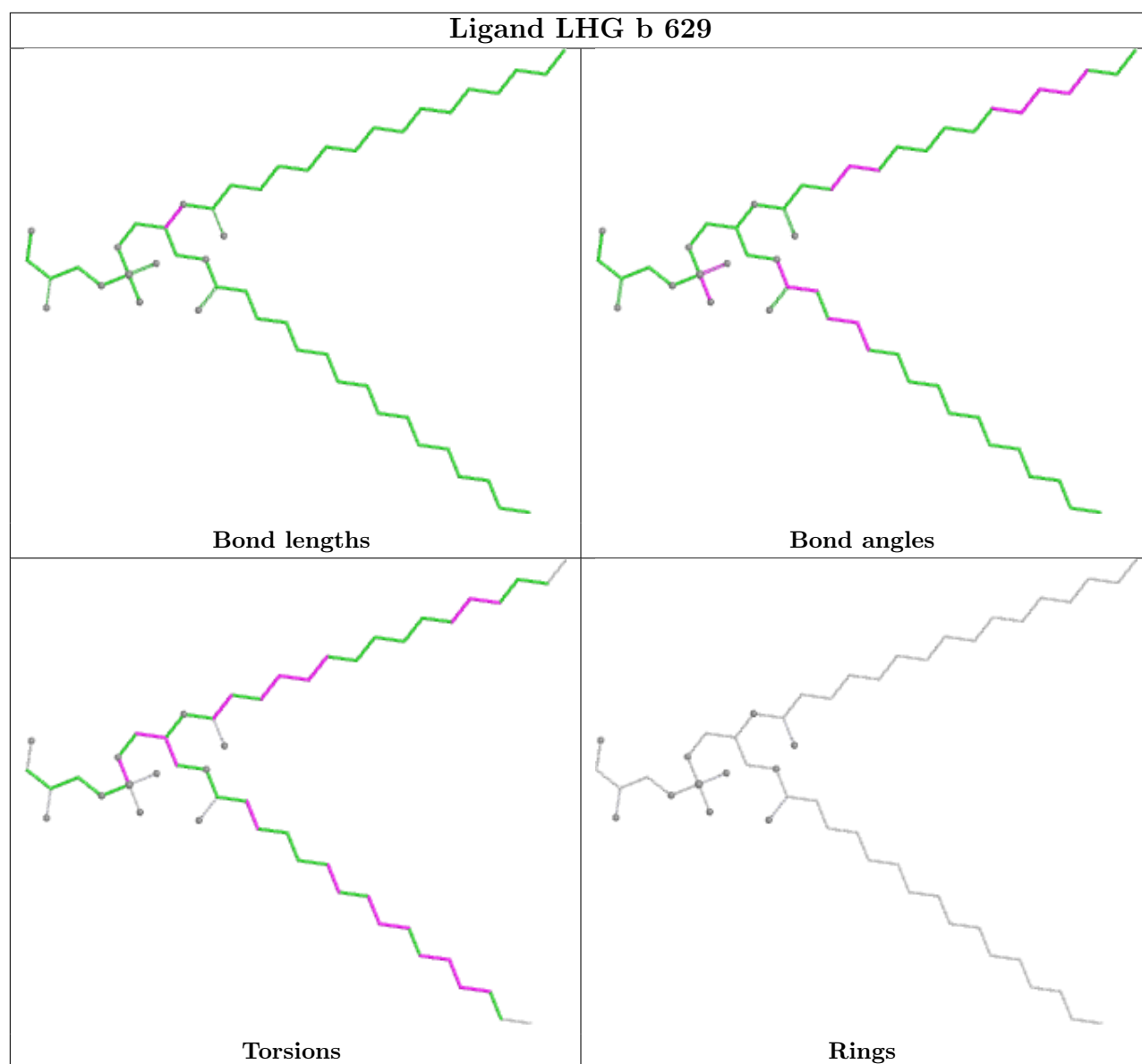


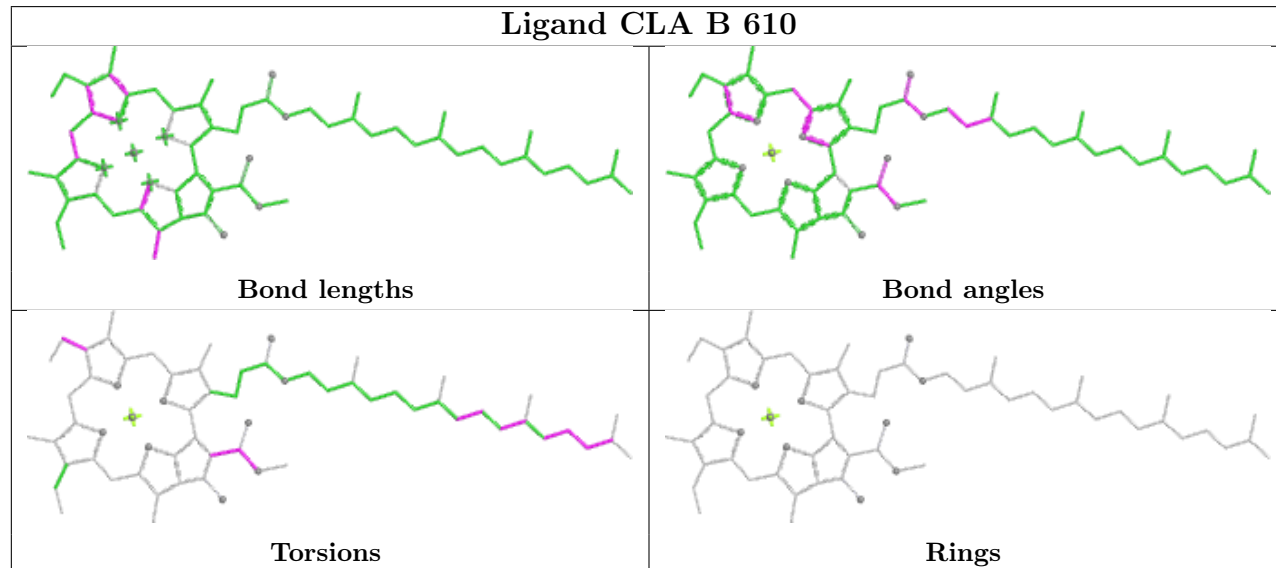
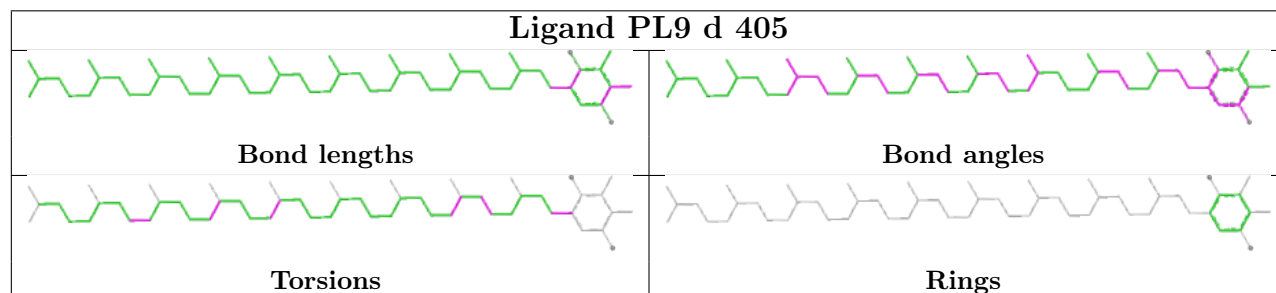
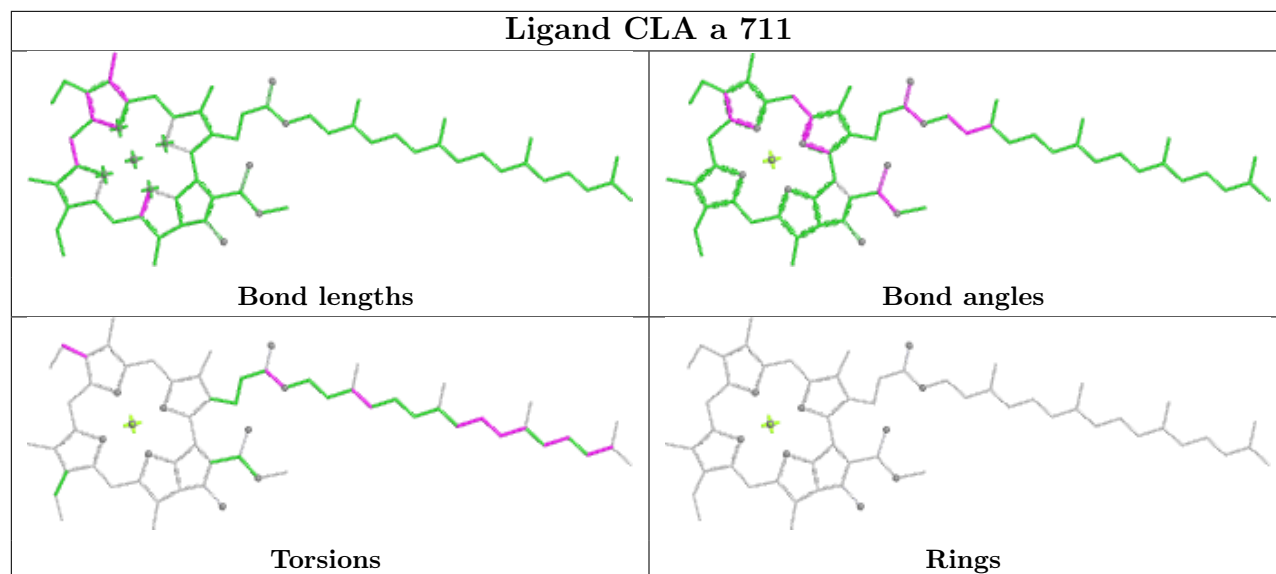
Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

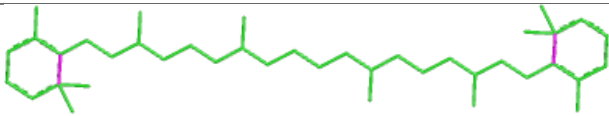
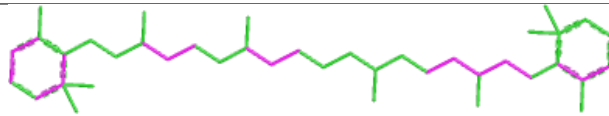
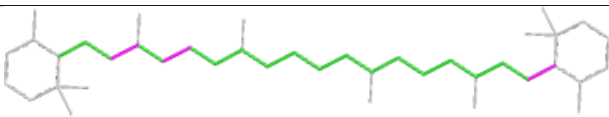
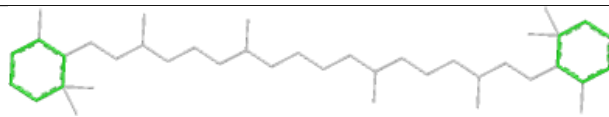
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

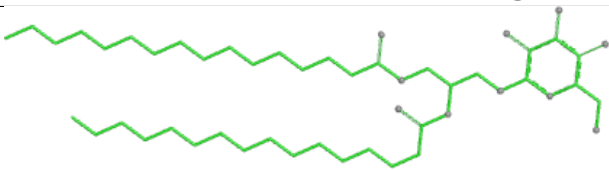
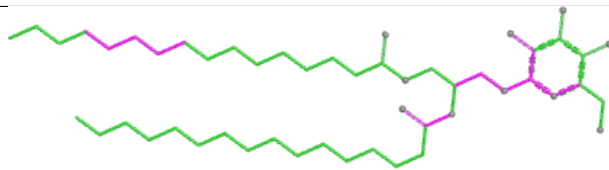
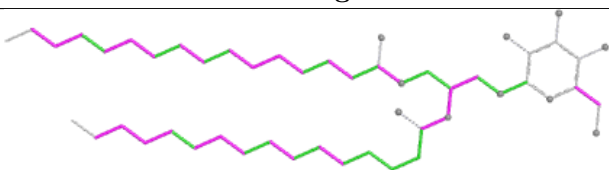
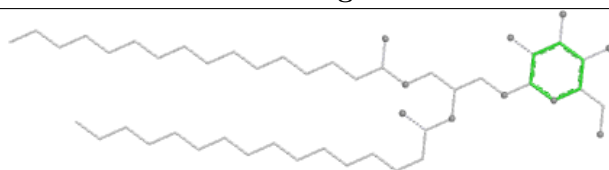
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

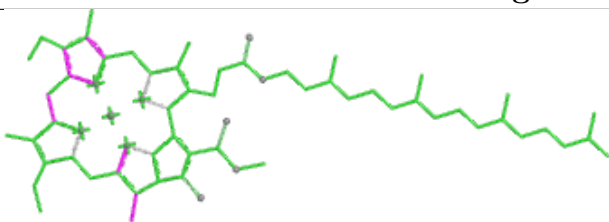
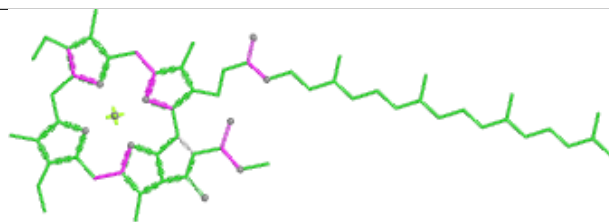
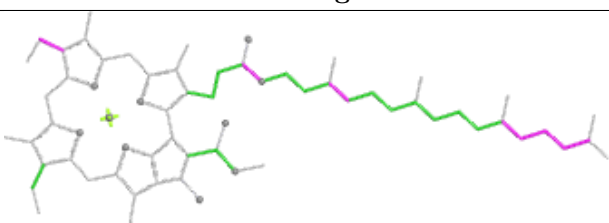
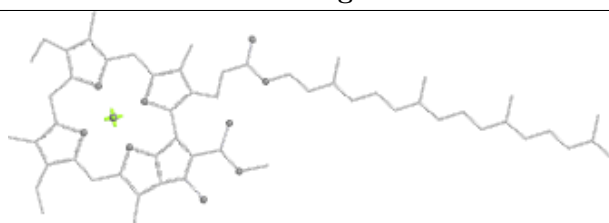
Ligand CLA a 708**Ligand CLA B 608**

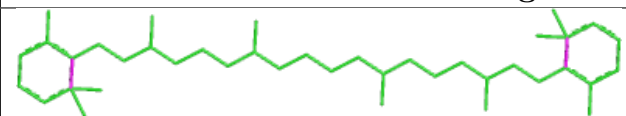
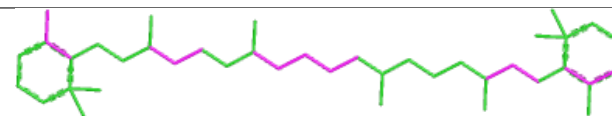
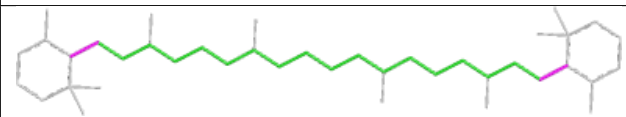
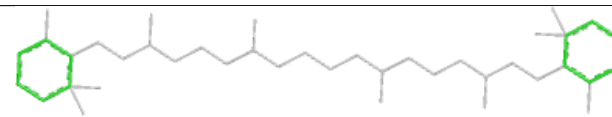


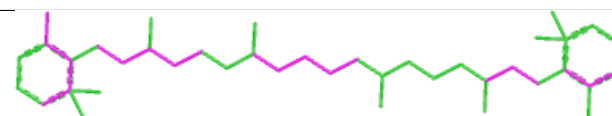
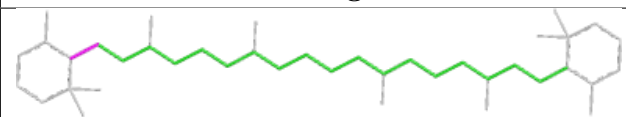
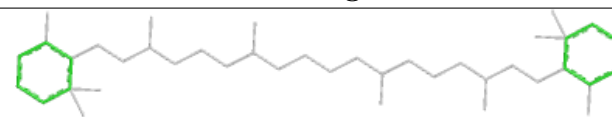


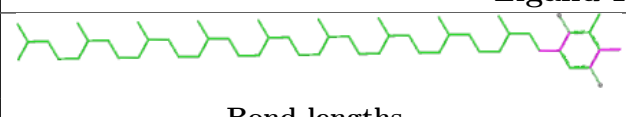
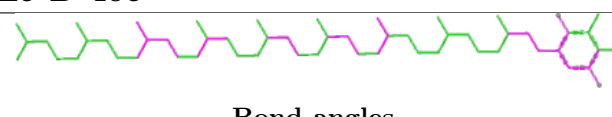
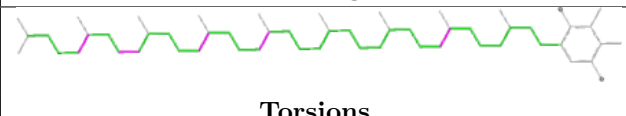
Ligand BCR H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

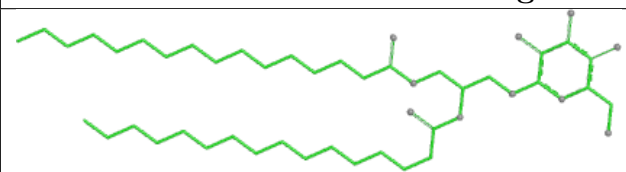
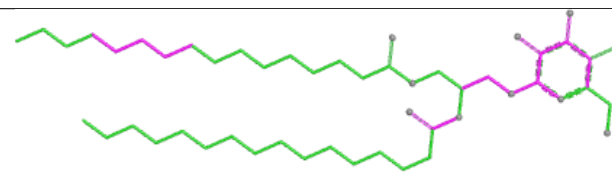
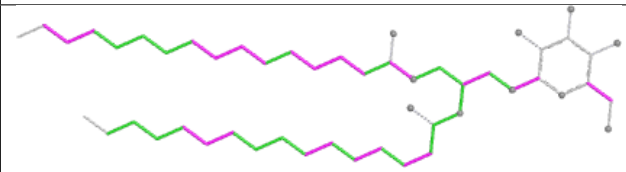
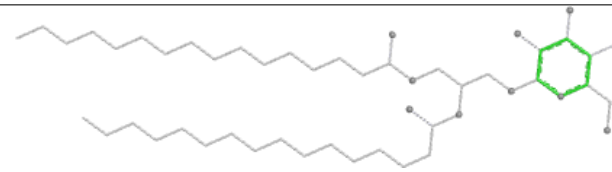
Ligand LMG a 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

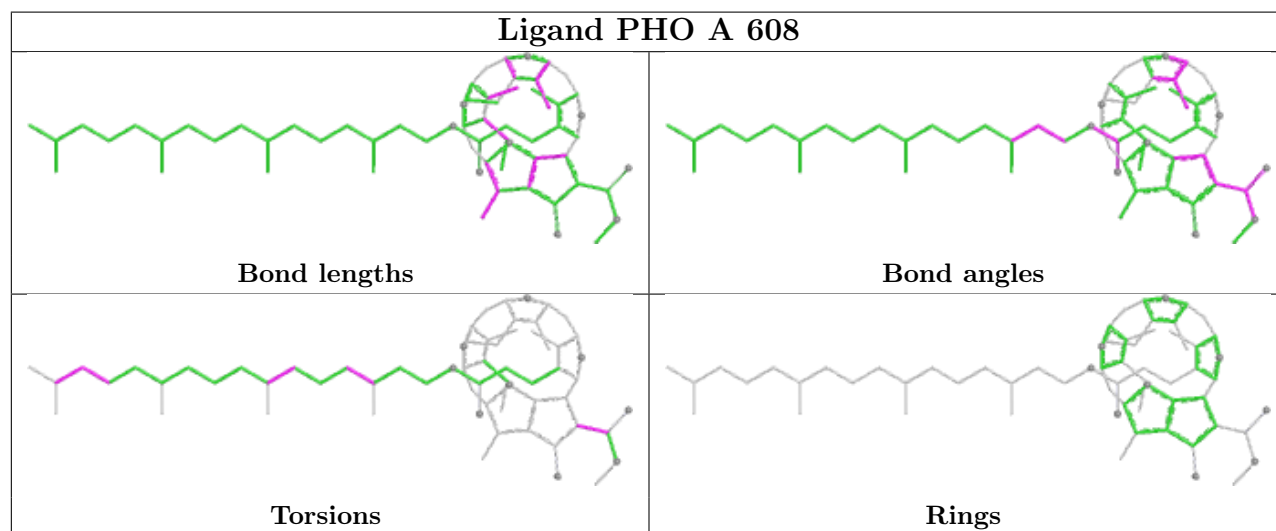
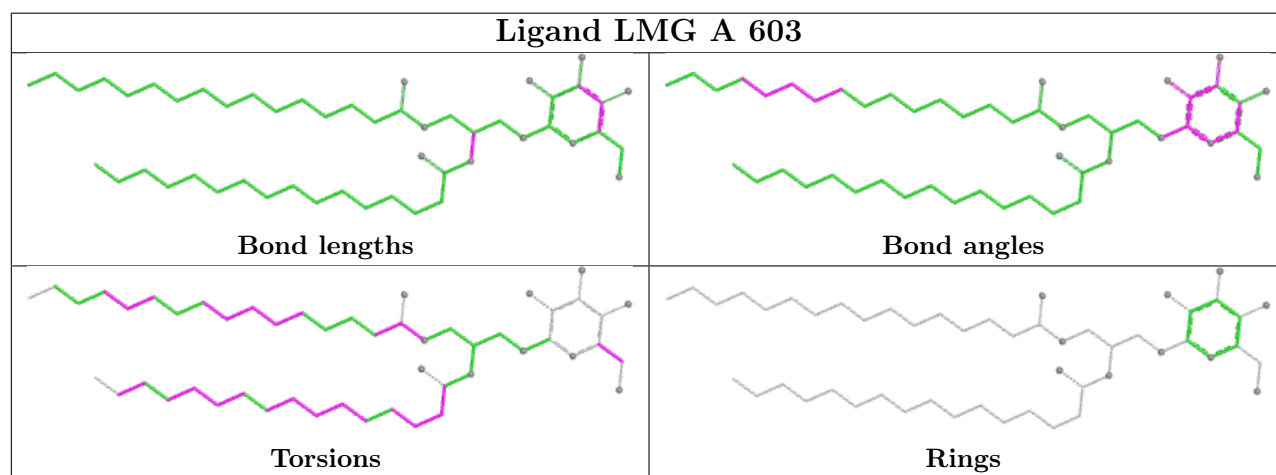
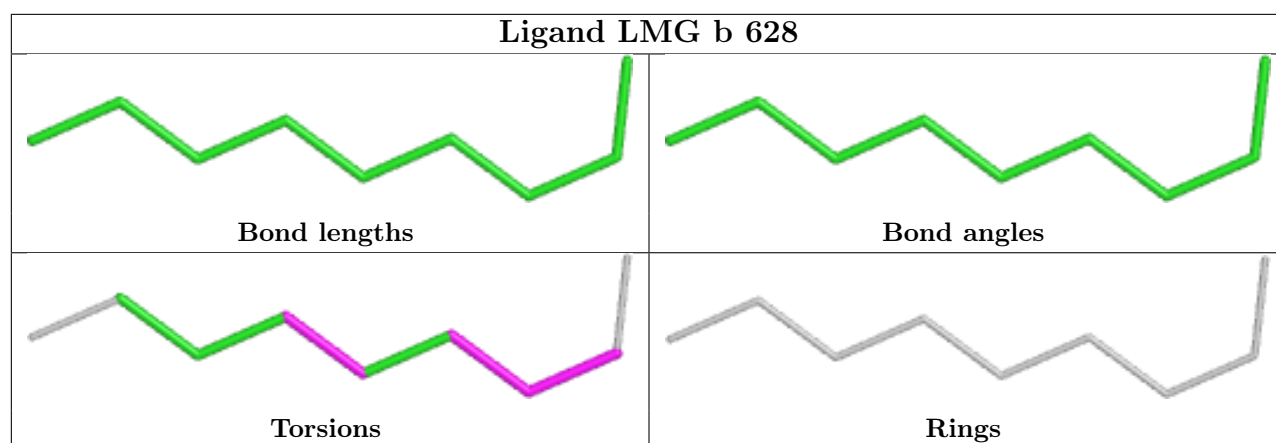
Ligand CLA b 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

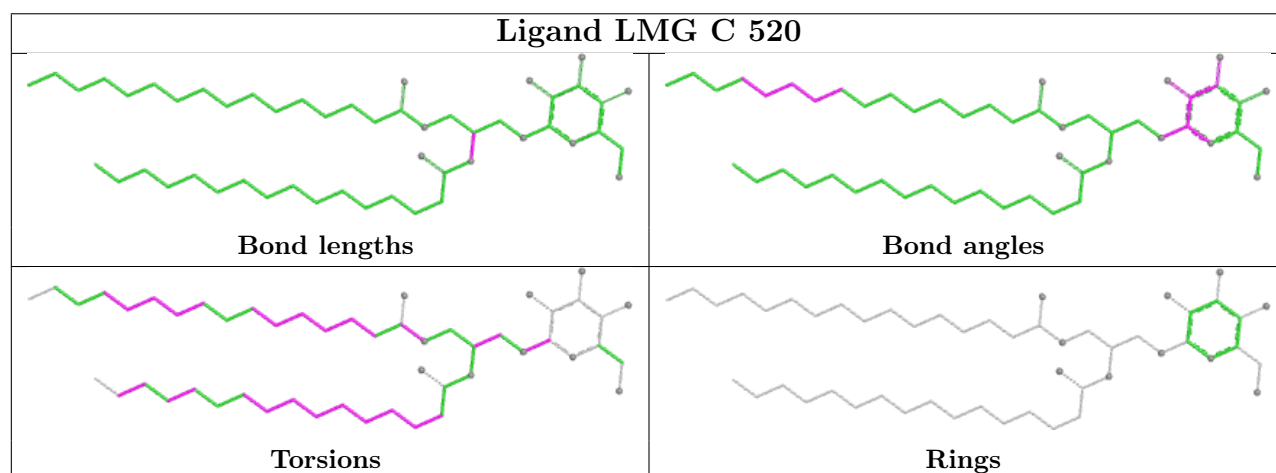
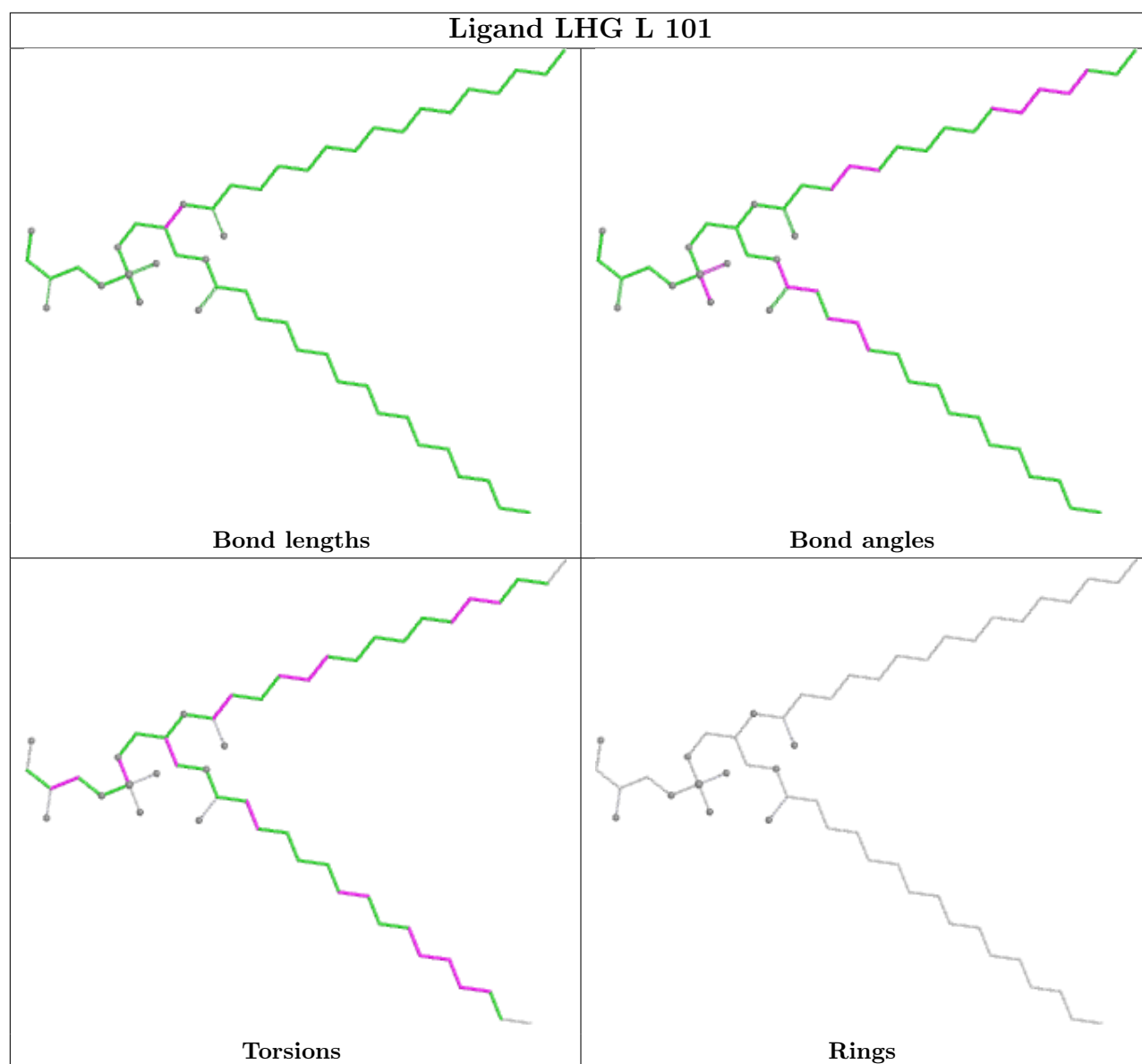
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

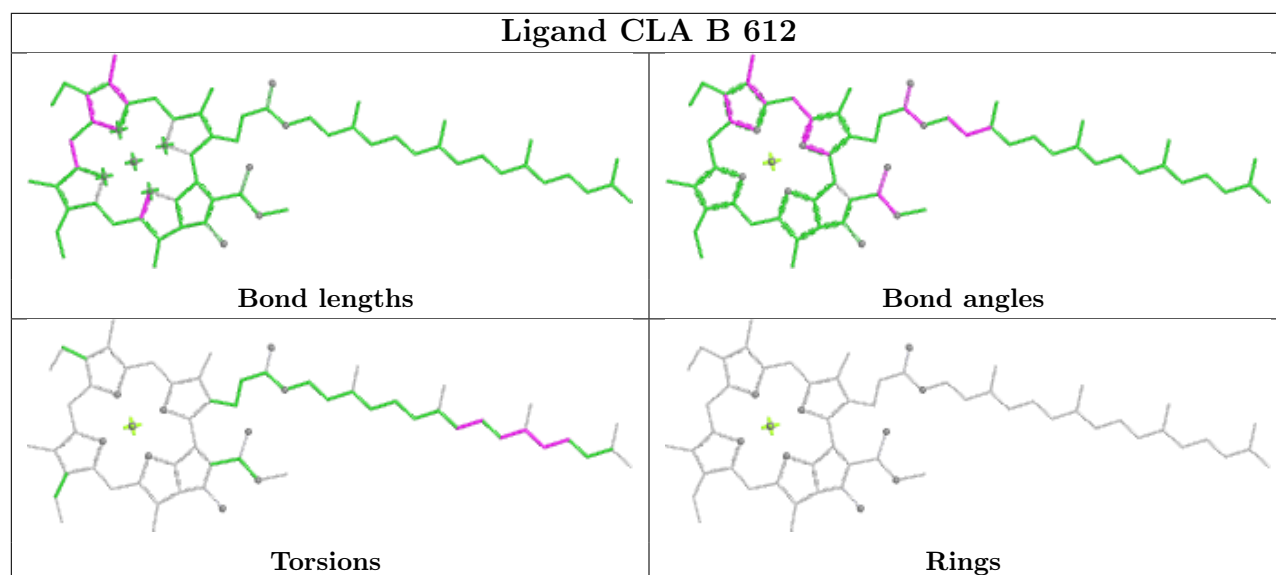
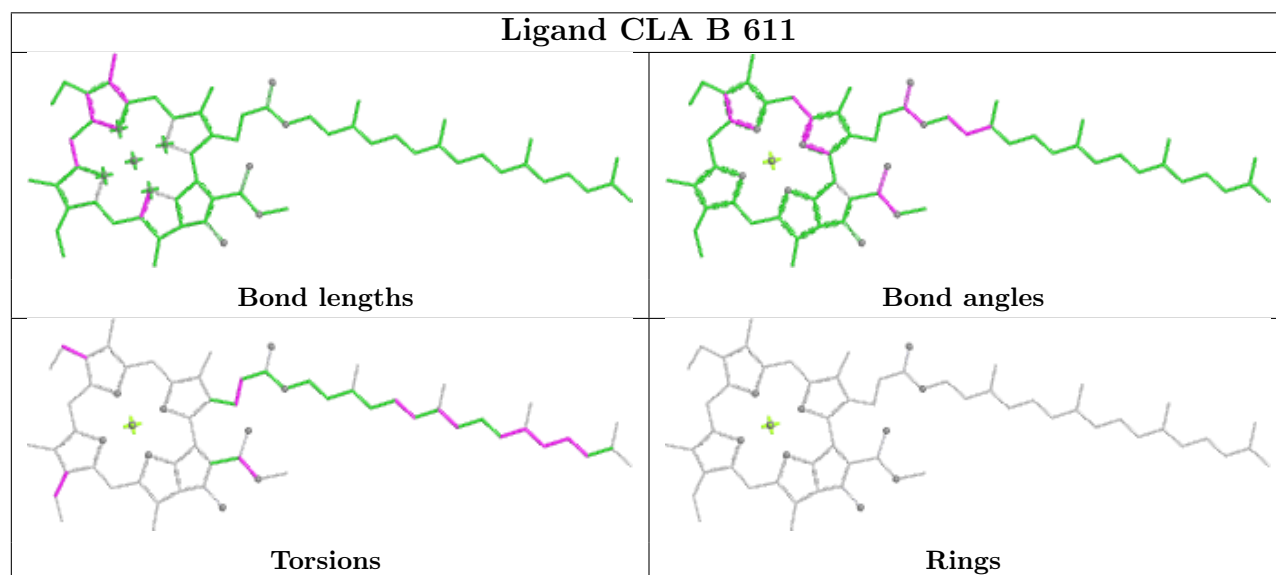
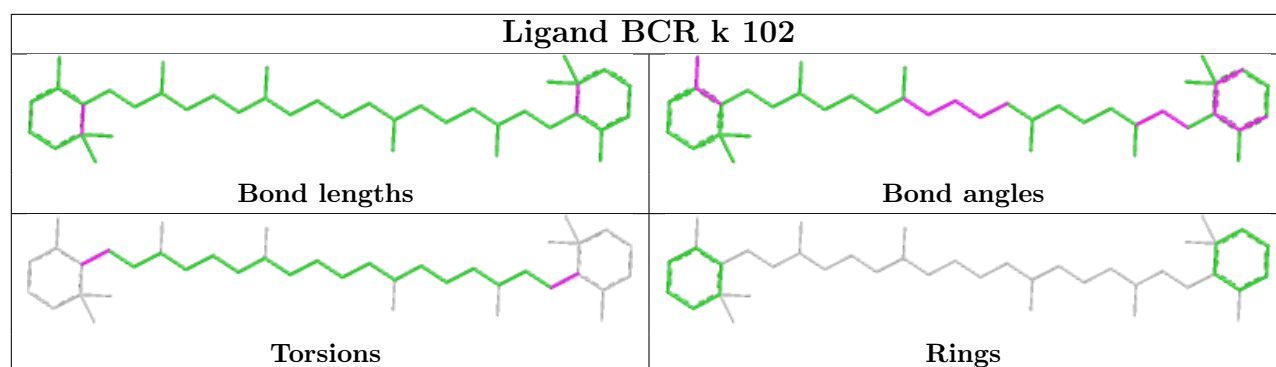
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Bond lengths	Bond angles
	
Torsions	Rings

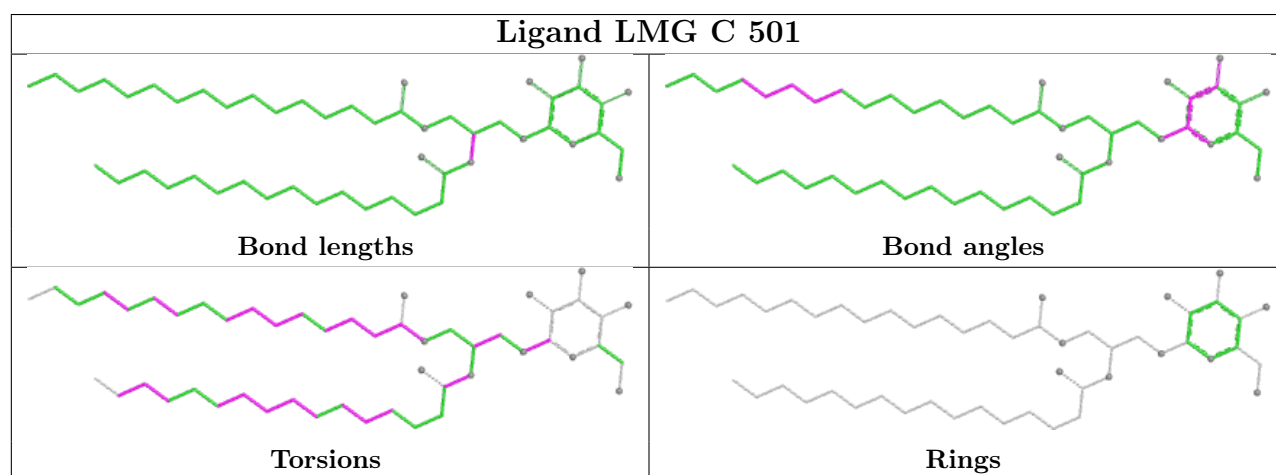
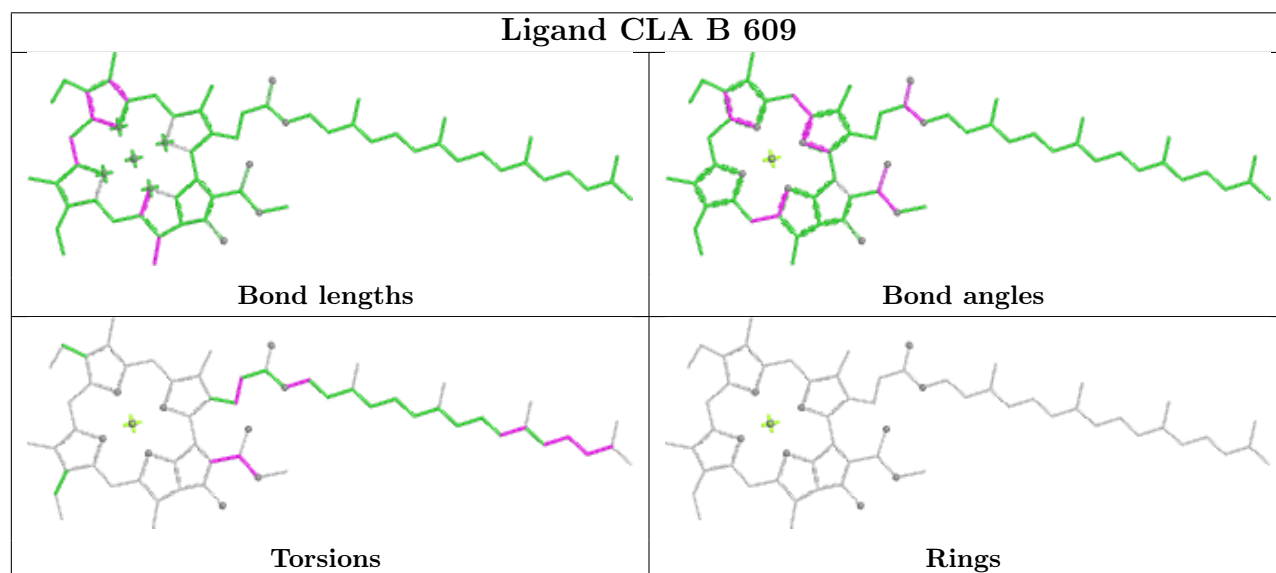
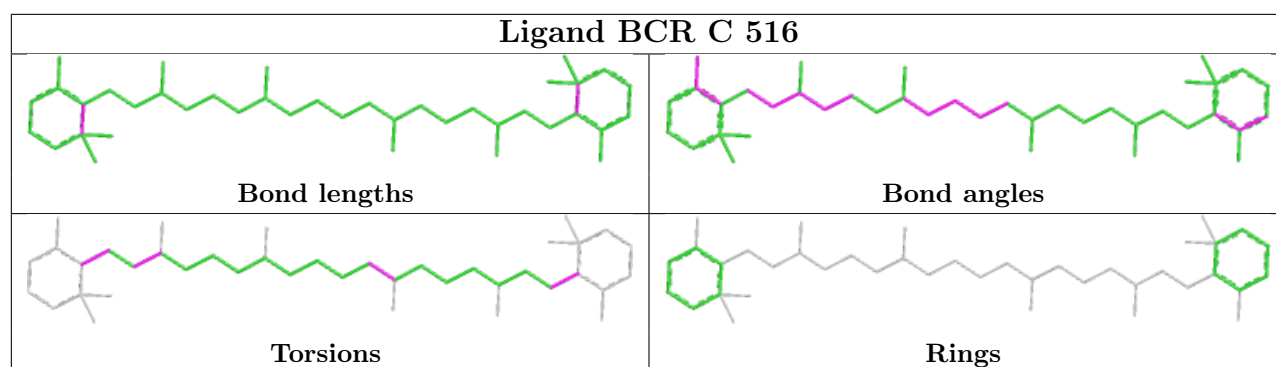
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Bond lengths	Bond angles
	
Torsions	Rings

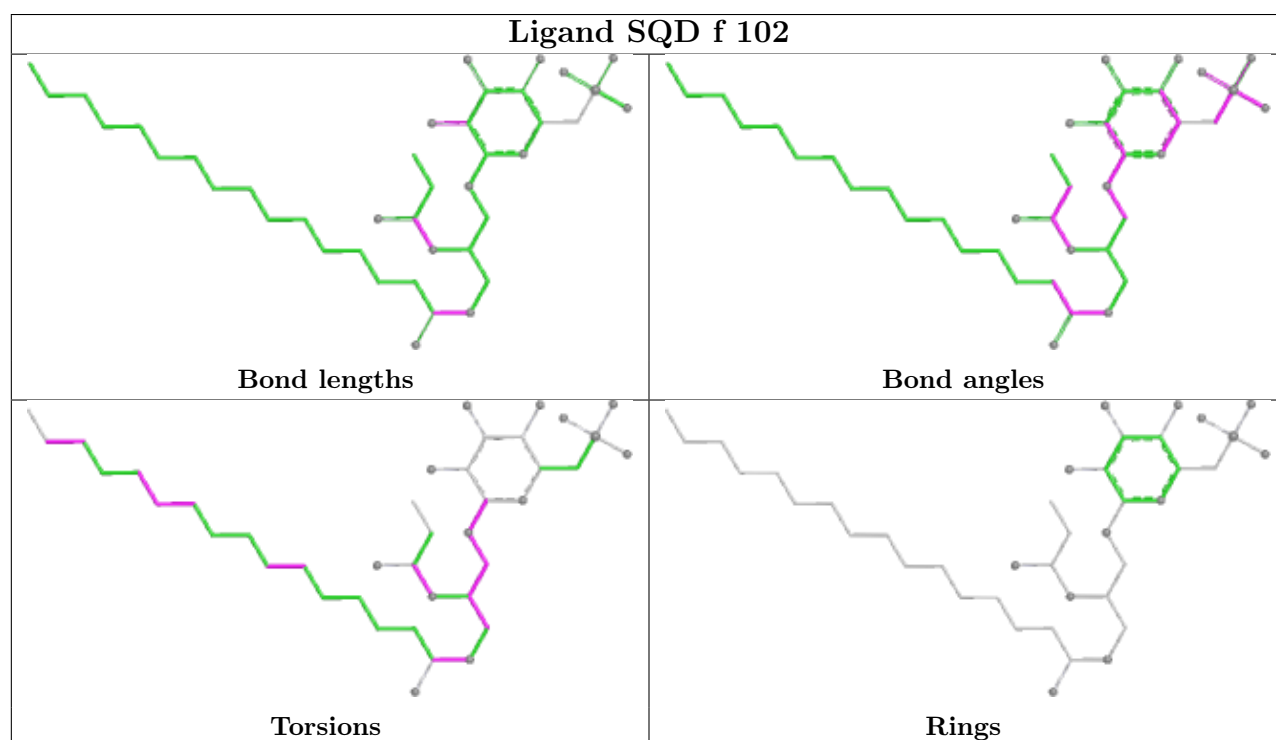
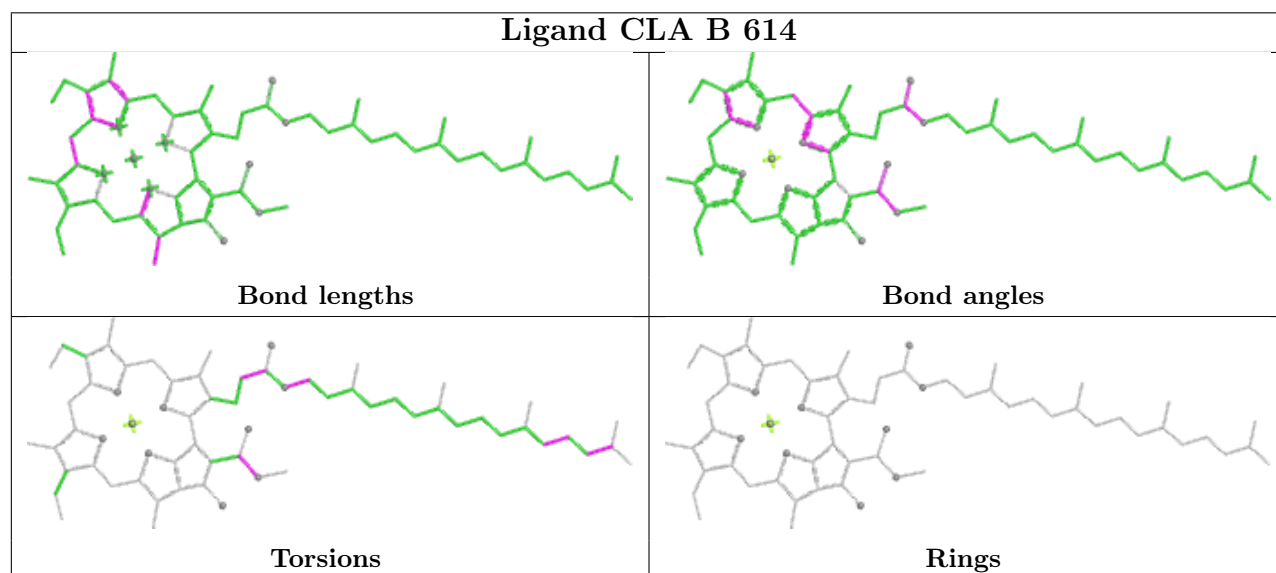
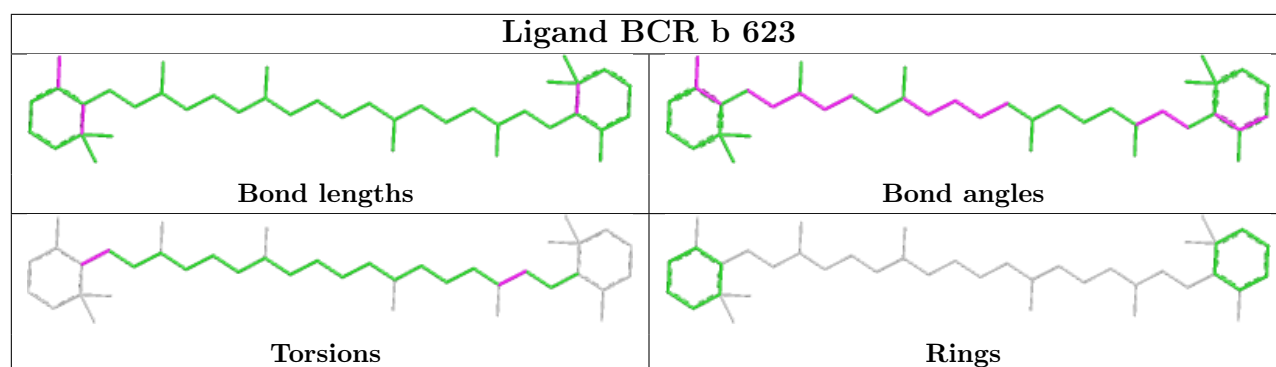
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Bond lengths	Bond angles
	
Torsions	Rings

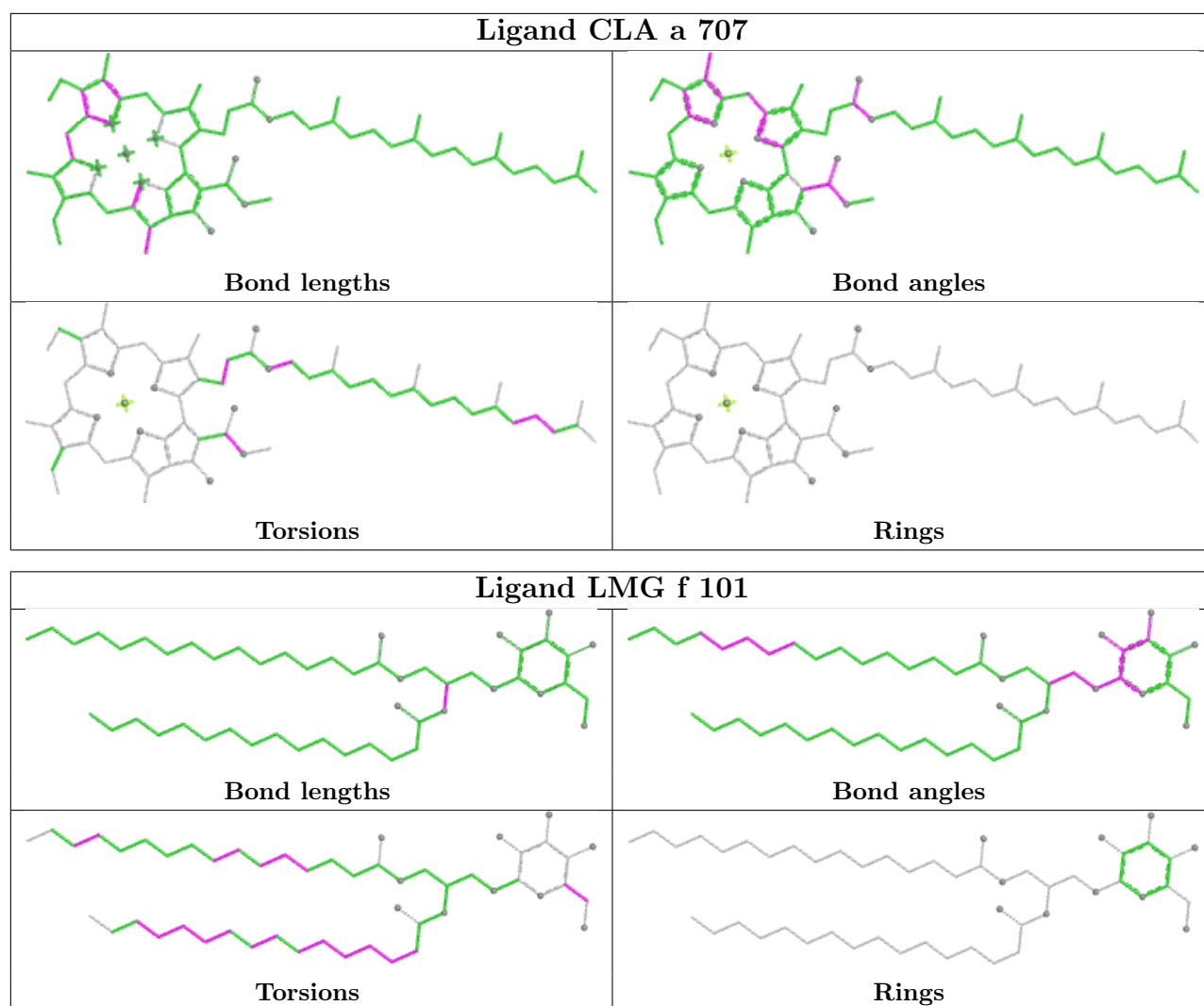




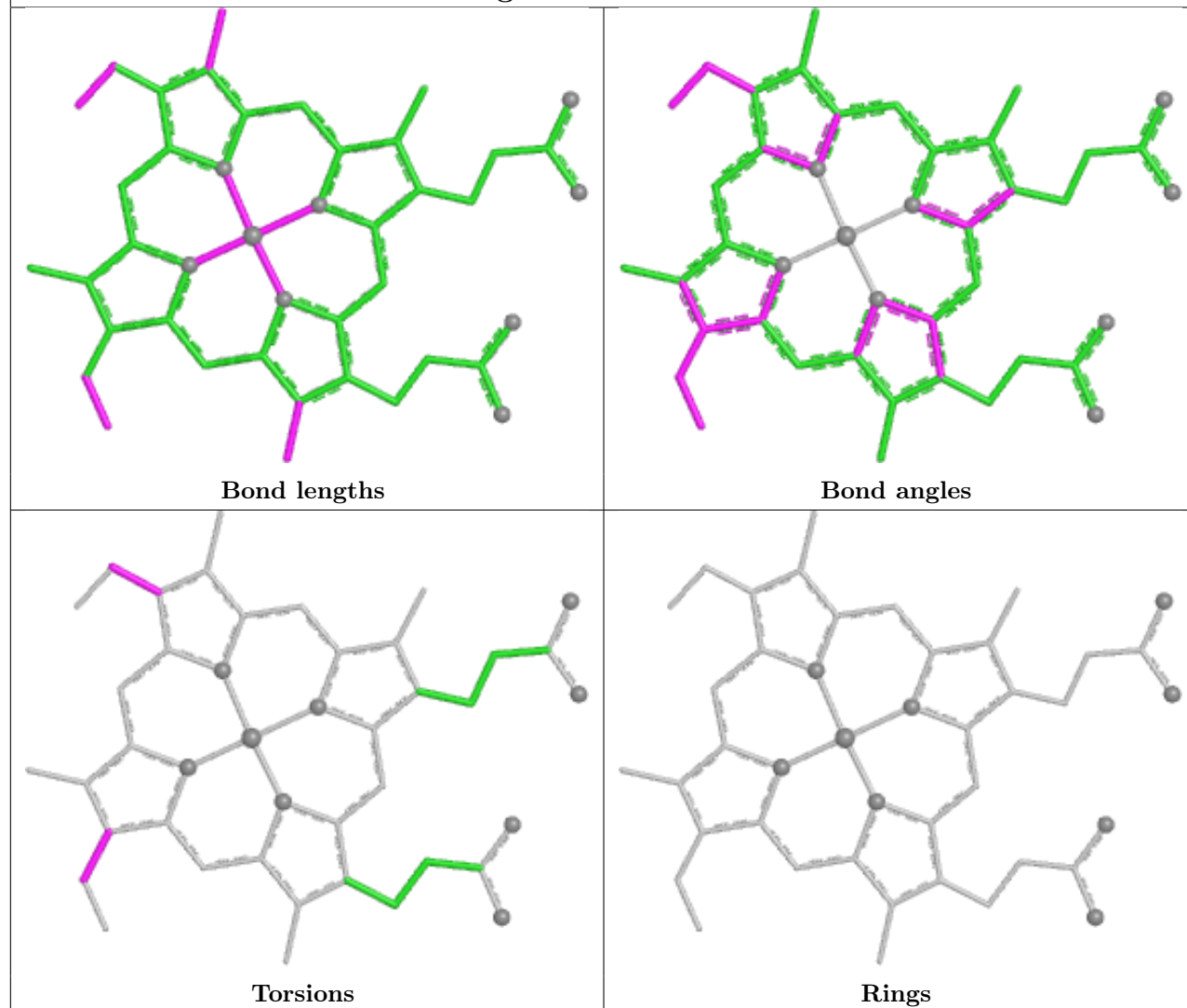




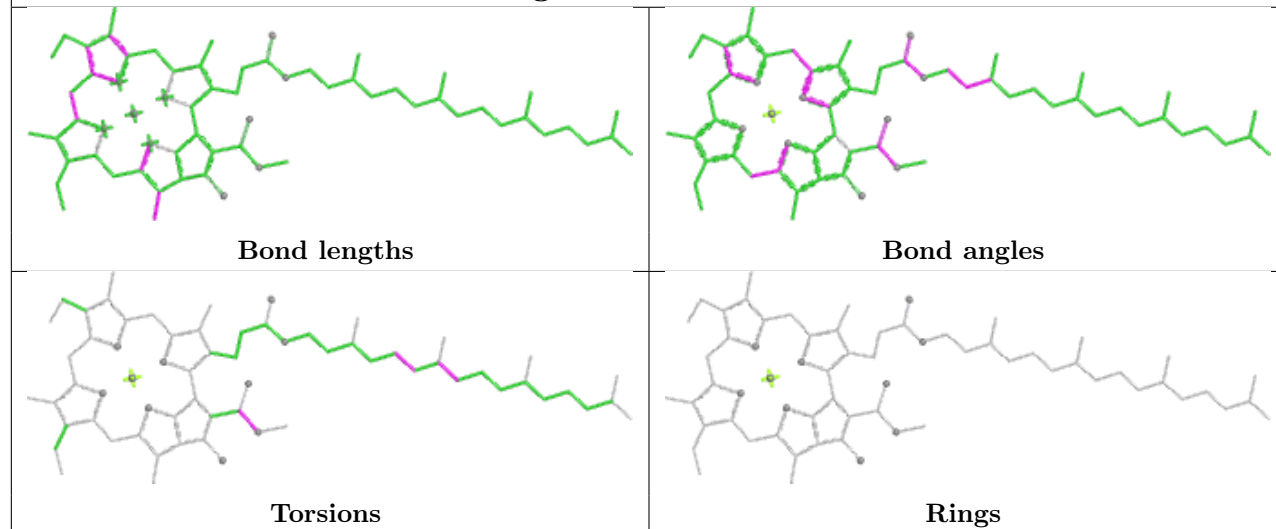


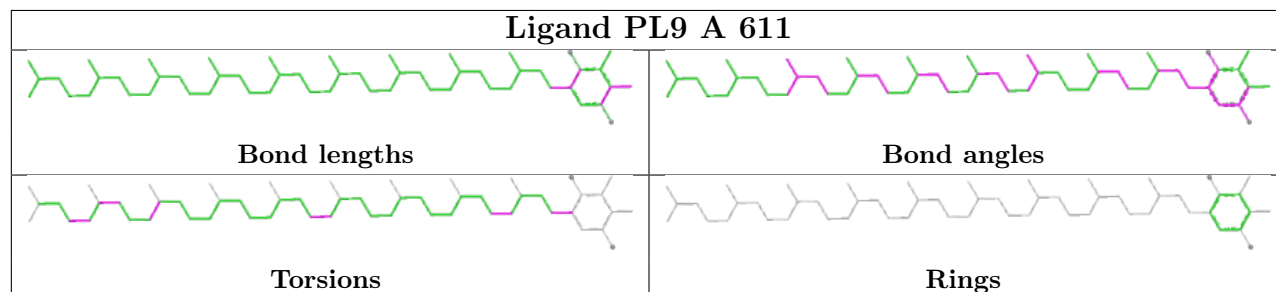
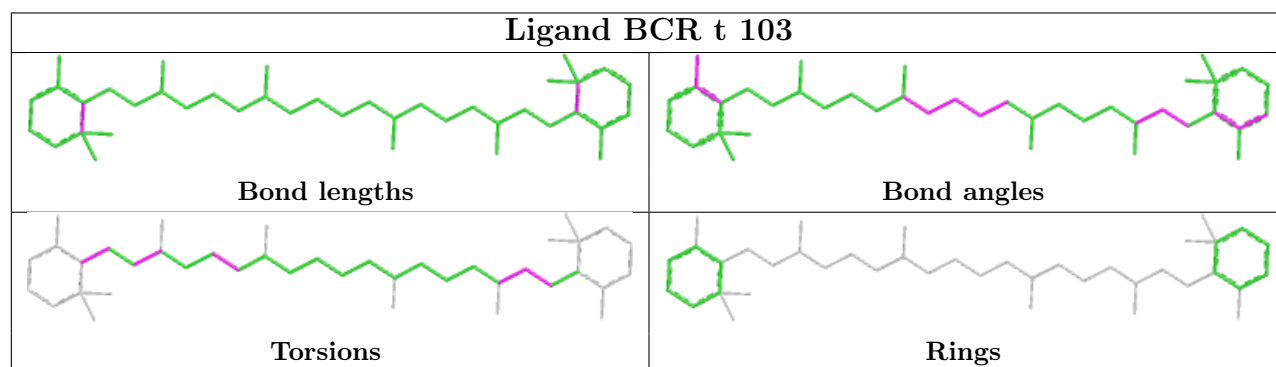
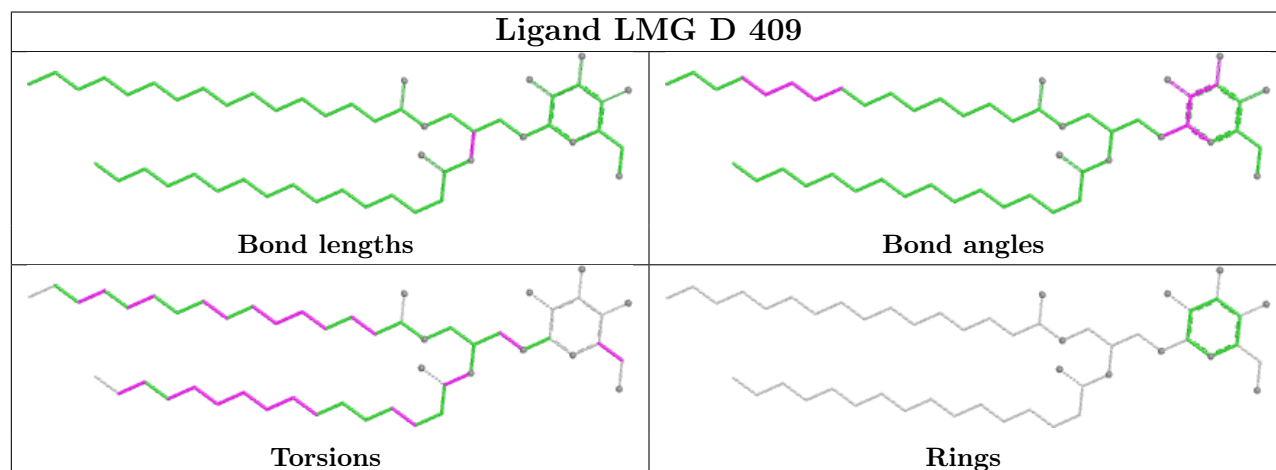
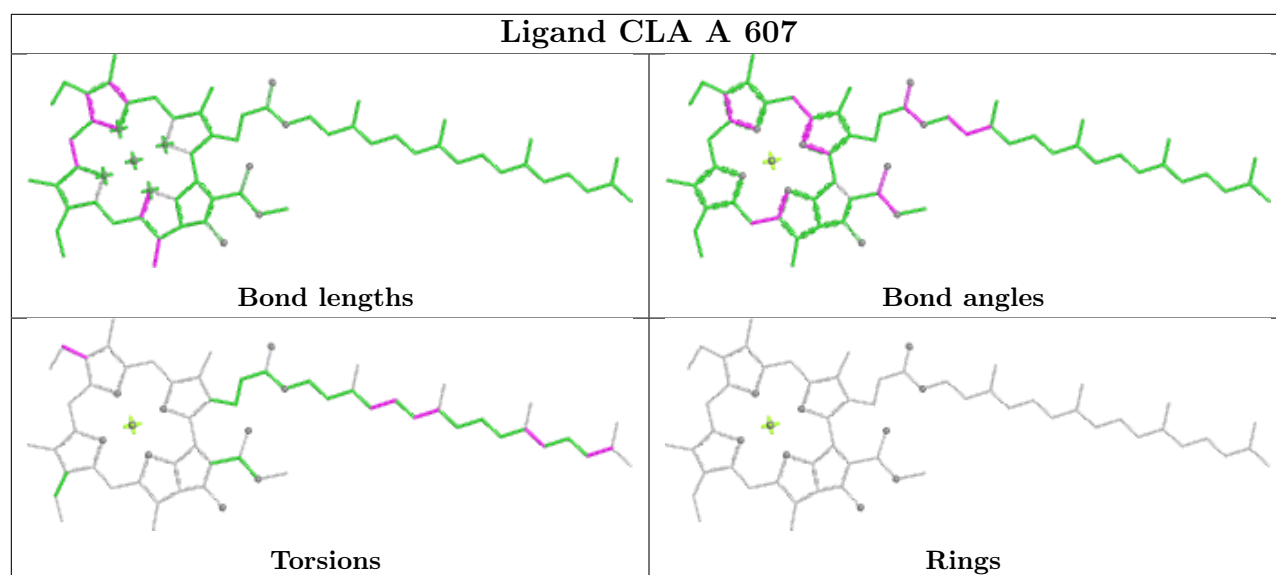


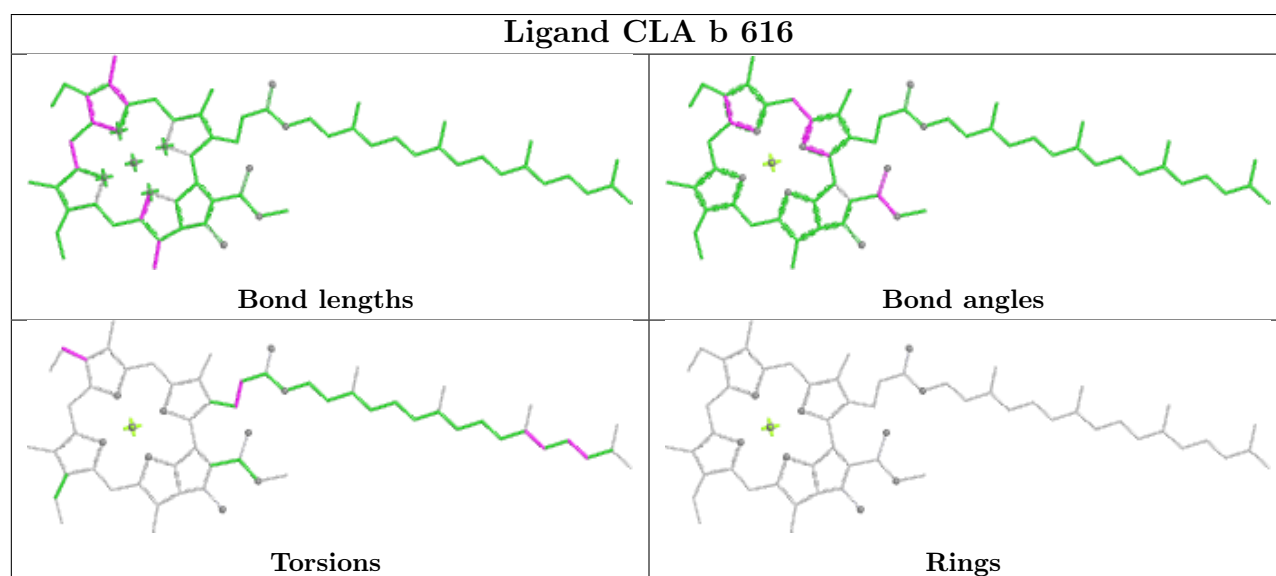
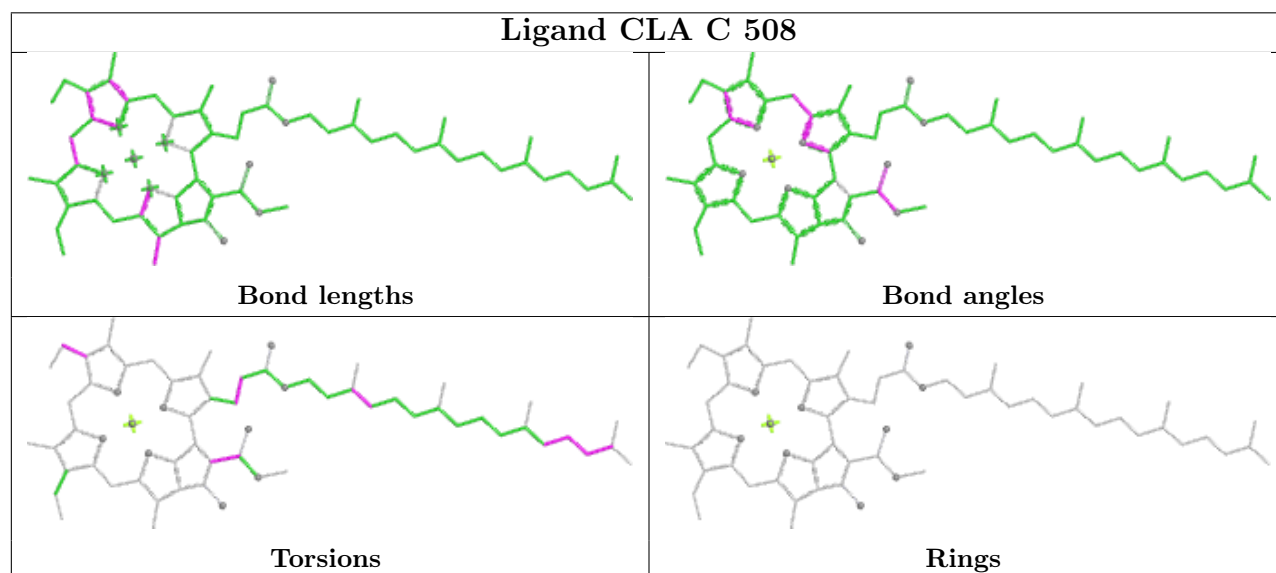
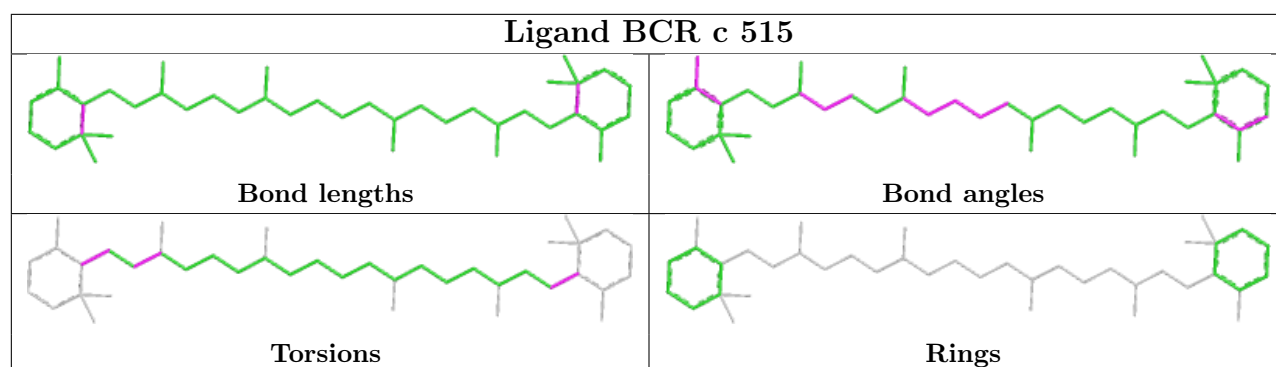
Ligand HEC v 201

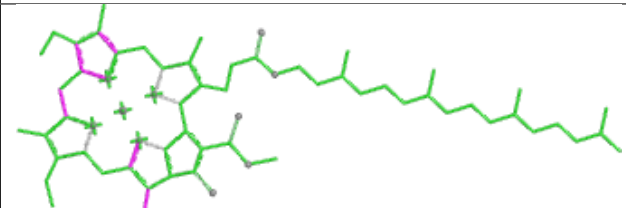
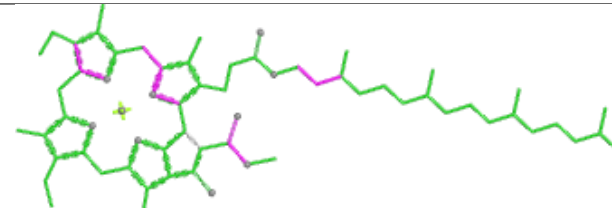
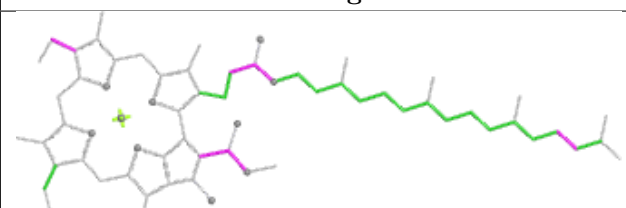
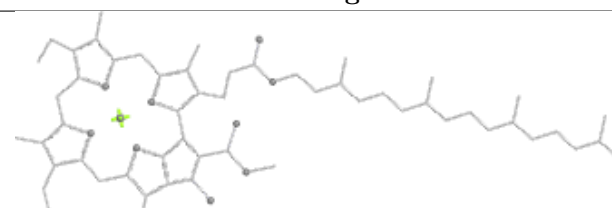


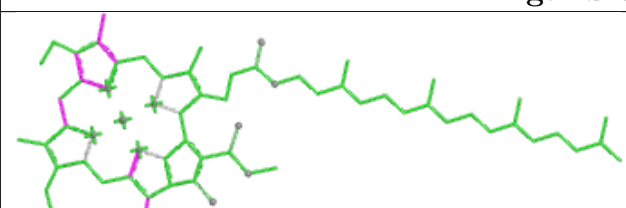
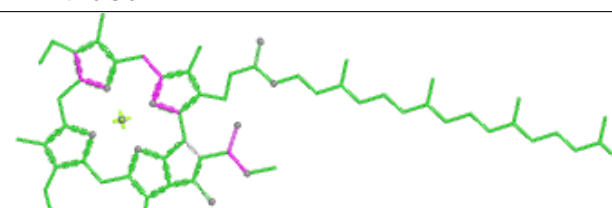
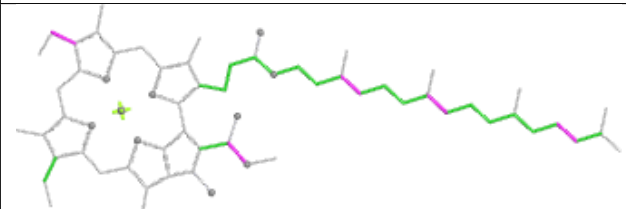
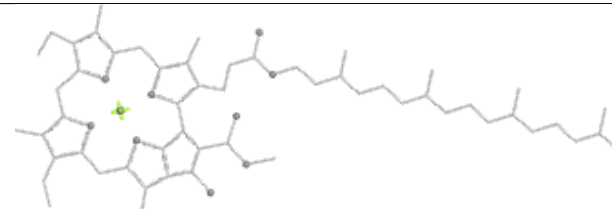
Ligand CLA C 509

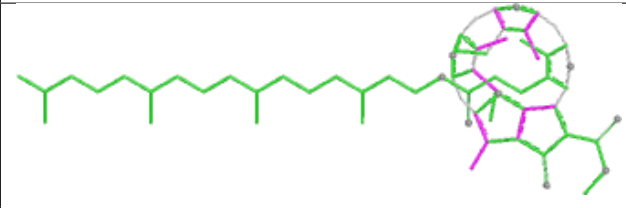
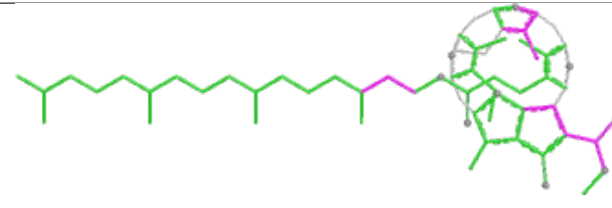
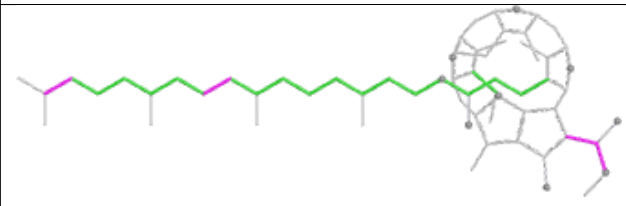
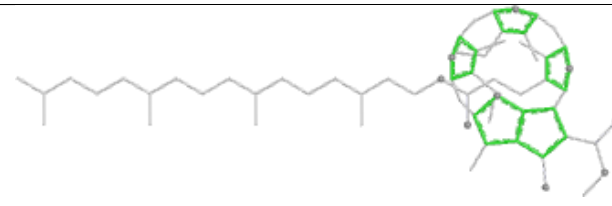


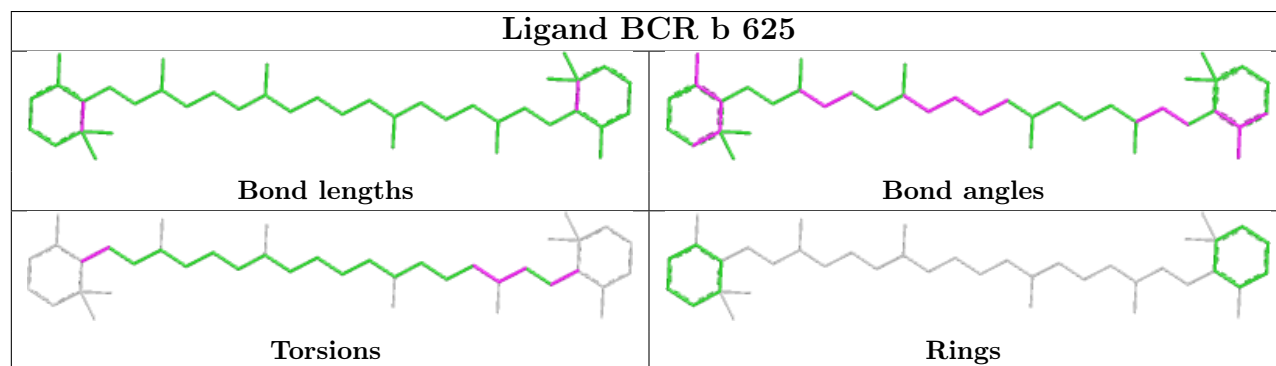
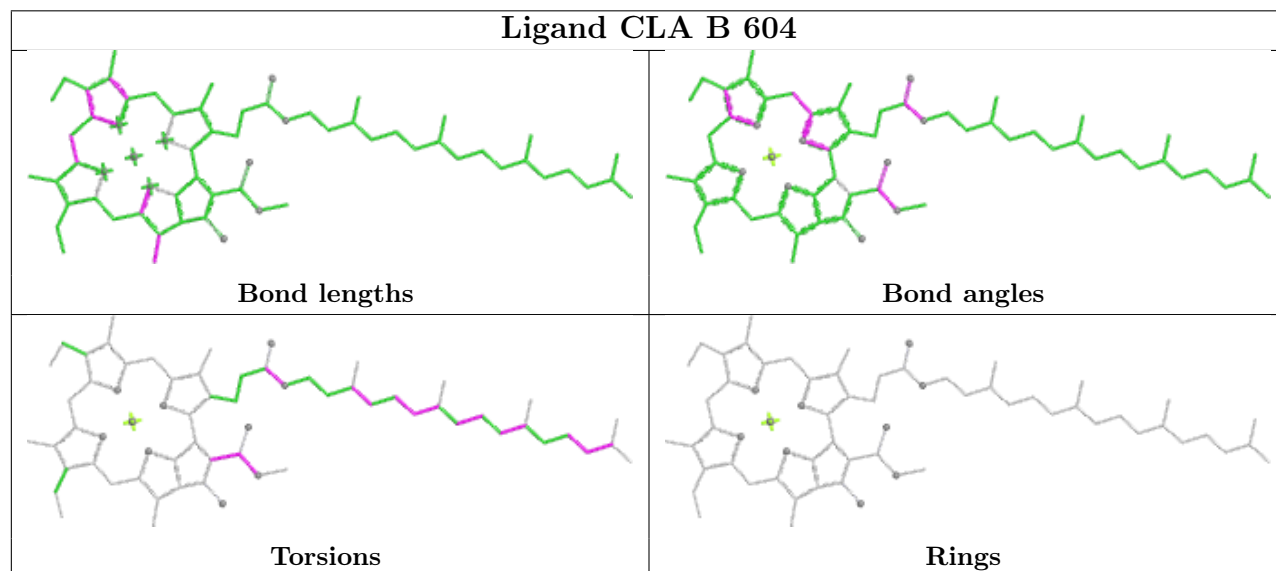
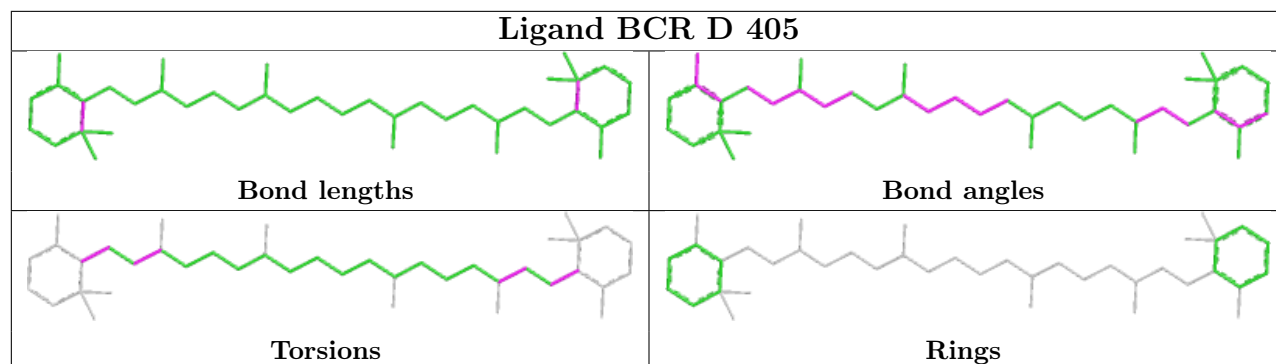


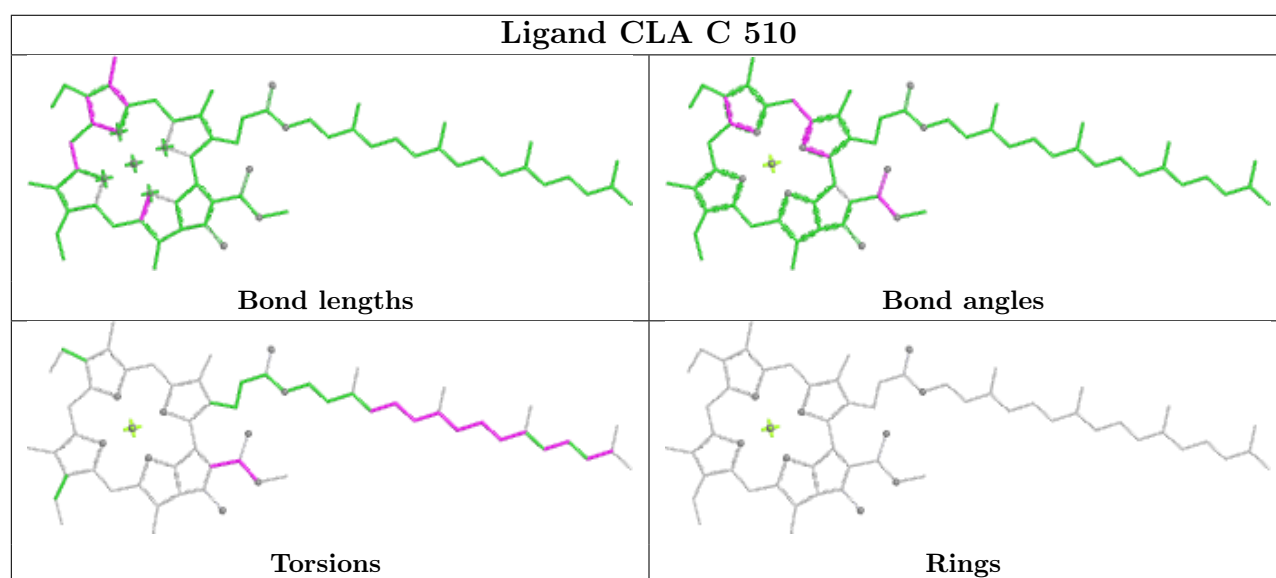
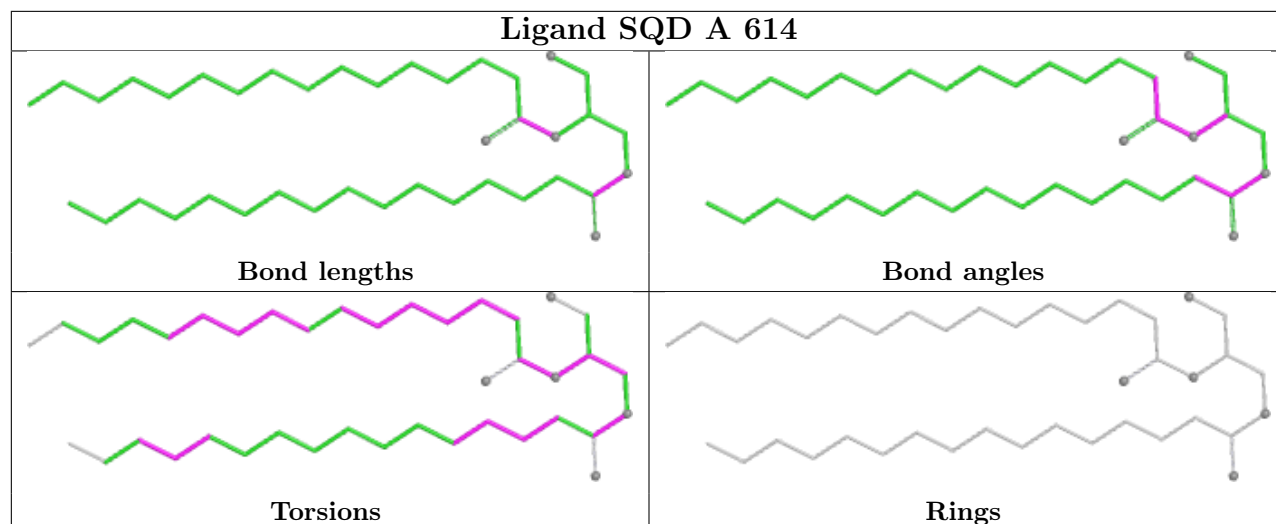


Ligand CLA b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

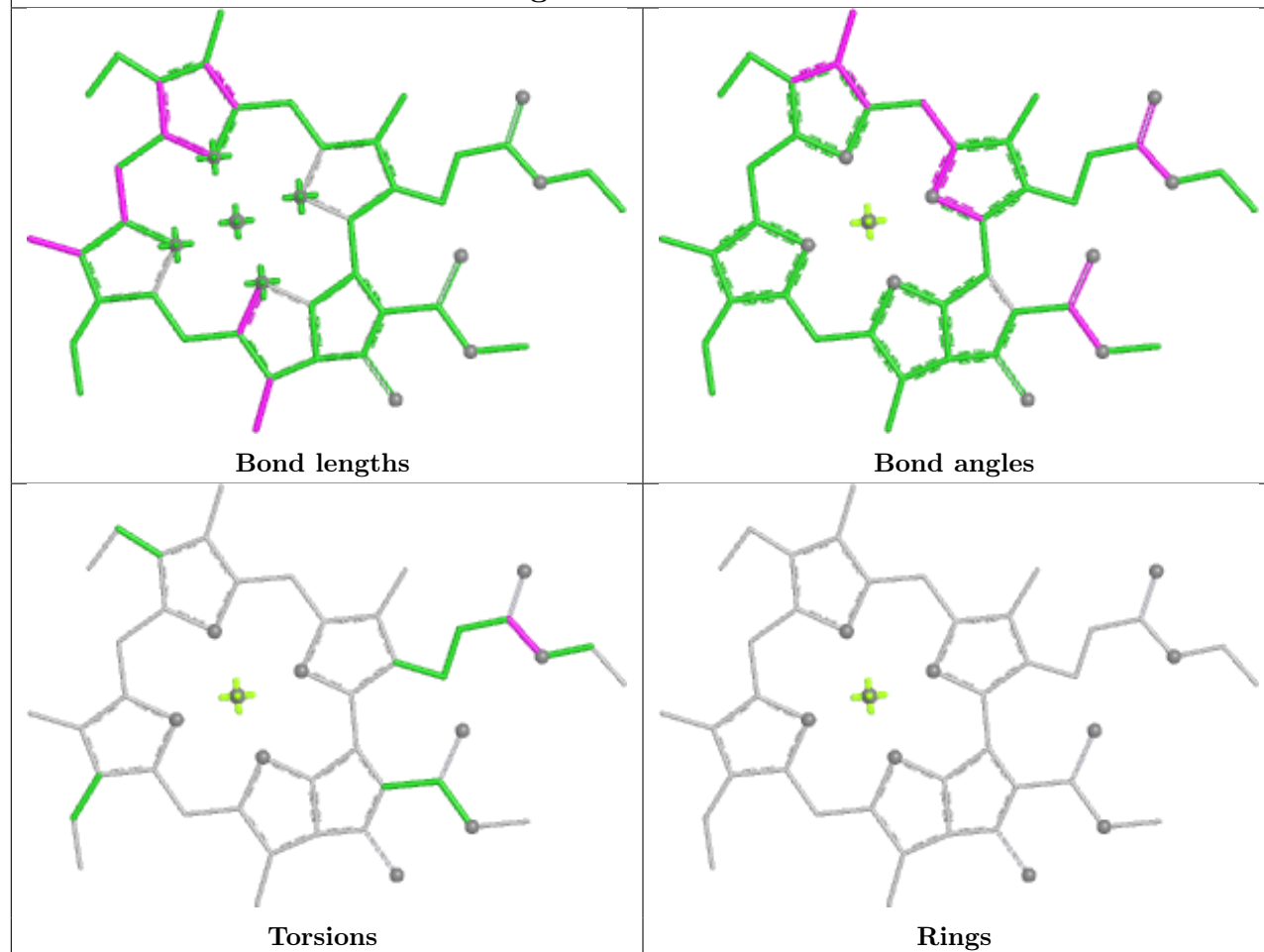
Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO a 710	
	
Bond lengths	Bond angles
	
Torsions	Rings

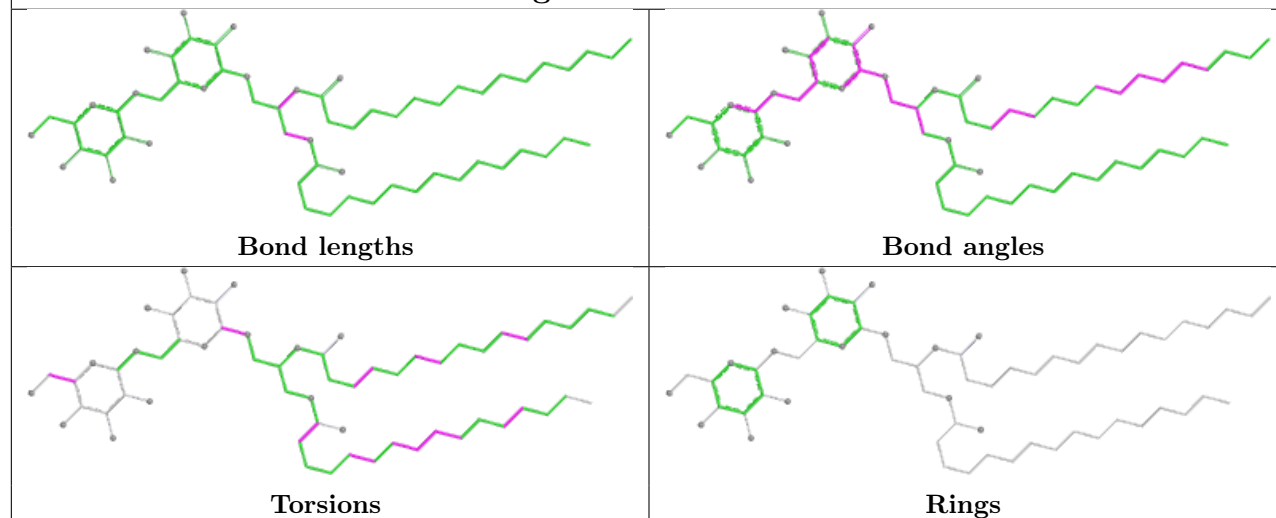


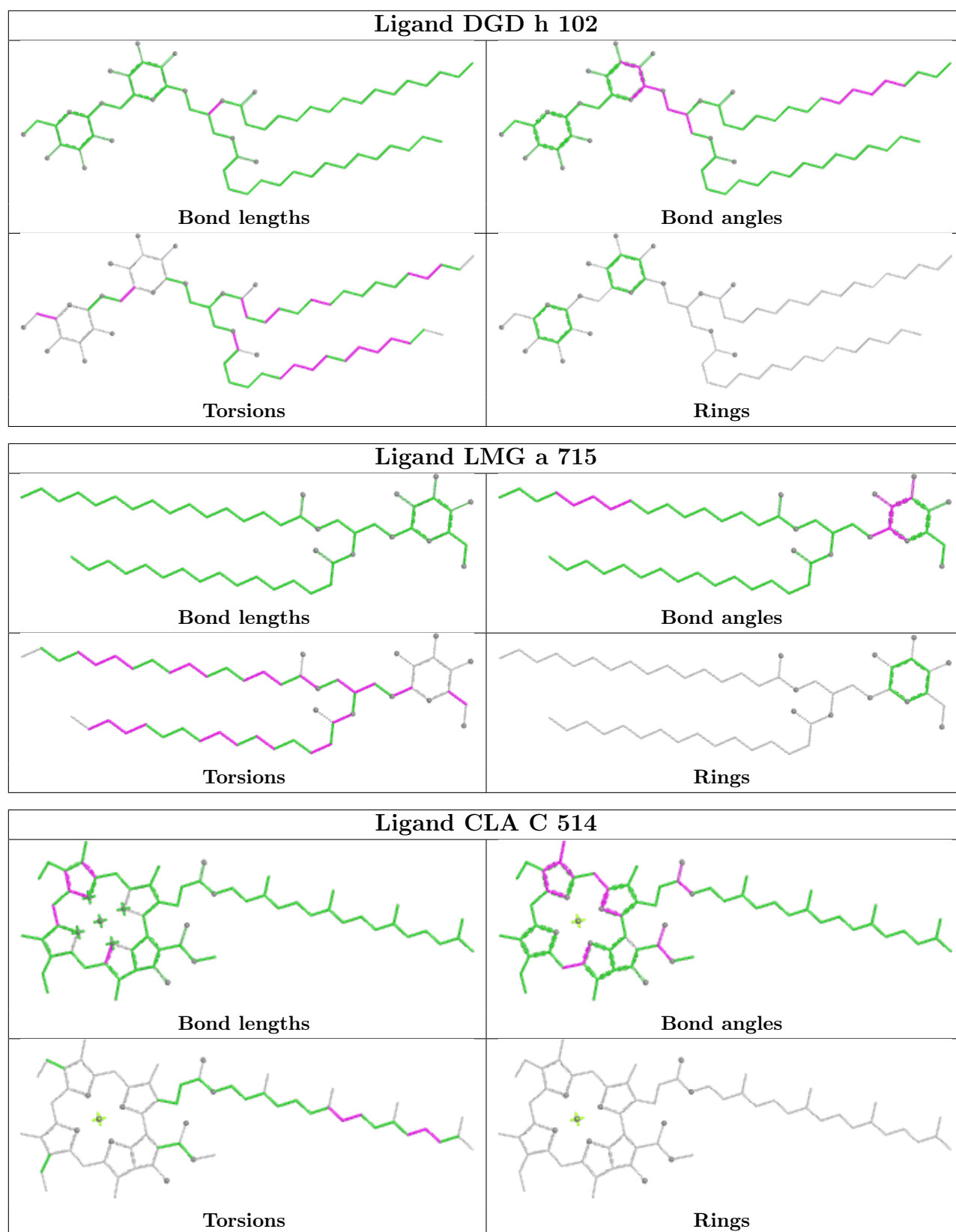


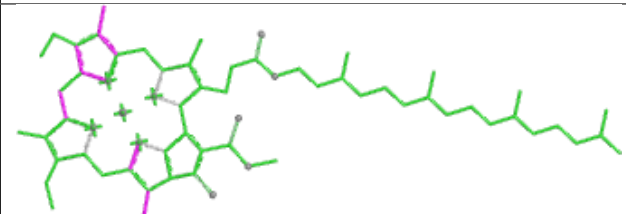
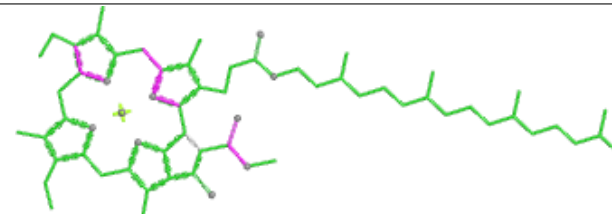
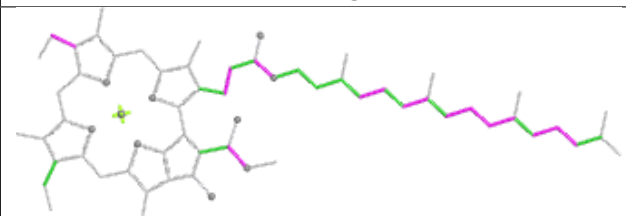
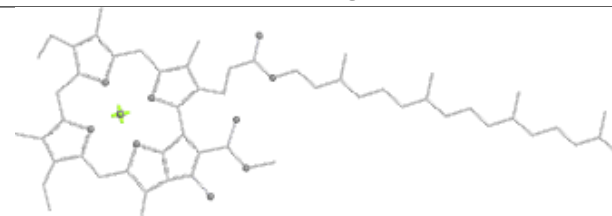
Ligand CLA b 622

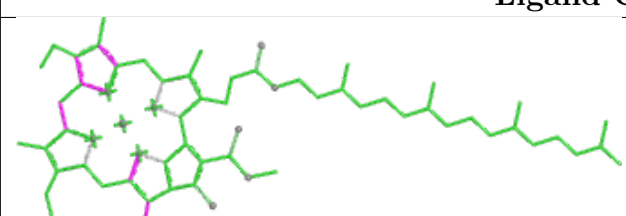
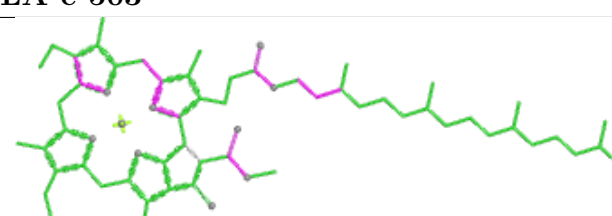
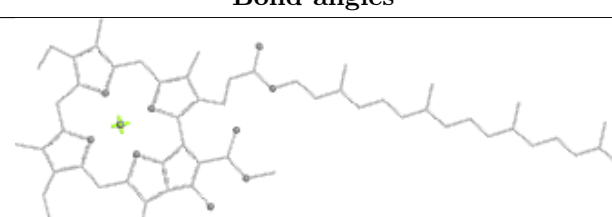


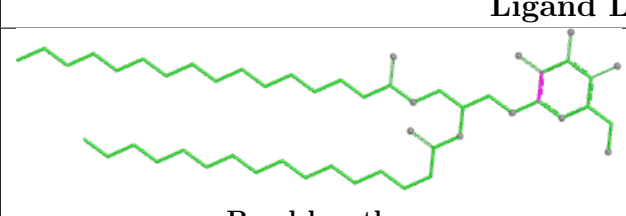
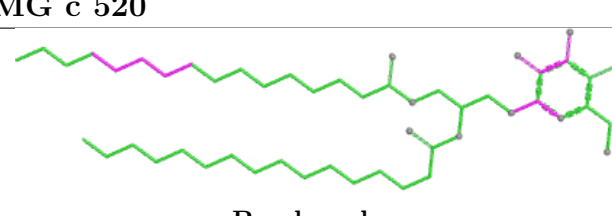
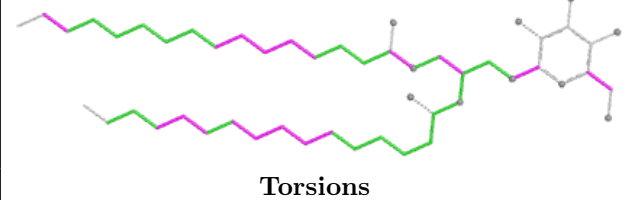
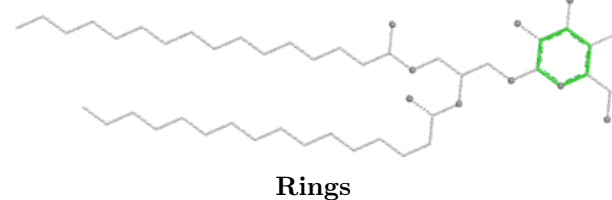
Ligand DGD c 518

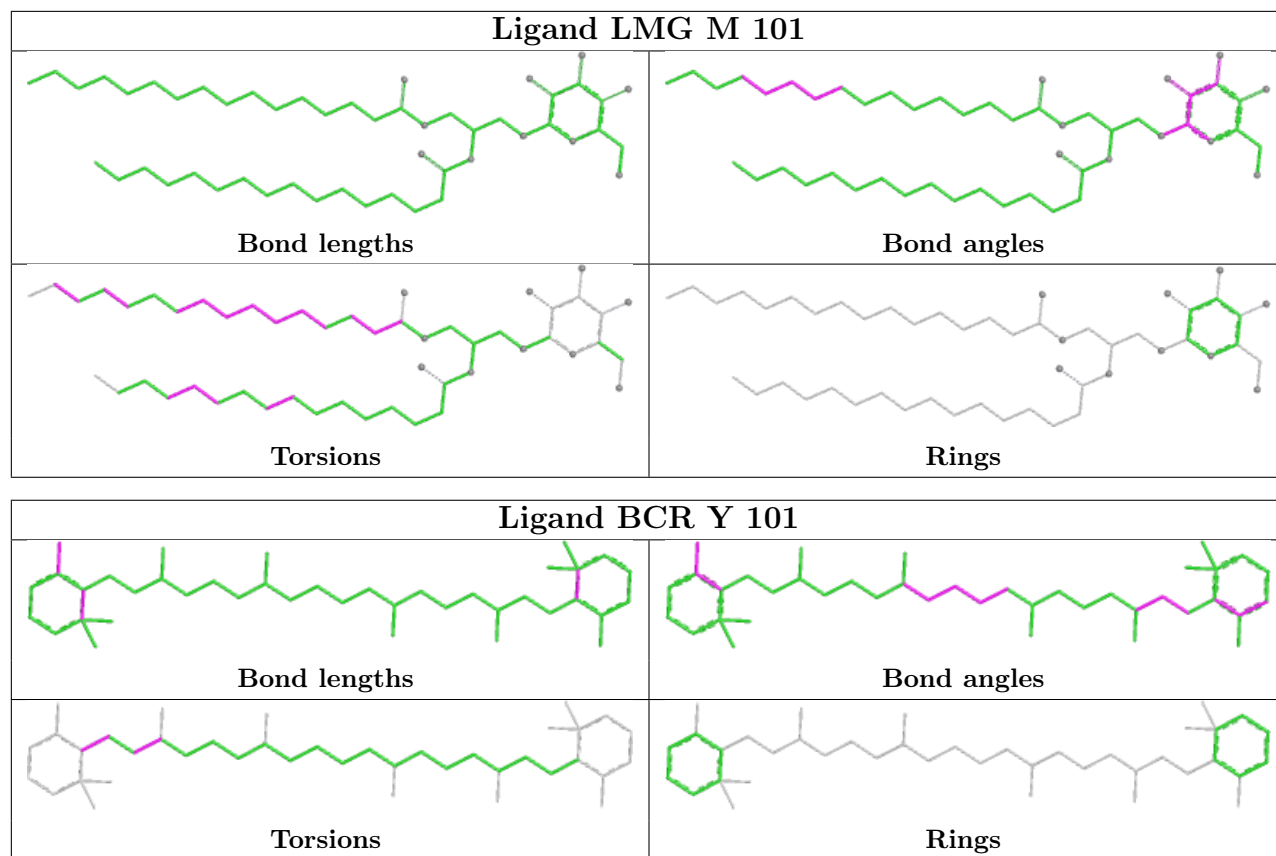


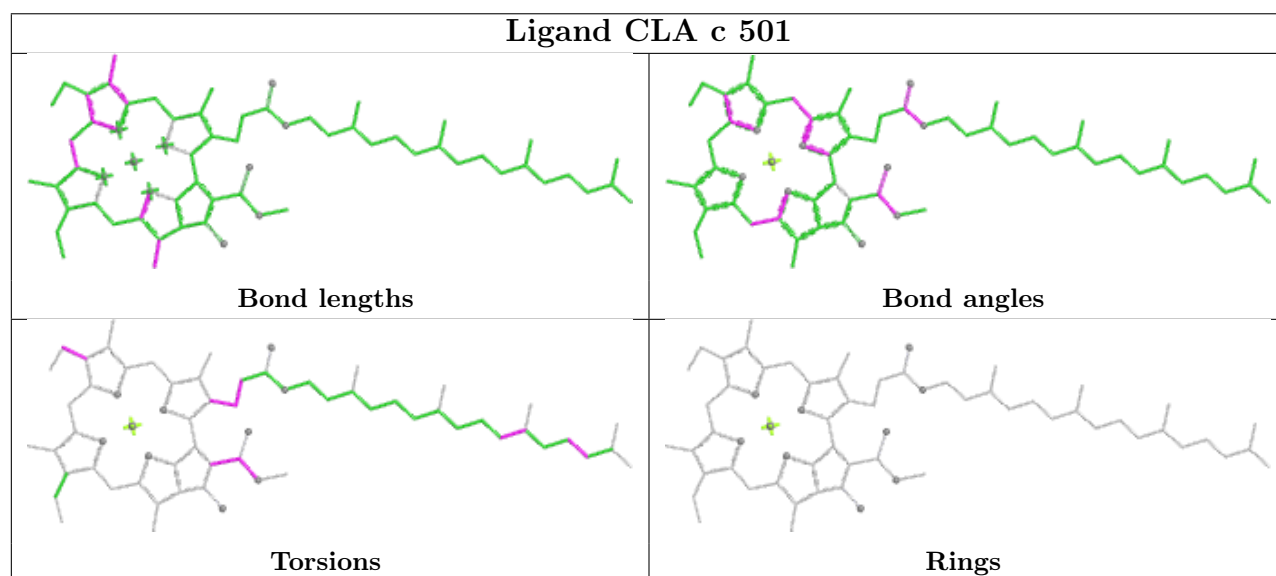
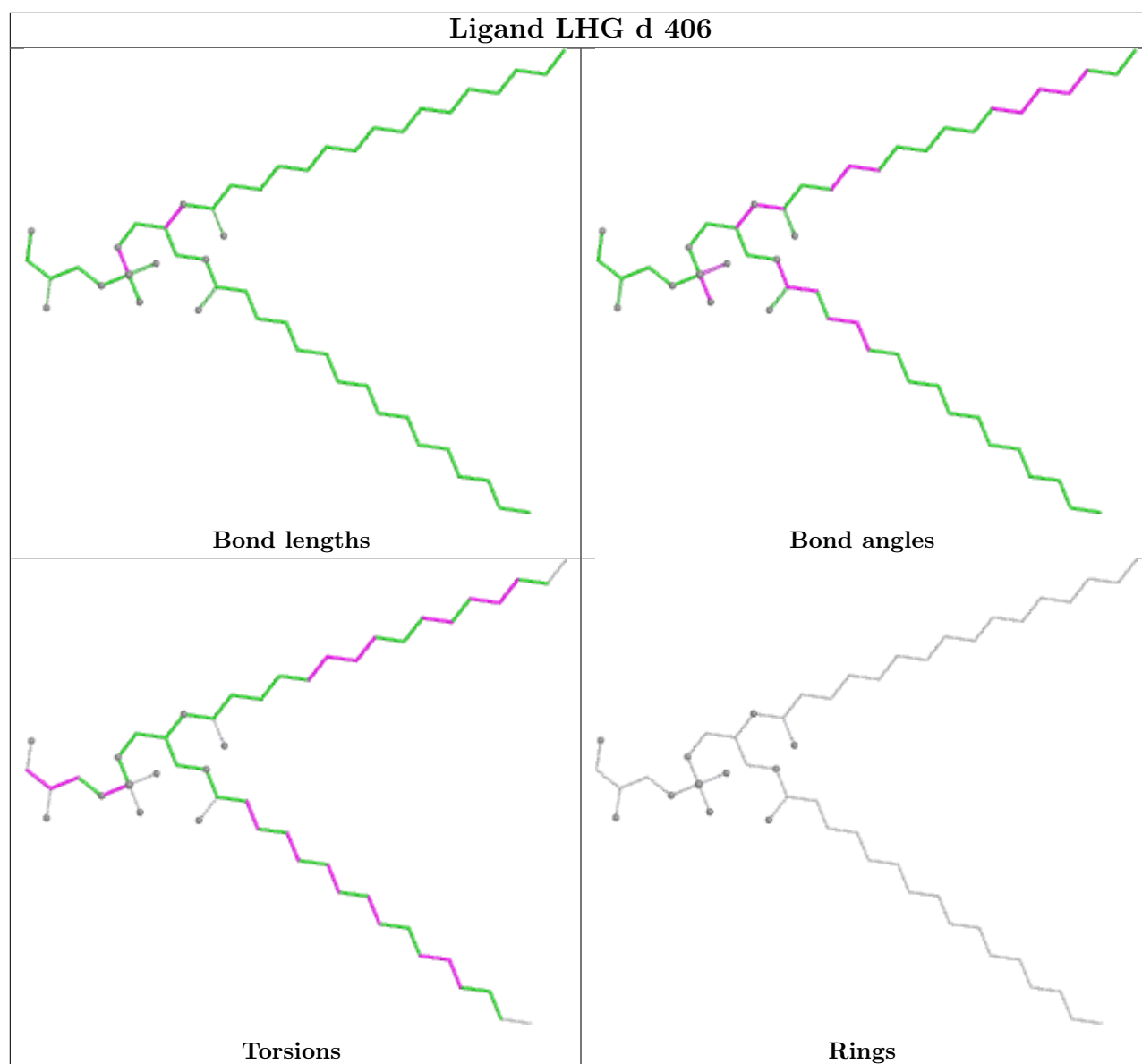


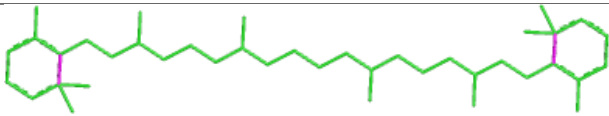
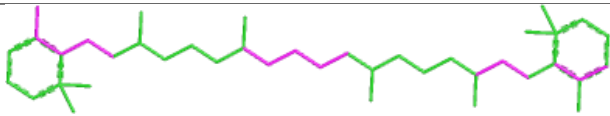
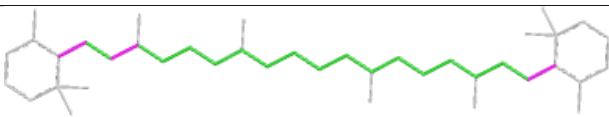
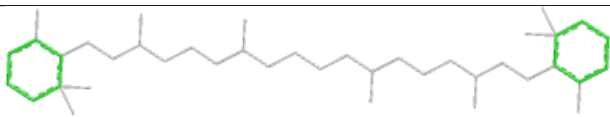
Ligand CLA B 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

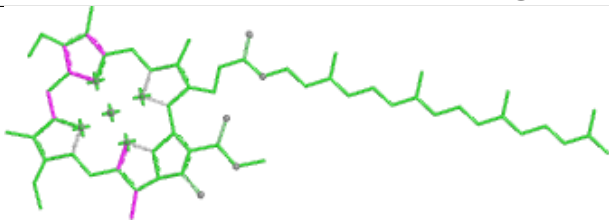
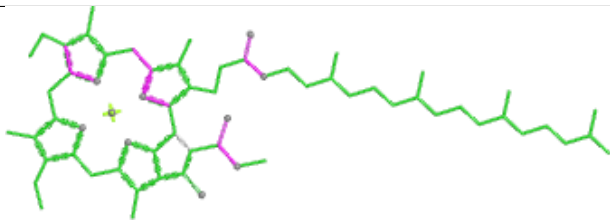
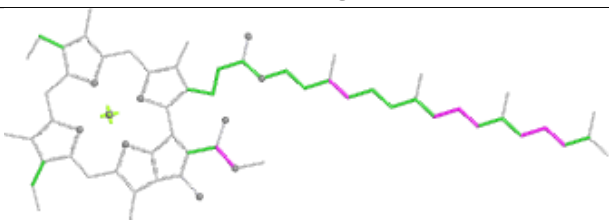
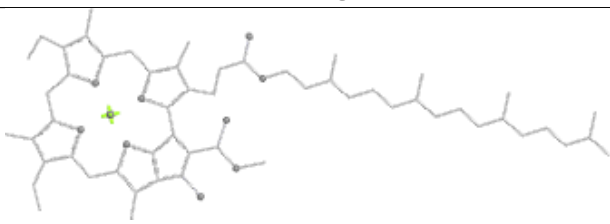
Ligand CLA c 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

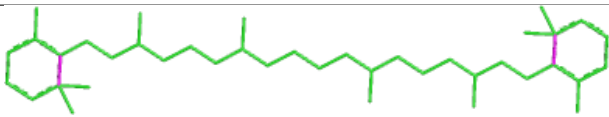
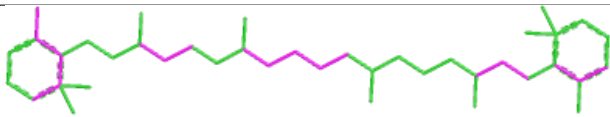
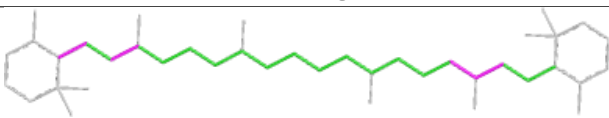
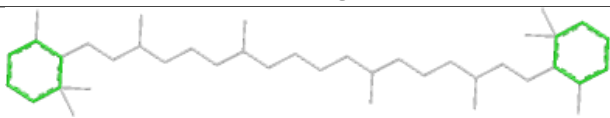
Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings



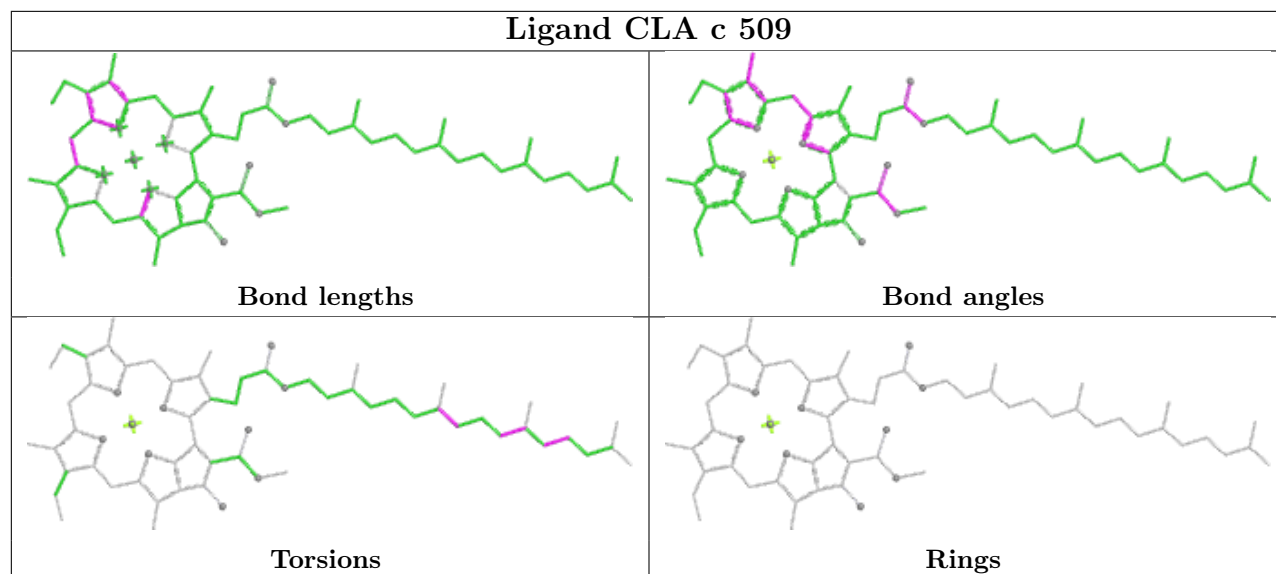


Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

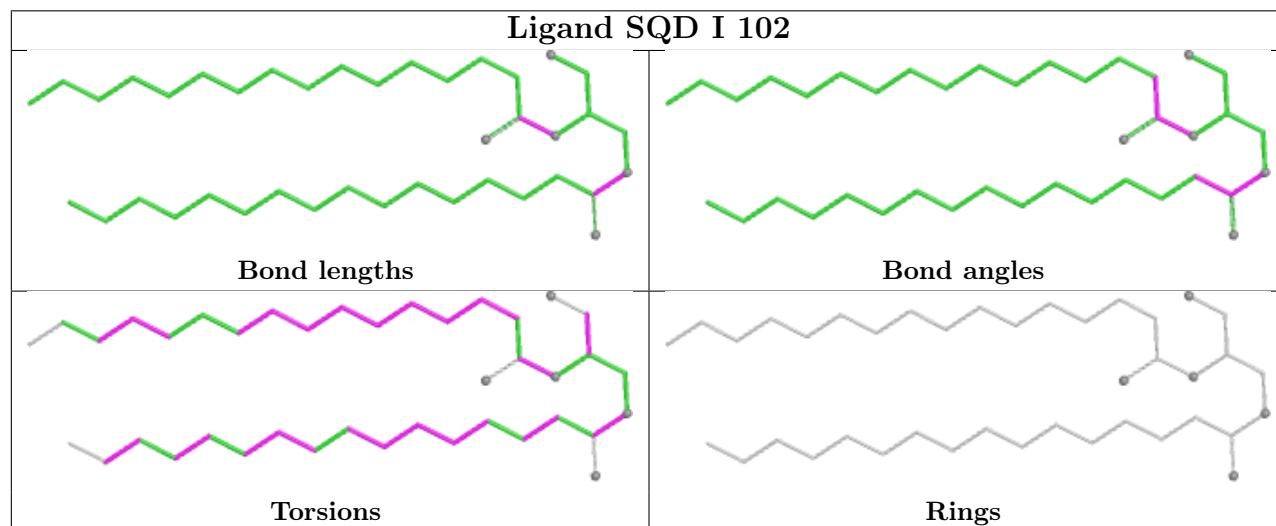
Ligand CLA b 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

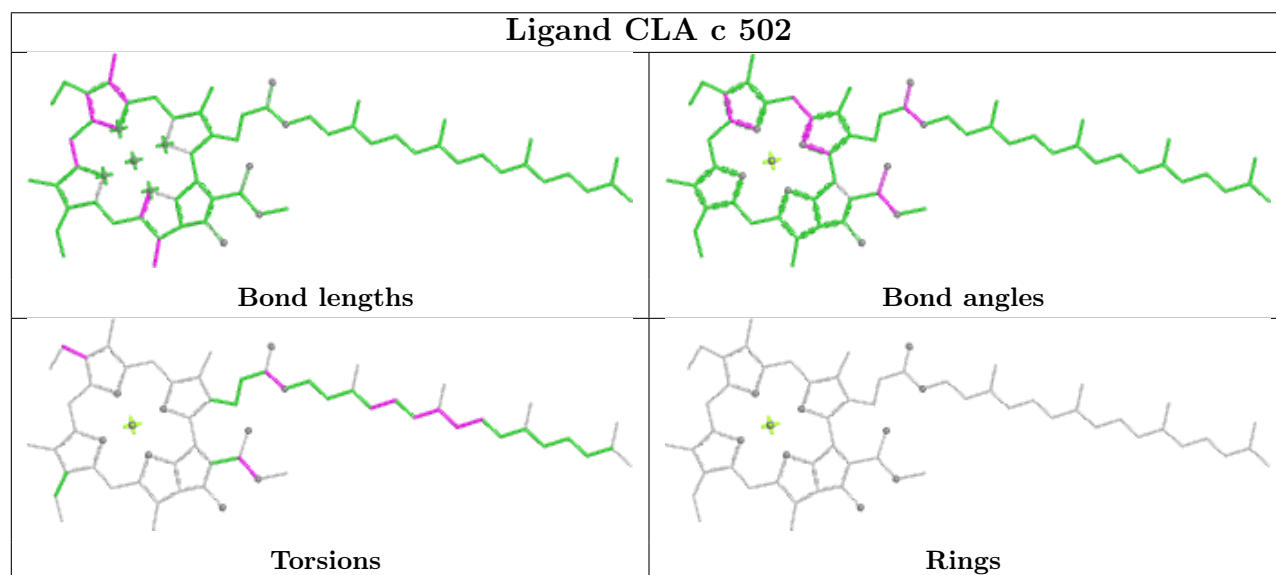
Ligand CLA c 509

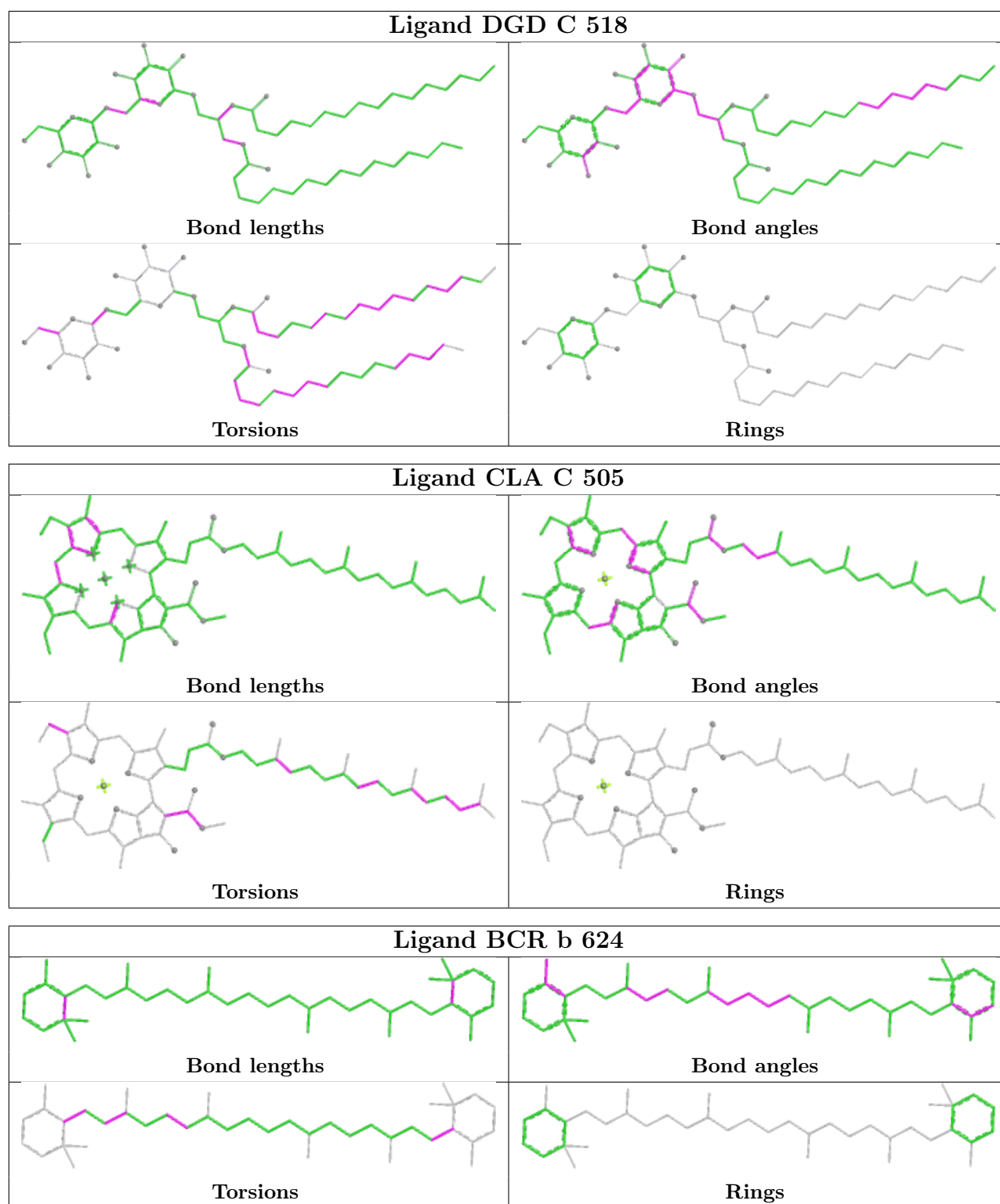


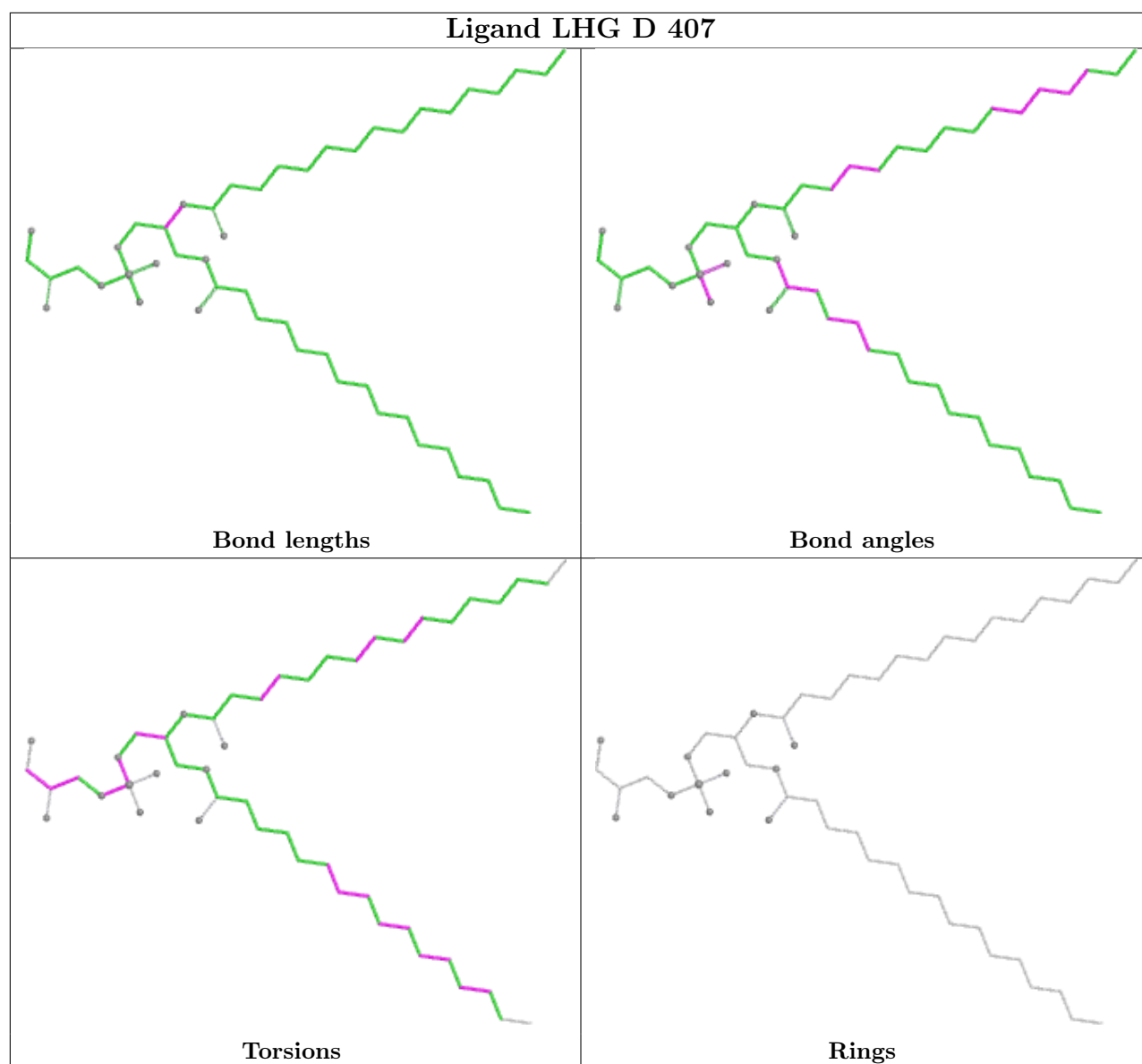
Ligand SQD I 102

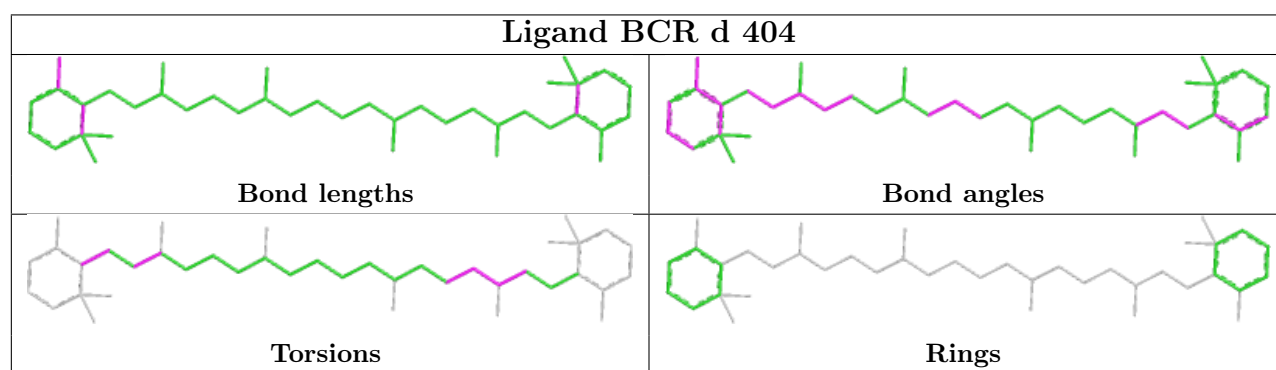
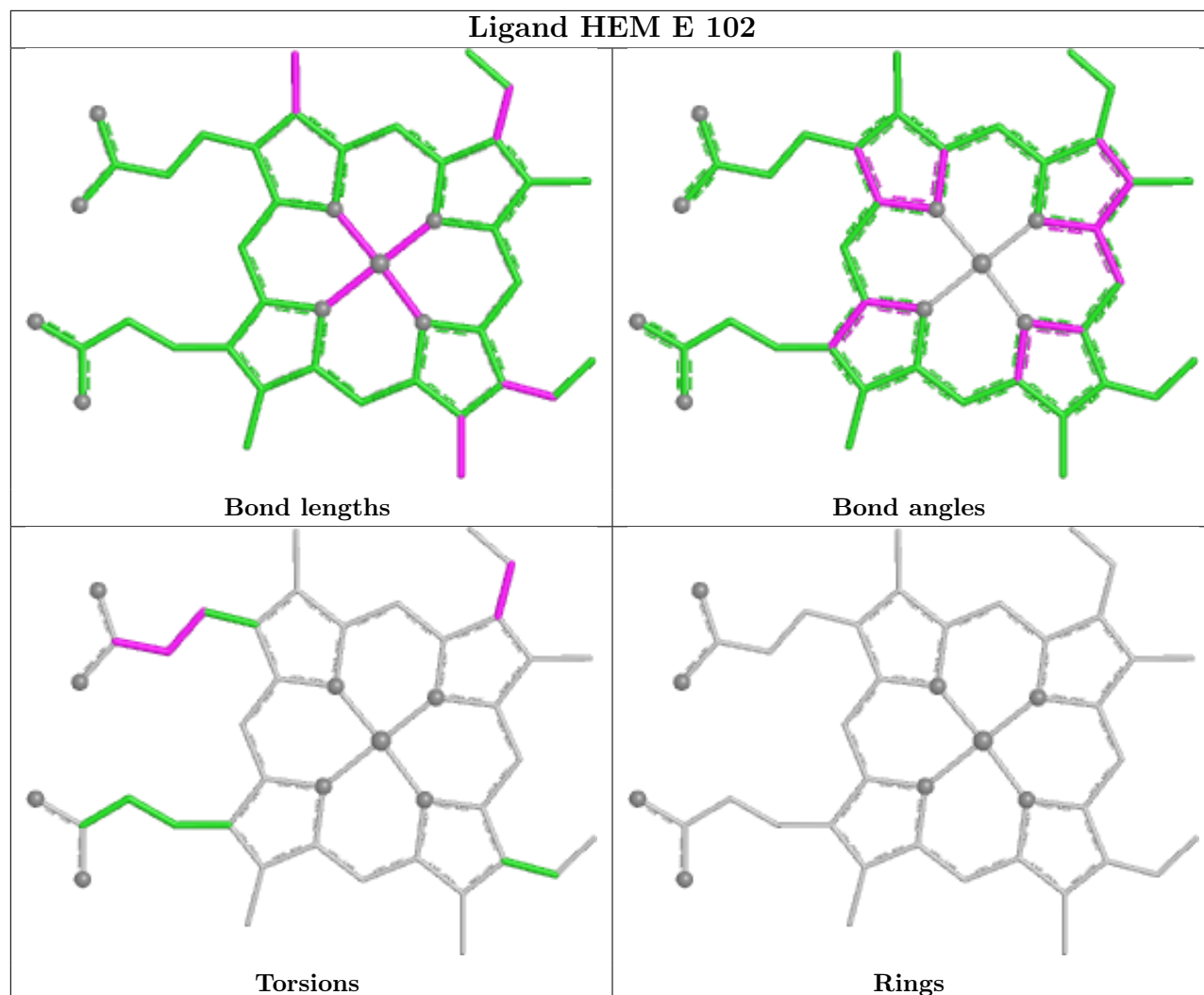


Ligand CLA c 502

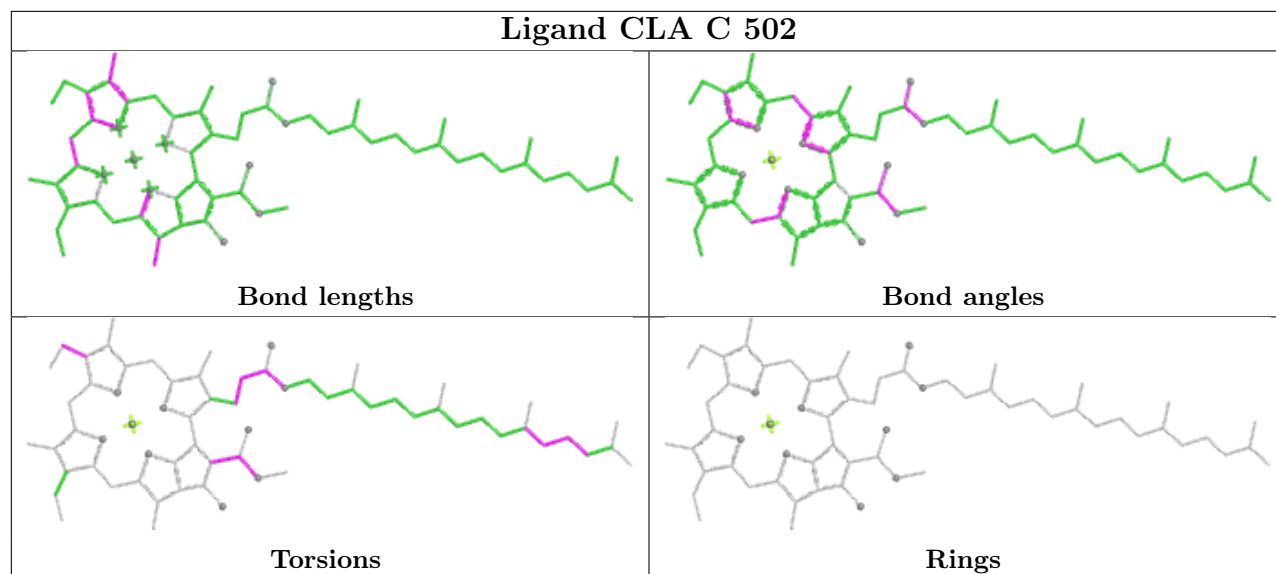




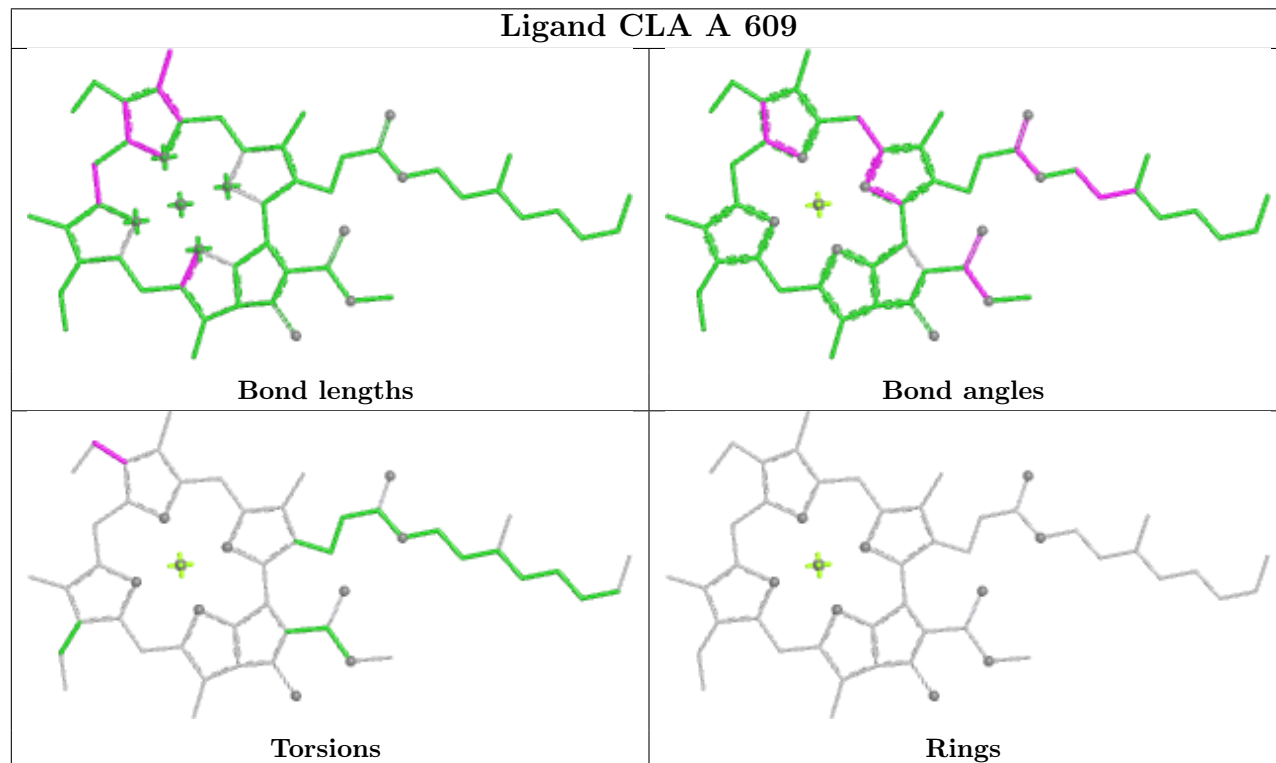


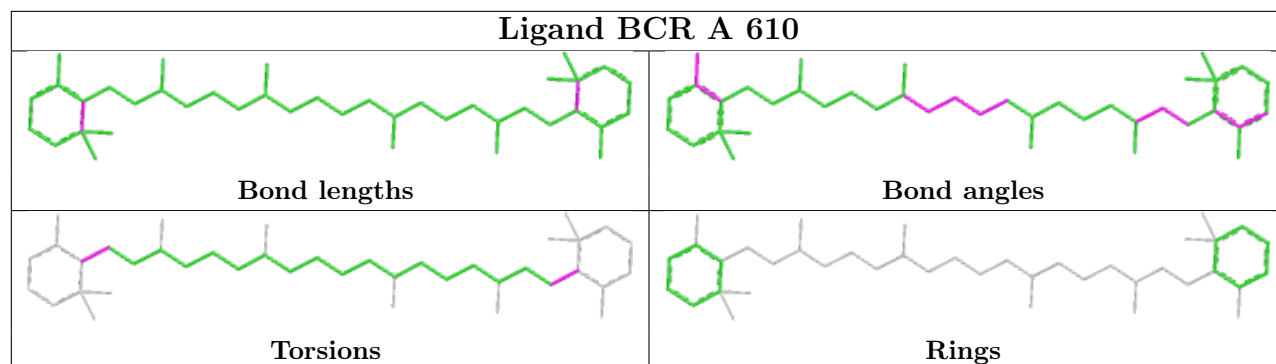
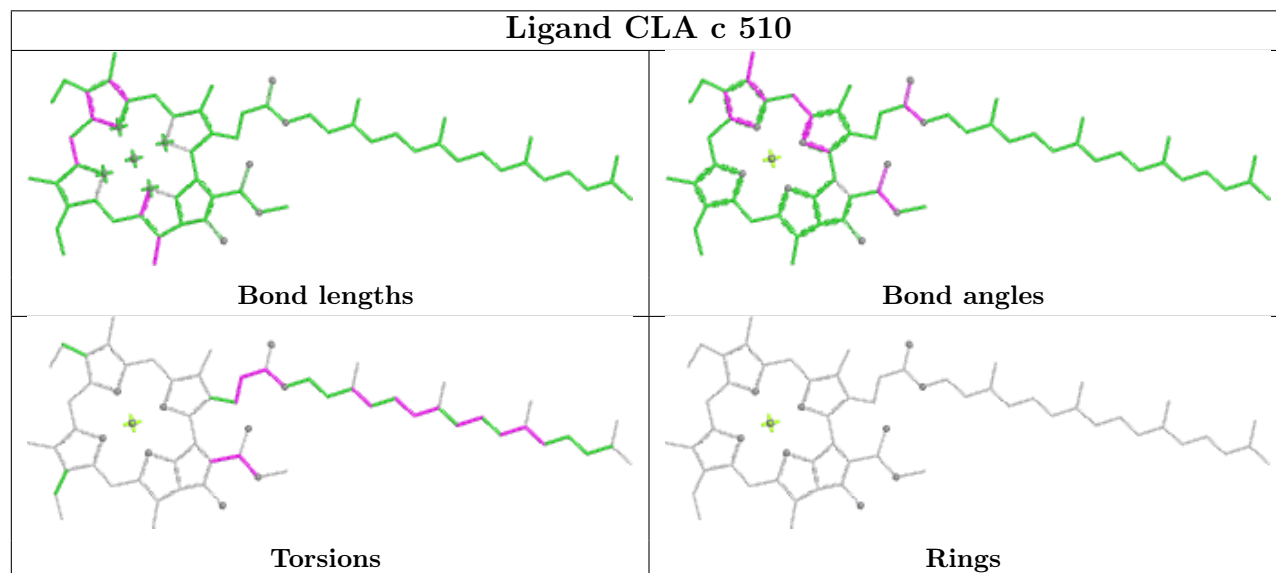
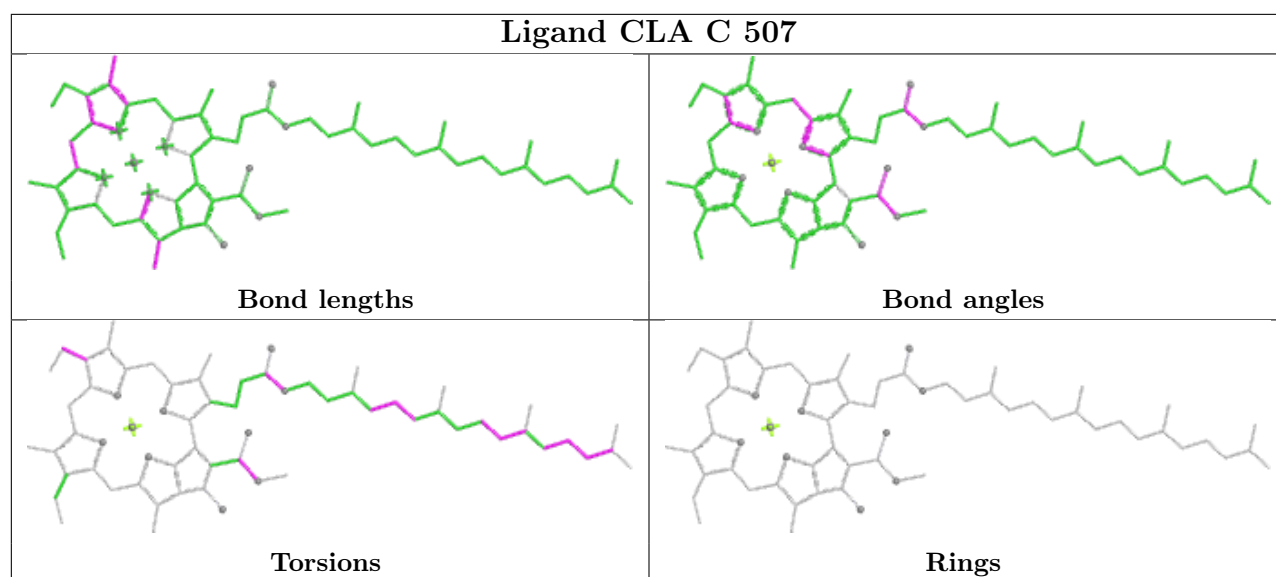


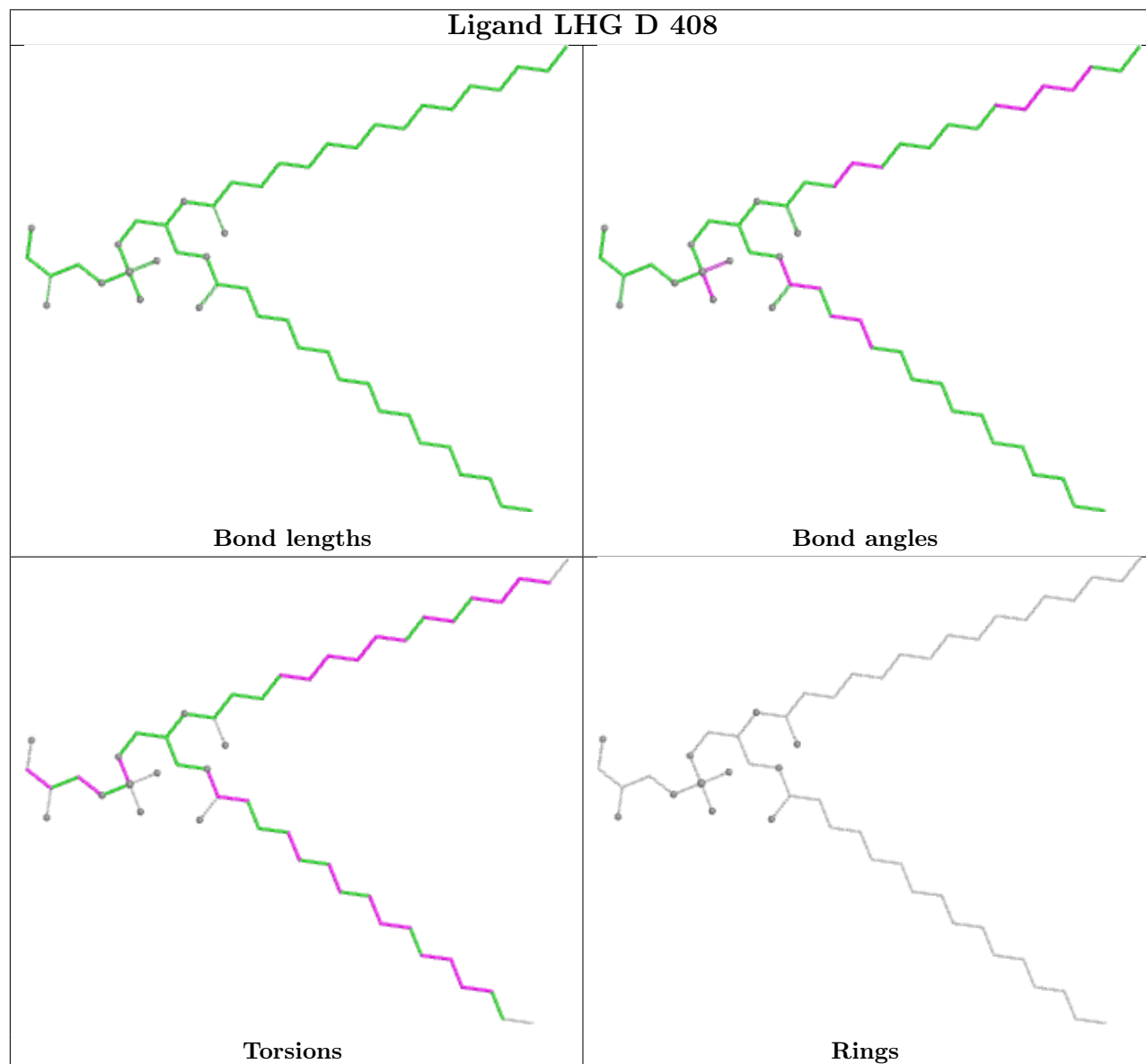
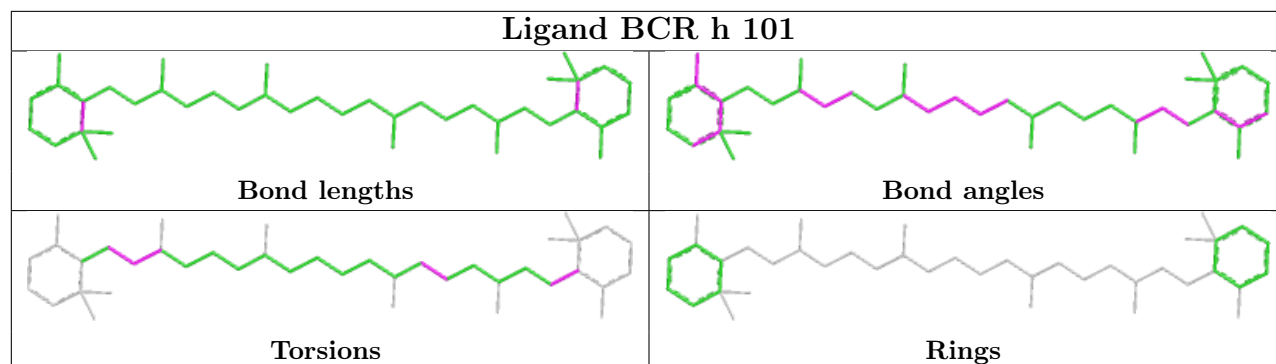
Ligand CLA C 502

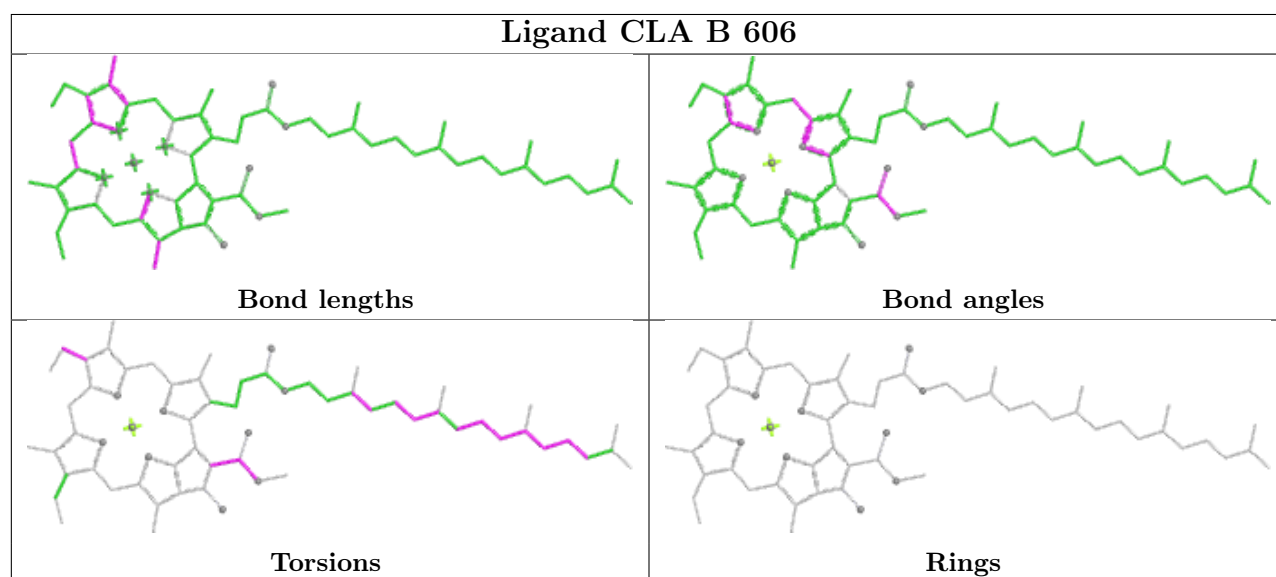
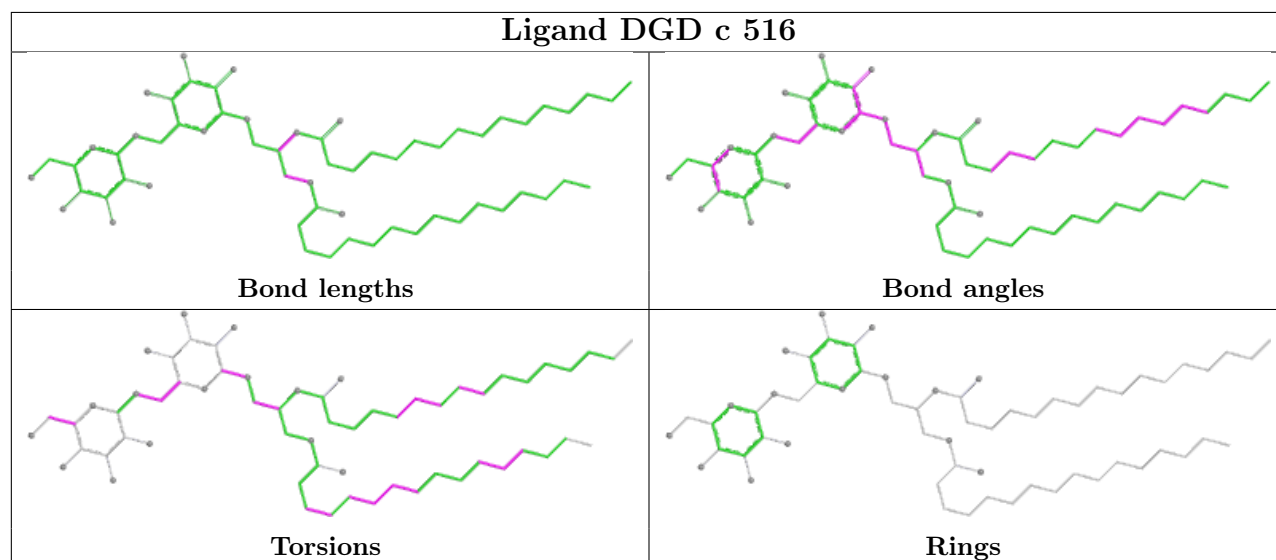
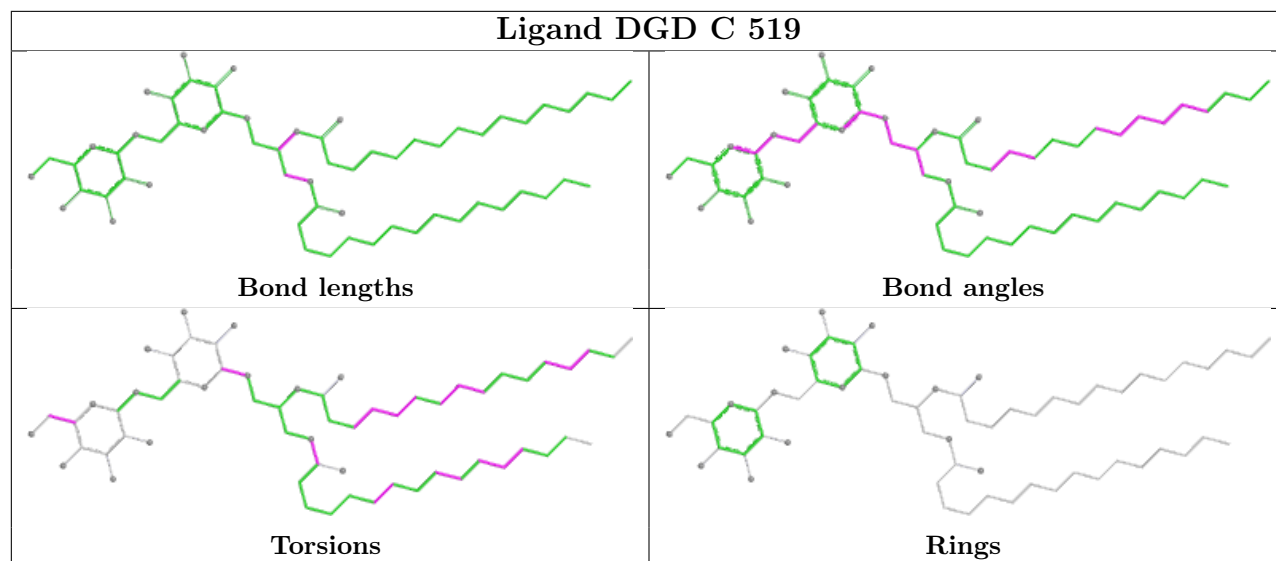


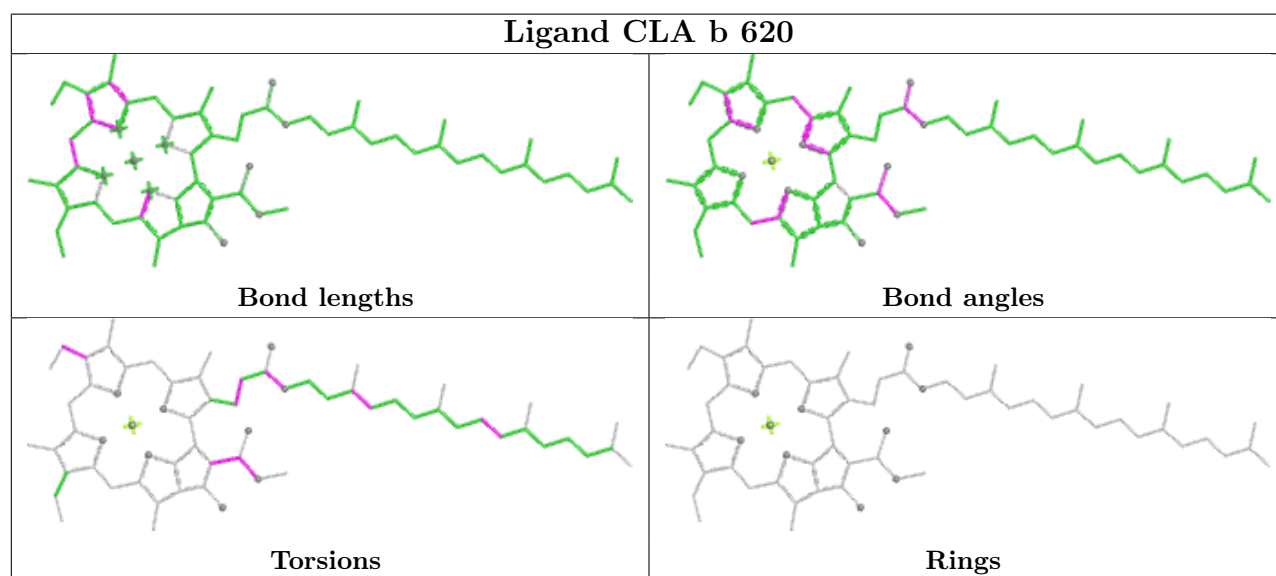
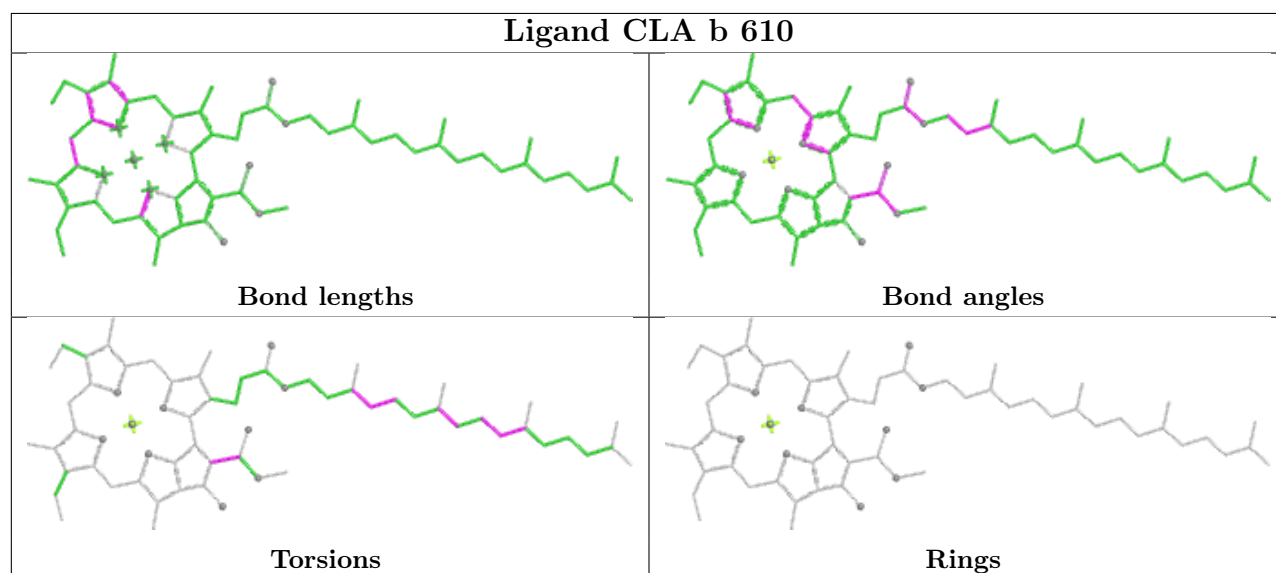
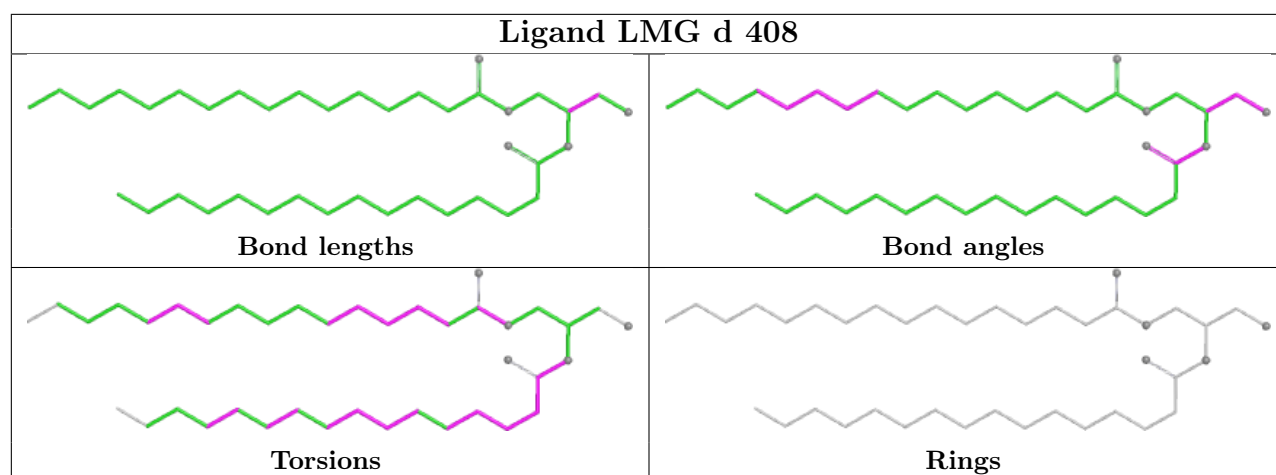
Ligand CLA A 609

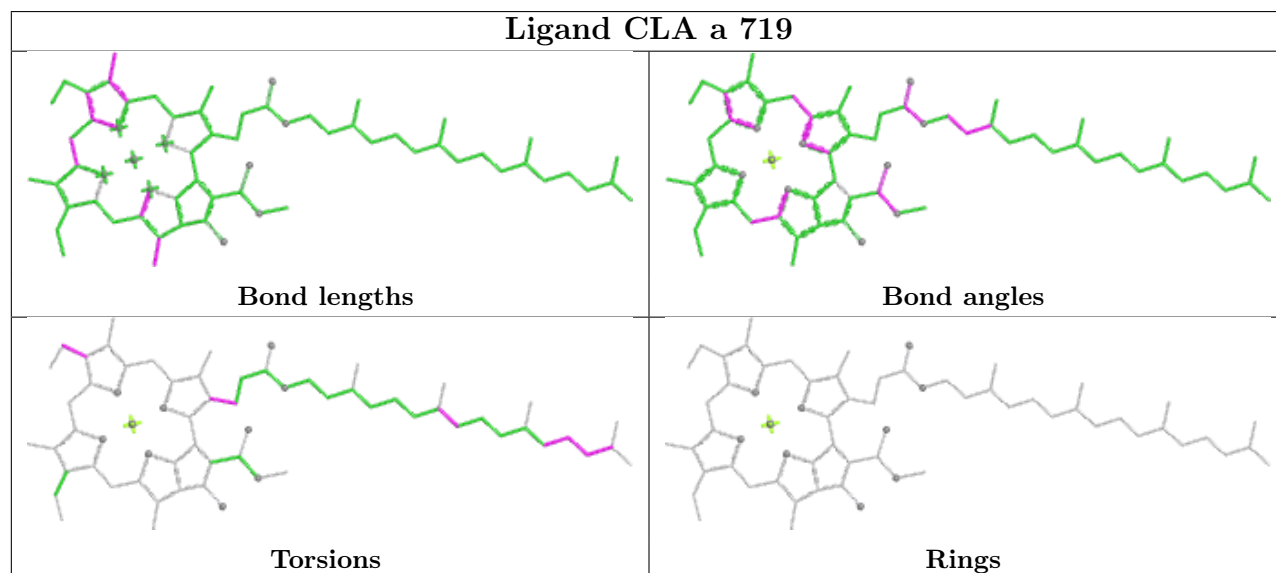
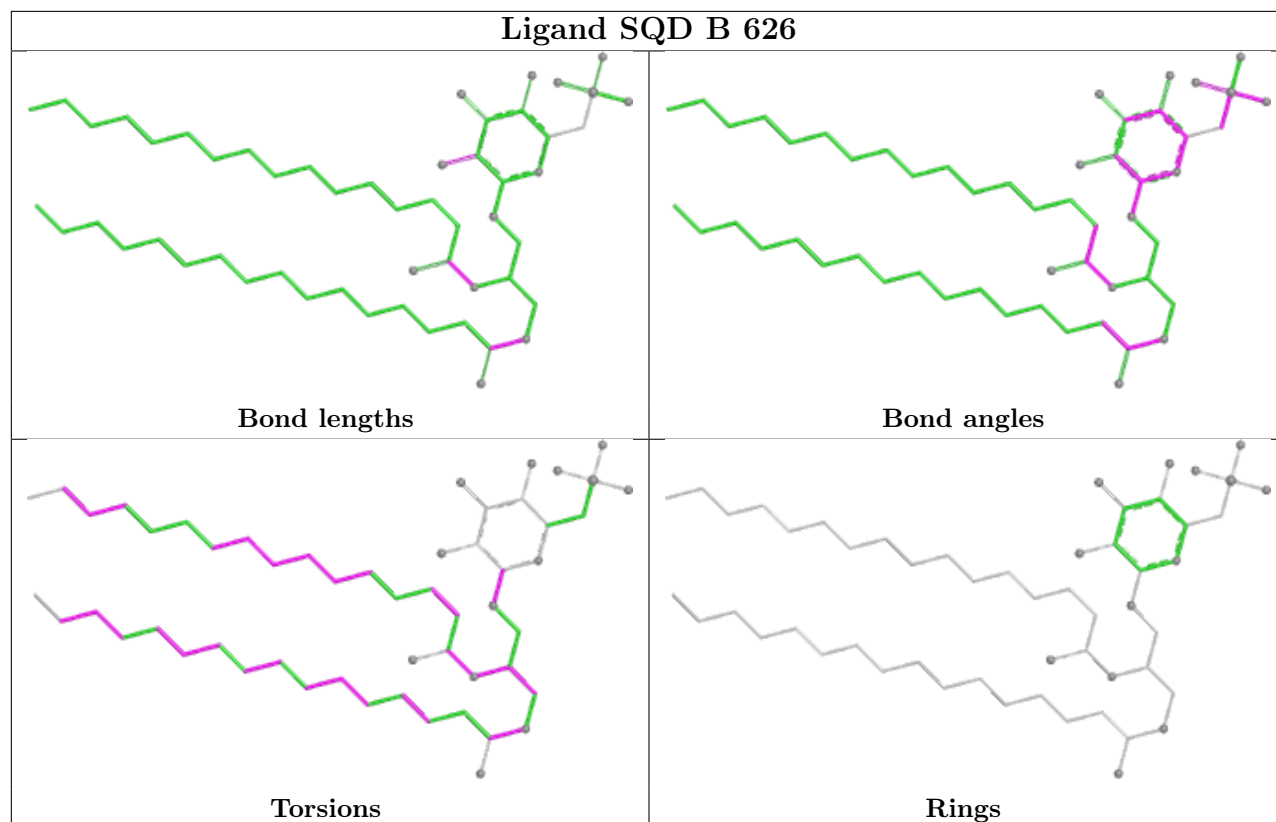




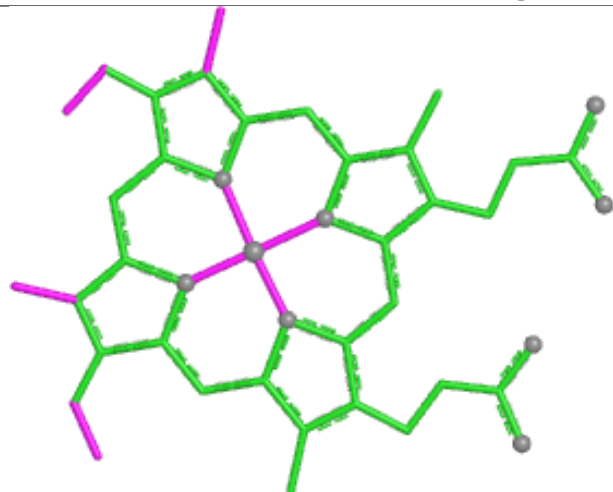




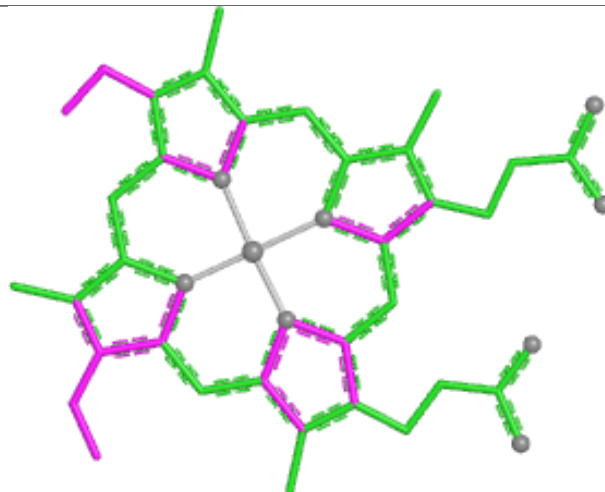




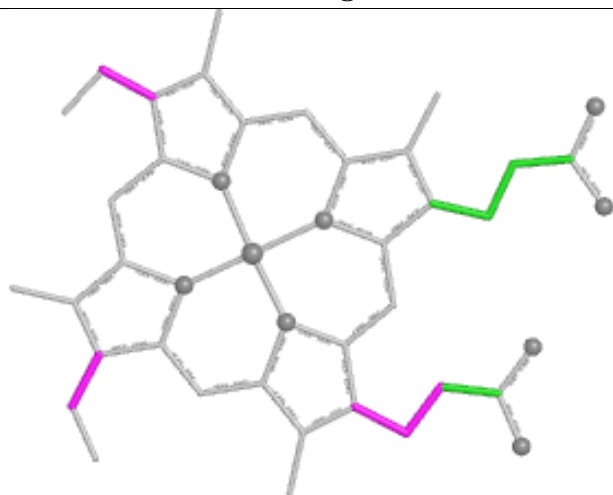
Ligand HEC V 201



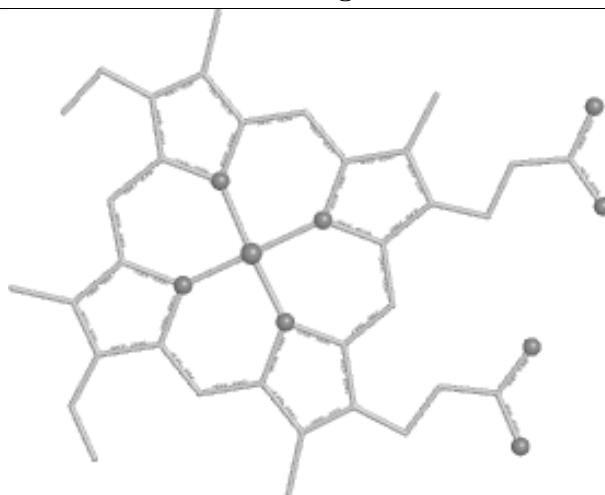
Bond lengths



Bond angles

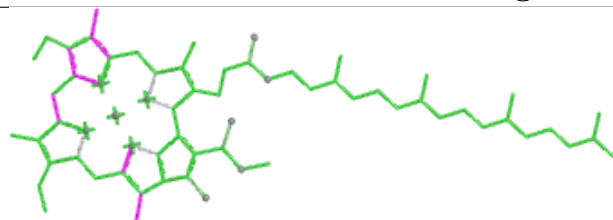


Torsions

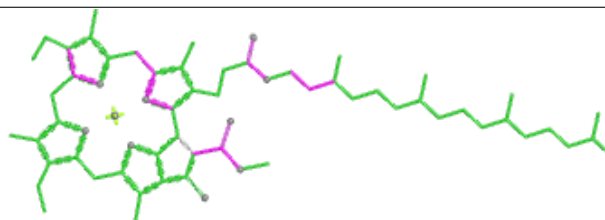


Rings

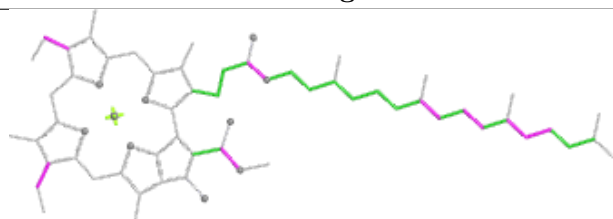
Ligand CLA B 605



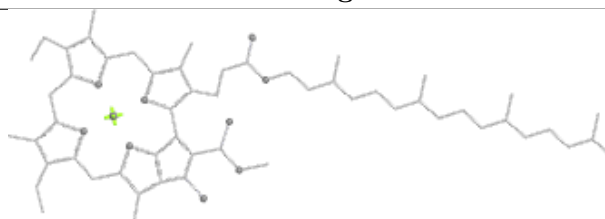
Bond lengths



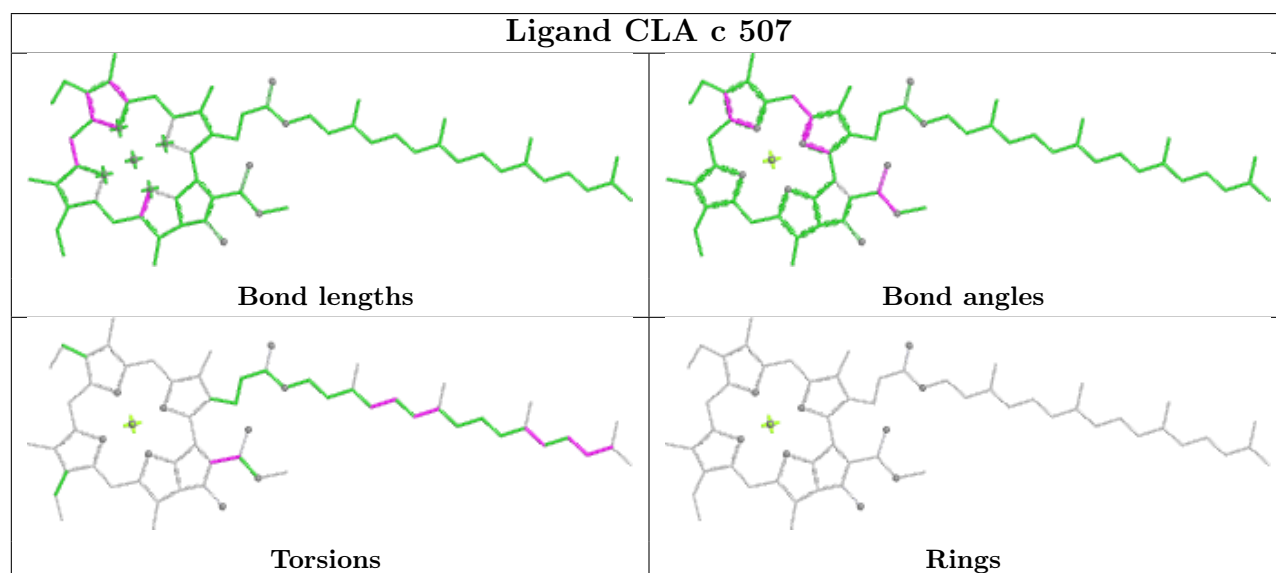
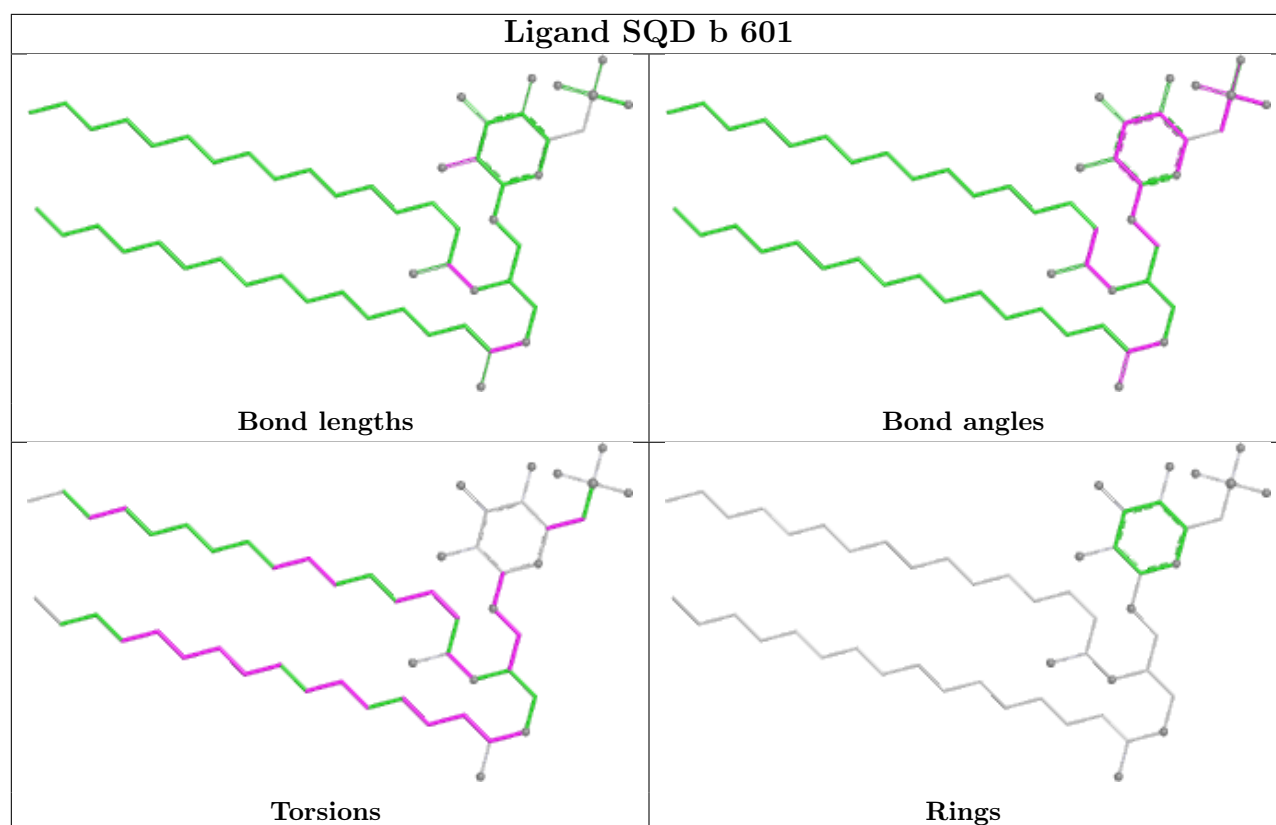
Bond angles

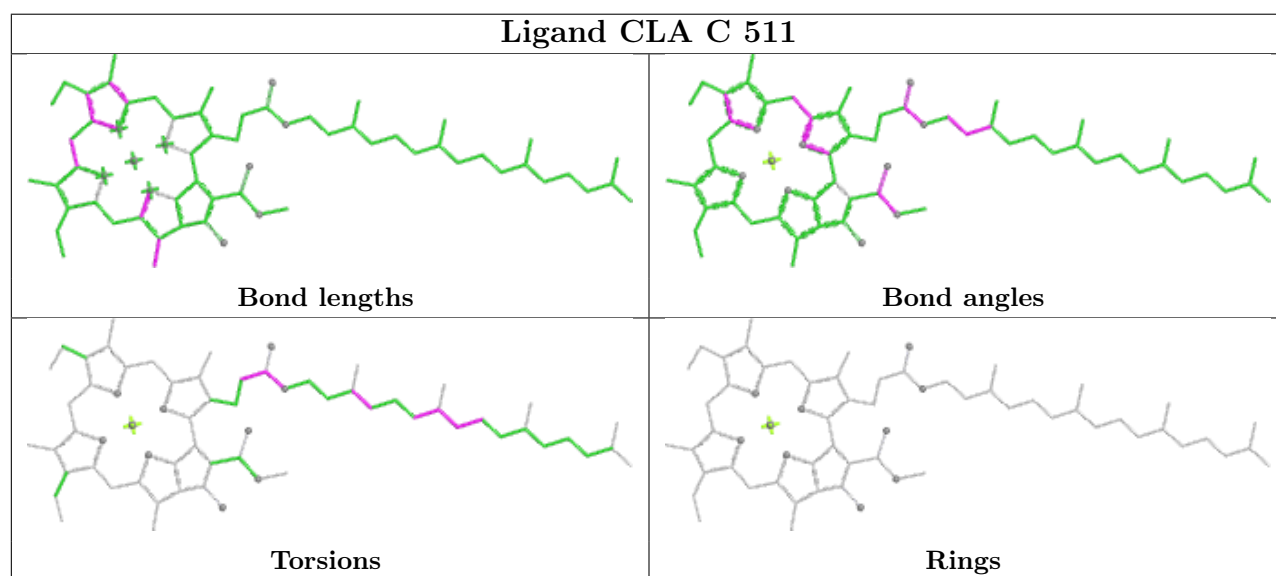
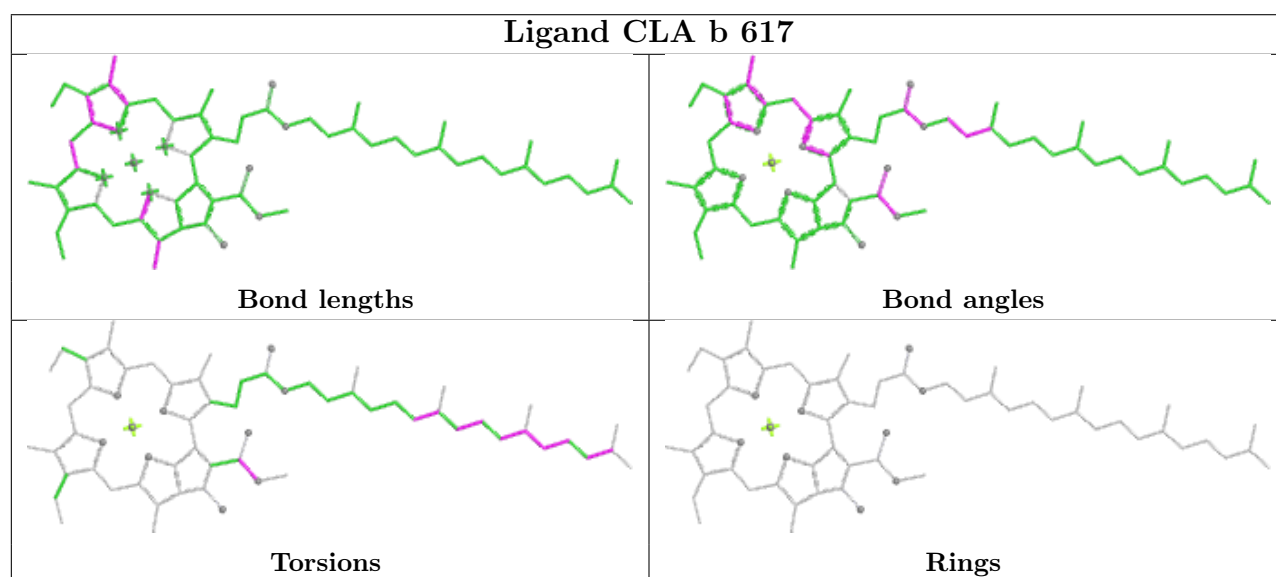
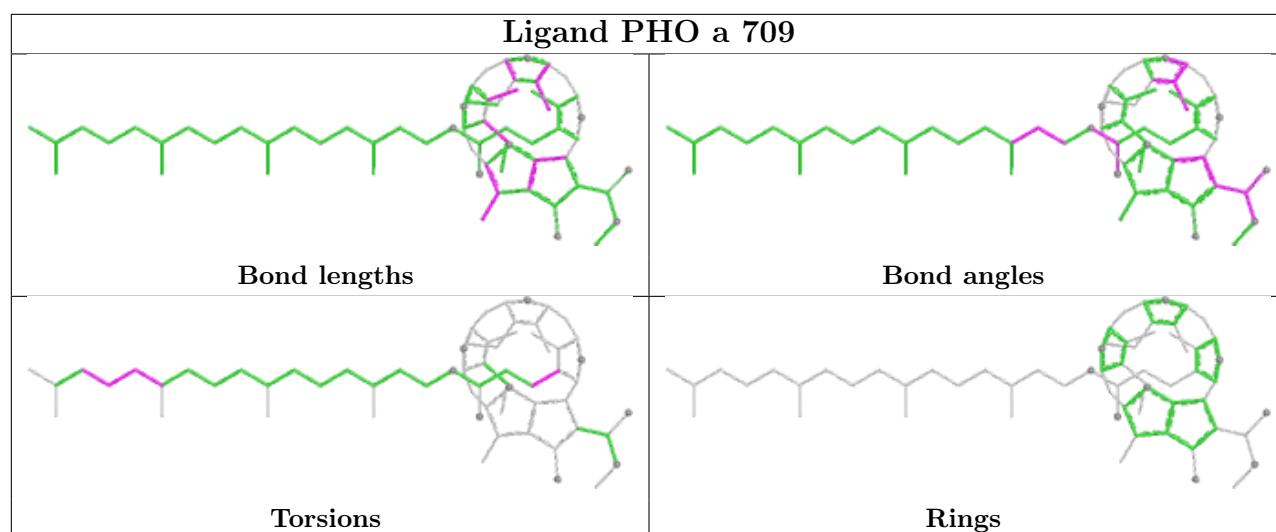


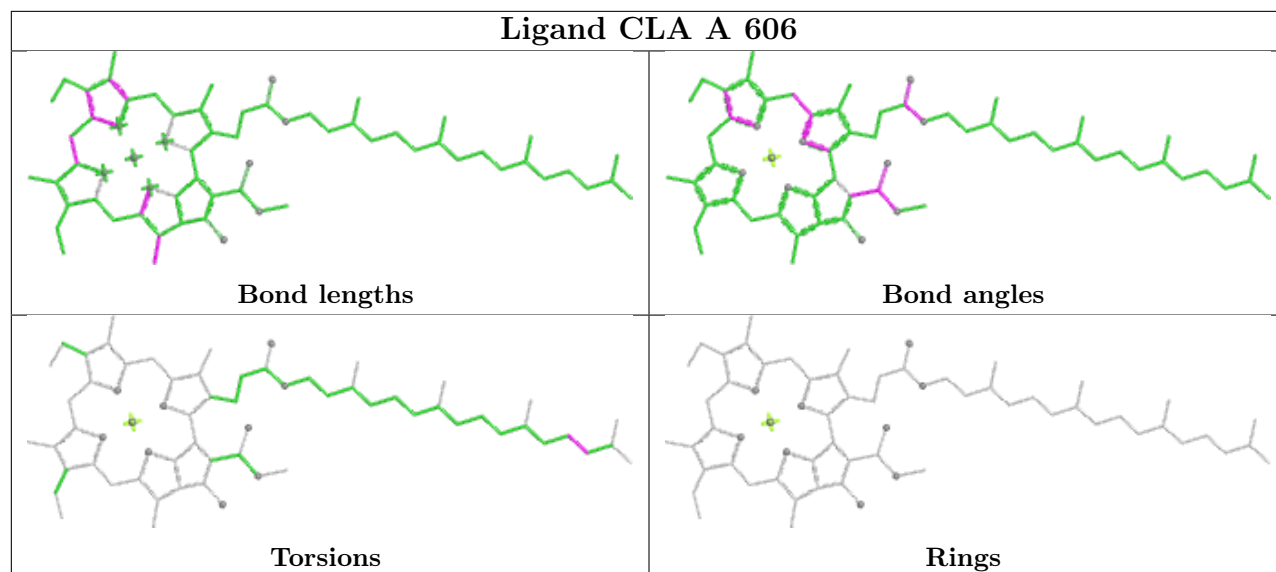
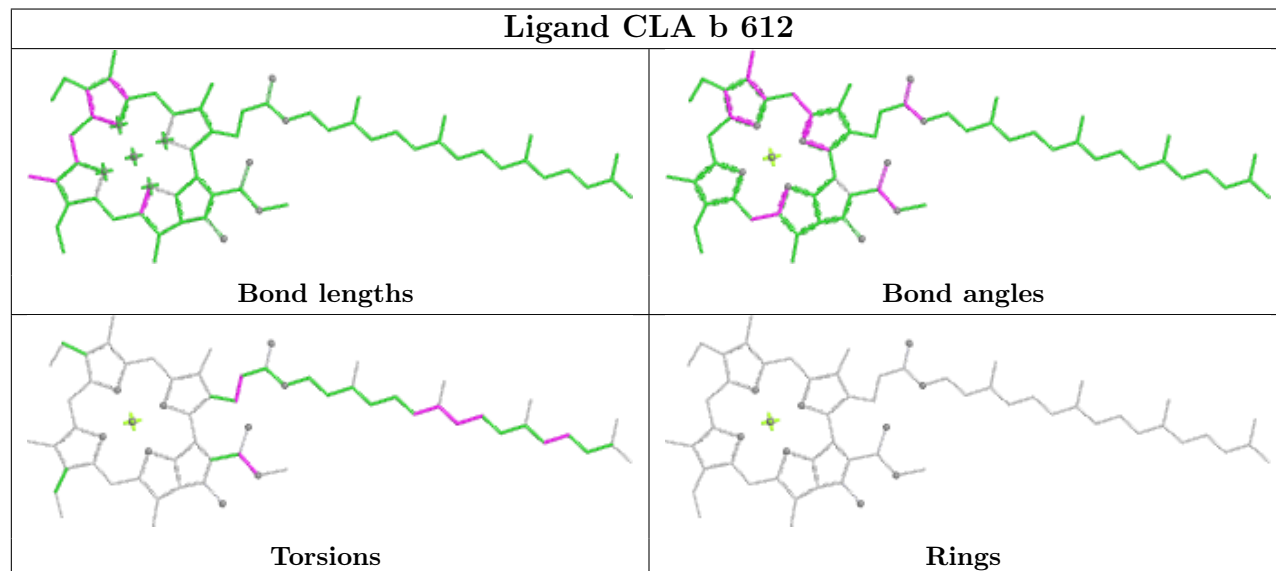
Torsions

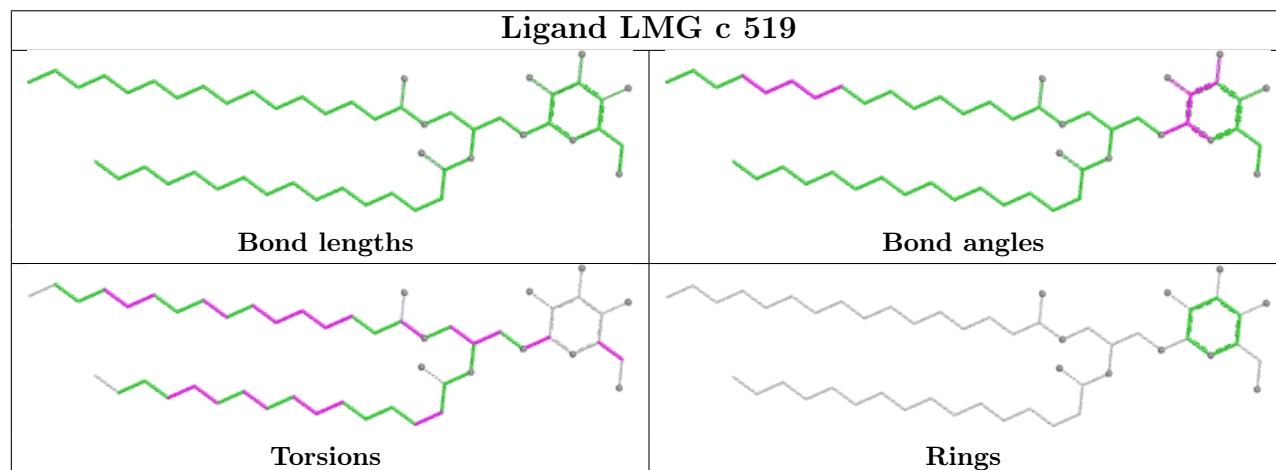
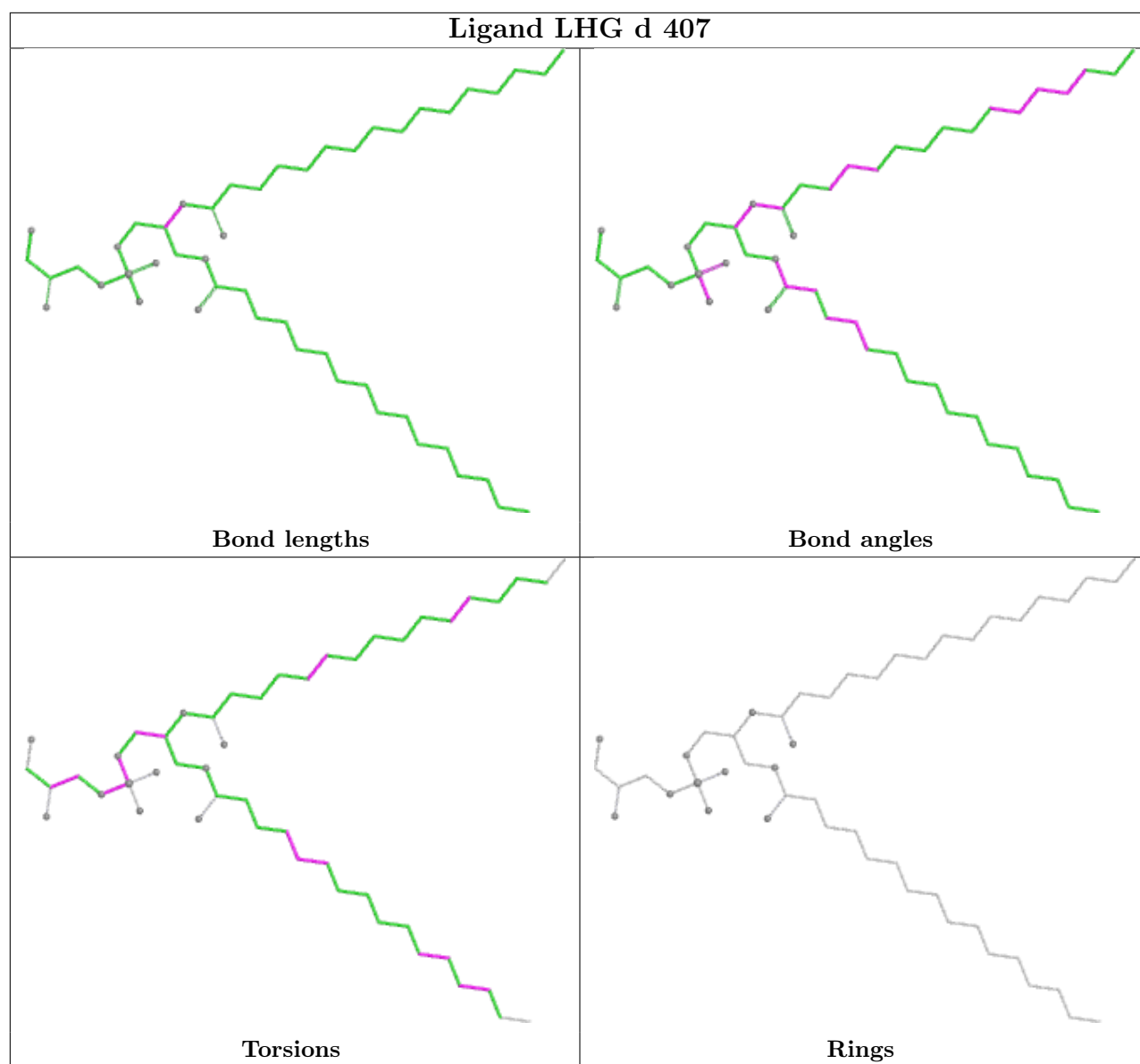


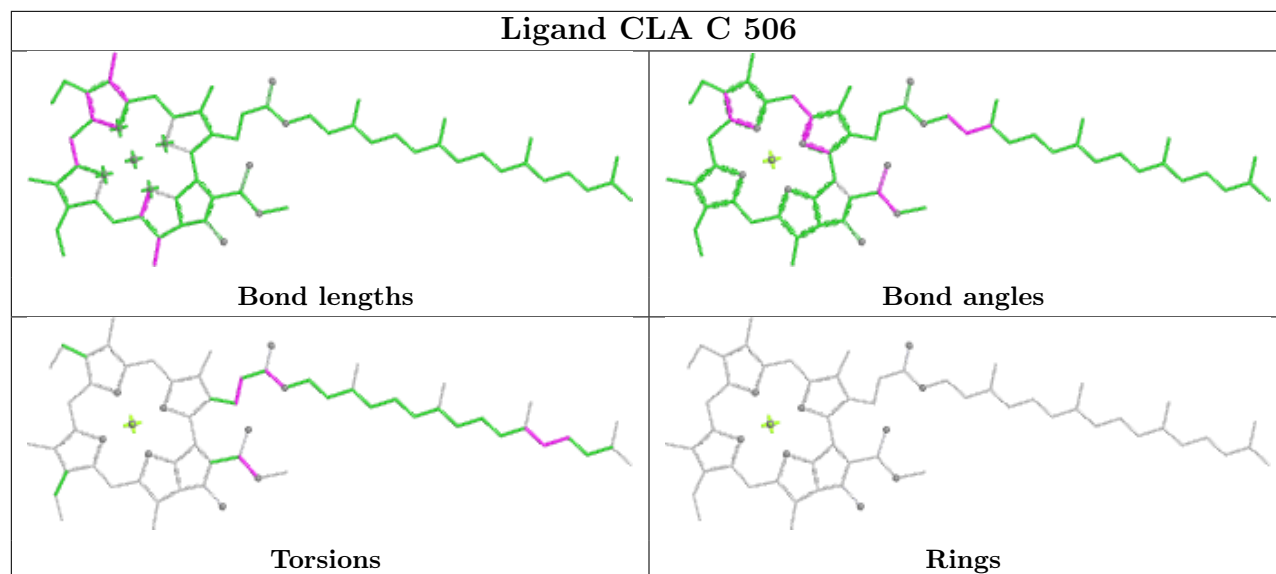
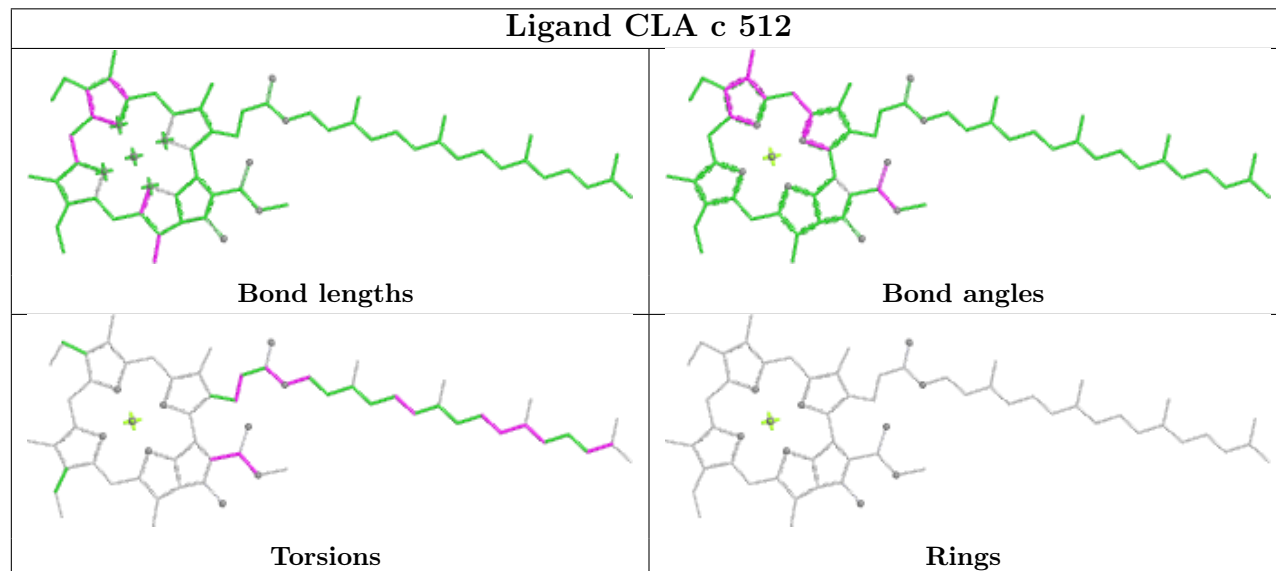
Rings

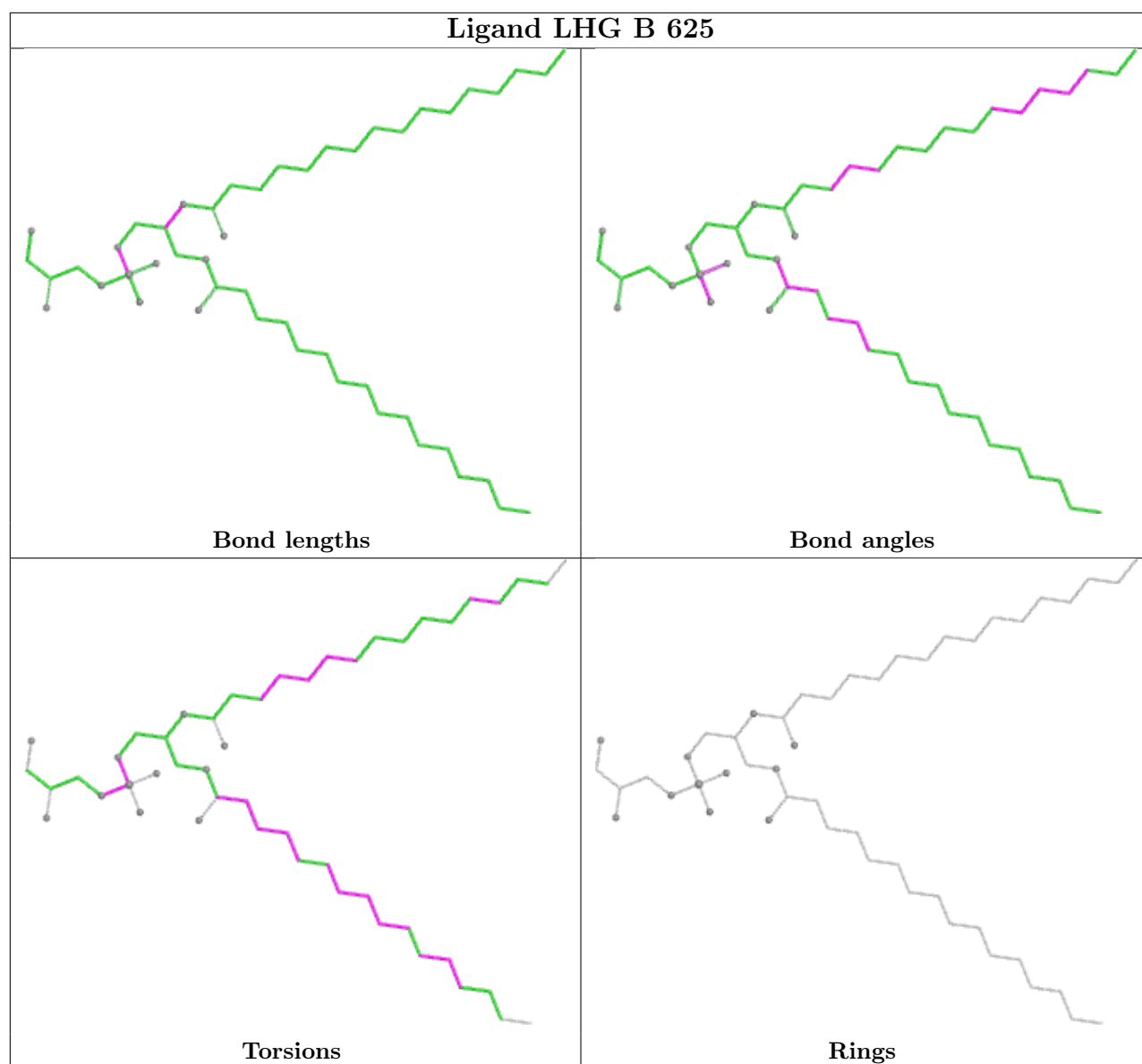


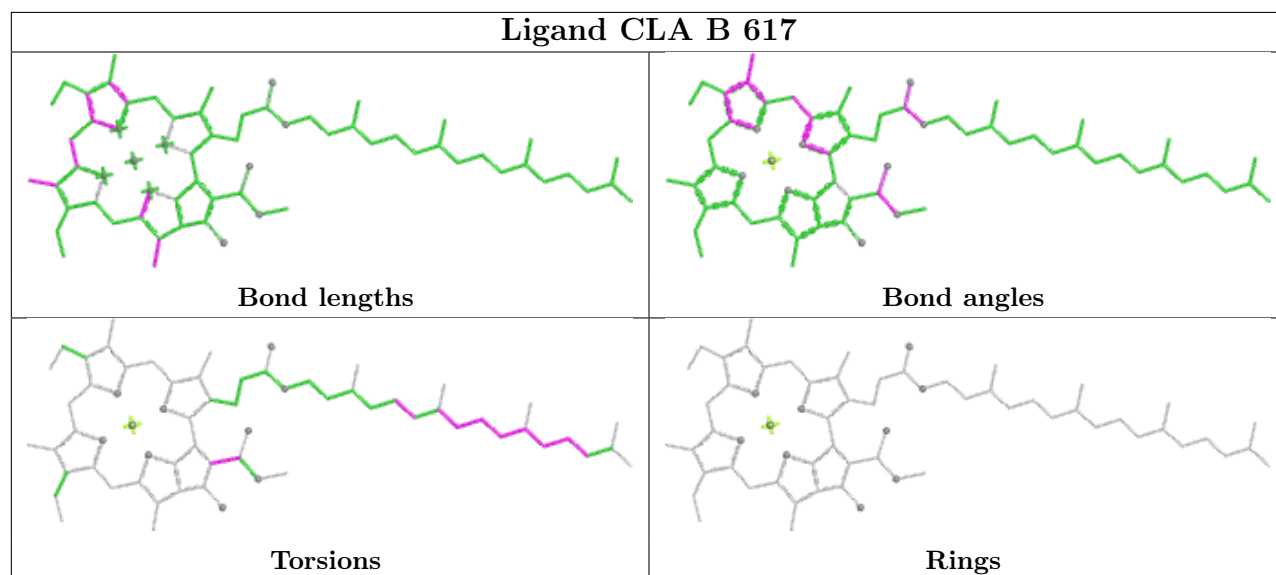
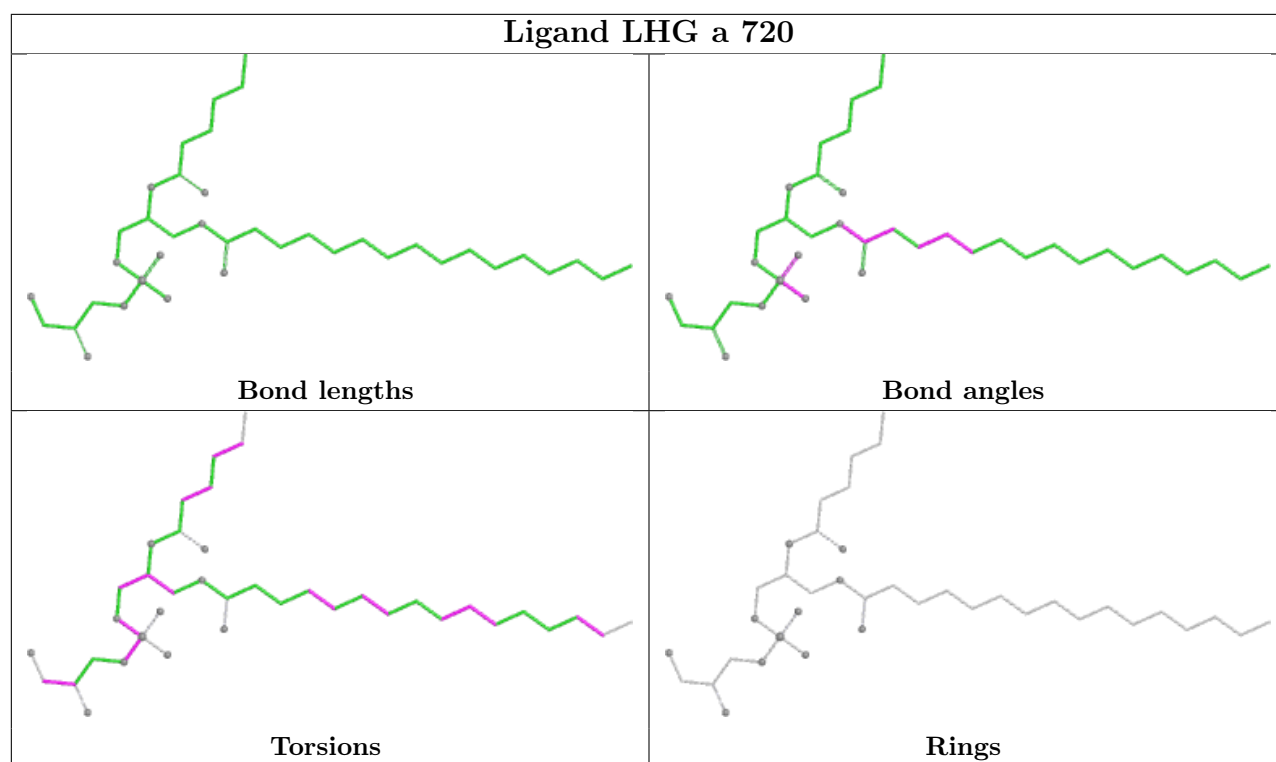


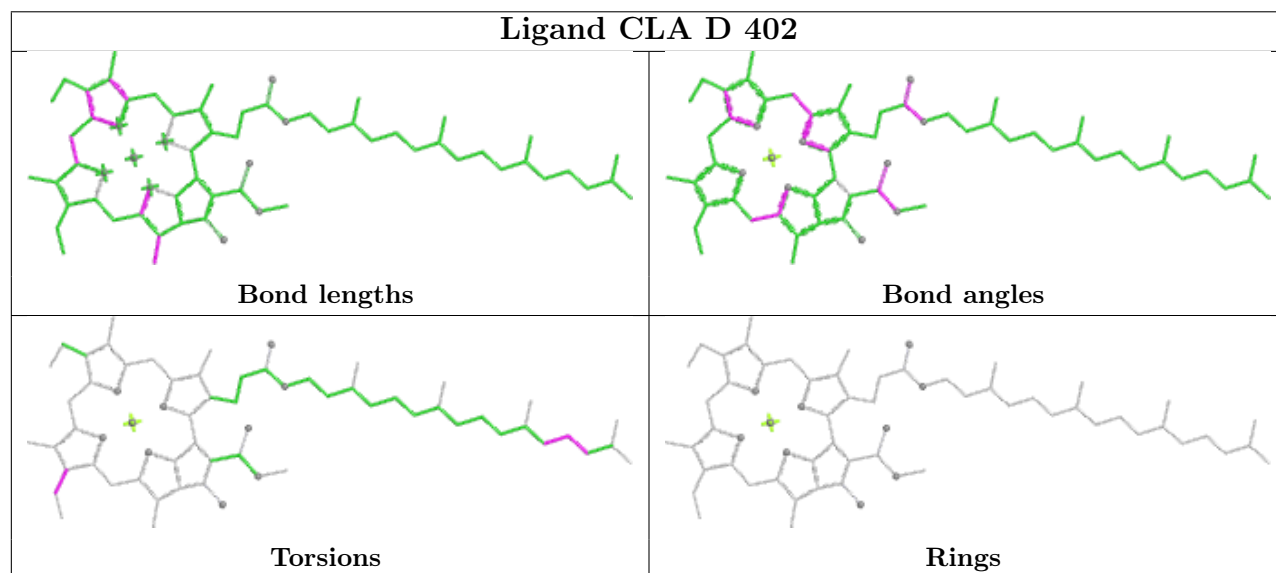
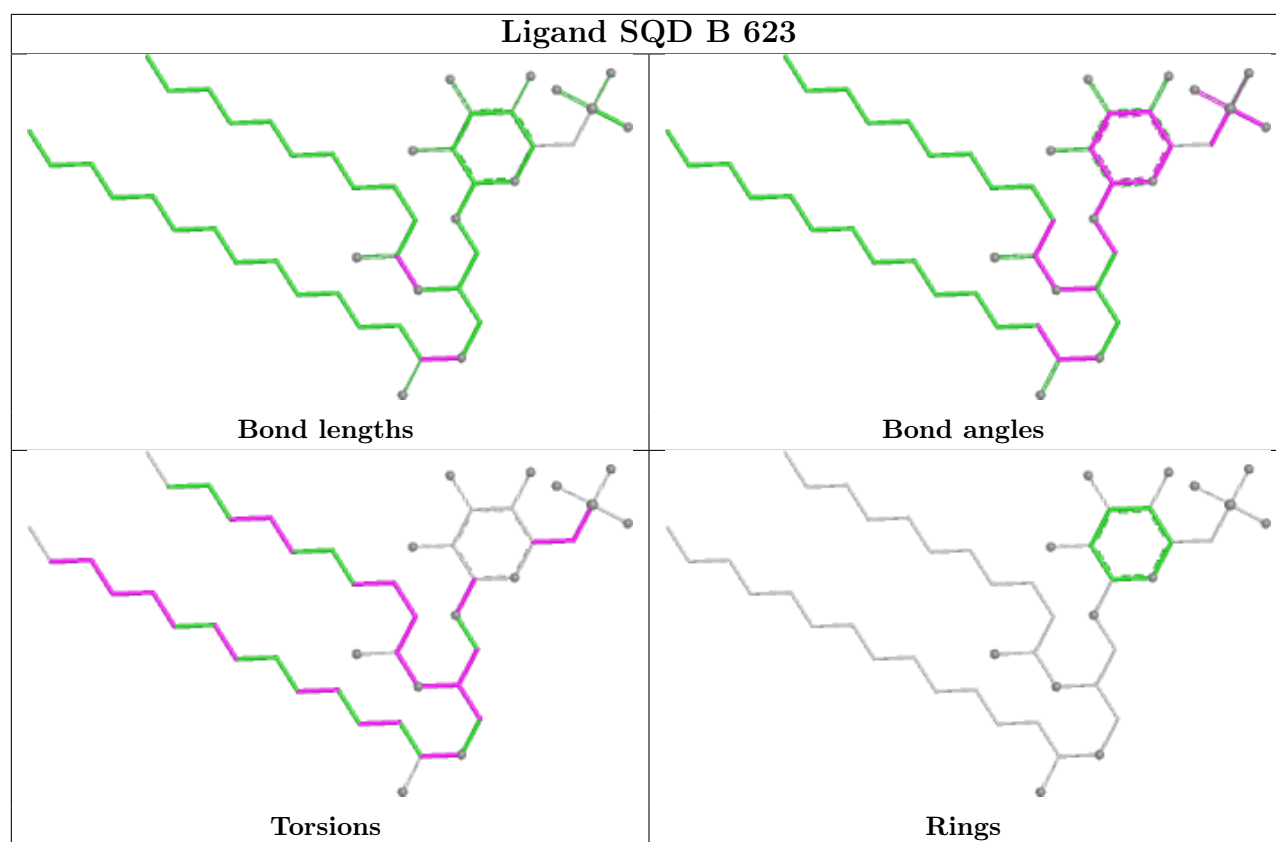
Ligand CLA A 606**Ligand CLA b 612**

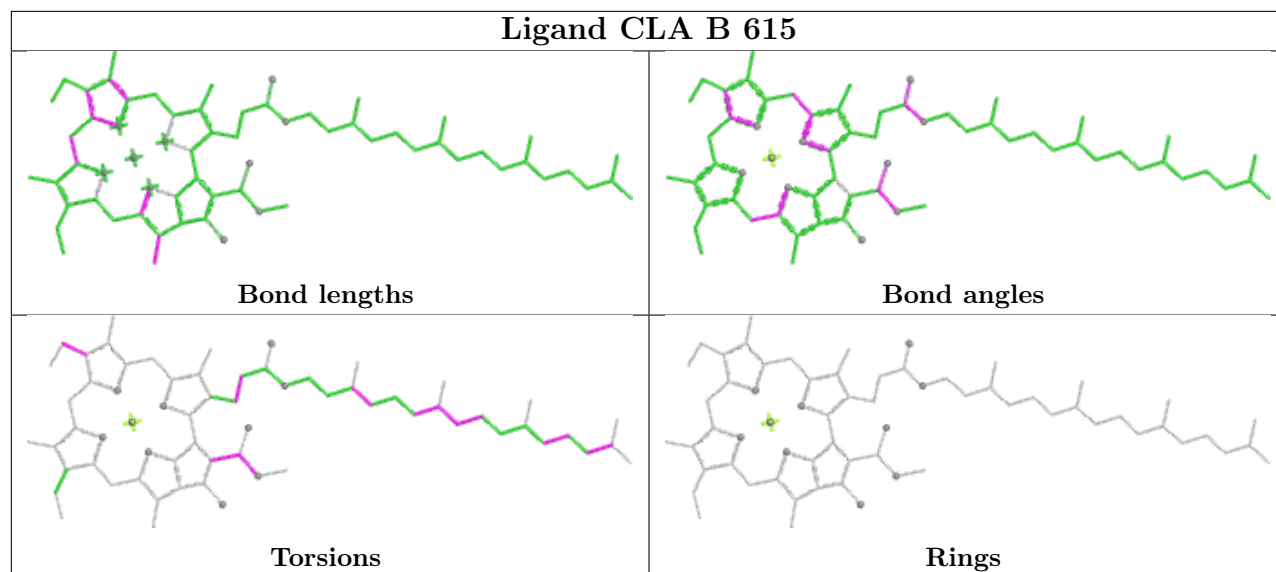
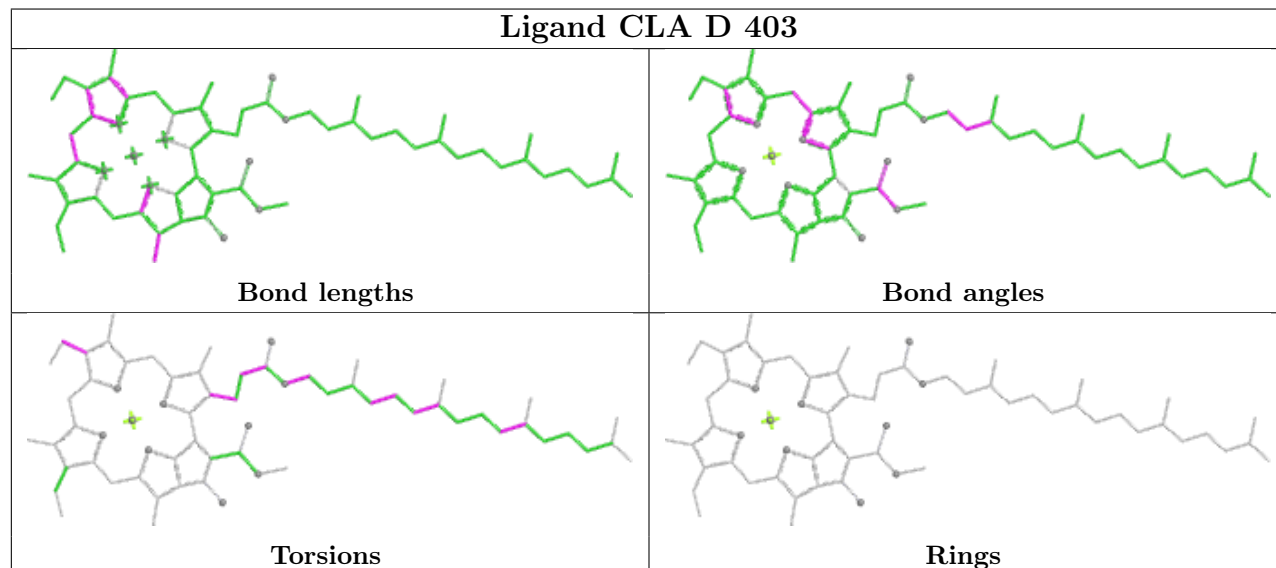


Ligand CLA C 506**Ligand CLA c 512**

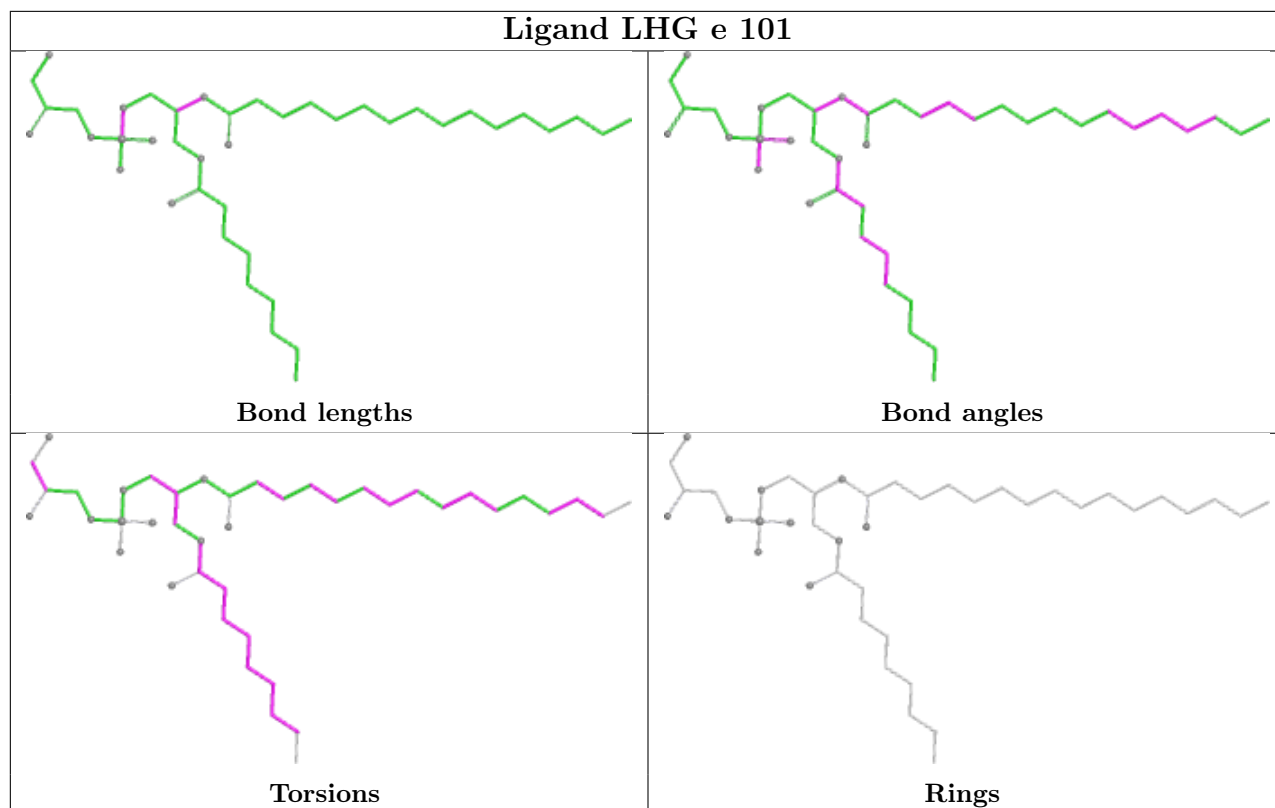




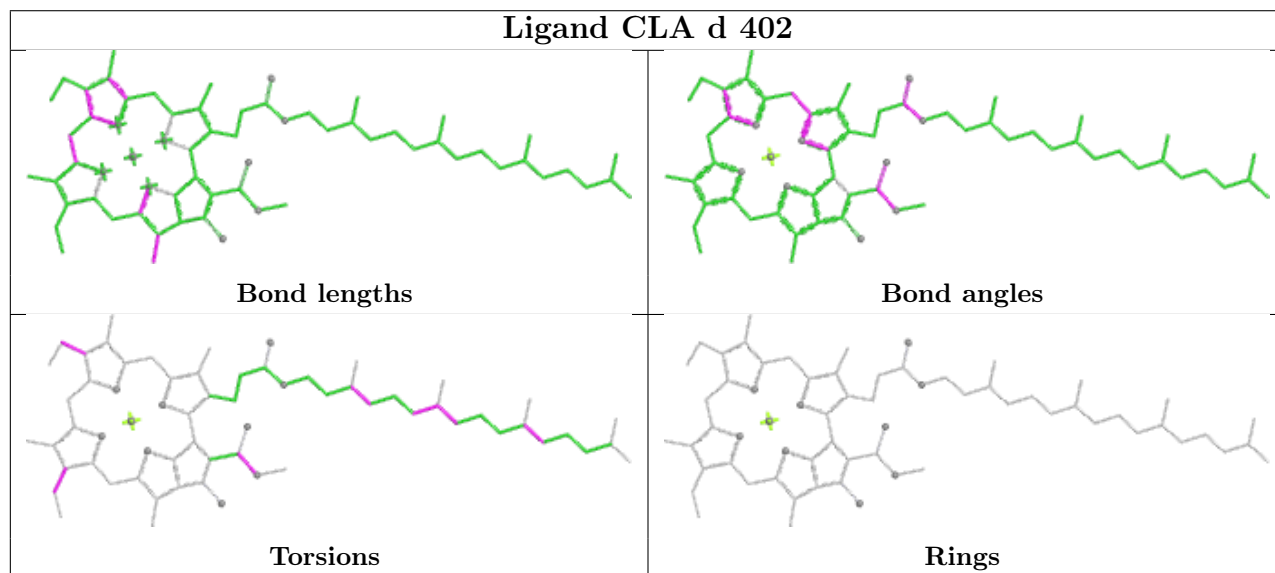


Ligand CLA B 615**Ligand CLA D 403**

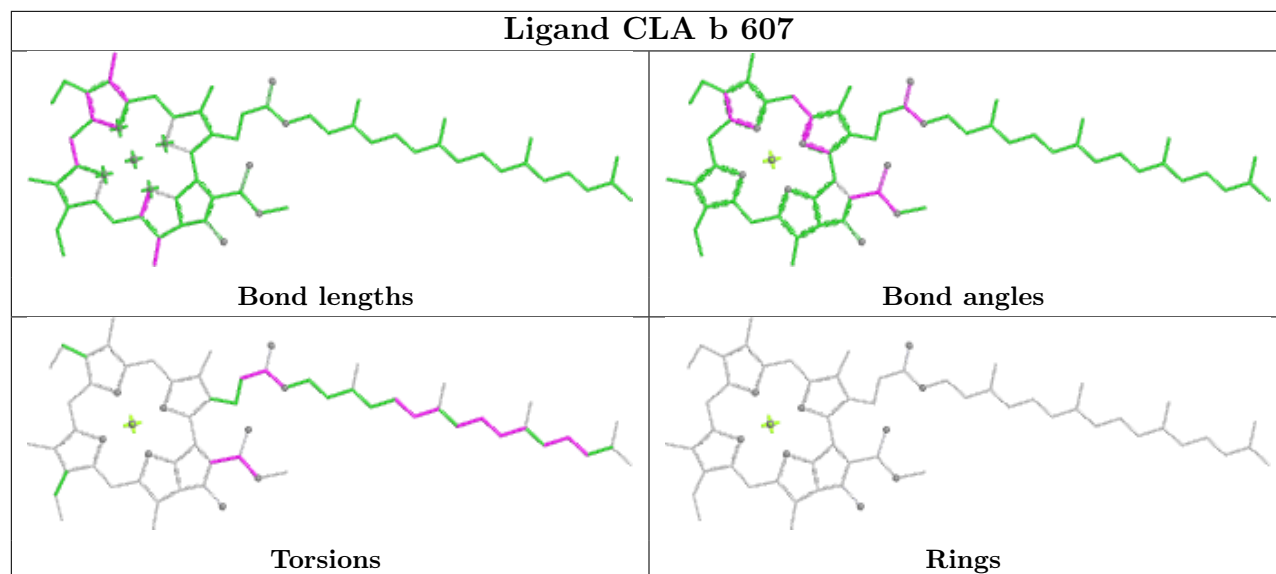
Ligand LHG e 101



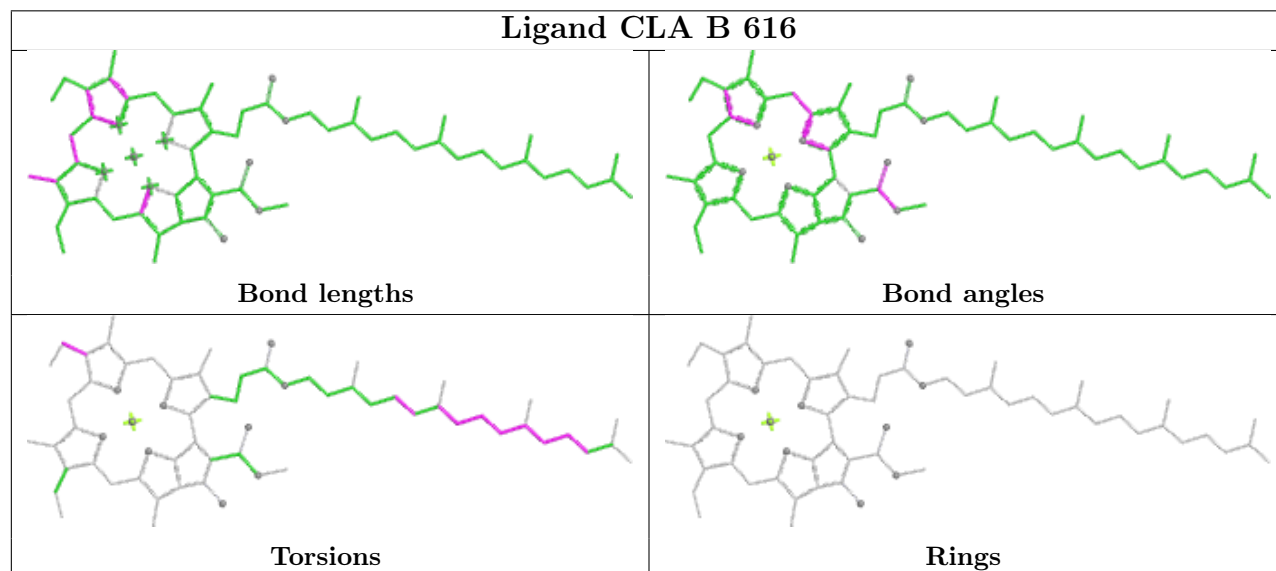
Ligand CLA d 402



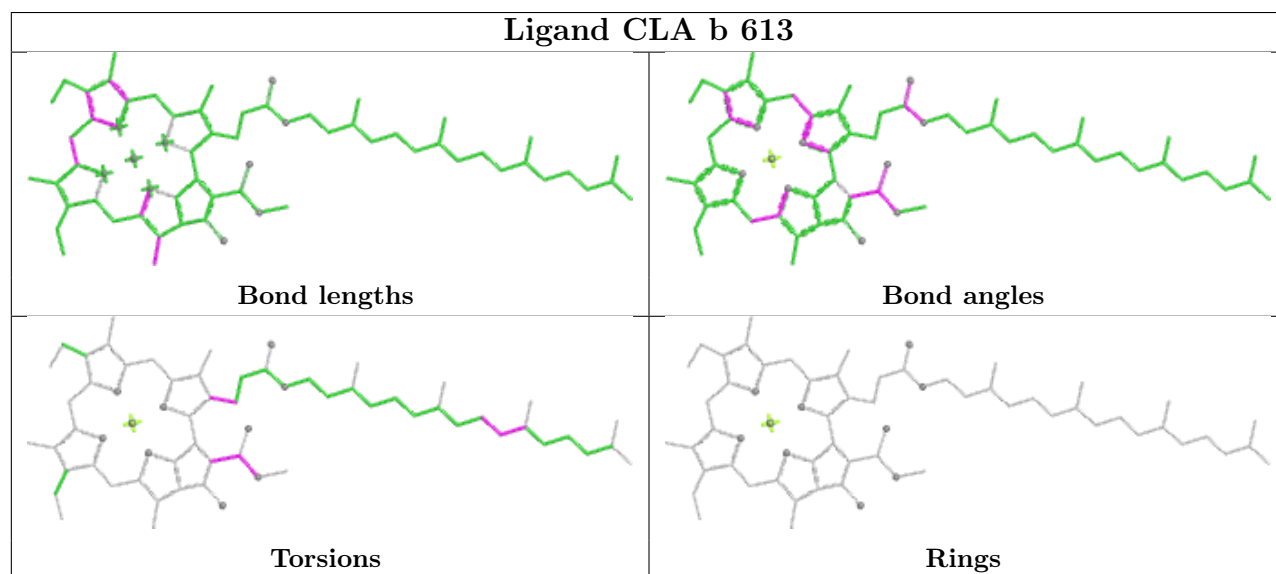
Ligand CLA b 607

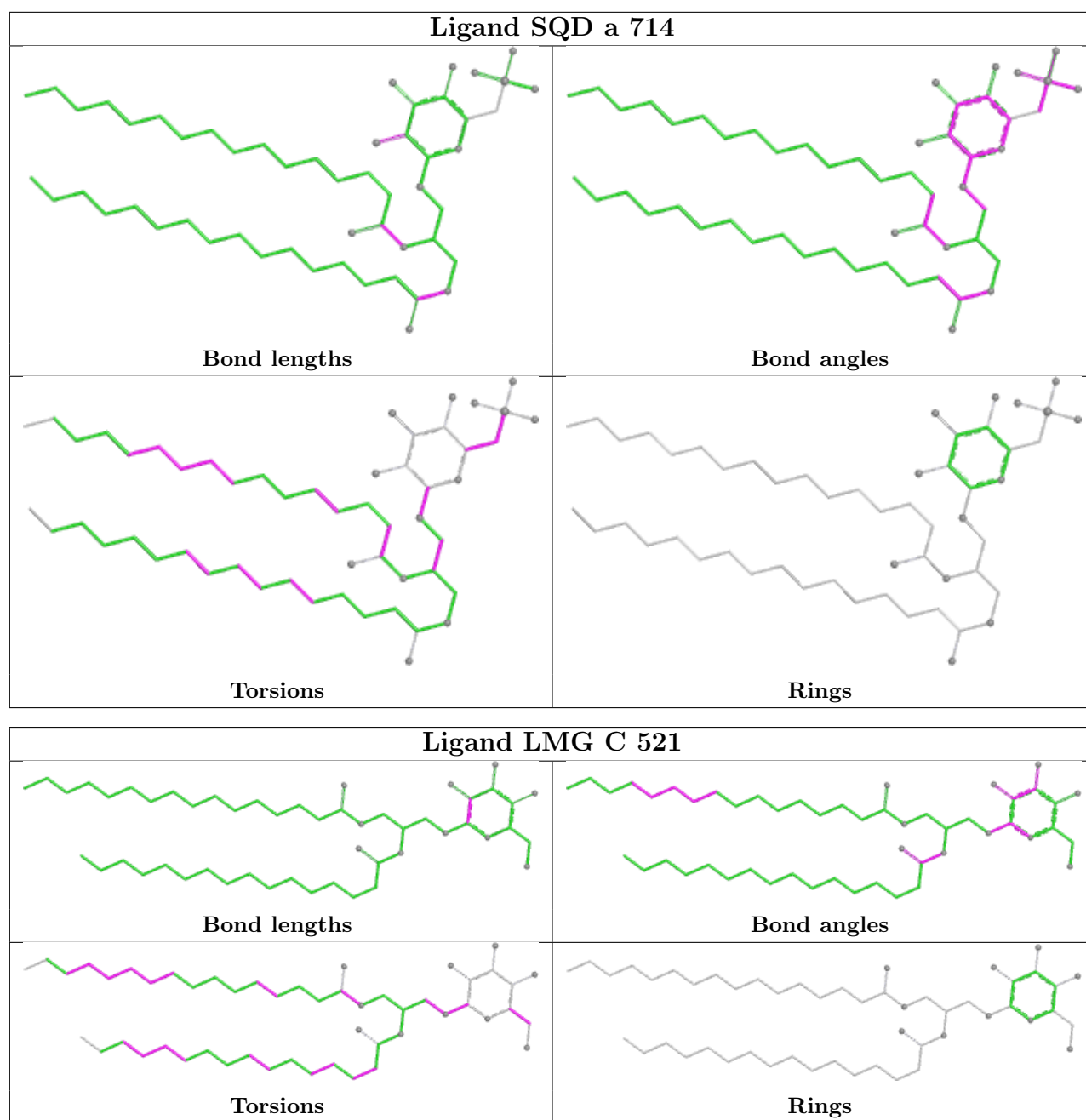


Ligand CLA B 616



Ligand CLA b 613





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%)	0.33	3 (0%) 81 74	38, 46, 69, 82	0
1	a	334/344 (97%)	0.43	13 (3%) 43 34	35, 48, 71, 82	0
2	B	504/510 (98%)	0.45	12 (2%) 59 49	38, 50, 74, 98	0
2	b	504/510 (98%)	0.51	27 (5%) 31 24	38, 50, 75, 93	1 (0%)
3	C	451/461 (97%)	0.51	9 (1%) 65 56	41, 54, 71, 90	0
3	c	451/461 (97%)	0.71	19 (4%) 40 32	39, 55, 74, 90	0
4	D	341/352 (96%)	0.29	3 (0%) 81 74	37, 48, 63, 82	0
4	d	341/352 (96%)	0.47	7 (2%) 63 54	40, 50, 67, 85	0
5	E	81/84 (96%)	0.85	5 (6%) 26 20	47, 67, 79, 85	0
5	e	82/84 (97%)	1.00	7 (8%) 16 12	52, 70, 85, 87	0
6	F	34/45 (75%)	0.63	0 100 100	54, 64, 78, 84	0
6	f	34/45 (75%)	0.73	1 (2%) 53 43	56, 63, 77, 80	0
7	H	63/63 (100%)	0.52	2 (3%) 50 40	43, 55, 68, 73	0
7	h	63/63 (100%)	0.56	2 (3%) 50 40	48, 56, 64, 68	0
8	I	35/38 (92%)	0.56	1 (2%) 53 43	43, 53, 83, 94	0
8	i	35/38 (92%)	0.60	4 (11%) 10 7	44, 51, 82, 89	0
9	J	36/40 (90%)	0.86	0 100 100	56, 64, 86, 99	0
9	j	36/40 (90%)	0.80	1 (2%) 55 45	55, 66, 85, 89	0
10	K	37/46 (80%)	0.94	2 (5%) 31 24	62, 68, 83, 89	0
10	k	37/46 (80%)	1.01	2 (5%) 31 24	60, 70, 84, 89	0
11	L	37/37 (100%)	0.18	0 100 100	34, 45, 82, 93	0
11	l	37/37 (100%)	0.32	1 (2%) 56 46	36, 47, 81, 90	0
12	M	32/36 (88%)	0.10	1 (3%) 51 41	38, 47, 71, 83	0
12	m	32/36 (88%)	0.15	0 100 100	36, 47, 71, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	0.62	11 (4%) 38 30	42, 57, 87, 106	0
13	o	244/272 (89%)	0.77	16 (6%) 24 18	43, 56, 89, 116	0
14	T	29/32 (90%)	0.25	1 (3%) 48 39	37, 46, 69, 87	0
14	t	29/32 (90%)	0.39	1 (3%) 48 39	38, 48, 70, 79	0
15	U	97/134 (72%)	0.48	2 (2%) 63 54	45, 58, 75, 86	0
15	u	97/134 (72%)	0.48	3 (3%) 51 41	47, 55, 69, 84	0
16	V	137/163 (84%)	0.58	1 (0%) 84 77	45, 55, 67, 85	0
16	v	137/163 (84%)	0.83	5 (3%) 46 37	49, 63, 79, 100	0
17	Y	27/46 (58%)	1.02	0 100 100	68, 75, 87, 95	0
17	y	30/46 (65%)	1.22	1 (3%) 49 39	69, 79, 89, 90	0
18	X	38/41 (92%)	0.50	1 (2%) 57 47	52, 60, 82, 93	0
18	x	38/41 (92%)	0.81	0 100 100	54, 63, 80, 92	0
19	Z	62/62 (100%)	1.44	15 (24%) 2 1	62, 76, 100, 113	0
19	z	62/62 (100%)	1.28	14 (22%) 2 1	67, 82, 101, 112	0
20	R	34/41 (82%)	1.75	11 (32%) 1 1	70, 82, 94, 95	0
20	r	34/41 (82%)	1.40	7 (20%) 2 2	70, 84, 94, 101	0
All	All	5310/5694 (93%)	0.57	211 (3%) 42 33	34, 53, 81, 116	1 (0%)

The worst 5 of 211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	453	ALA	6.0
3	C	142	GLU	5.7
4	D	238	THR	4.8
2	B	488	PRO	4.7
19	Z	7	LEU	4.7

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
14	FME	t	1	10/11	0.88	0.11	42,56,71,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.89	0.13	49,61,69,69	0
8	FME	I	1	10/11	0.89	0.14	50,60,70,76	0
14	FME	T	1	10/11	0.91	0.10	51,58,70,77	0
12	FME	m	1	10/11	0.92	0.11	52,59,74,79	0
12	FME	M	1	10/11	0.92	0.15	54,63,77,87	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
29	SQD	I	102	40/54	0.67	0.23	44,69,94,102	0
32	LHG	E	101	49/49	0.69	0.21	48,77,92,95	0
30	UNL	j	101	9/-	0.70	0.28	52,61,65,65	0
30	UNL	b	603	11/-	0.71	0.20	44,54,62,62	0
30	UNL	a	717	7/-	0.72	0.23	48,53,61,67	0
30	UNL	b	606	13/-	0.73	0.22	45,51,57,59	0
29	SQD	B	623	47/54	0.73	0.17	44,61,109,124	0
30	UNL	I	101	9/-	0.73	0.21	44,52,61,61	0
30	UNL	H	101	8/-	0.75	0.21	43,53,58,64	0
23	LMG	b	627	51/55	0.76	0.18	51,70,80,82	0
30	UNL	a	716	4/-	0.76	0.20	31,46,50,51	0
23	LMG	C	521	51/55	0.76	0.19	49,71,81,91	0
30	UNL	z	101	11/-	0.76	0.24	48,65,72,72	0
30	UNL	a	718	13/-	0.76	0.19	45,54,61,62	0
32	LHG	e	101	42/49	0.76	0.18	57,76,98,101	0
30	UNL	A	613	7/-	0.77	0.20	34,49,53,55	0
23	LMG	c	520	51/55	0.77	0.21	61,75,95,100	0
23	LMG	B	621	51/55	0.78	0.18	52,70,78,88	0
23	LMG	C	501	51/55	0.78	0.19	46,67,81,88	0
23	LMG	C	520	51/55	0.78	0.20	43,74,86,89	0
23	LMG	A	603	51/55	0.78	0.19	40,62,77,83	0
30	UNL	B	601	12/-	0.79	0.16	31,49,56,56	0
30	UNL	i	101	22/-	0.79	0.18	36,50,58,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	LMG	b	626	51/55	0.80	0.17	38,56,72,77	0
29	SQD	b	601	54/54	0.80	0.15	45,66,94,105	0
29	SQD	A	614	40/54	0.80	0.18	47,59,68,72	0
23	LMG	a	701	51/55	0.80	0.16	42,64,87,90	0
23	LMG	a	715	51/55	0.81	0.16	47,65,85,91	0
29	SQD	B	626	54/54	0.81	0.16	46,67,90,99	0
23	LMG	d	408	40/55	0.81	0.16	47,61,84,89	0
23	LMG	b	628	9/55	0.81	0.15	36,50,54,54	0
30	UNL	M	102	6/-	0.81	0.19	45,51,51,53	0
28	PL9	a	713	55/55	0.82	0.19	57,68,77,84	0
23	LMG	c	519	51/55	0.82	0.20	42,75,90,91	0
25	CLA	b	607	65/65	0.82	0.16	48,63,81,91	0
30	UNL	t	102	5/-	0.82	0.15	32,38,43,47	0
27	BCR	k	101	40/40	0.82	0.18	53,69,78,78	0
28	PL9	A	611	55/55	0.82	0.19	46,68,78,83	0
30	UNL	b	605	13/-	0.82	0.18	42,54,62,62	0
25	CLA	B	602	65/65	0.83	0.15	44,62,75,80	0
29	SQD	f	102	41/54	0.83	0.17	54,73,85,89	0
27	BCR	D	405	40/40	0.83	0.17	48,61,77,81	0
25	CLA	C	514	65/65	0.83	0.15	44,73,81,89	0
30	UNL	B	622	6/-	0.83	0.19	40,51,56,56	0
27	BCR	b	602	40/40	0.84	0.15	45,53,70,76	0
30	UNL	M	103	16/-	0.84	0.16	41,51,57,58	0
25	CLA	B	617	65/65	0.85	0.15	39,52,80,84	0
27	BCR	t	103	40/40	0.85	0.16	36,47,60,63	0
25	CLA	c	506	65/65	0.85	0.15	47,57,79,92	0
25	CLA	c	512	65/65	0.85	0.17	60,67,89,91	0
25	CLA	c	513	65/65	0.85	0.15	57,68,82,96	0
27	BCR	C	515	40/40	0.85	0.17	53,63,72,76	0
25	CLA	C	505	65/65	0.85	0.16	48,63,71,79	0
29	SQD	D	410	43/54	0.85	0.16	56,75,87,96	0
23	LMG	M	101	51/55	0.85	0.14	34,58,74,77	0
27	BCR	d	404	40/40	0.85	0.17	45,59,70,77	0
33	DGD	c	517	62/66	0.85	0.17	54,61,81,92	0
30	UNL	B	624	11/-	0.86	0.18	34,49,52,53	0
30	UNL	m	101	5/-	0.86	0.13	36,39,42,45	0
30	UNL	m	102	12/-	0.86	0.14	41,47,50,52	0
30	UNL	t	101	10/-	0.86	0.14	26,44,49,50	0
27	BCR	c	514	40/40	0.86	0.17	61,67,74,75	0
27	BCR	H	102	40/40	0.86	0.15	41,54,62,62	0
25	CLA	C	513	65/65	0.86	0.15	52,66,80,86	0
27	BCR	k	102	40/40	0.86	0.18	53,65,81,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	SQD	a	714	54/54	0.86	0.16	48,68,83,90	0
23	LMG	f	101	51/55	0.87	0.16	48,58,84,93	0
30	UNL	d	401	22/-	0.87	0.16	39,54,63,66	0
25	CLA	c	504	58/65	0.87	0.14	52,59,66,67	0
27	BCR	Y	101	40/40	0.87	0.15	46,66,71,72	0
30	UNL	b	604	11/-	0.87	0.18	38,48,57,59	0
25	CLA	C	507	65/65	0.87	0.14	44,55,75,88	0
25	CLA	C	512	65/65	0.88	0.14	52,60,69,71	0
23	LMG	D	409	51/55	0.88	0.15	39,61,82,88	0
27	BCR	h	101	40/40	0.88	0.15	40,54,68,71	0
25	CLA	c	503	65/65	0.88	0.14	48,61,68,73	0
27	BCR	b	623	40/40	0.88	0.14	42,53,60,61	0
33	DGD	C	518	62/66	0.88	0.13	51,62,81,88	0
27	BCR	b	624	40/40	0.88	0.13	38,49,58,59	0
33	DGD	h	102	62/66	0.88	0.14	41,55,63,66	0
27	BCR	B	618	40/40	0.89	0.13	37,52,60,63	0
27	BCR	B	620	40/40	0.89	0.14	39,48,56,71	0
27	BCR	b	625	40/40	0.89	0.12	36,49,55,58	0
29	SQD	A	612	52/54	0.89	0.16	45,67,80,92	0
25	CLA	C	506	65/65	0.89	0.12	41,51,57,60	0
32	LHG	B	625	49/49	0.89	0.14	41,51,58,61	0
32	LHG	D	408	49/49	0.89	0.15	42,59,72,84	0
27	BCR	c	515	40/40	0.89	0.13	38,53,64,72	0
25	CLA	C	504	65/65	0.89	0.12	43,57,62,68	0
25	CLA	c	511	65/65	0.89	0.14	50,62,71,74	0
33	DGD	H	103	62/66	0.89	0.13	39,49,59,62	0
25	CLA	C	510	65/65	0.89	0.14	45,57,64,68	0
25	CLA	B	605	65/65	0.89	0.13	35,47,62,73	0
25	CLA	B	609	65/65	0.90	0.12	32,45,51,59	0
25	CLA	c	505	65/65	0.90	0.13	41,52,60,69	0
25	CLA	B	615	65/65	0.90	0.12	38,48,67,73	0
25	CLA	a	711	65/65	0.90	0.13	34,46,79,87	0
25	CLA	C	511	65/65	0.90	0.13	44,57,64,70	0
28	PL9	D	406	55/55	0.90	0.14	31,43,52,55	0
25	CLA	b	610	65/65	0.90	0.13	37,47,59,62	0
28	PL9	d	405	55/55	0.90	0.13	32,41,53,56	0
25	CLA	b	612	65/65	0.90	0.13	32,46,56,69	0
33	DGD	C	519	62/66	0.90	0.13	43,56,67,76	0
25	CLA	b	613	65/65	0.90	0.12	37,44,55,58	0
33	DGD	c	516	62/66	0.90	0.14	34,50,68,76	0
25	CLA	B	607	65/65	0.90	0.13	41,50,64,75	0
33	DGD	c	518	62/66	0.90	0.14	44,57,76,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	BCR	C	516	40/40	0.90	0.13	42,51,58,58	0
27	BCR	B	619	40/40	0.91	0.12	35,47,51,52	0
25	CLA	C	509	65/65	0.91	0.14	46,55,91,100	0
25	CLA	B	616	65/65	0.91	0.11	42,51,60,64	0
25	CLA	b	620	65/65	0.91	0.12	35,52,61,64	0
25	CLA	b	621	65/65	0.91	0.12	38,49,55,60	0
25	CLA	b	622	47/65	0.91	0.11	40,48,58,64	0
27	BCR	K	101	40/40	0.91	0.14	51,60,70,75	0
25	CLA	A	607	65/65	0.91	0.14	31,46,91,99	0
25	CLA	C	503	65/65	0.91	0.12	43,56,62,68	0
25	CLA	B	610	65/65	0.91	0.11	36,51,58,63	0
25	CLA	B	611	65/65	0.91	0.12	40,47,55,60	0
25	CLA	c	507	65/65	0.91	0.11	41,50,61,67	0
25	CLA	c	508	65/65	0.91	0.13	46,57,72,82	0
25	CLA	c	509	65/65	0.91	0.13	49,57,70,73	0
32	LHG	a	720	39/49	0.91	0.13	41,54,65,66	0
25	CLA	c	510	65/65	0.91	0.13	43,54,63,68	0
33	DGD	C	517	62/66	0.91	0.12	36,46,65,71	0
25	CLA	a	707	65/65	0.91	0.11	33,47,51,53	0
25	CLA	B	614	65/65	0.91	0.11	34,43,57,69	0
25	CLA	A	606	65/65	0.91	0.11	29,43,48,53	0
25	CLA	d	402	65/65	0.91	0.12	35,45,51,55	0
25	CLA	d	403	65/65	0.91	0.12	45,54,65,66	0
26	PHO	D	401	64/64	0.91	0.11	37,46,55,59	0
25	CLA	C	508	65/65	0.91	0.12	41,50,57,66	0
26	PHO	a	710	64/64	0.92	0.12	38,46,55,62	0
27	BCR	A	610	40/40	0.92	0.10	31,44,52,56	0
25	CLA	c	502	65/65	0.92	0.12	45,55,67,81	0
25	CLA	B	612	65/65	0.92	0.11	32,42,49,54	0
25	CLA	C	502	65/65	0.92	0.12	38,50,57,64	0
25	CLA	b	608	65/65	0.92	0.12	39,49,60,64	0
25	CLA	A	609	54/65	0.92	0.11	34,43,60,71	0
25	CLA	B	604	65/65	0.92	0.12	33,44,54,57	0
32	LHG	L	101	49/49	0.92	0.11	39,50,57,64	0
25	CLA	D	402	65/65	0.92	0.11	31,41,47,51	0
32	LHG	b	629	49/49	0.92	0.11	36,50,57,64	0
32	LHG	d	406	49/49	0.92	0.12	32,53,61,65	0
25	CLA	b	614	65/65	0.92	0.11	39,48,58,60	0
25	CLA	b	615	65/65	0.92	0.11	42,50,55,60	0
27	BCR	a	712	40/40	0.92	0.12	26,44,53,54	0
25	CLA	b	616	65/65	0.92	0.12	34,42,50,56	0
25	CLA	b	617	65/65	0.92	0.11	36,45,50,57	0

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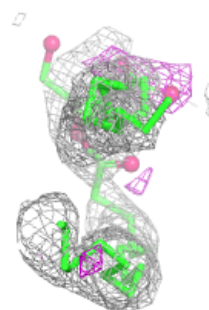
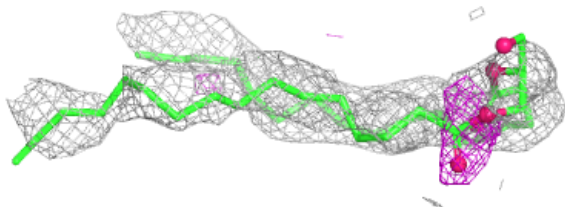
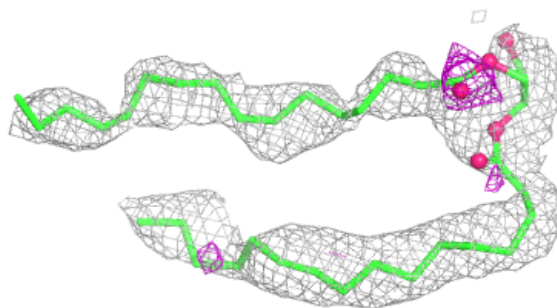
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CLA	b	619	65/65	0.92	0.11	31,42,59,67	0
25	CLA	D	403	65/65	0.92	0.11	33,42,54,61	0
25	CLA	D	404	65/65	0.92	0.12	34,44,80,84	0
25	CLA	B	608	65/65	0.92	0.11	30,42,52,56	0
34	HEM	E	102	43/43	0.92	0.12	52,66,76,80	0
34	HEM	e	102	43/43	0.92	0.14	60,71,81,91	0
25	CLA	b	611	65/65	0.93	0.10	30,46,52,56	0
32	LHG	d	407	49/49	0.93	0.12	36,46,54,61	0
25	CLA	b	618	65/65	0.93	0.11	32,43,50,52	0
25	CLA	a	719	65/65	0.93	0.11	32,43,49,54	0
31	BCT	A	615	4/4	0.93	0.11	46,49,51,54	0
31	BCT	a	706	4/4	0.93	0.09	50,56,56,59	0
25	CLA	B	606	65/65	0.93	0.11	37,45,52,53	0
32	LHG	D	407	49/49	0.93	0.10	34,49,59,60	0
25	CLA	B	613	65/65	0.93	0.11	36,43,55,59	0
25	CLA	b	609	65/65	0.93	0.11	34,45,55,61	0
26	PHO	a	709	64/64	0.93	0.10	26,41,47,50	0
25	CLA	c	501	65/65	0.93	0.11	37,49,55,59	0
25	CLA	B	603	65/65	0.93	0.11	42,52,59,62	0
26	PHO	A	608	64/64	0.94	0.10	32,40,46,50	0
25	CLA	a	708	65/65	0.94	0.11	37,47,89,101	0
24	CL	A	605	1/1	0.94	0.11	51,51,51,51	0
35	HEC	V	201	43/43	0.94	0.11	41,51,57,63	0
35	HEC	v	201	43/43	0.94	0.11	46,58,64,72	0
24	CL	a	704	1/1	0.95	0.09	59,59,59,59	0
24	CL	a	705	1/1	0.96	0.11	50,50,50,50	0
24	CL	A	604	1/1	0.97	0.07	39,39,39,39	0
22	FE2	a	703	1/1	0.98	0.07	60,60,60,60	0
21	OEX	A	601	10/10	0.98	0.06	42,54,59,60	0
21	OEX	a	702	10/10	0.98	0.05	44,52,59,60	0
22	FE2	A	602	1/1	0.99	0.05	60,60,60,60	0

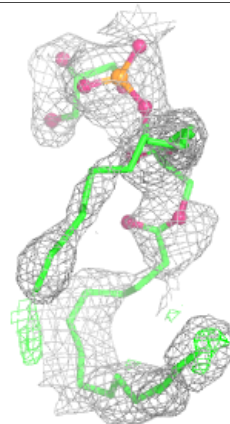
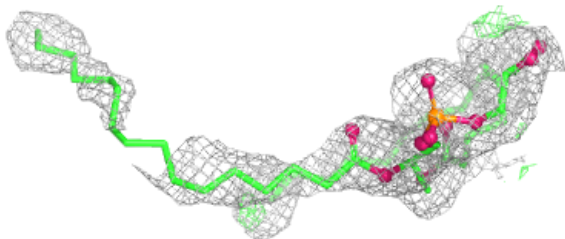
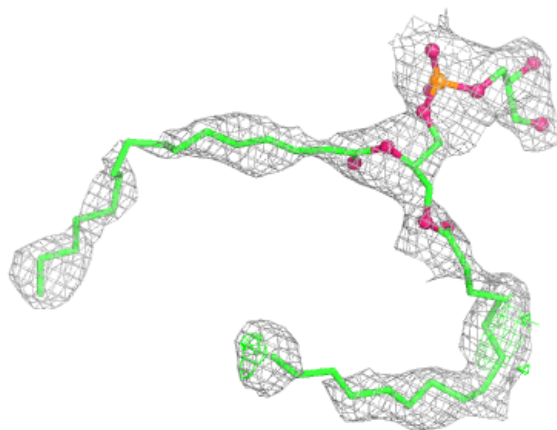
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SQD I 102:

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

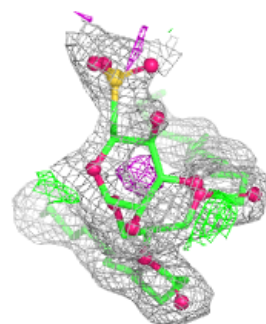
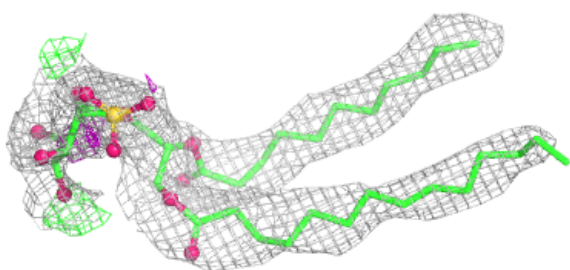
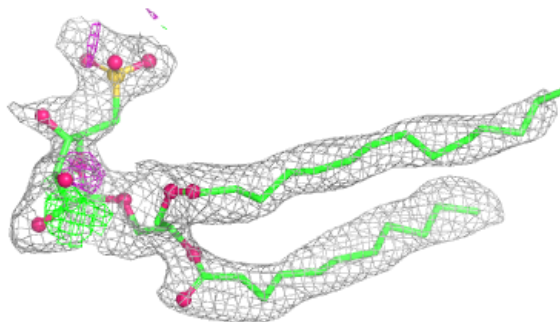
**Electron density around LHG E 101:**

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

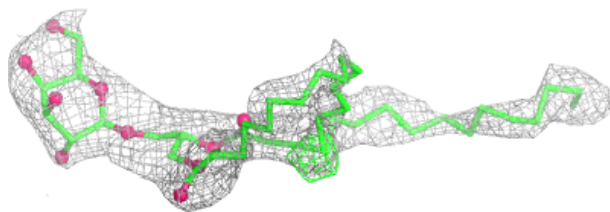
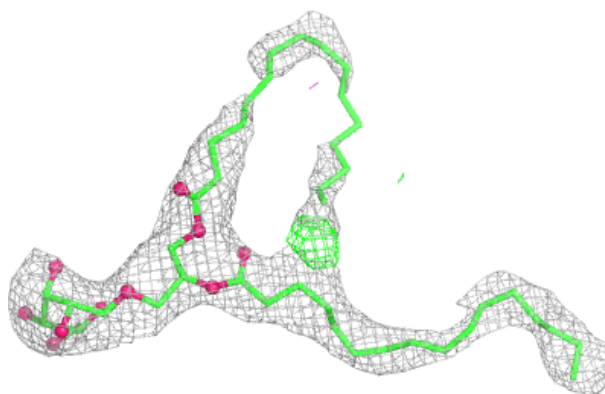


Electron density around SQD B 623:

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

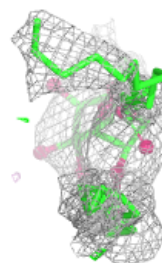
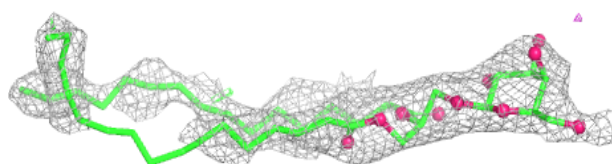
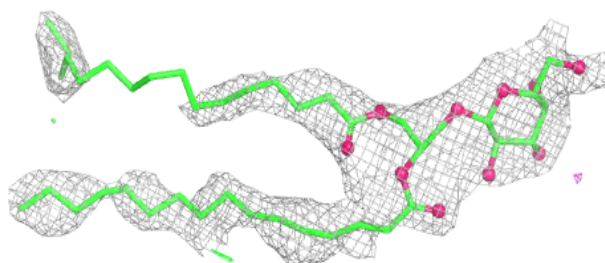
**Electron density around LMG b 627:**

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

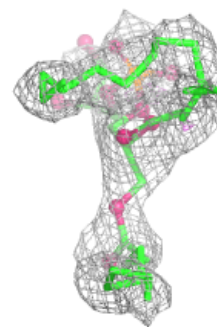
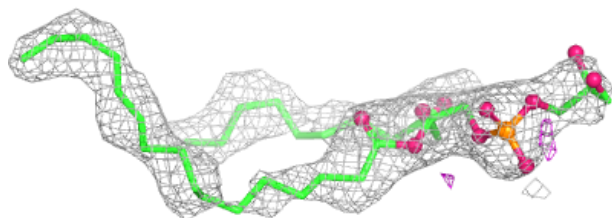
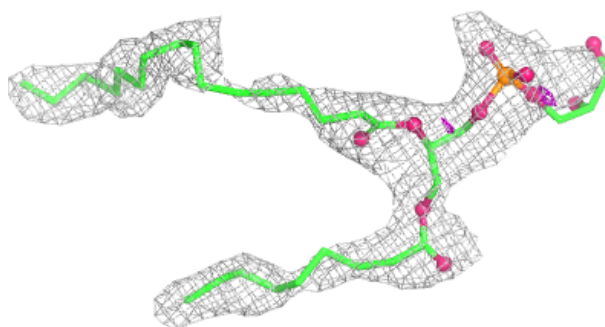


Electron density around LMG C 521:

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

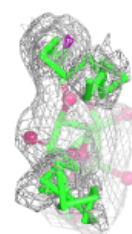
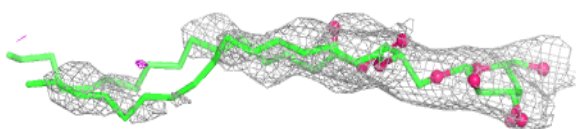
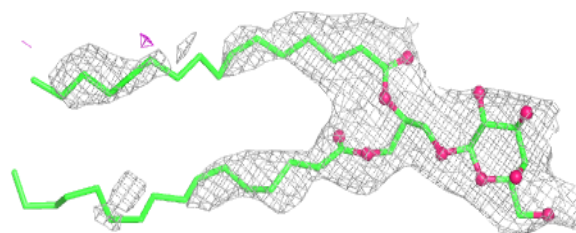
**Electron density around LHG e 101:**

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

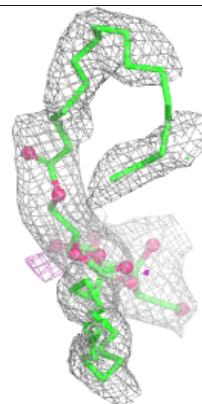
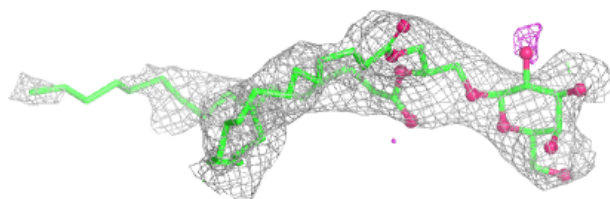
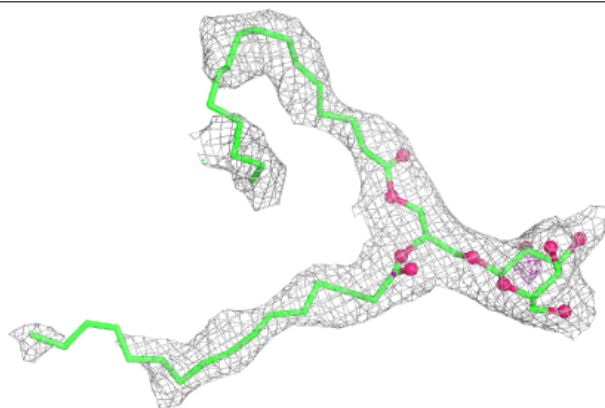


Electron density around LMG c 520:

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

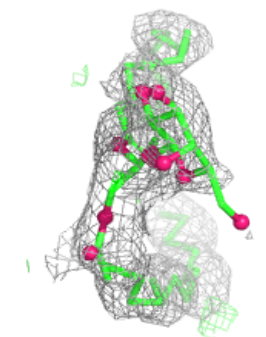
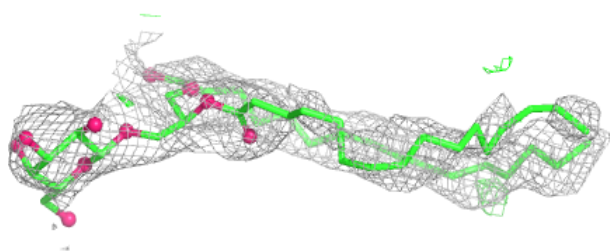
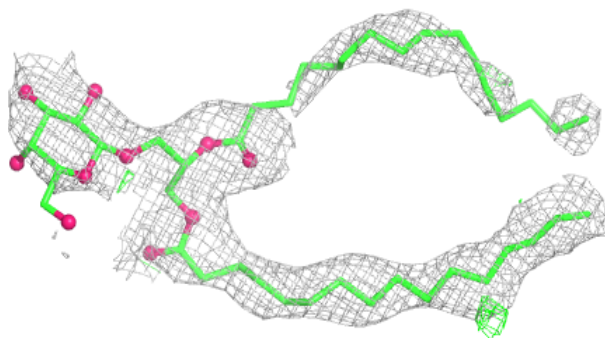
**Electron density around LMG B 621:**

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

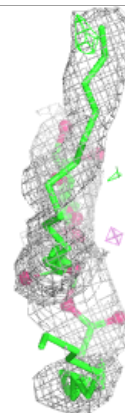
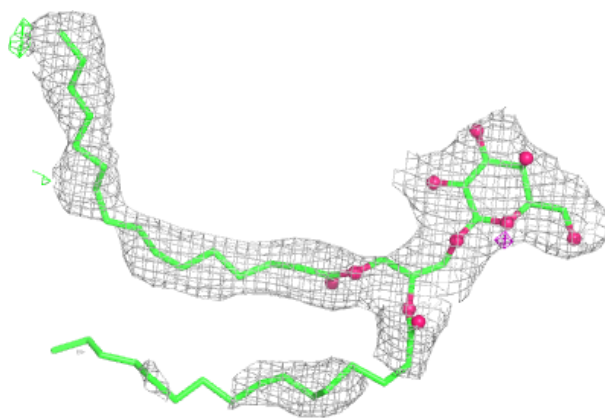


Electron density around LMG C 501:

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

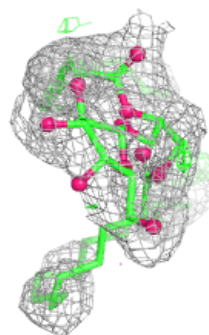
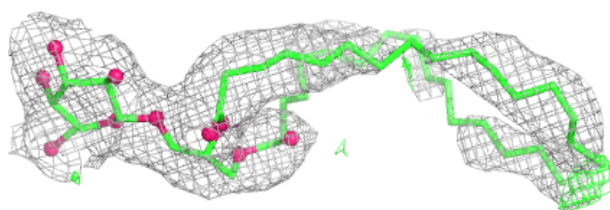
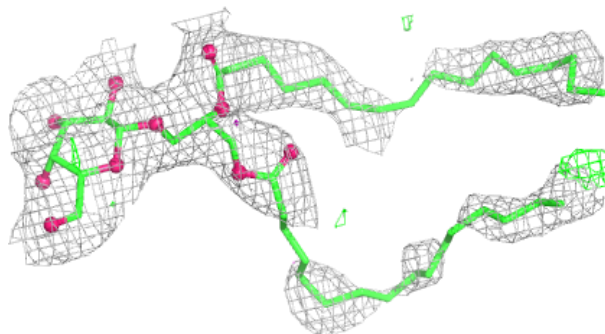
**Electron density around LMG C 520:**

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



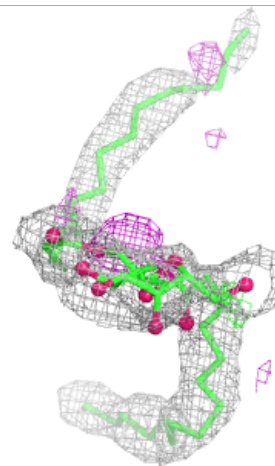
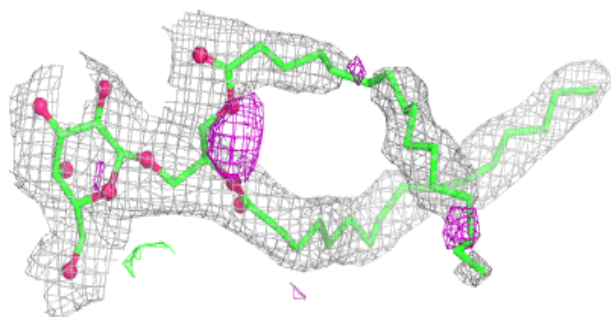
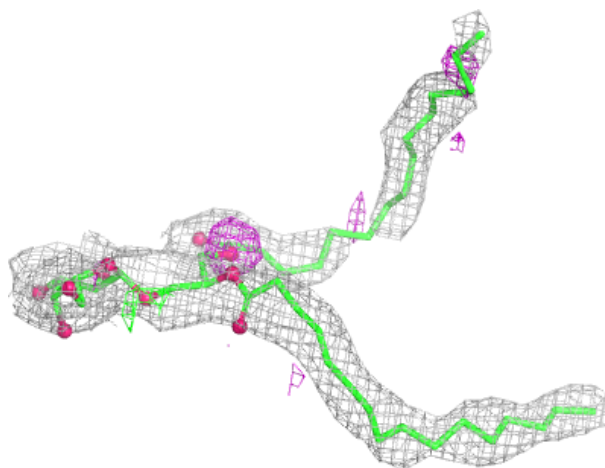
Electron density around LMG A 603:

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



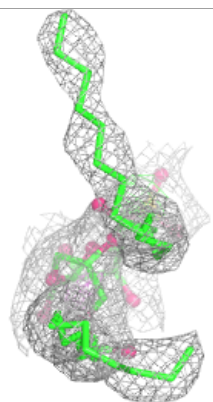
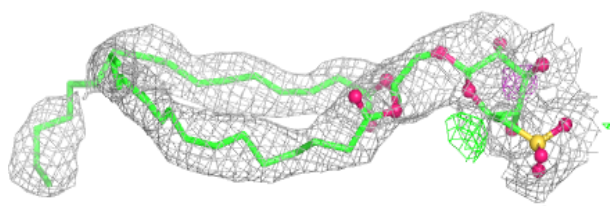
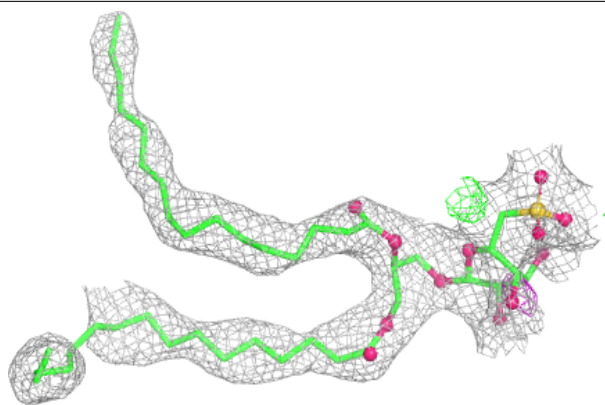
Electron density around LMG b 626:

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

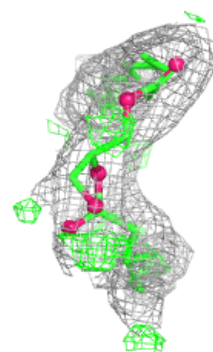
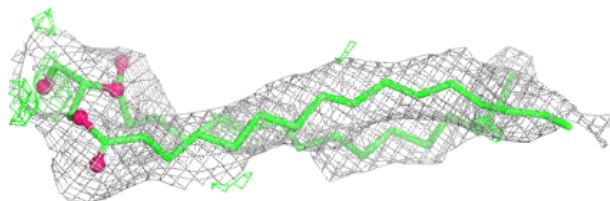
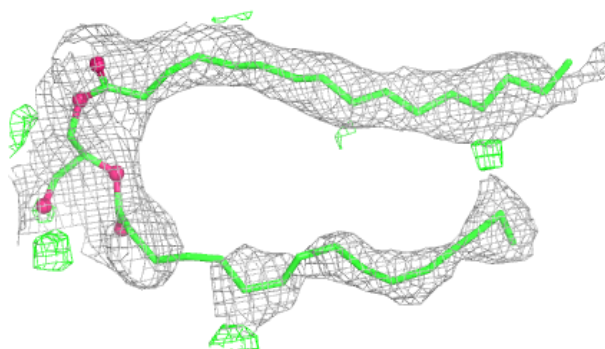


Electron density around SQD b 601:

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

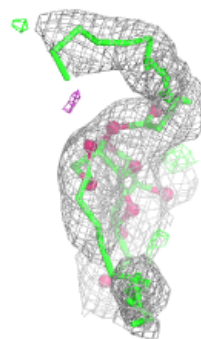
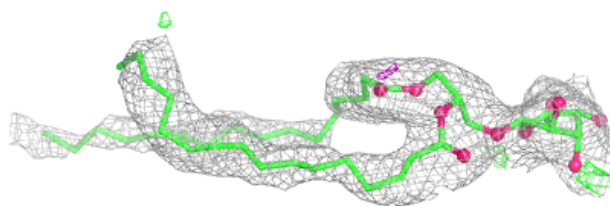
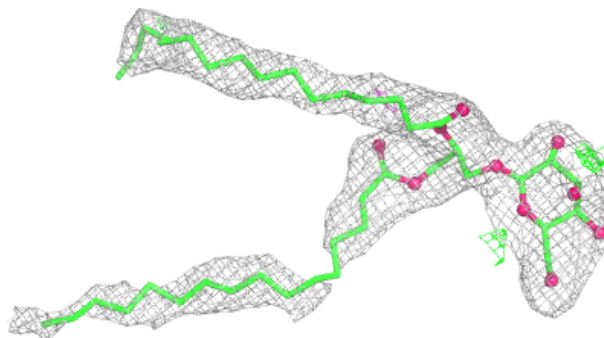
**Electron density around SQD A 614:**

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

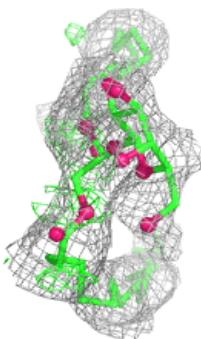
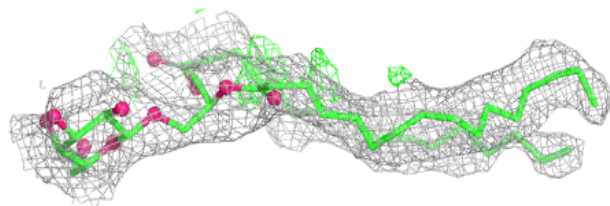
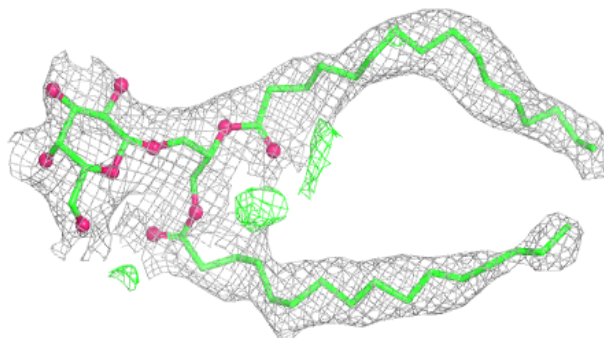


Electron density around LMG a 701:

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

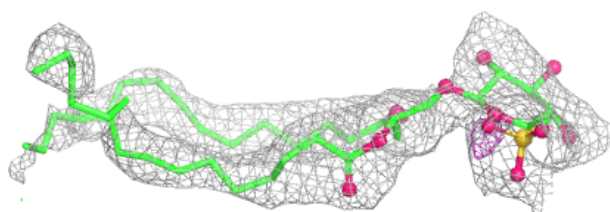
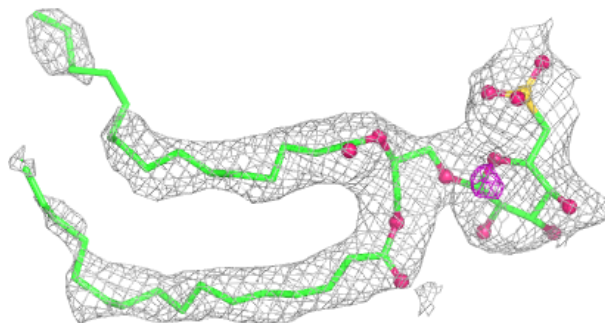
**Electron density around LMG a 715:**

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

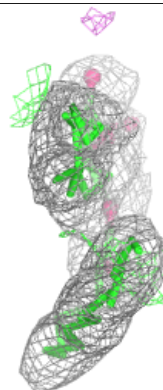
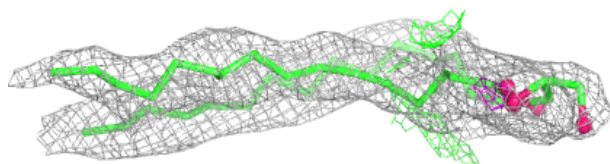
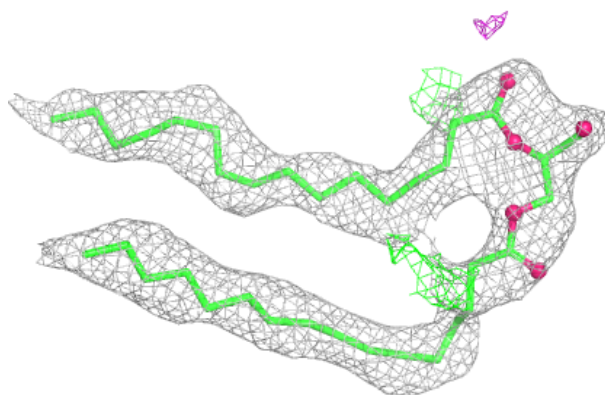


Electron density around SQD B 626:

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

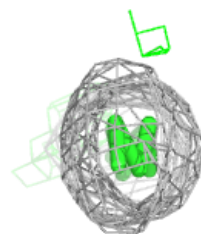
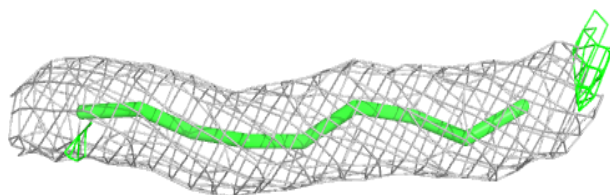
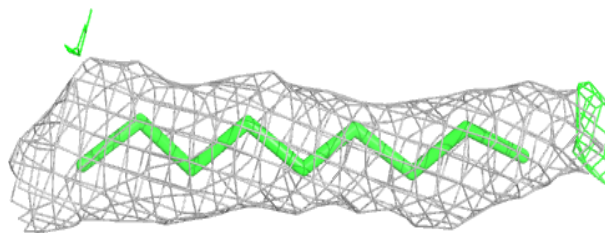
**Electron density around LMG d 408:**

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

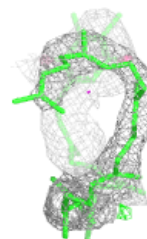
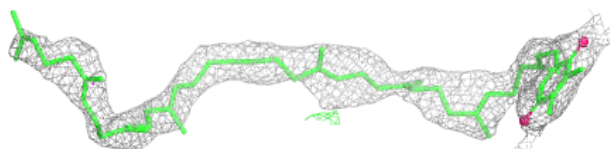
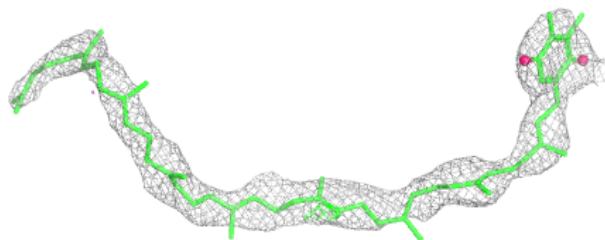


Electron density around LMG b 628:

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

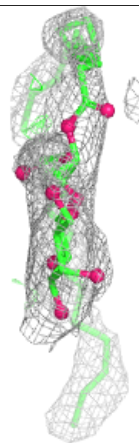
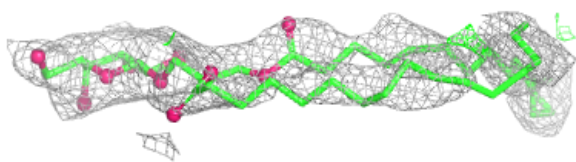
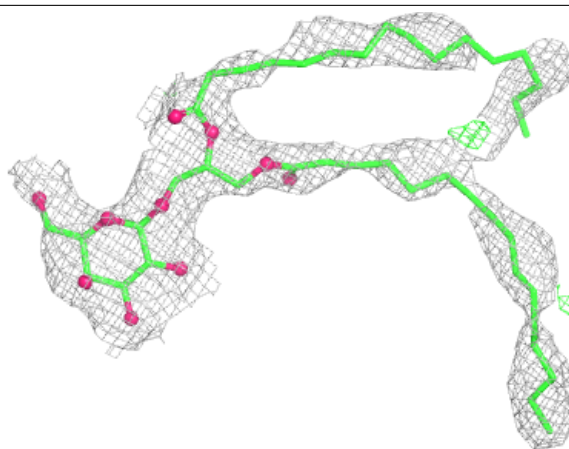
**Electron density around PL9 a 713:**

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



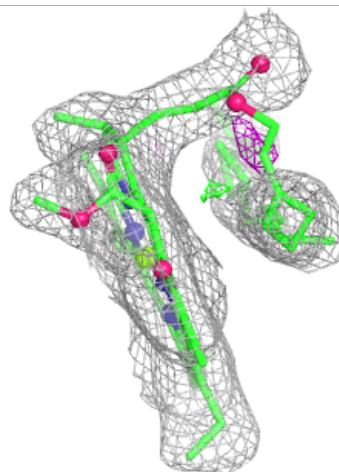
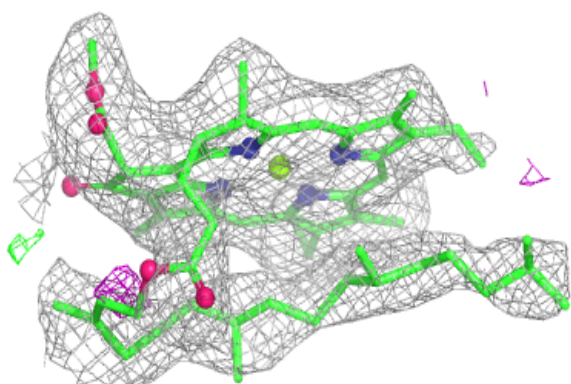
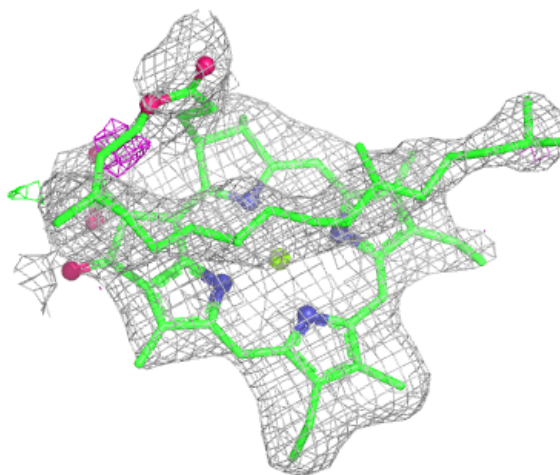
Electron density around LMG c 519:

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



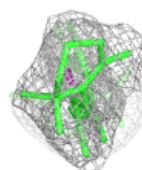
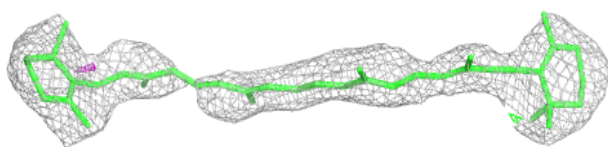
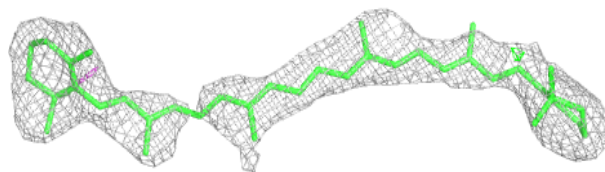
Electron density around CLA b 607:

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

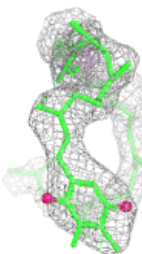
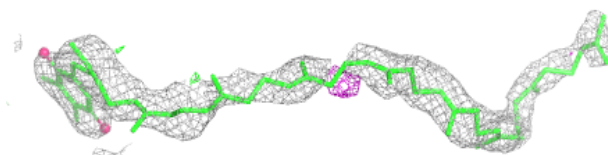
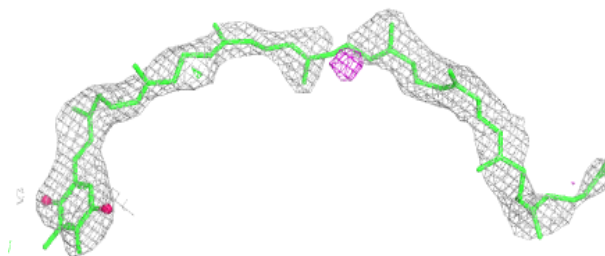


Electron density around BCR k 101:

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

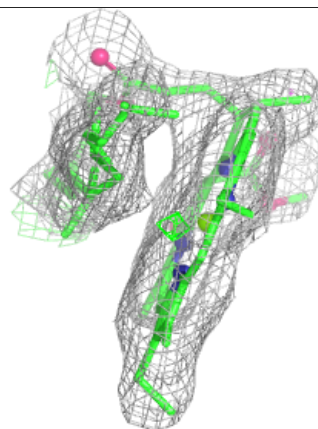
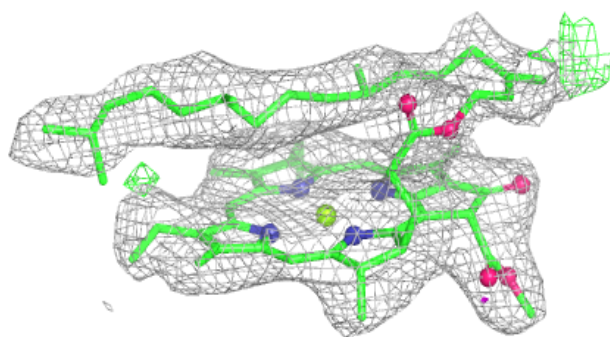
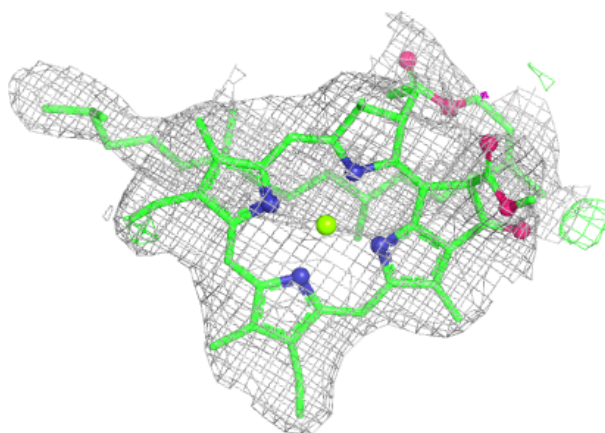
**Electron density around PL9 A 611:**

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

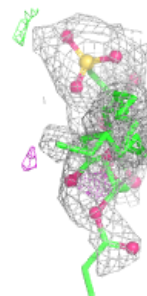
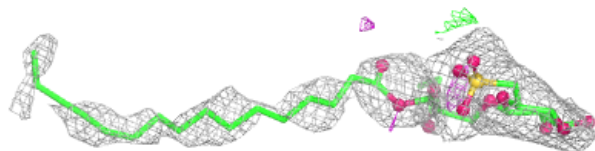
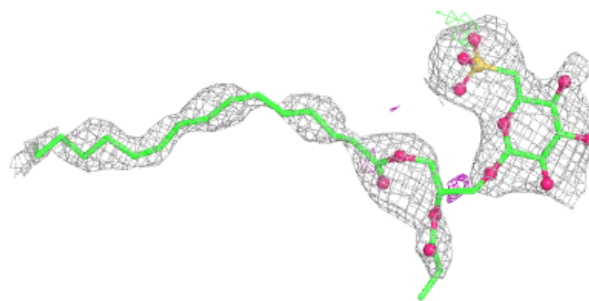


Electron density around CLA B 602:

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

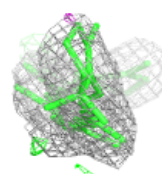
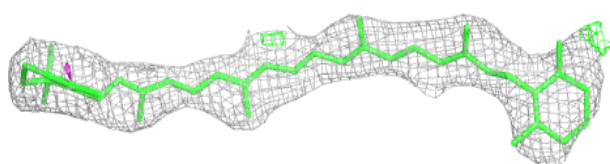
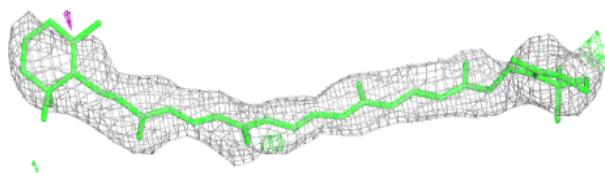
**Electron density around SQD f 102:**

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

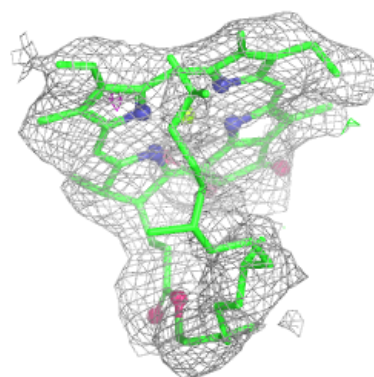
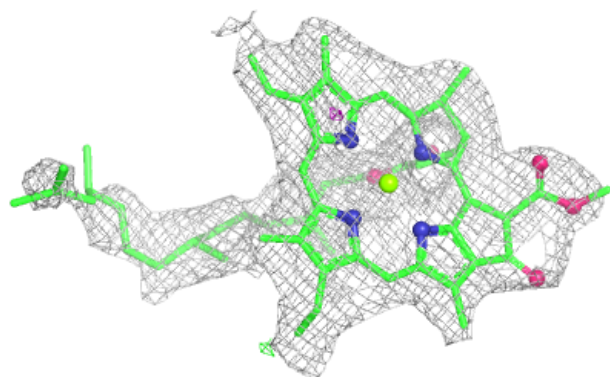
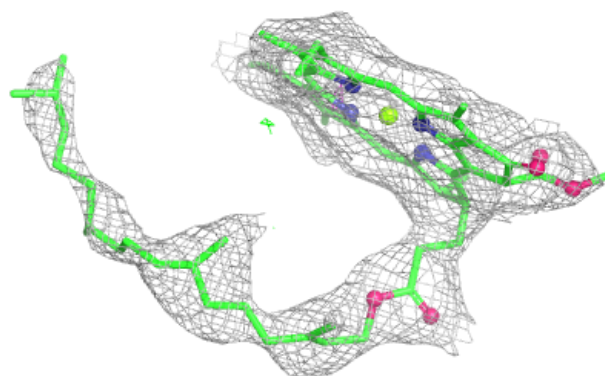


Electron density around BCR D 405:

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

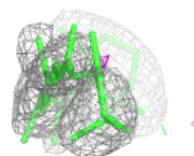
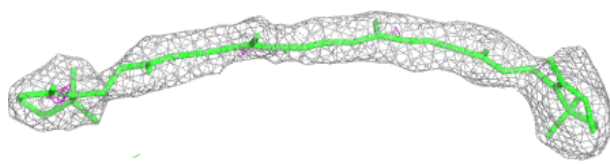
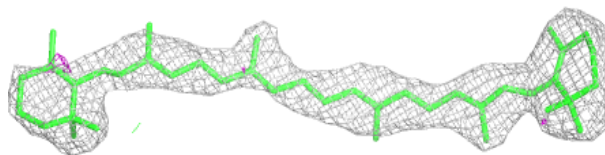
**Electron density around CLA C 514:**

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

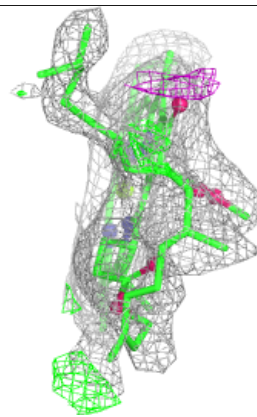
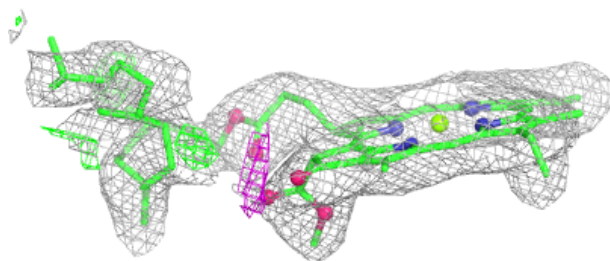
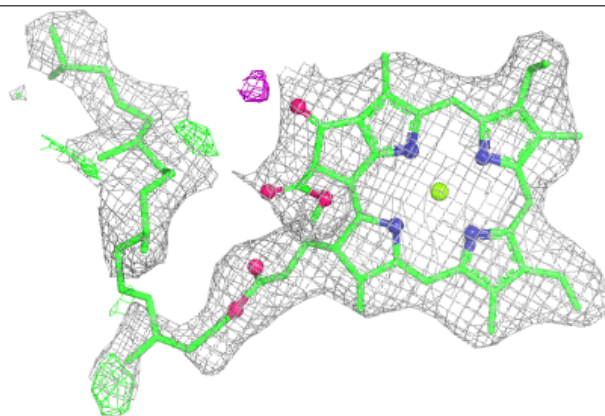


Electron density around BCR b 602:

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

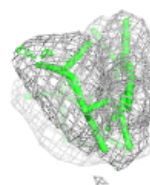
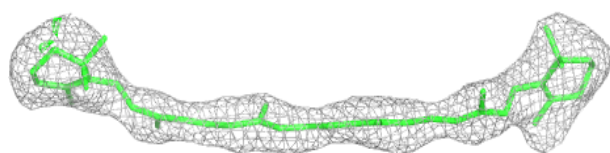
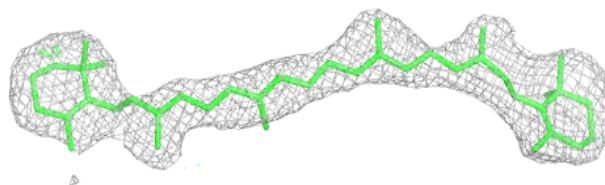
**Electron density around CLA B 617:**

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

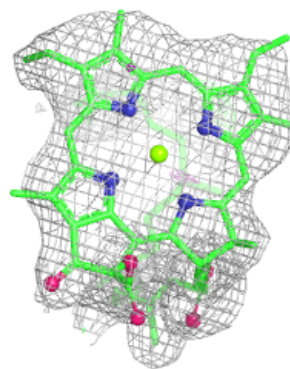
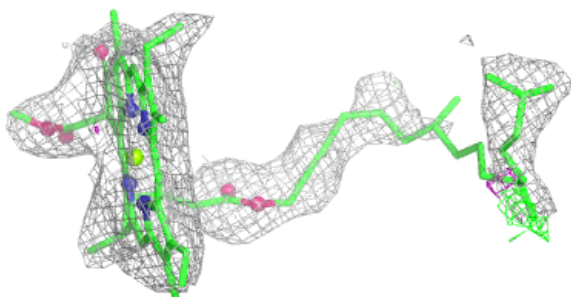
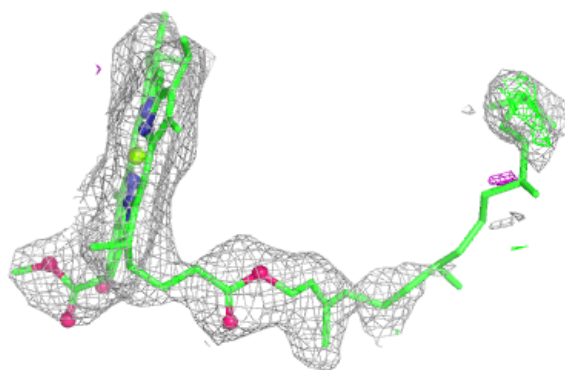


Electron density around BCR t 103:

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

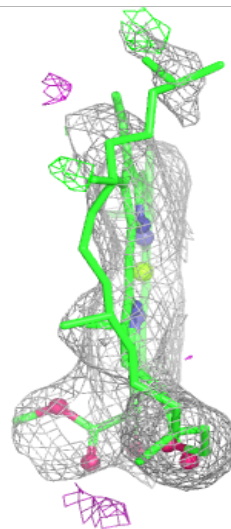
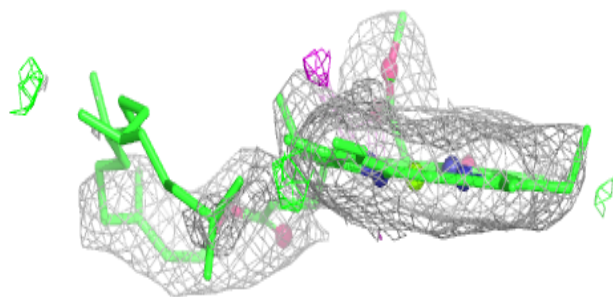
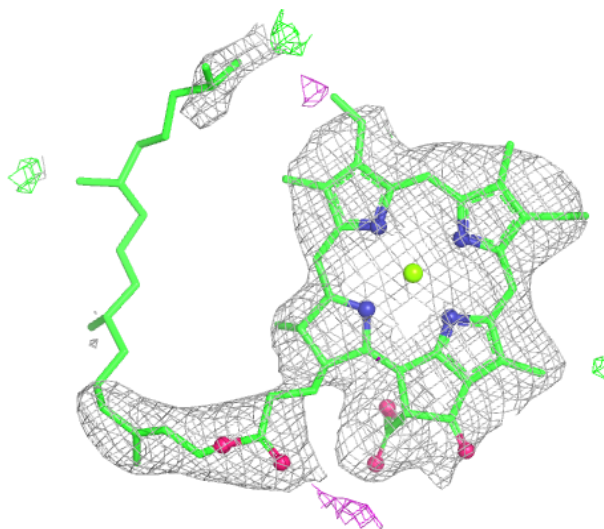
**Electron density around CLA c 506:**

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



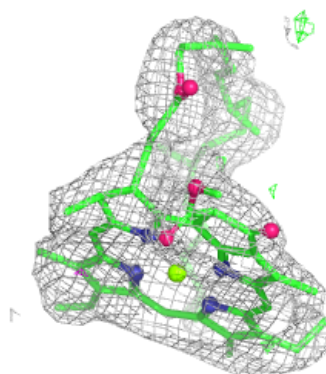
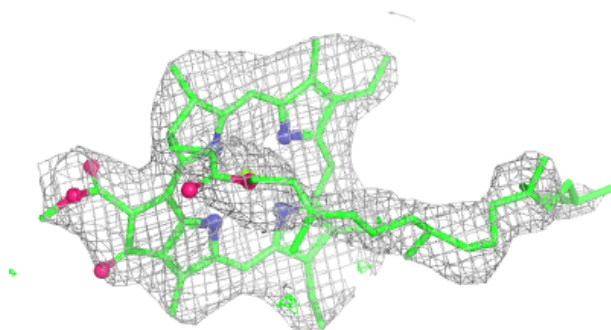
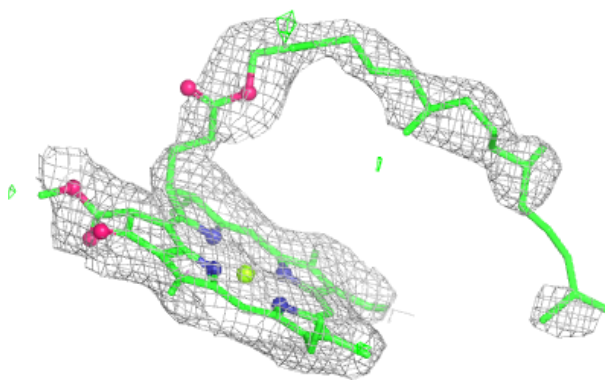
Electron density around CLA c 512:

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

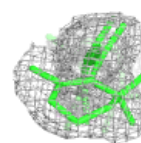
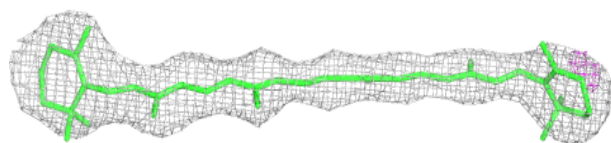
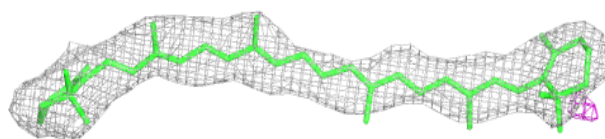


Electron density around CLA c 513:

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

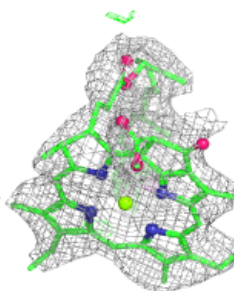
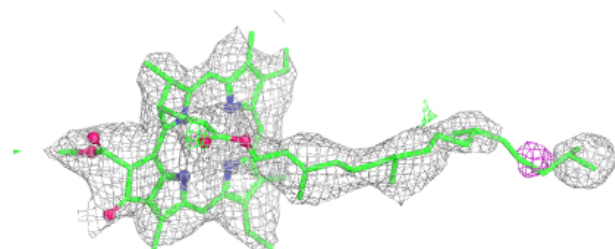
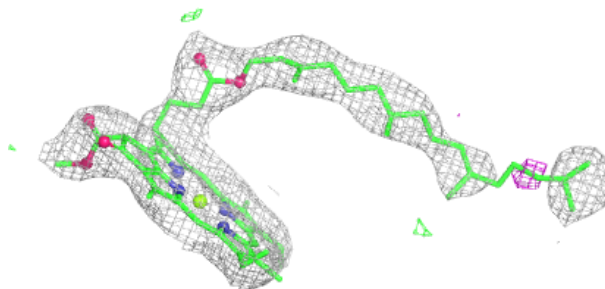
**Electron density around BCR C 515:**

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

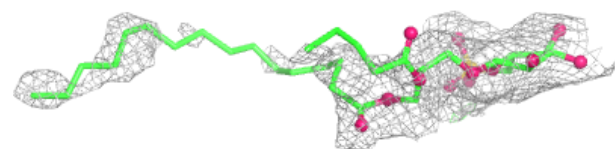
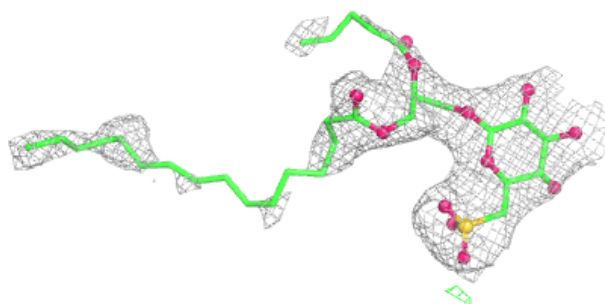


Electron density around CLA C 505:

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

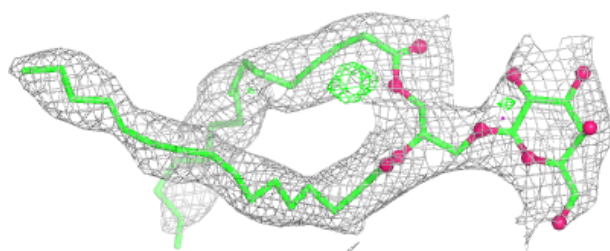
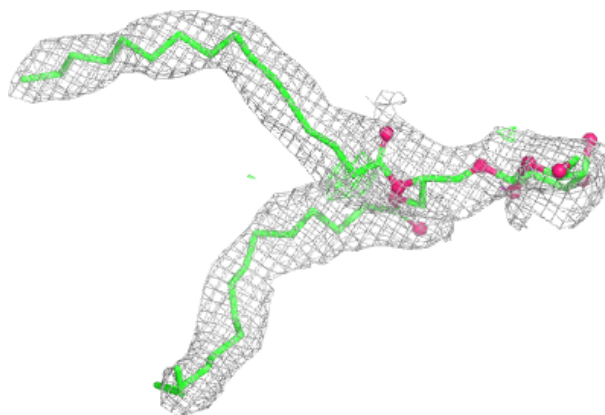
**Electron density around SQD D 410:**

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

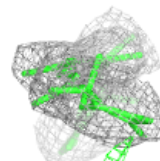
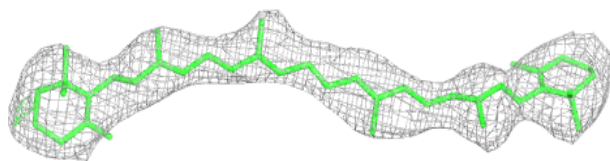
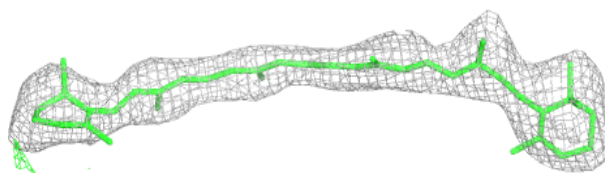


Electron density around LMG M 101:

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

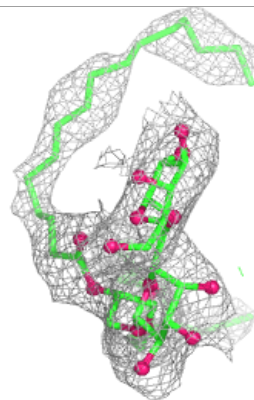
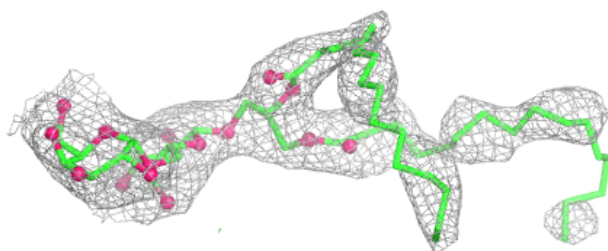
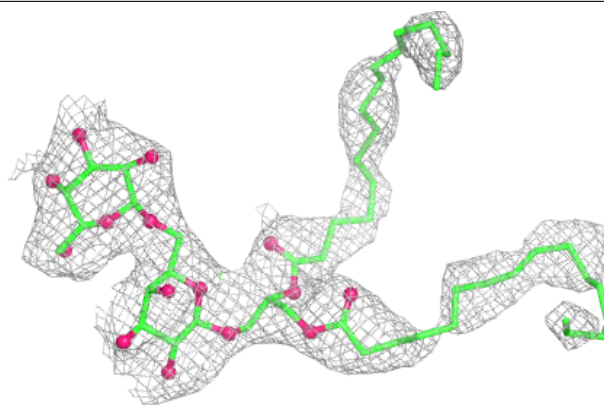
**Electron density around BCR d 404:**

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

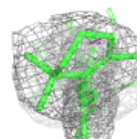
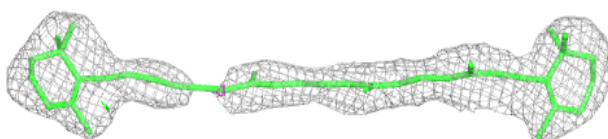
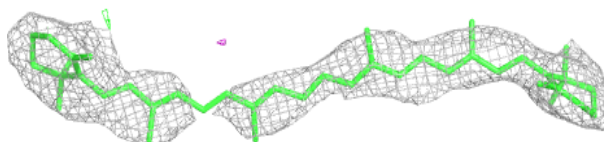


Electron density around DGD c 517:

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

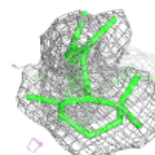
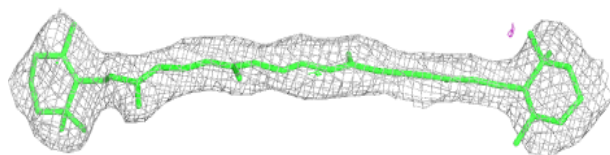
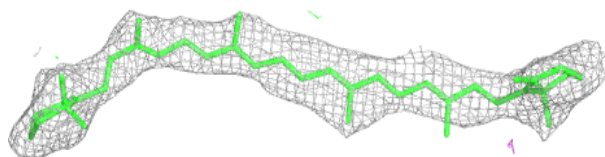
**Electron density around BCR c 514:**

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



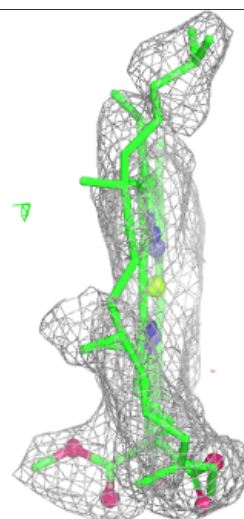
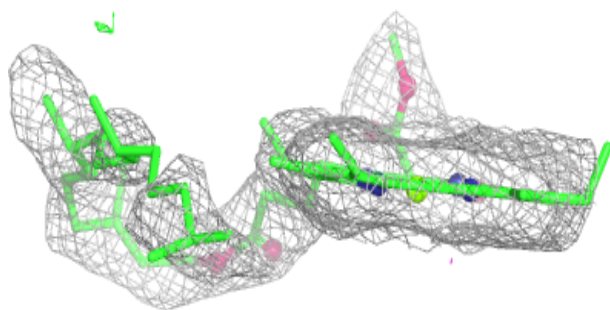
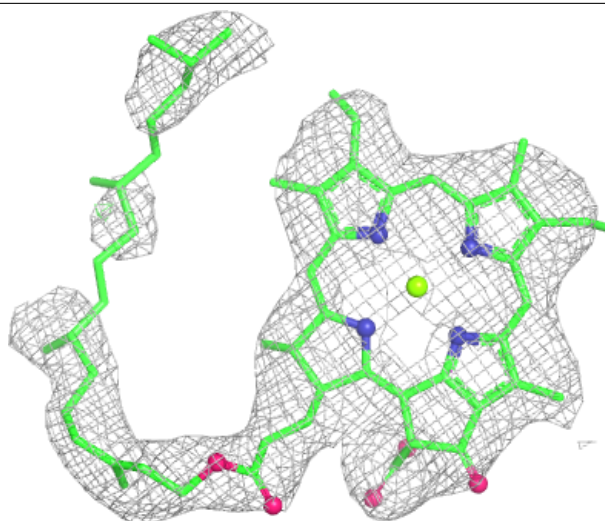
Electron density around BCR H 102:

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



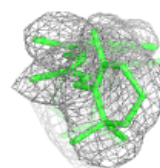
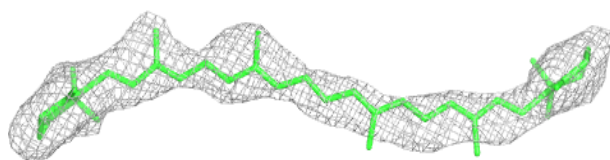
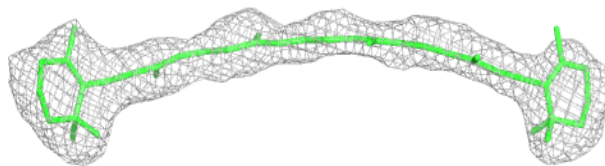
Electron density around CLA C 513:

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

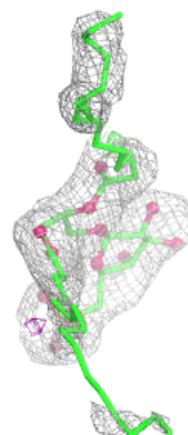
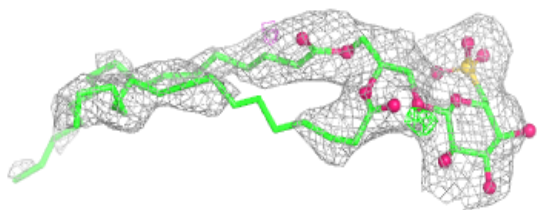
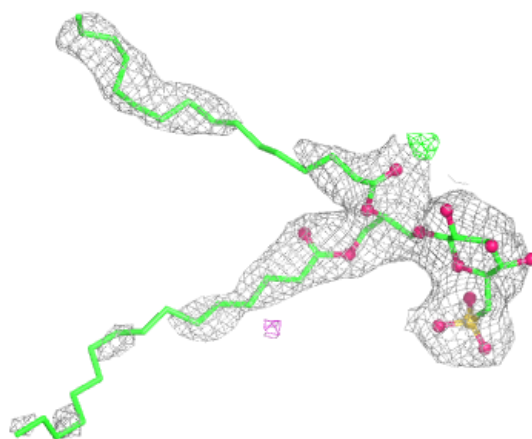


Electron density around BCR k 102:

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

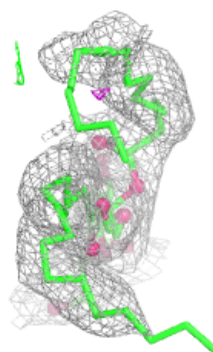
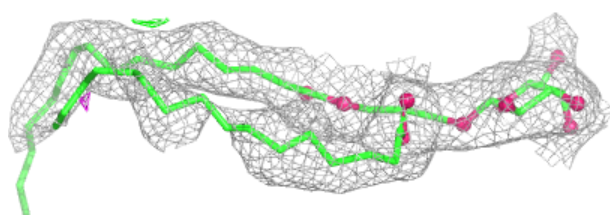
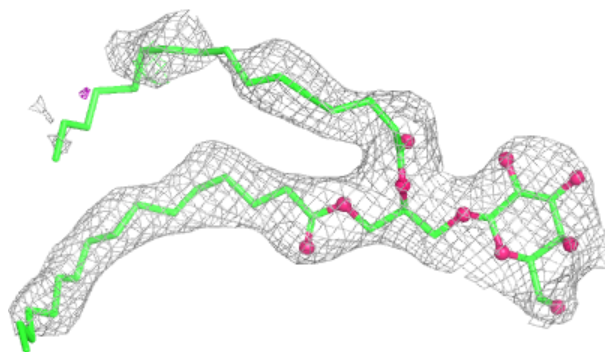
**Electron density around SQD a 714:**

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

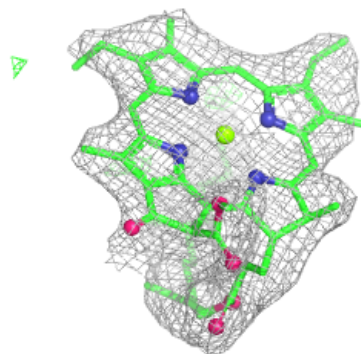
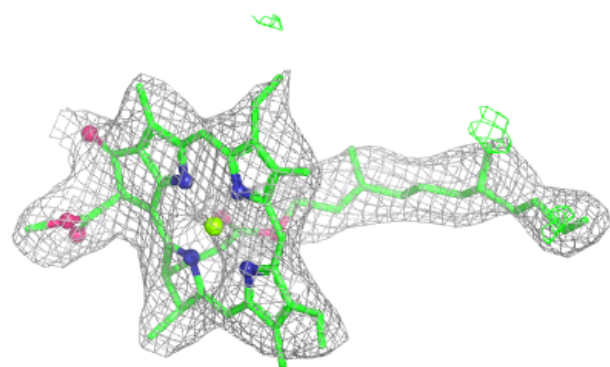
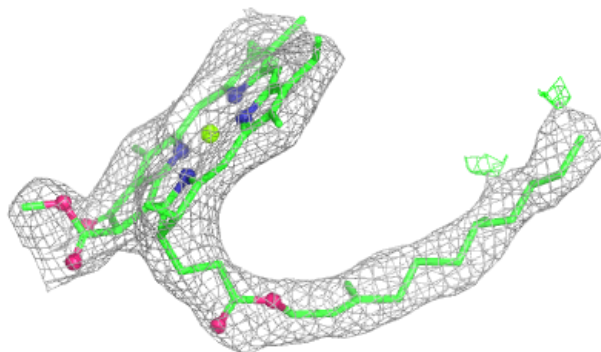


Electron density around LMG f 101:

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

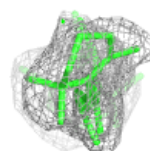
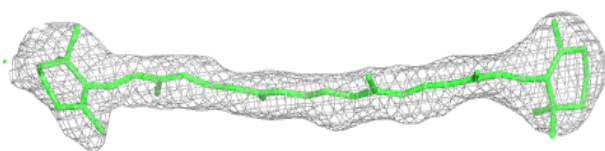
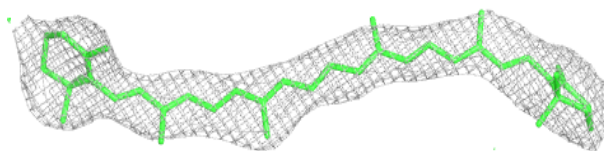
**Electron density around CLA c 504:**

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

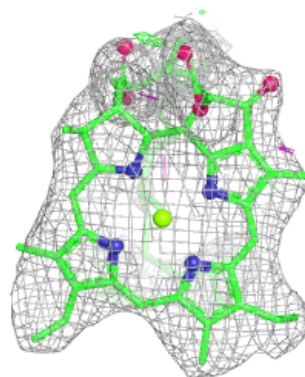
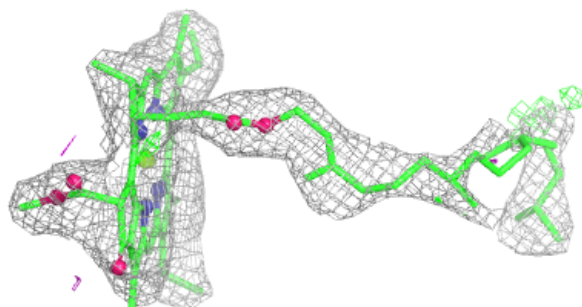
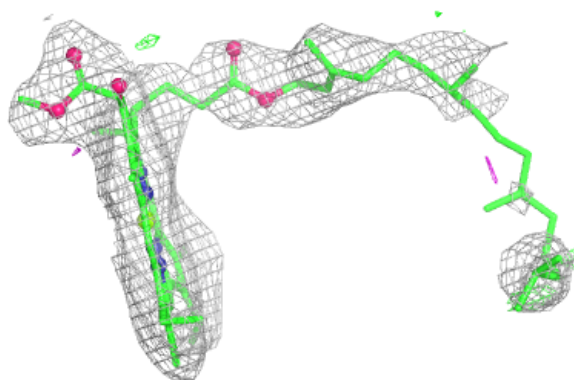


Electron density around BCR Y 101:

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

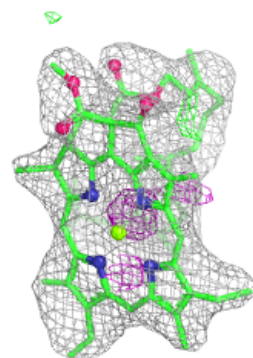
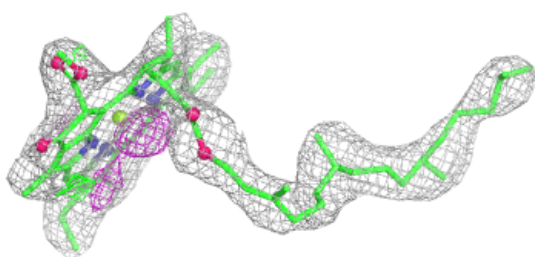
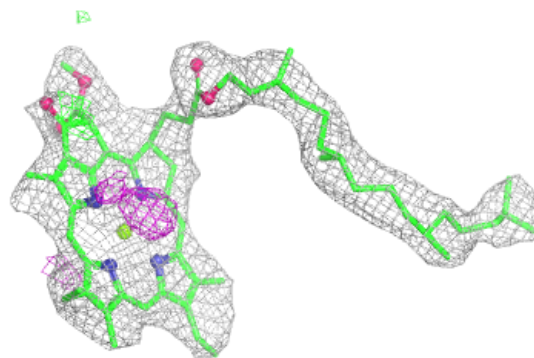
**Electron density around CLA C 507:**

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

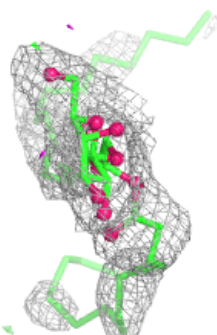
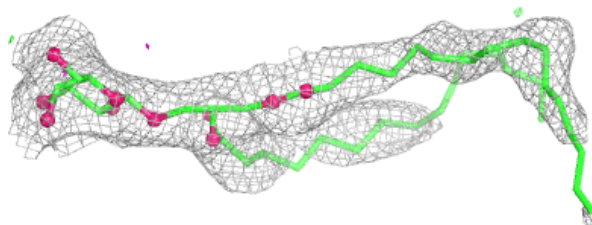
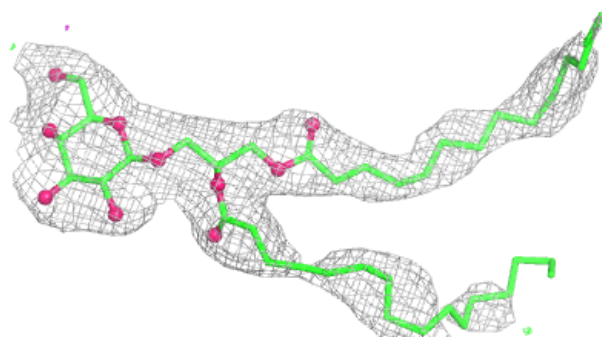


Electron density around CLA C 512:

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

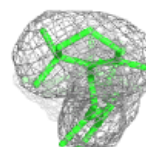
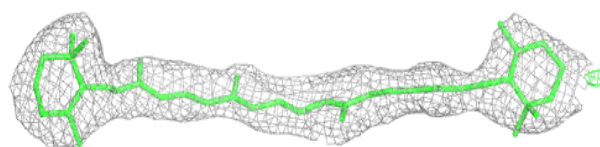
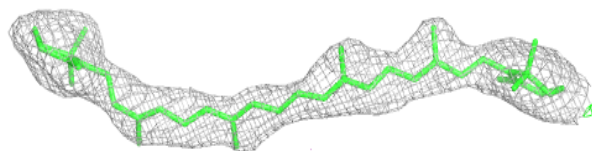
**Electron density around LMG D 409:**

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



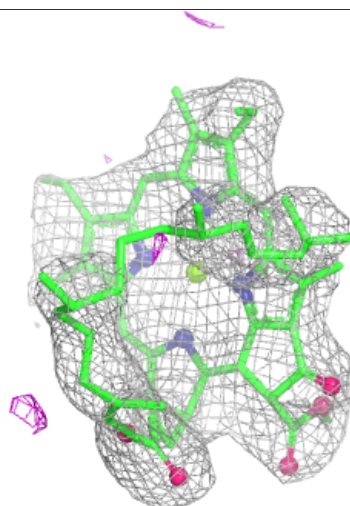
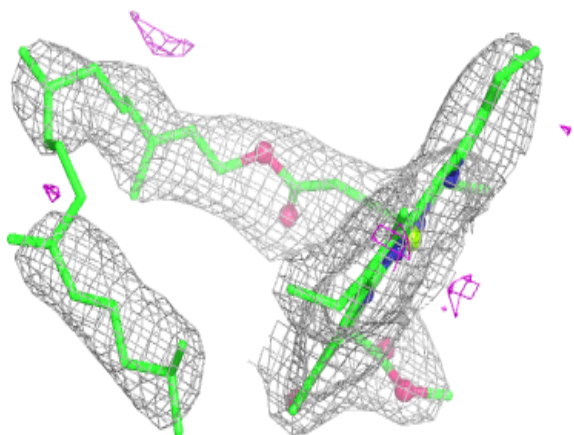
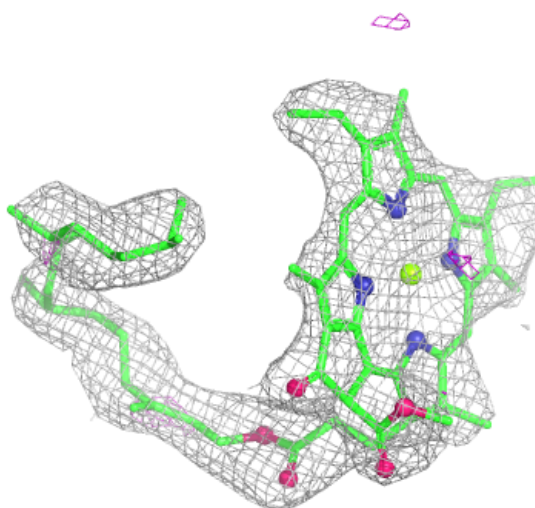
Electron density around BCR h 101:

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



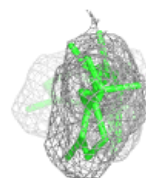
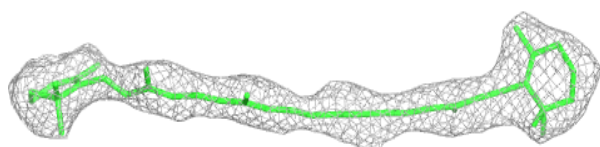
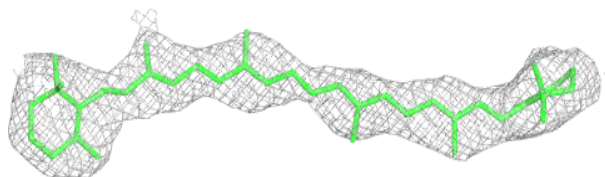
Electron density around CLA c 503:

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

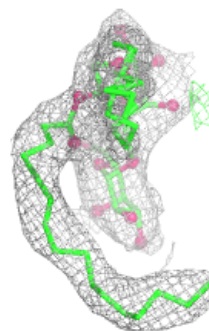
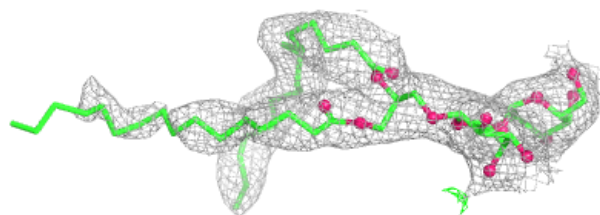
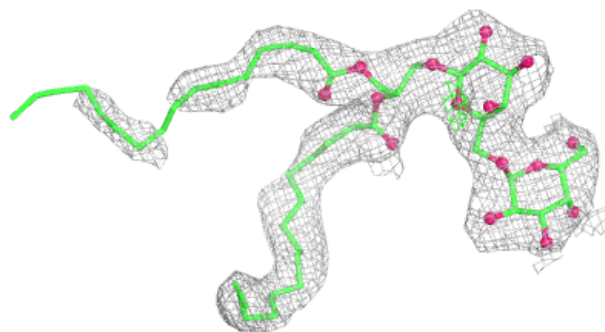


Electron density around BCR b 623:

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

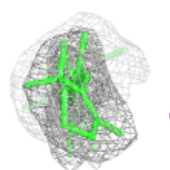
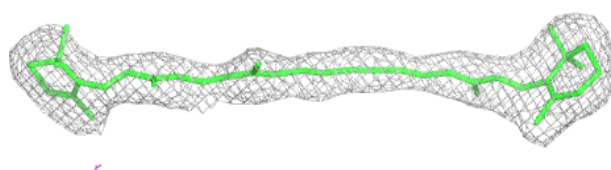
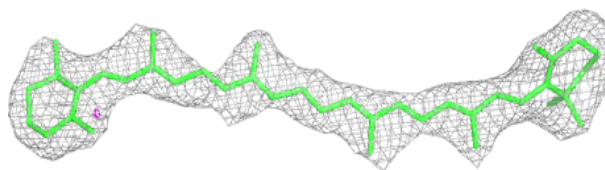
**Electron density around DGD C 518:**

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

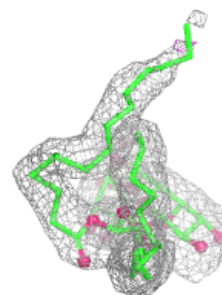
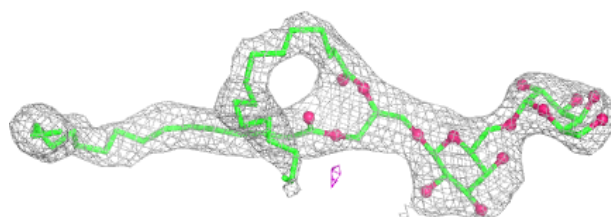


Electron density around BCR b 624:

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

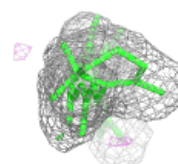
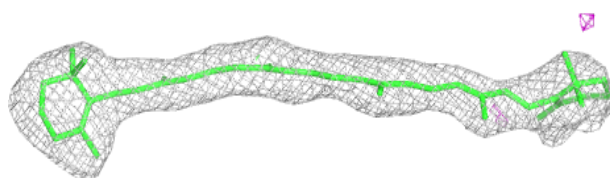
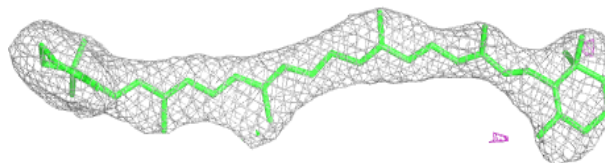
**Electron density around DGD h 102:**

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

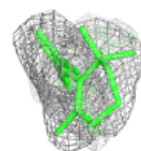
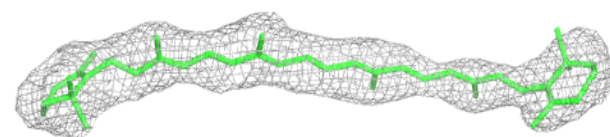
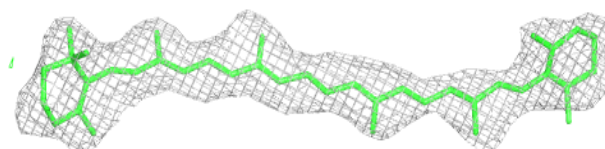


Electron density around BCR B 618:

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

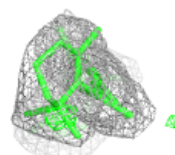
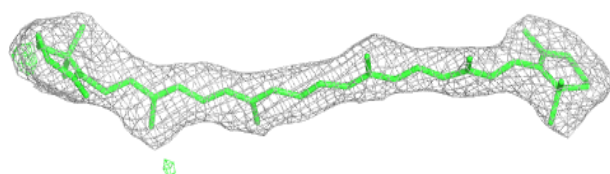
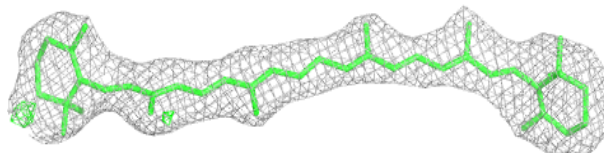
**Electron density around BCR B 620:**

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

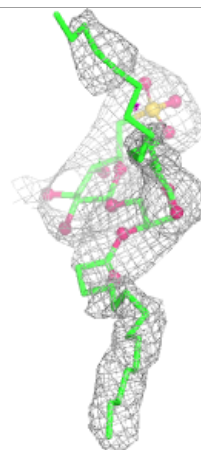
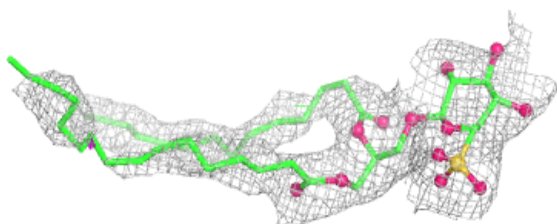
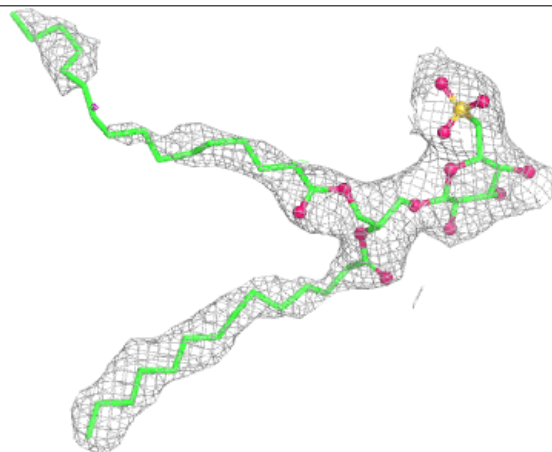


Electron density around BCR b 625:

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

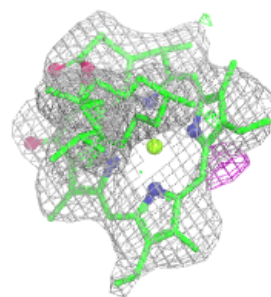
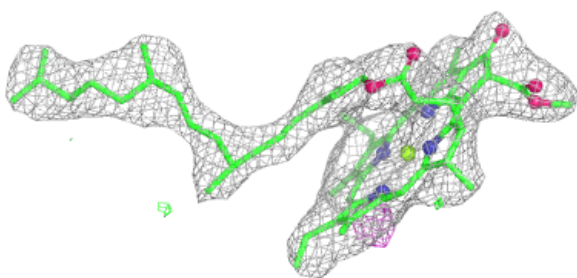
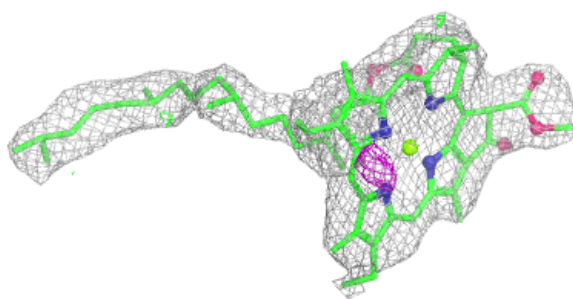
**Electron density around SQD A 612:**

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

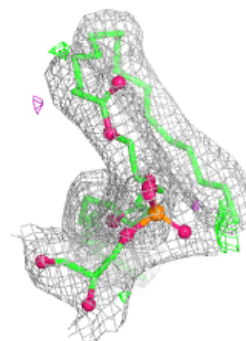
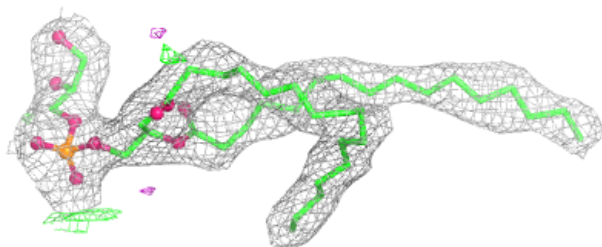
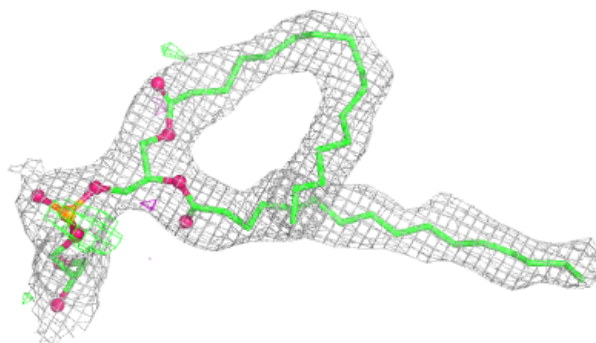


Electron density around CLA C 506:

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

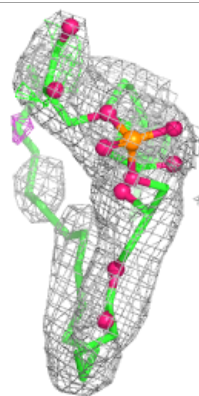
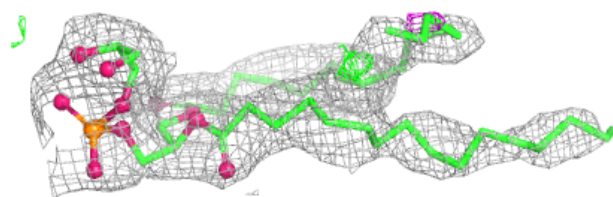
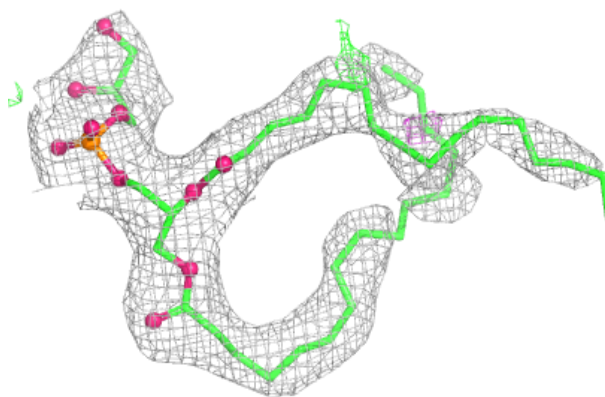
**Electron density around LHG B 625:**

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

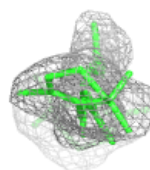
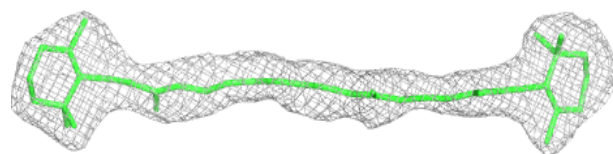
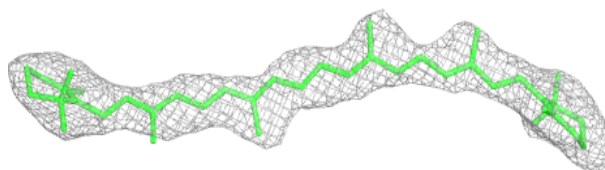


Electron density around LHG D 408:

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

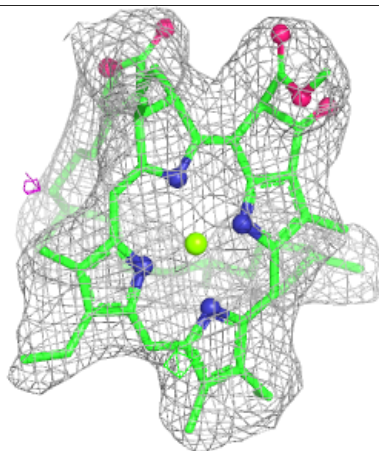
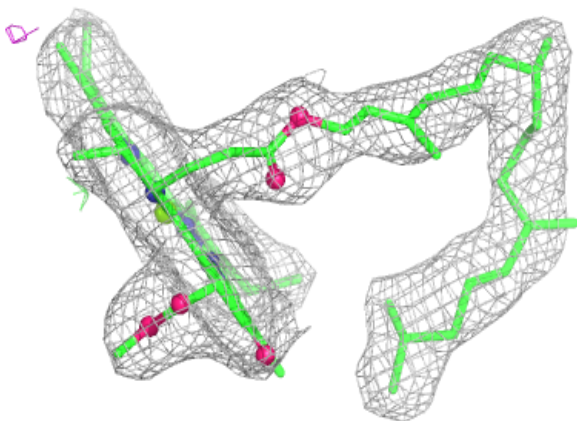
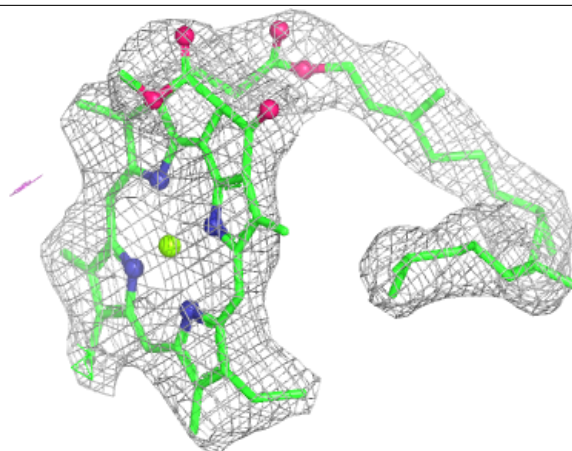
**Electron density around BCR c 515:**

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



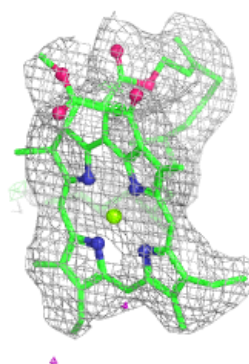
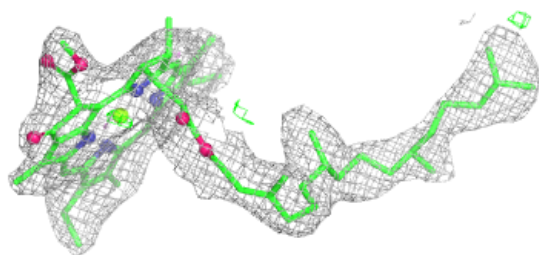
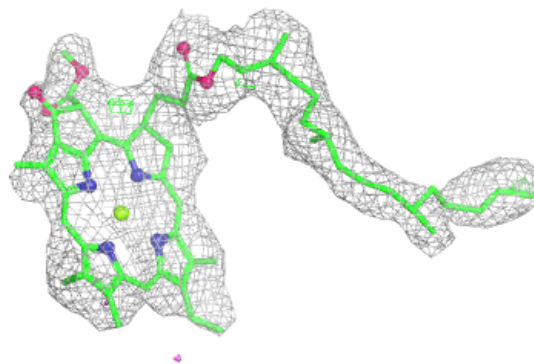
Electron density around CLA C 504:

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

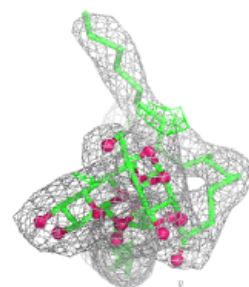
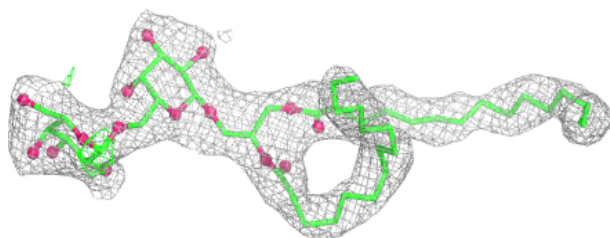
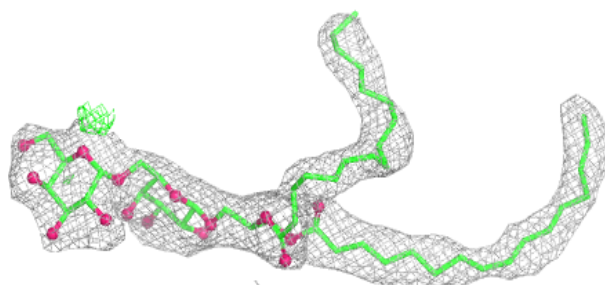


Electron density around CLA c 511:

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

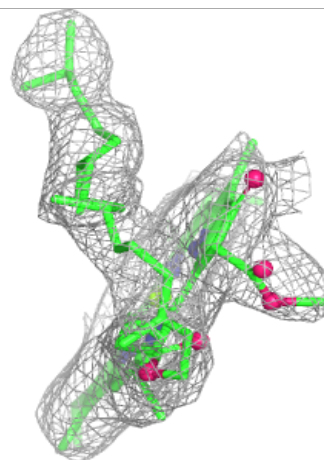
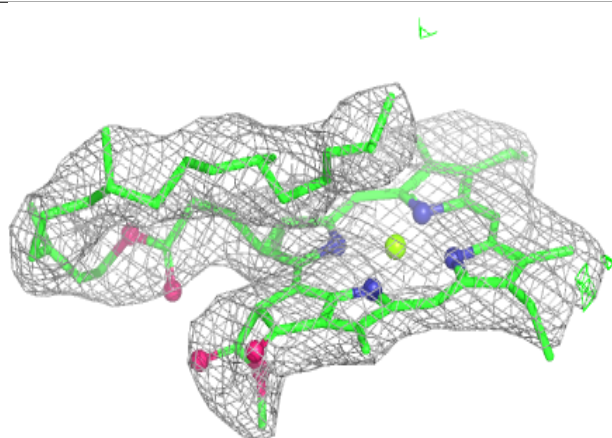
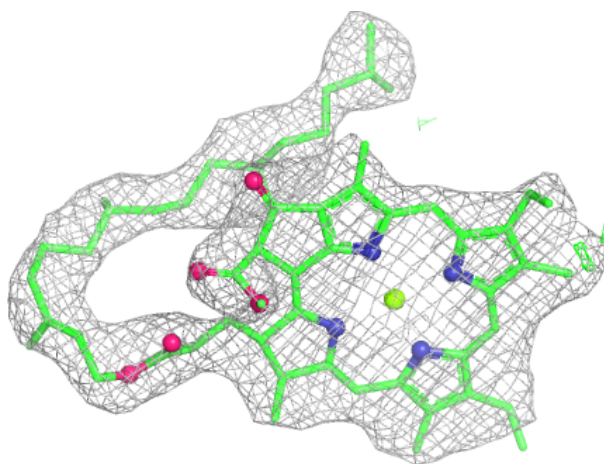
**Electron density around DGD H 103:**

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



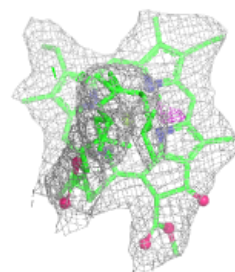
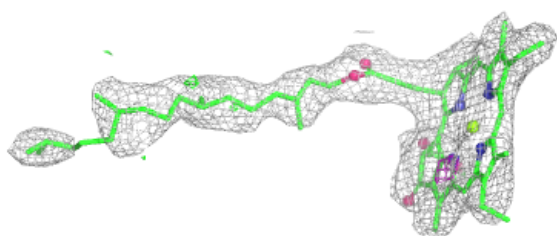
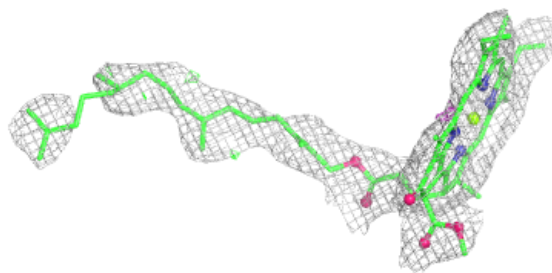
Electron density around CLA C 510:

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

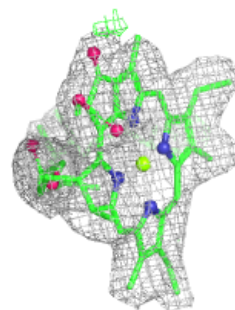
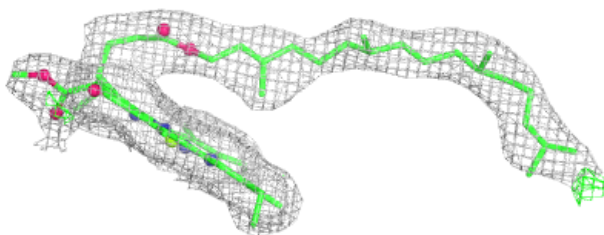
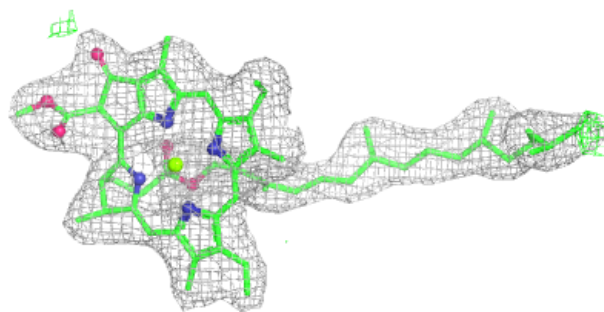


Electron density around CLA B 605:

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

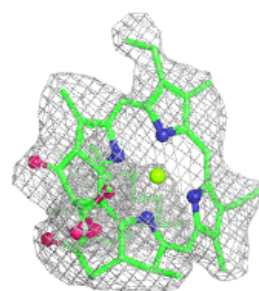
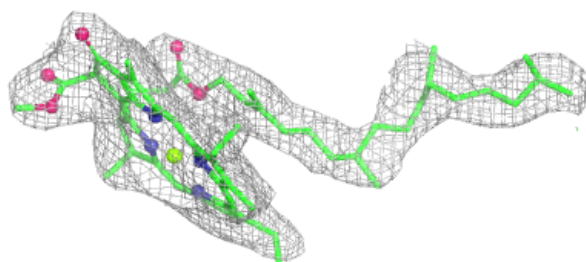
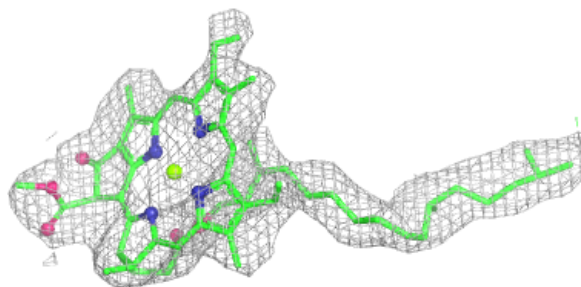
**Electron density around CLA B 609:**

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

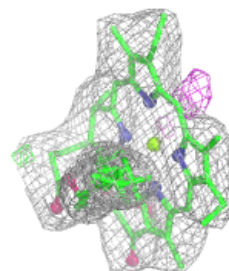
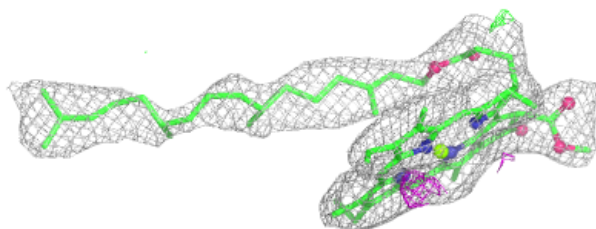
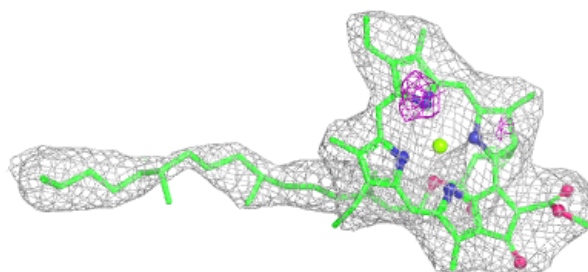


Electron density around CLA c 505:

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

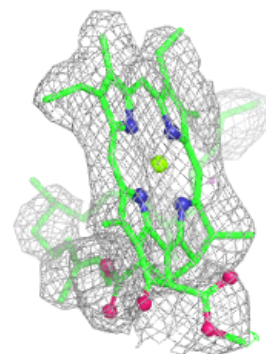
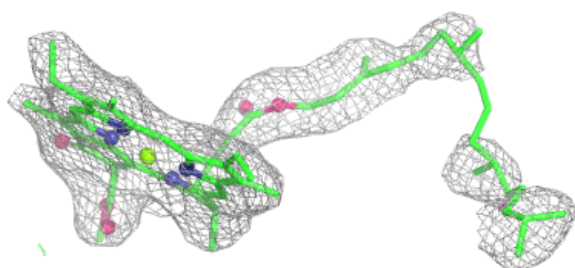
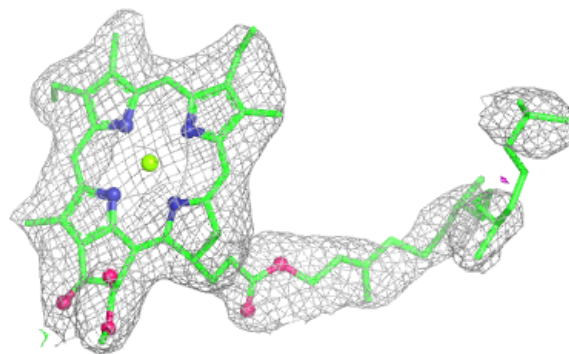
**Electron density around CLA B 615:**

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



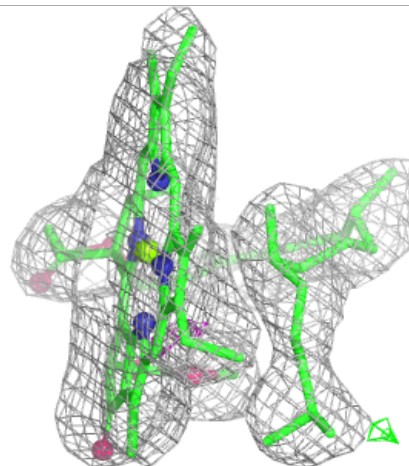
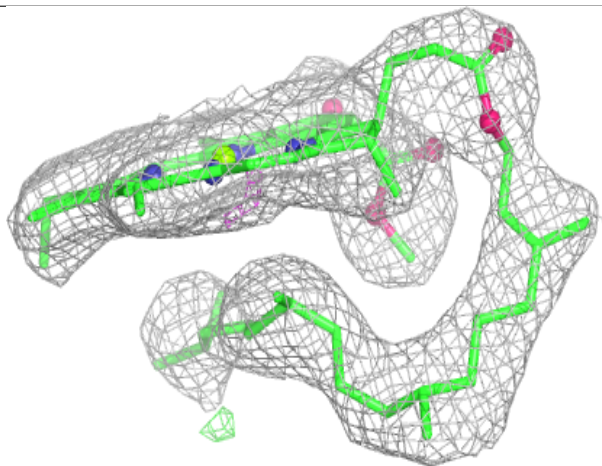
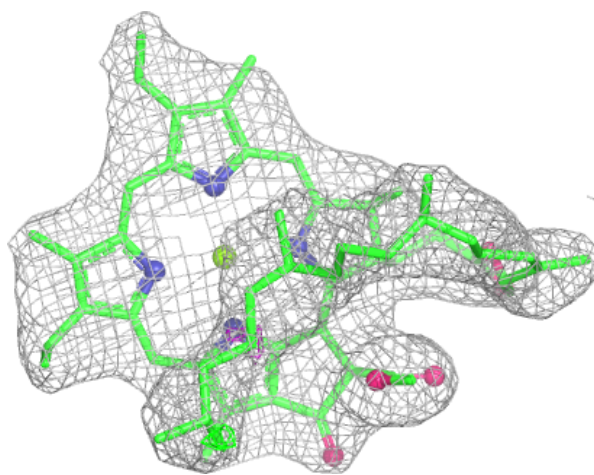
Electron density around CLA a 711:

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



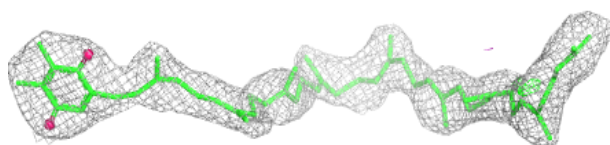
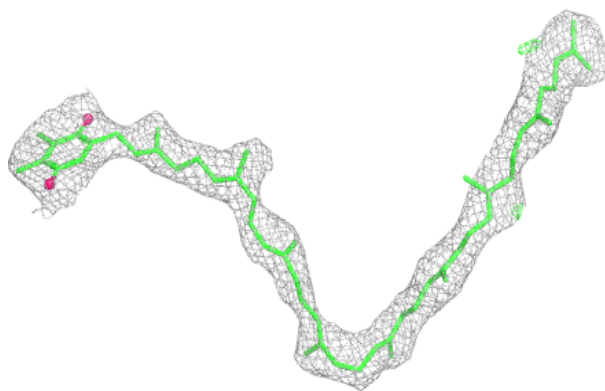
Electron density around CLA C 511:

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

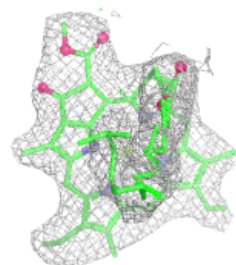
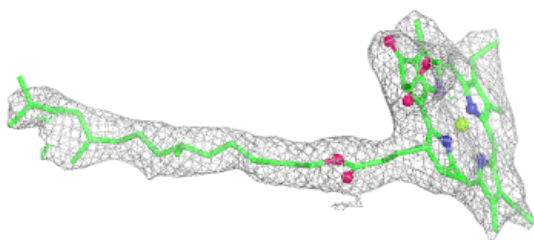
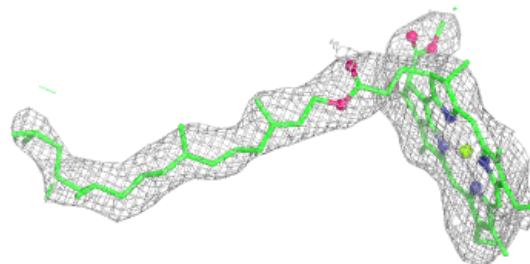


Electron density around PL9 D 406:

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

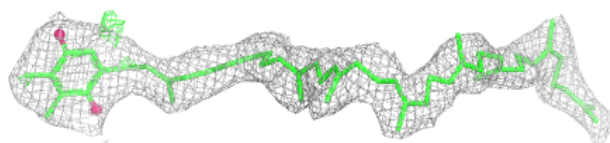
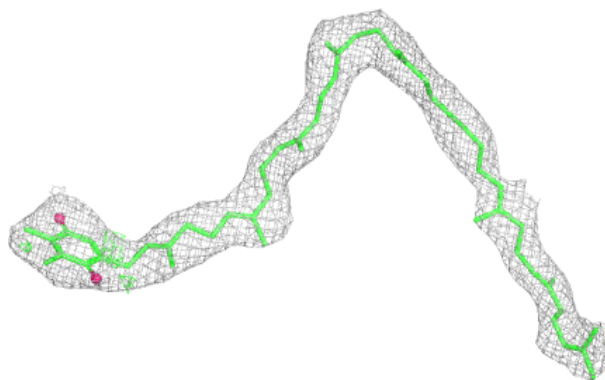
**Electron density around CLA b 610:**

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

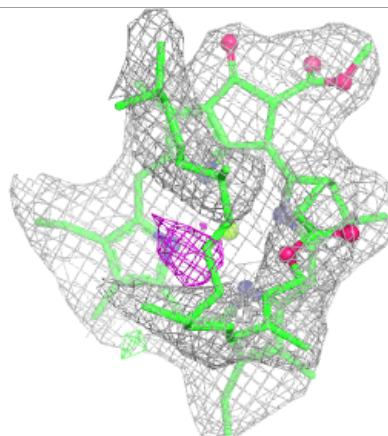
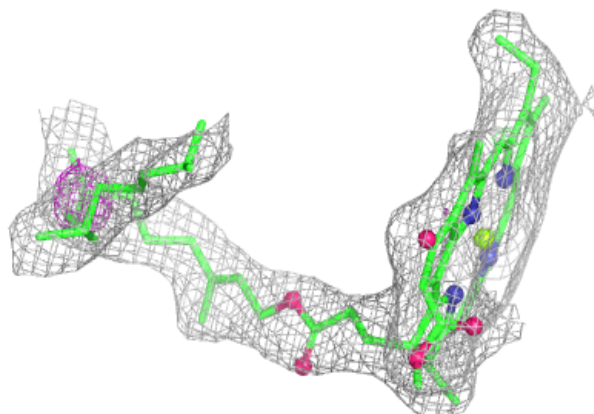
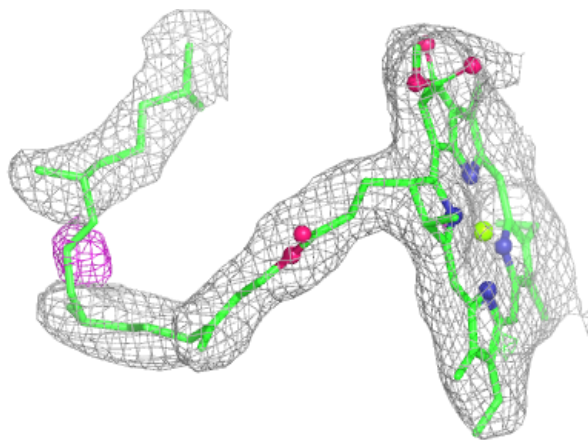


Electron density around PL9 d 405:

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

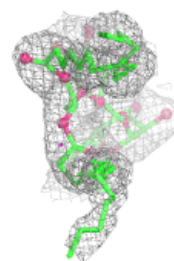
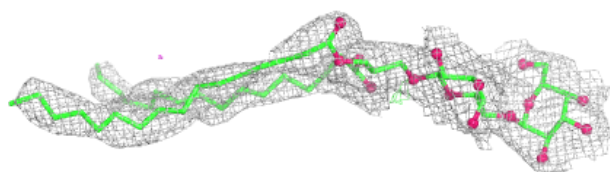
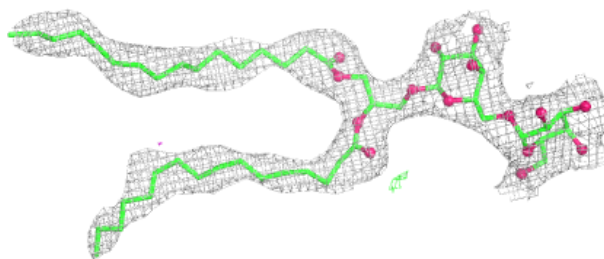
**Electron density around CLA b 612:**

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

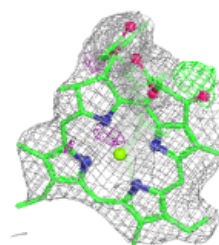
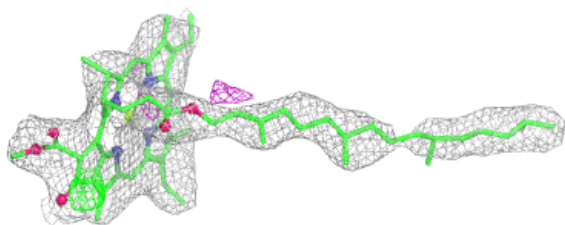
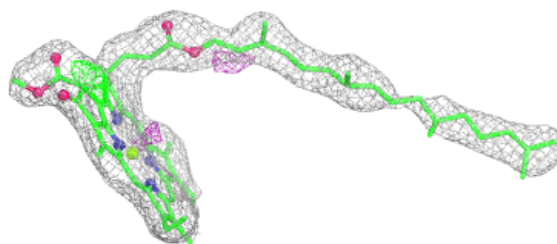


Electron density around DGD C 519:

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

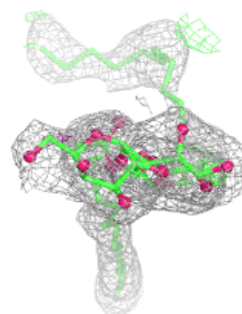
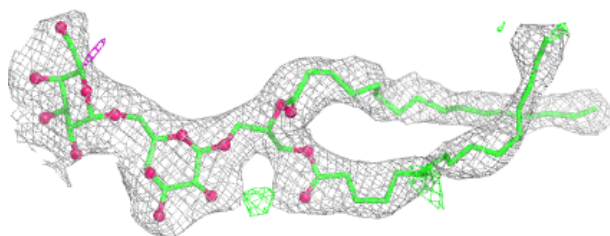
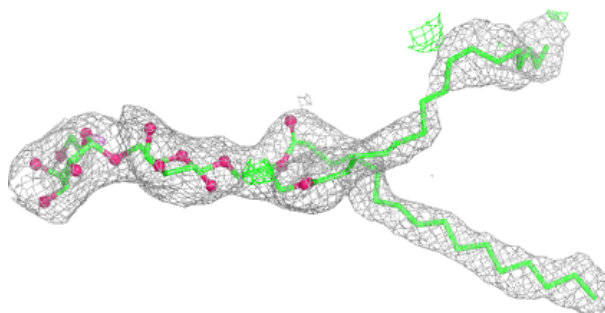
**Electron density around CLA b 613:**

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

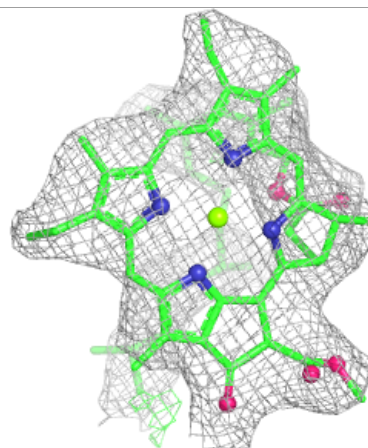
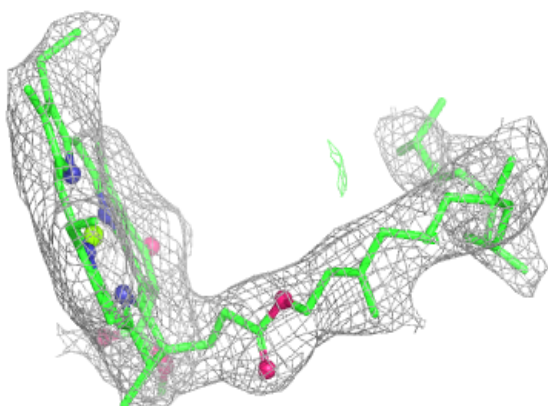
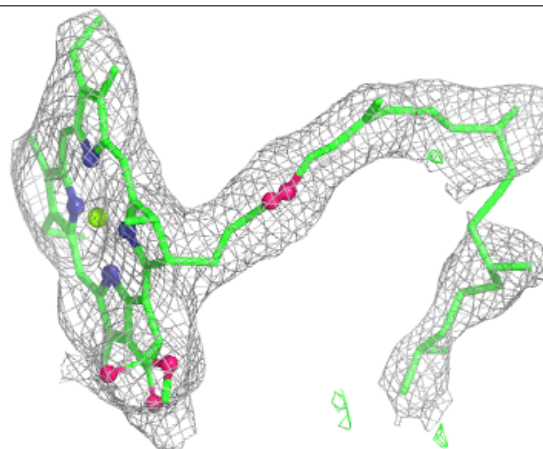


Electron density around DGD c 516:

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

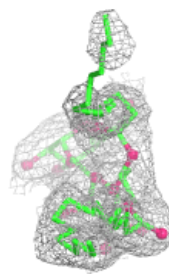
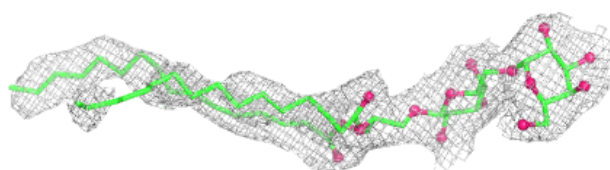
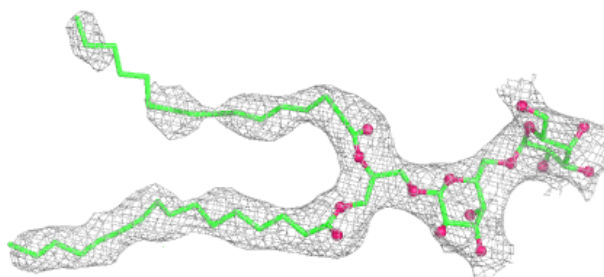
**Electron density around CLA B 607:**

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

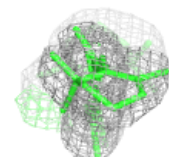
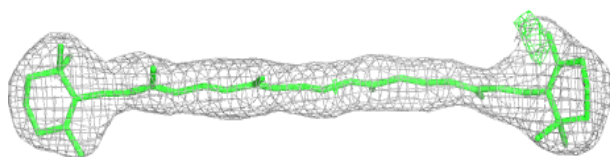


Electron density around DGD c 518:

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

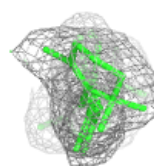
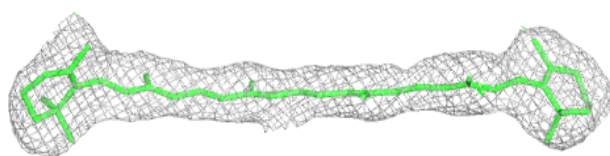
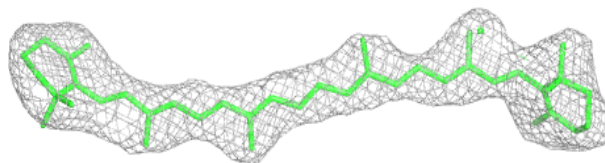
**Electron density around BCR C 516:**

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

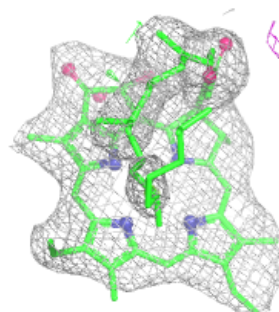
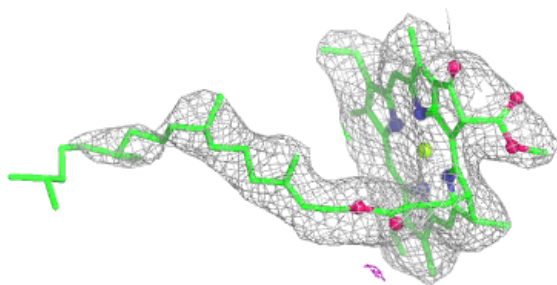
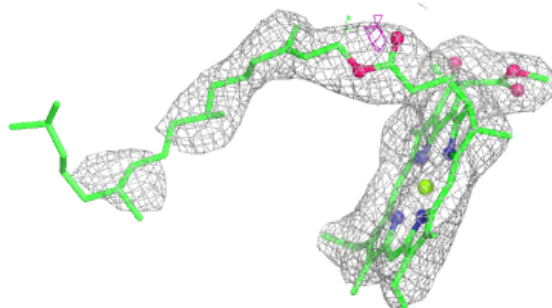


Electron density around BCR B 619:

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

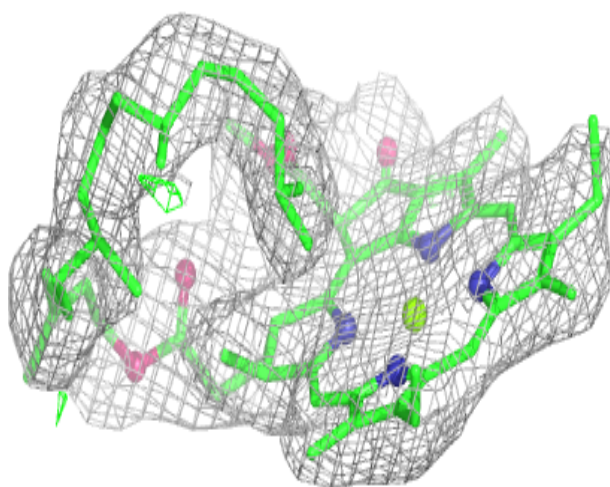
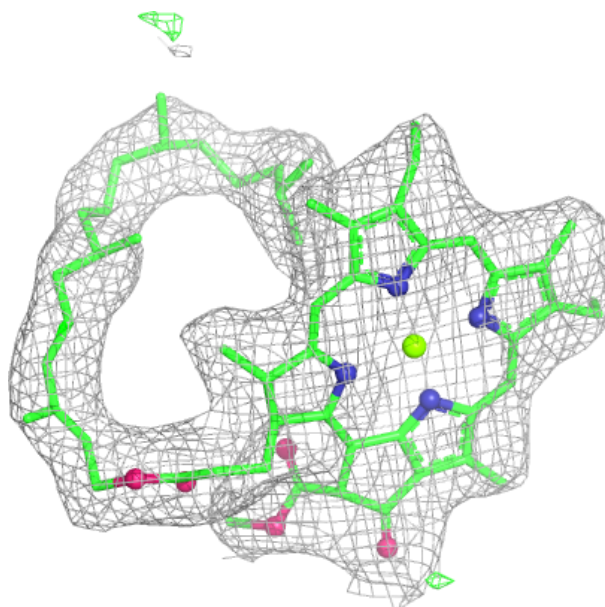
**Electron density around CLA C 509:**

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



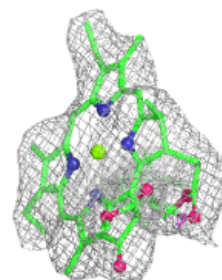
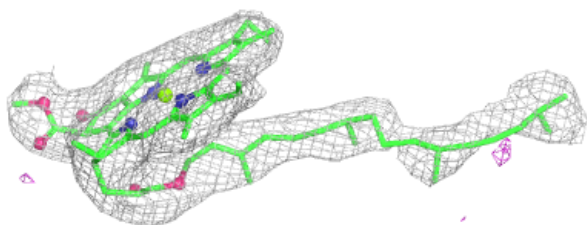
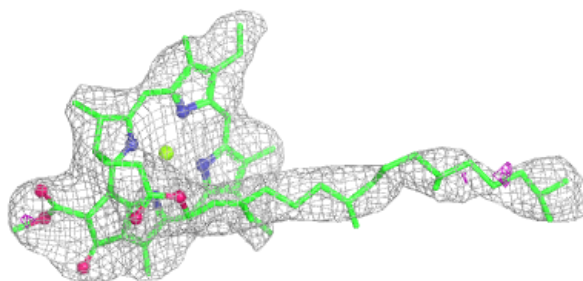
Electron density around CLA B 616:

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



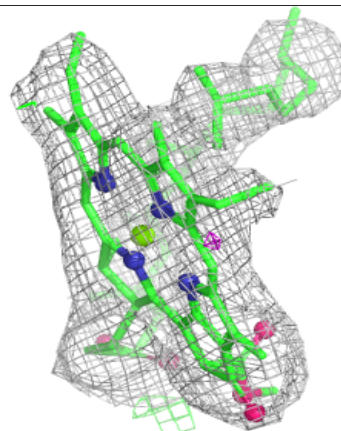
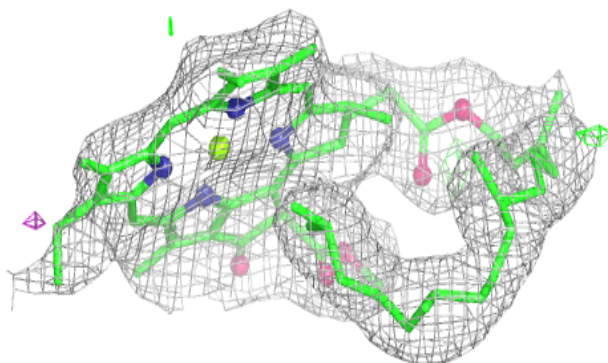
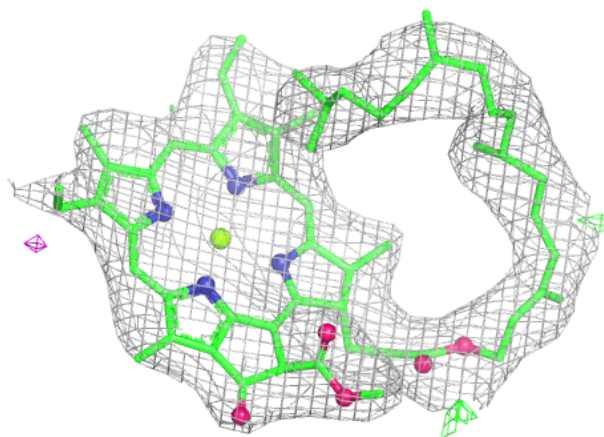
Electron density around CLA b 620:

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



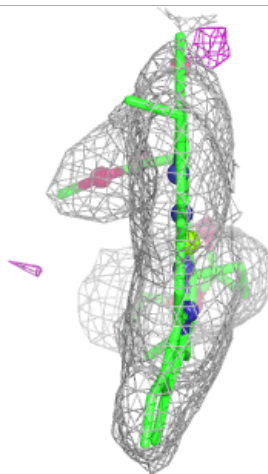
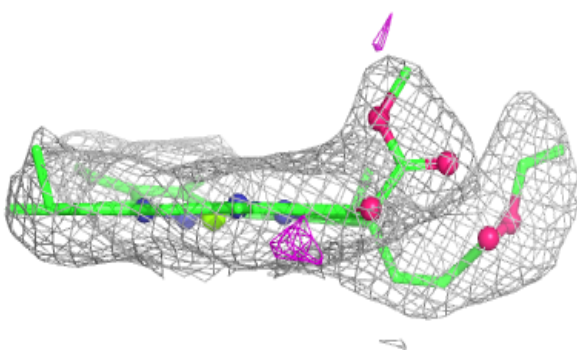
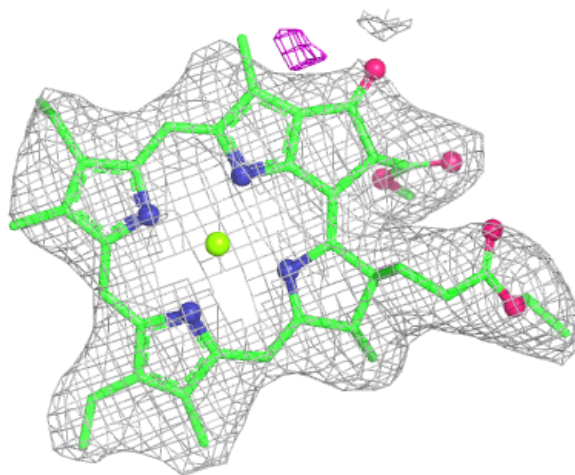
Electron density around CLA b 621:

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



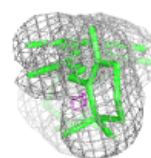
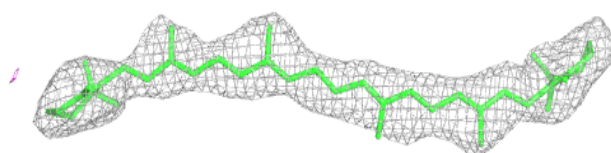
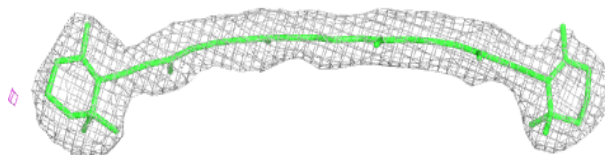
Electron density around CLA b 622:

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

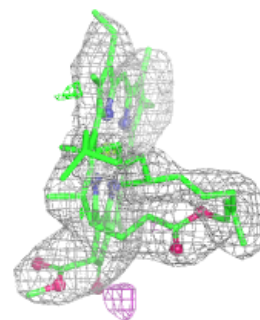
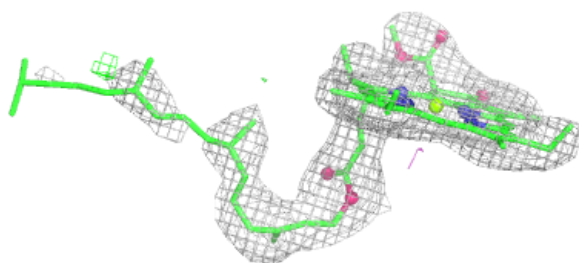
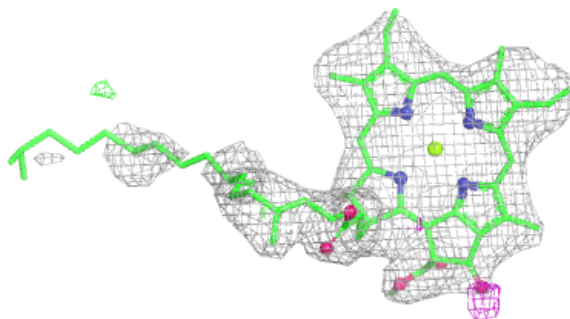


Electron density around BCR K 101:

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

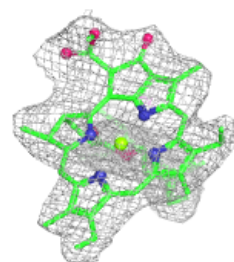
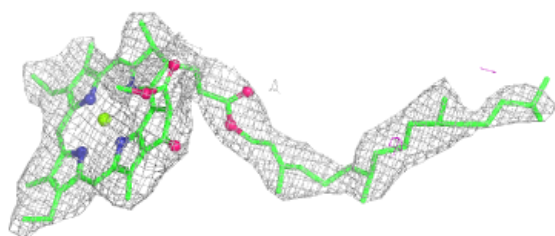
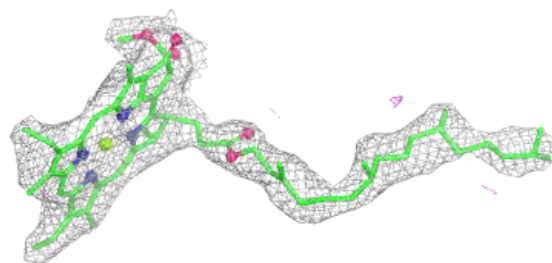
**Electron density around CLA A 607:**

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

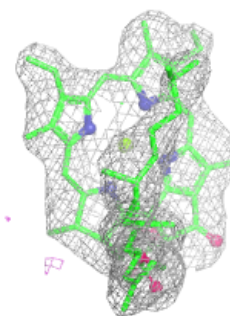
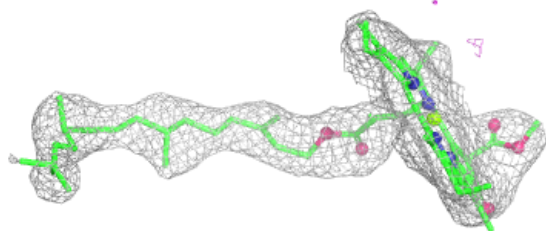
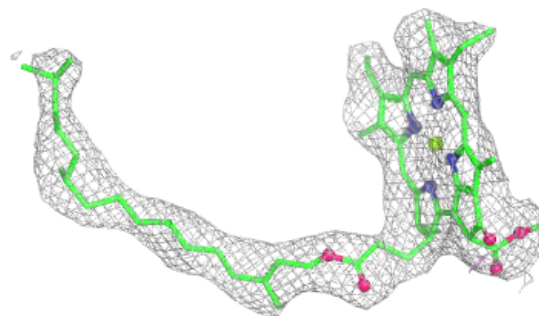


Electron density around CLA C 503:

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

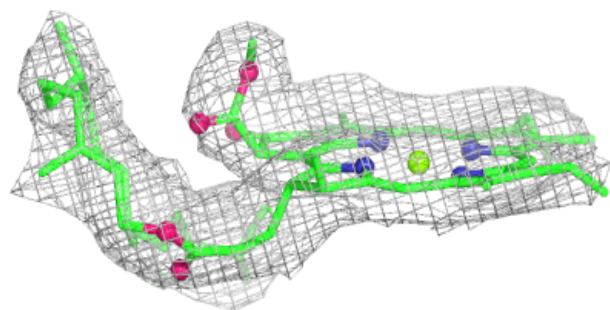
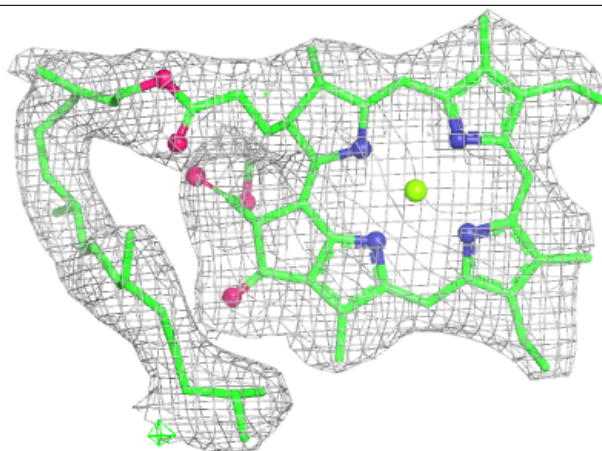
**Electron density around CLA B 610:**

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



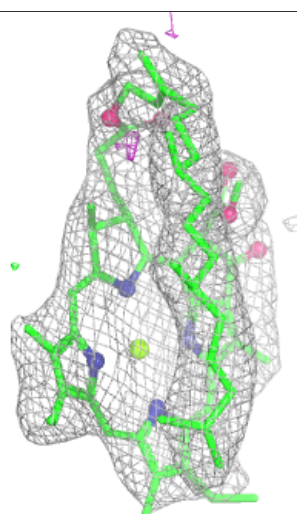
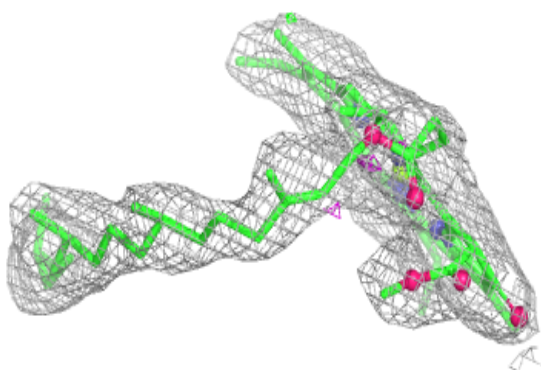
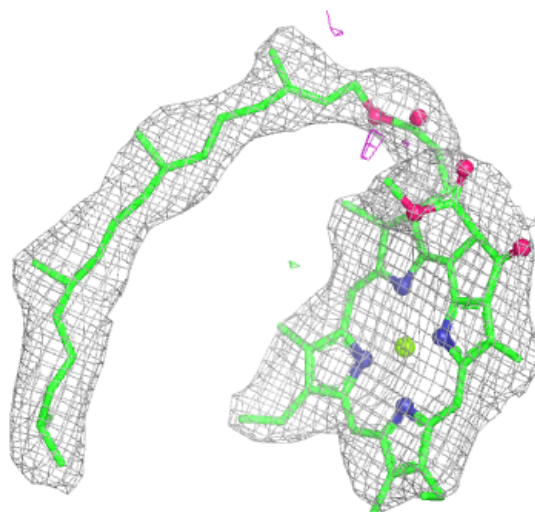
Electron density around CLA B 611:

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



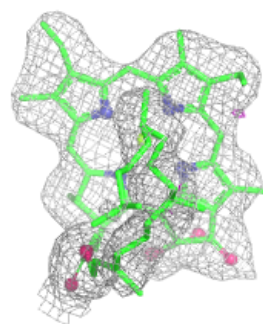
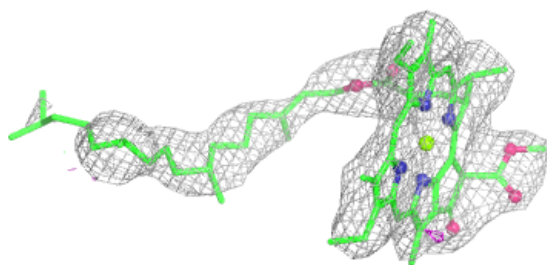
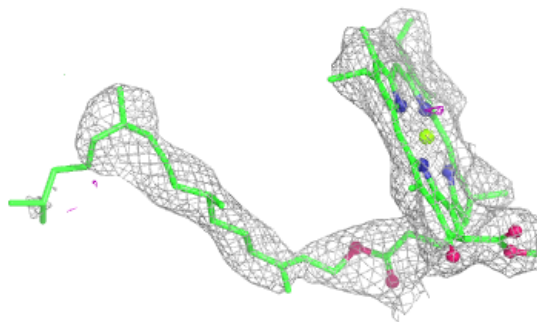
Electron density around CLA c 507:

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



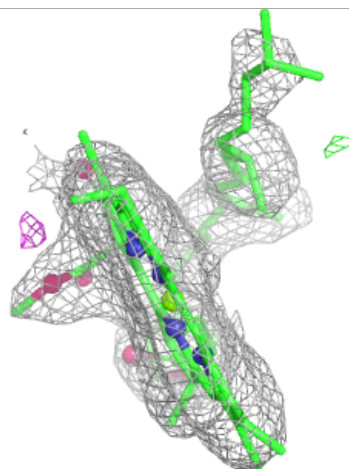
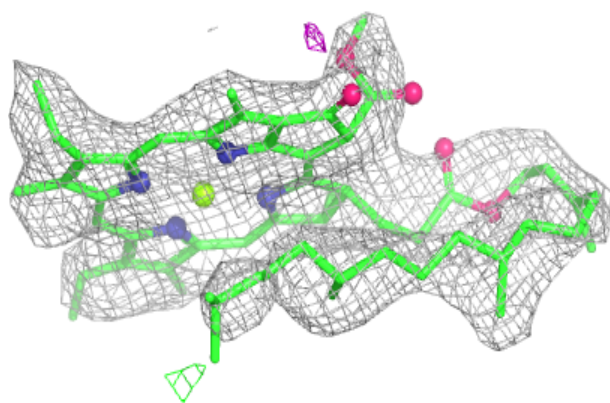
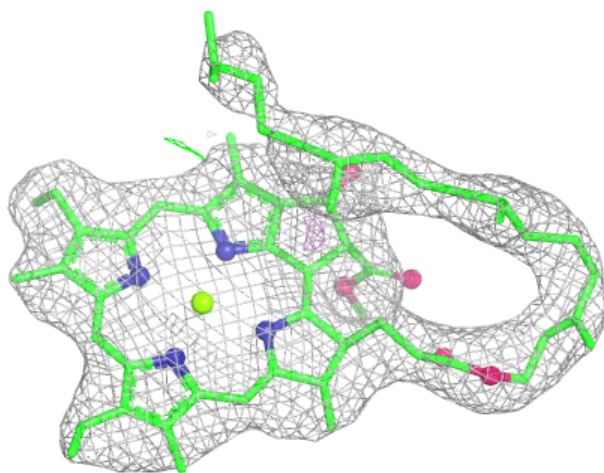
Electron density around CLA c 508:

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



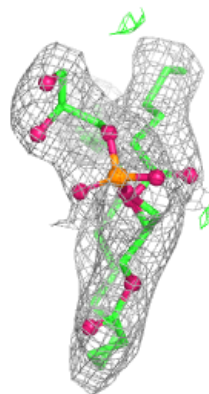
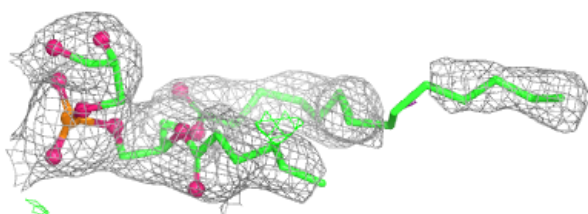
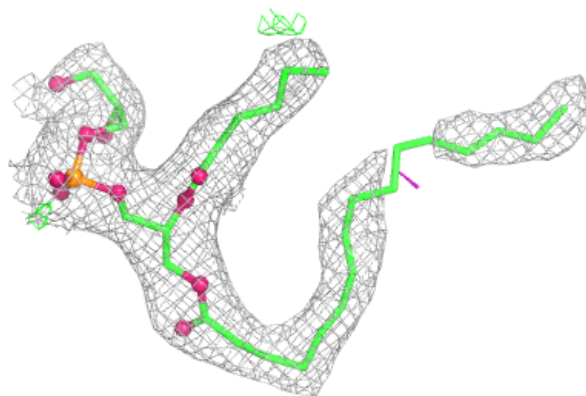
Electron density around CLA c 509:

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

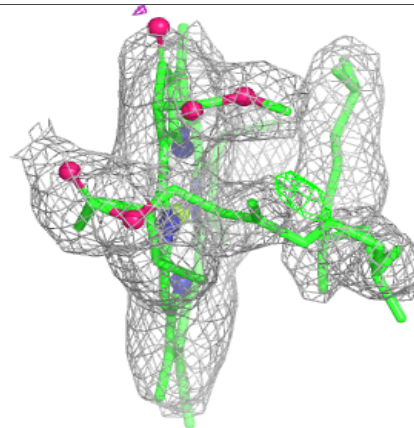
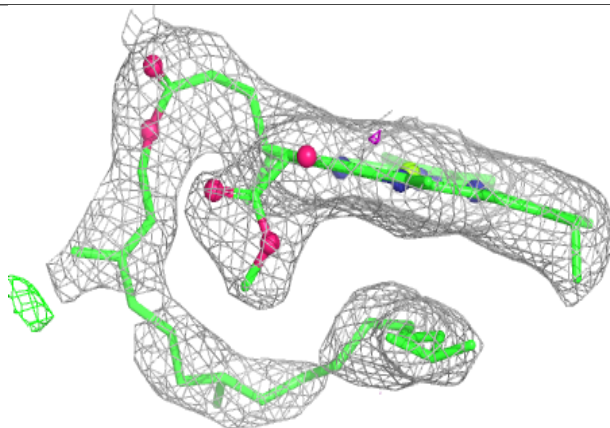
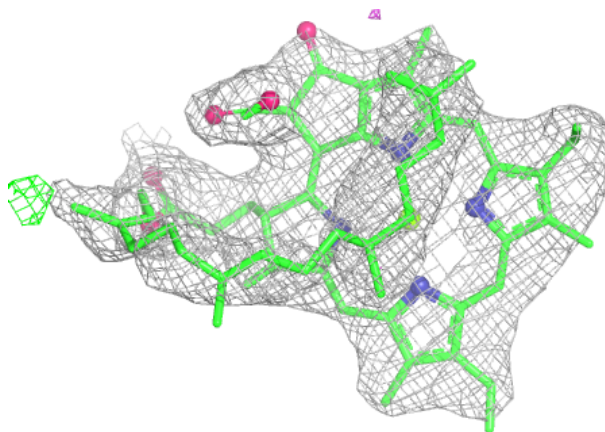


Electron density around LHG a 720:

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

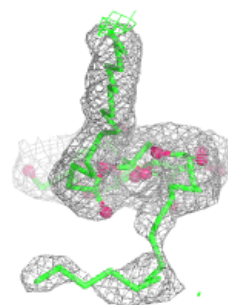
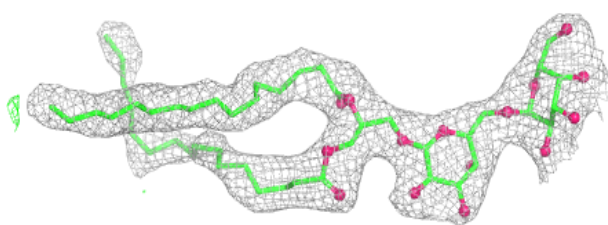
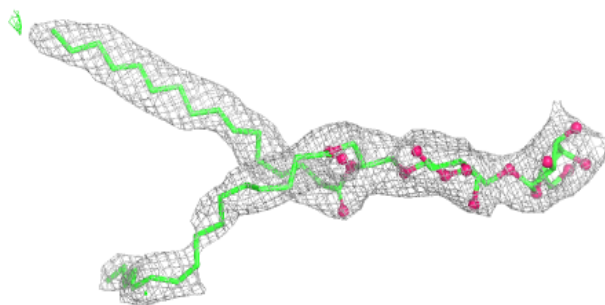
**Electron density around CLA c 510:**

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

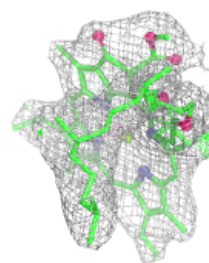
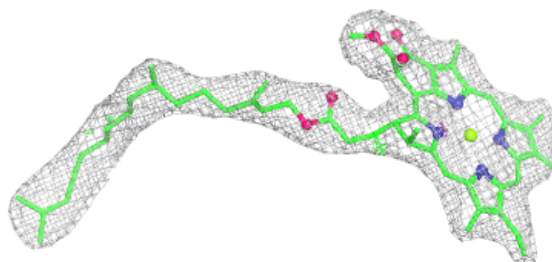


Electron density around DGD C 517:

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

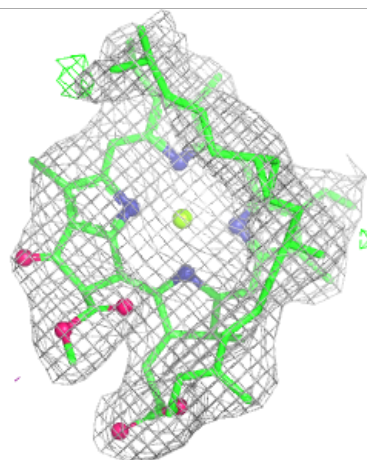
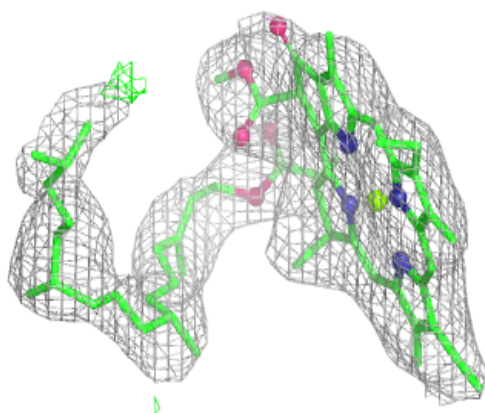
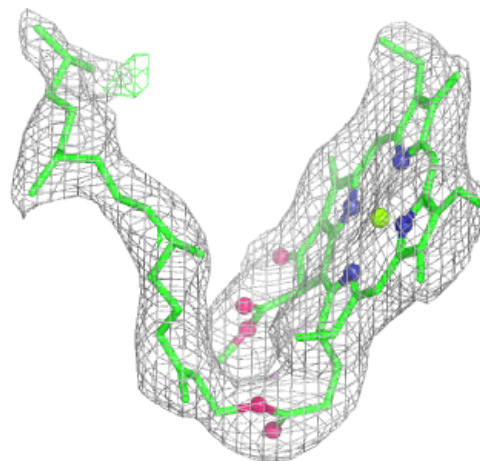
**Electron density around CLA a 707:**

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



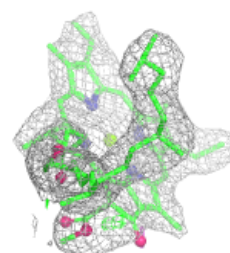
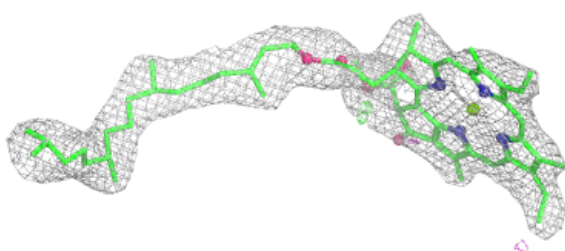
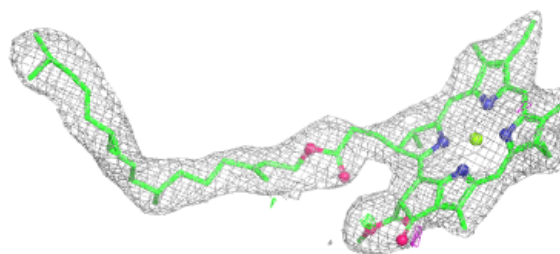
Electron density around CLA B 614:

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

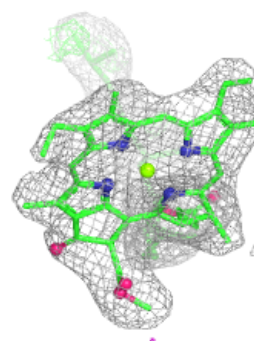
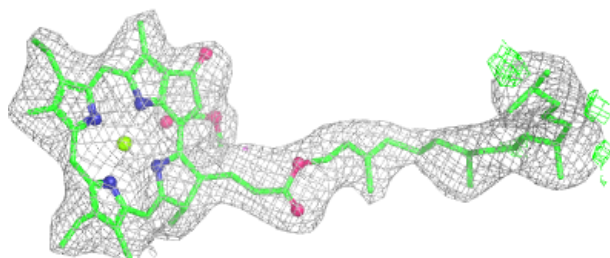
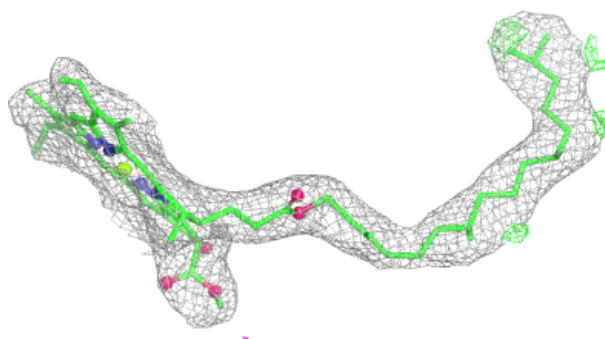


Electron density around CLA A 606:

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

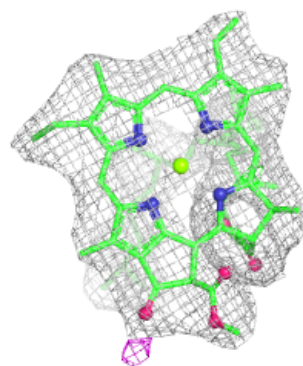
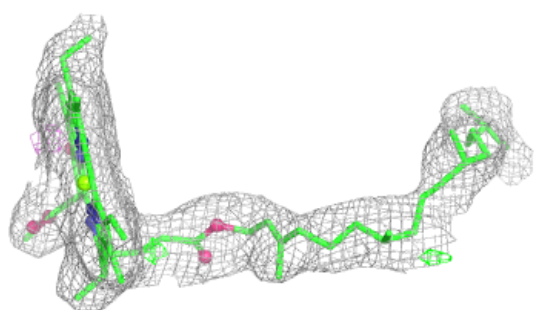
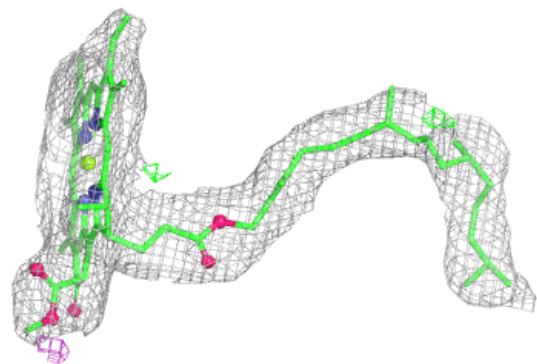
**Electron density around CLA d 402:**

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

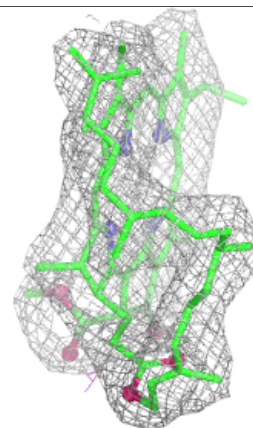
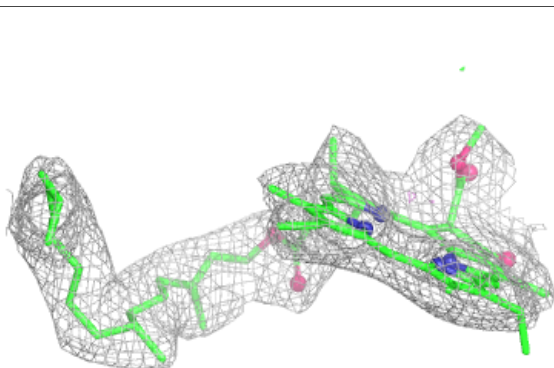
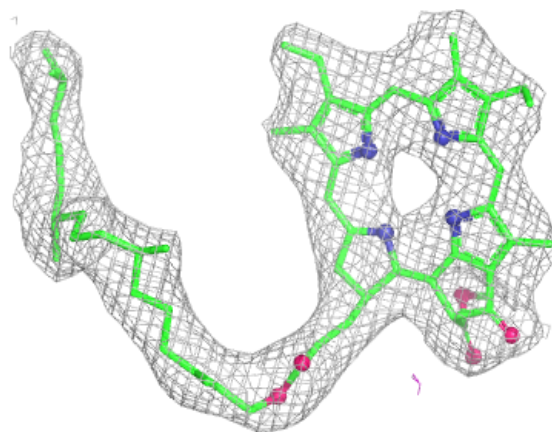


Electron density around CLA d 403:

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

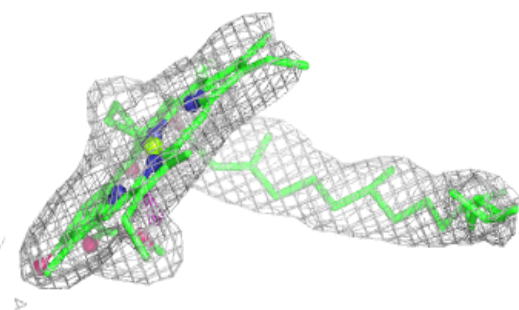
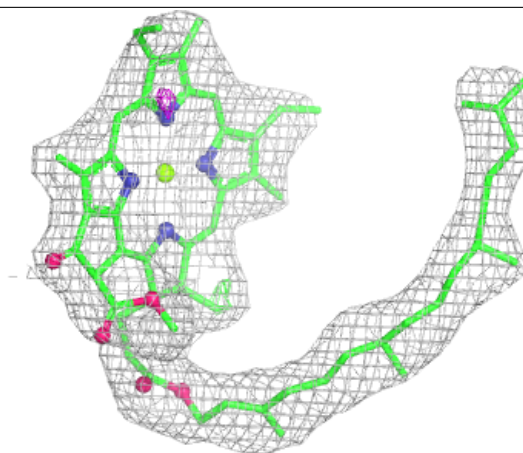
**Electron density around PHO D 401:**

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



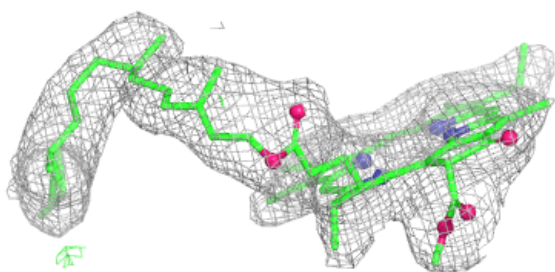
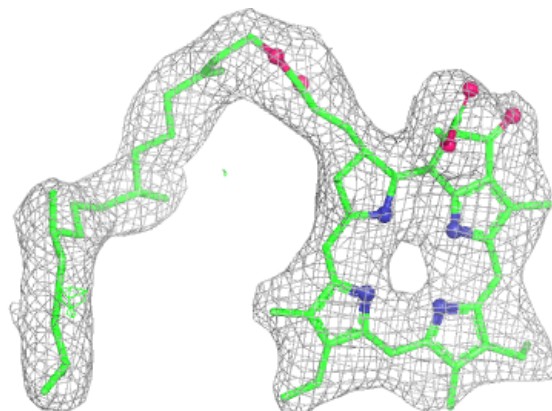
Electron density around CLA C 508:

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

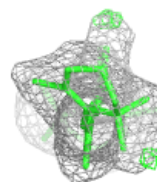
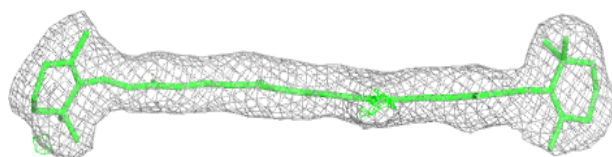
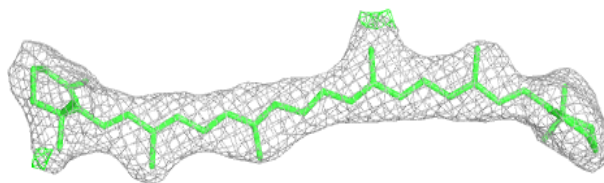


Electron density around PHO a 710:

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

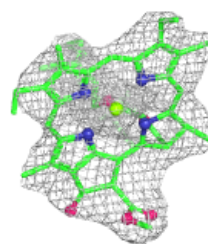
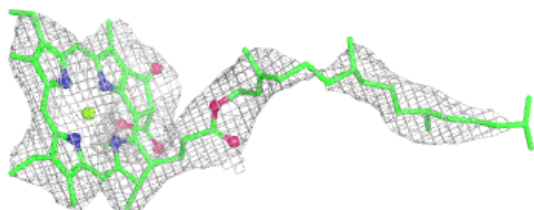
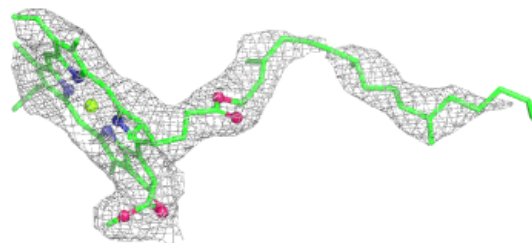
**Electron density around BCR A 610:**

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



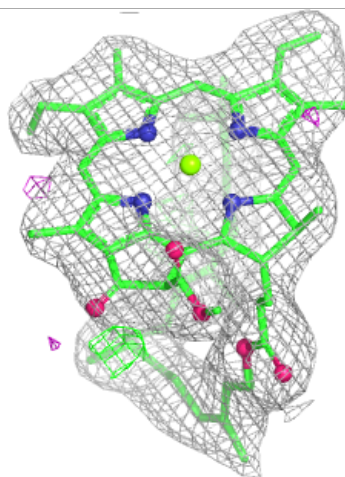
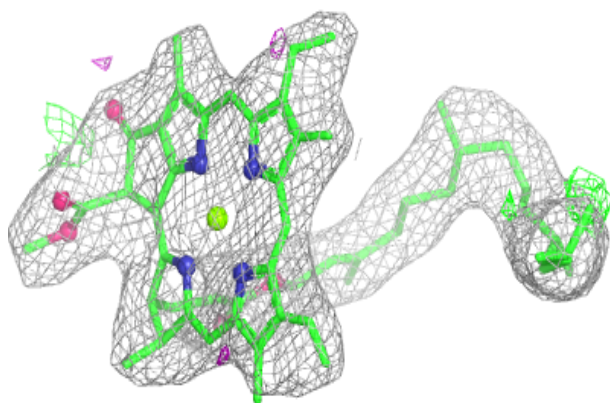
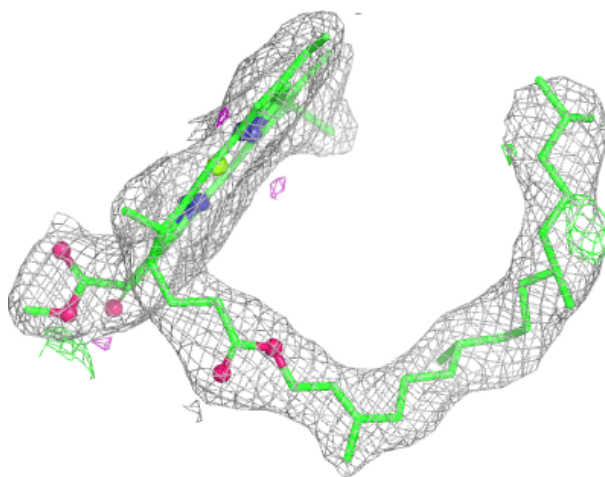
Electron density around CLA c 502:

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



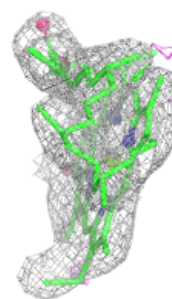
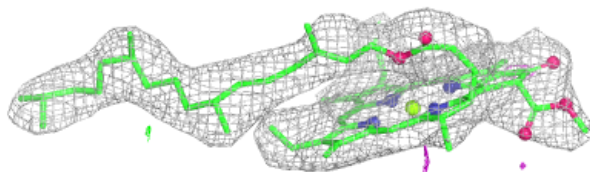
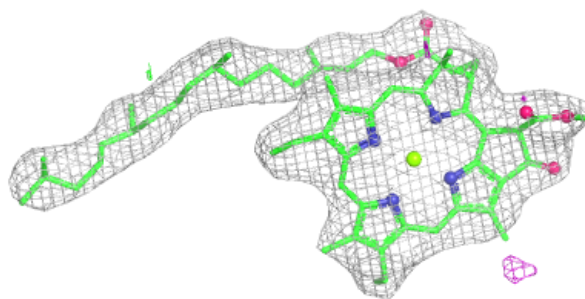
Electron density around CLA B 612:

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

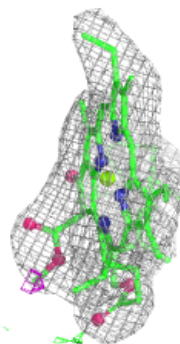
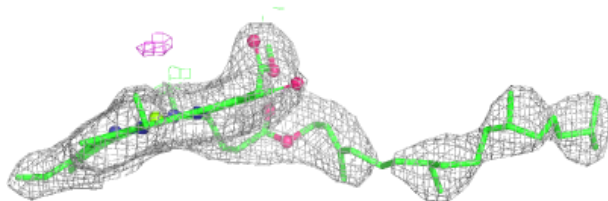
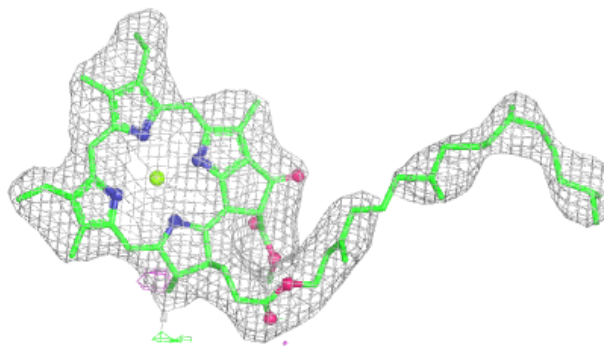


Electron density around CLA C 502:

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

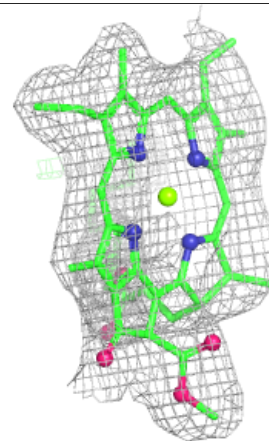
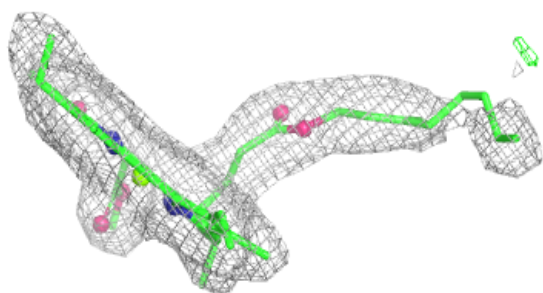
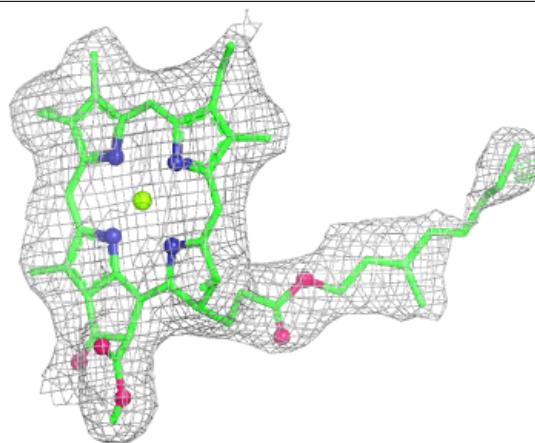
**Electron density around CLA b 608:**

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



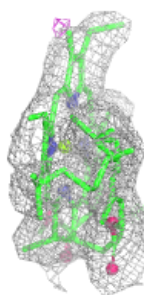
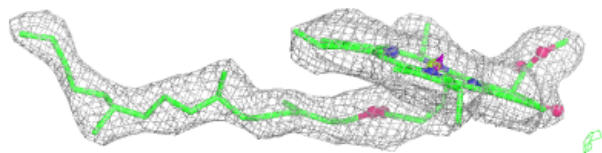
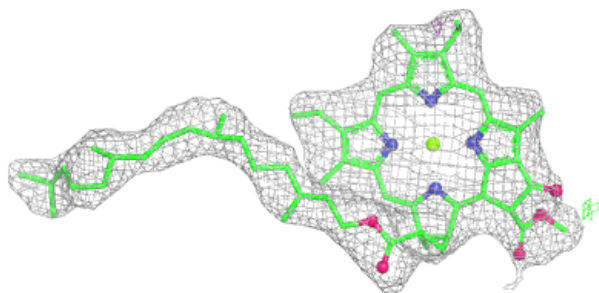
Electron density around CLA A 609:

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



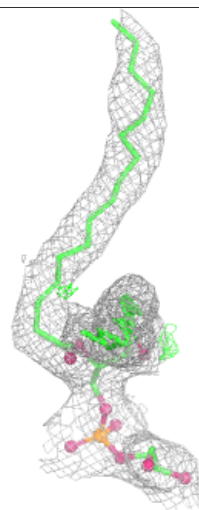
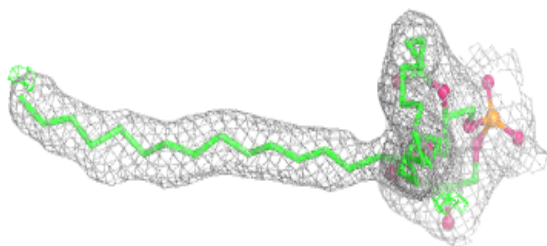
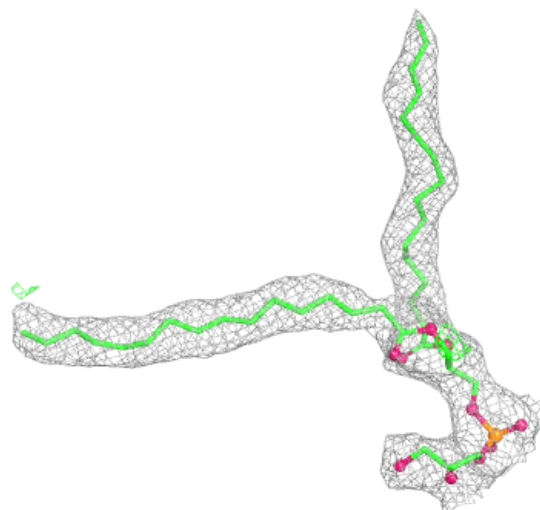
Electron density around CLA B 604:

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



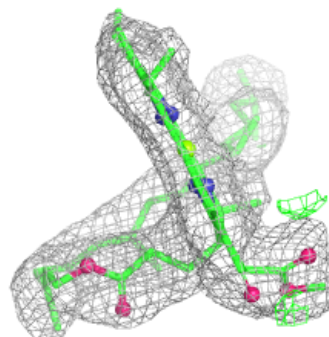
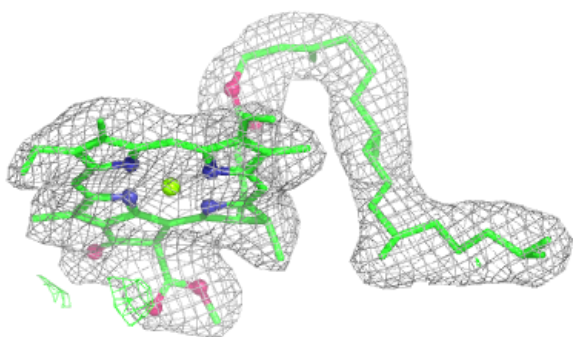
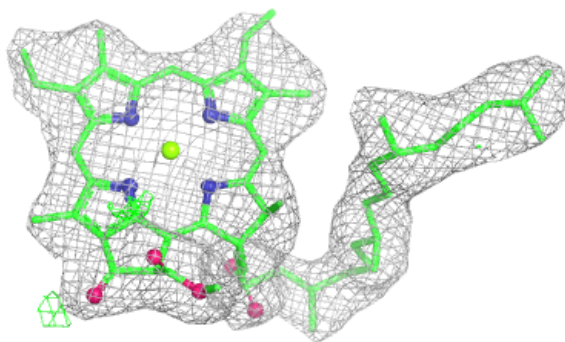
Electron density around LHG L 101:

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



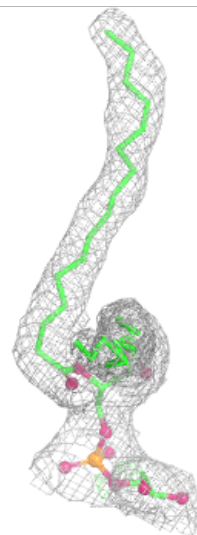
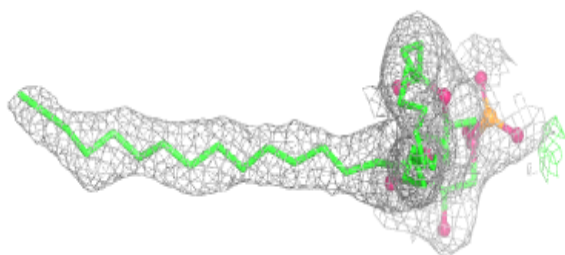
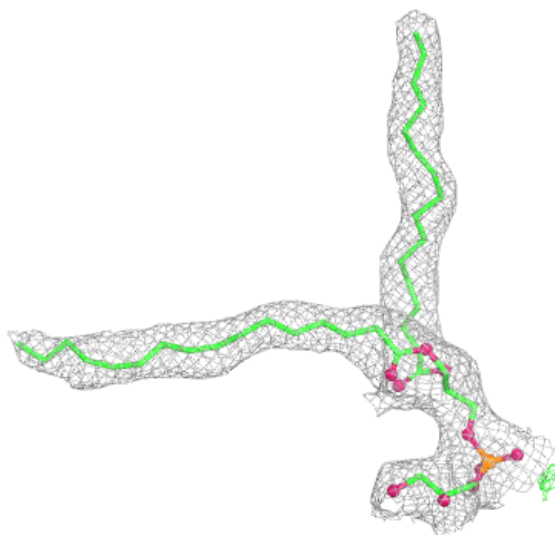
Electron density around CLA D 402:

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



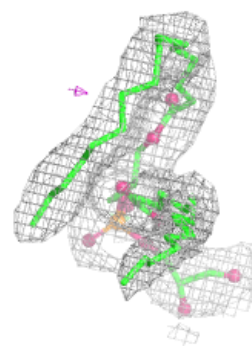
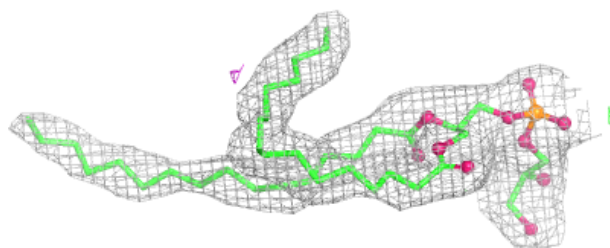
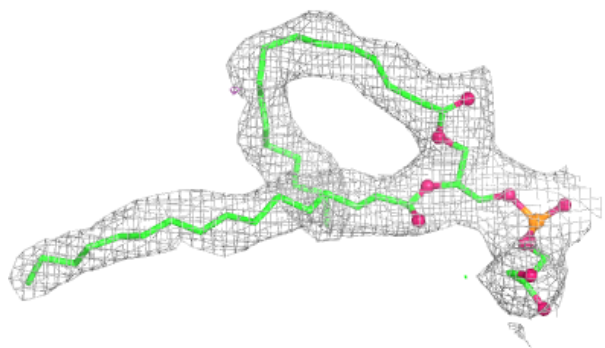
Electron density around LHG b 629:

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

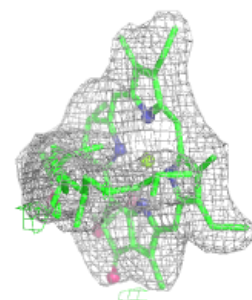
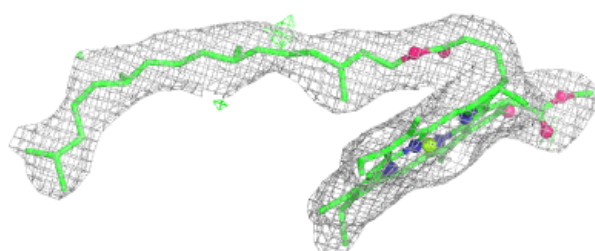
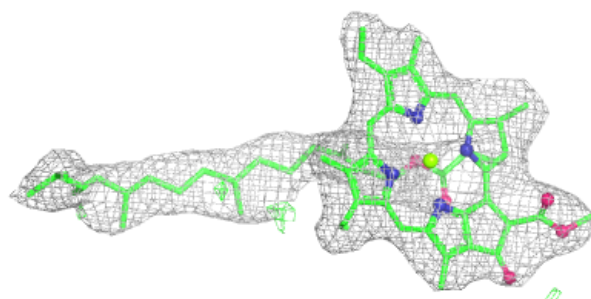


Electron density around LHG d 406:

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

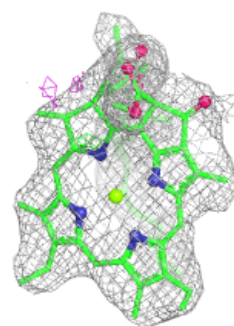
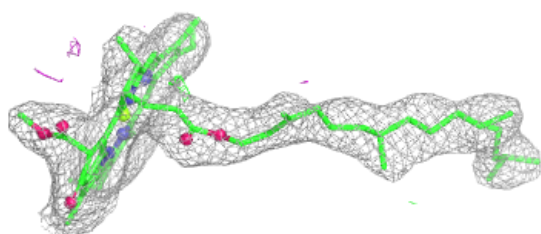
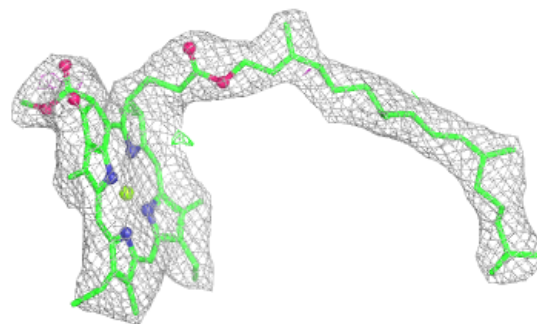
**Electron density around CLA b 614:**

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

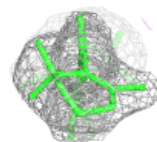
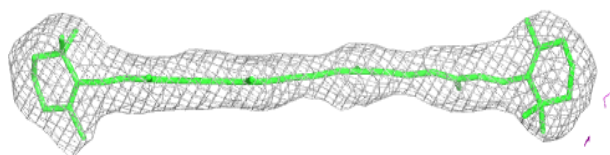
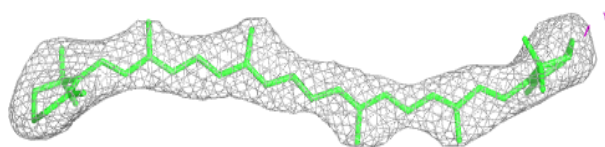


Electron density around CLA b 615:

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

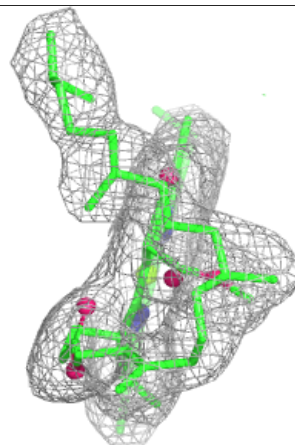
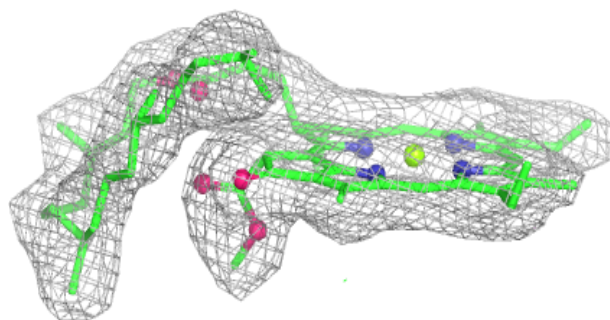
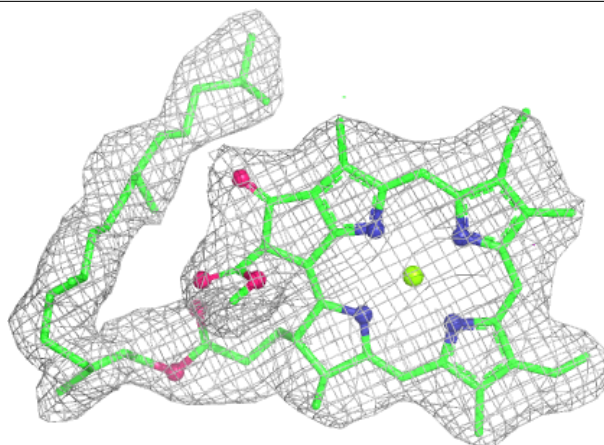
**Electron density around BCR a 712:**

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



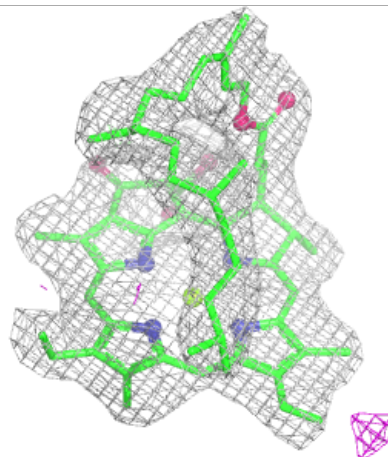
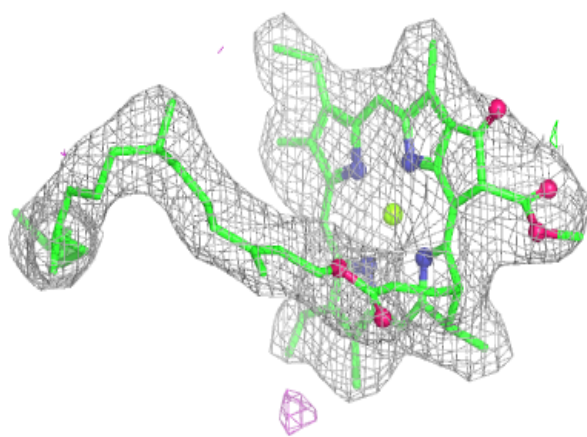
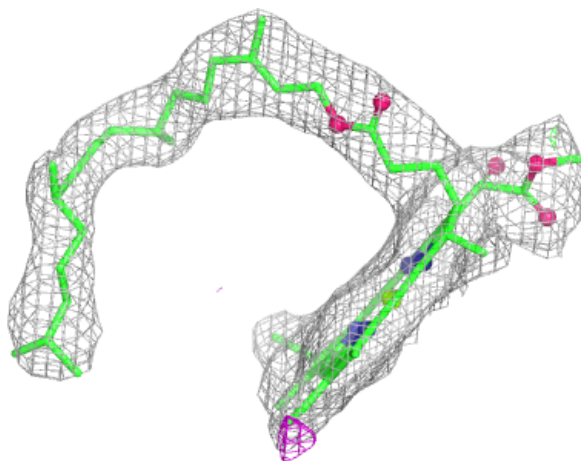
Electron density around CLA b 616:

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



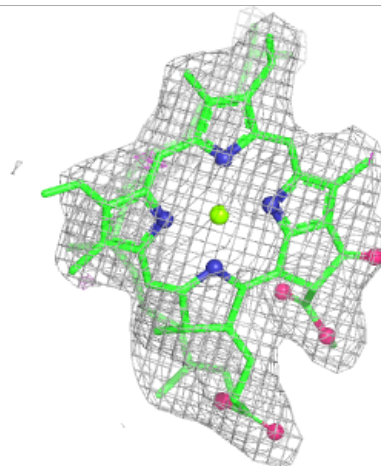
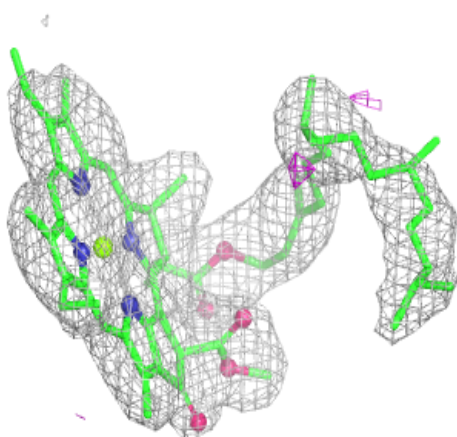
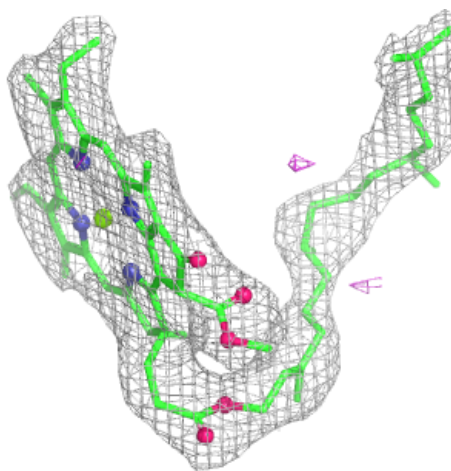
Electron density around CLA b 617:

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



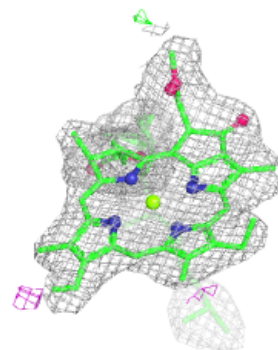
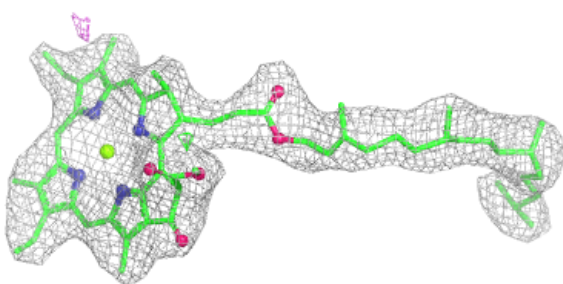
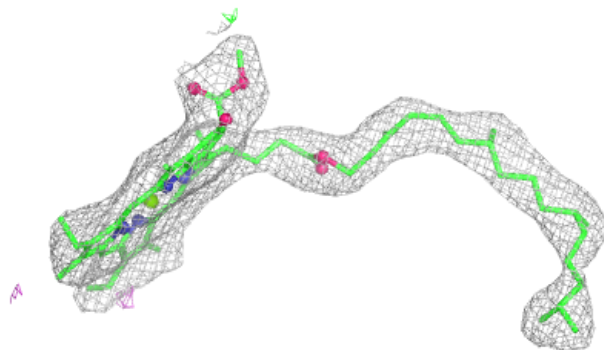
Electron density around CLA b 619:

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

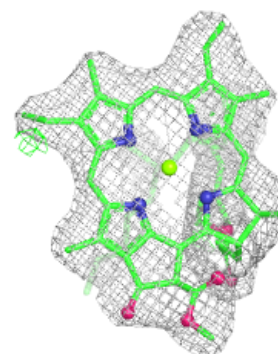
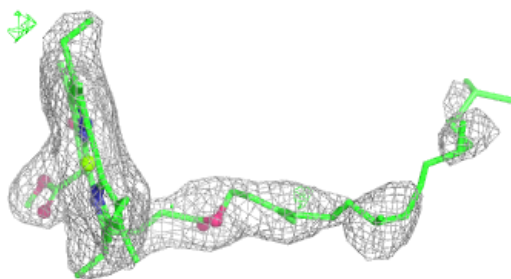
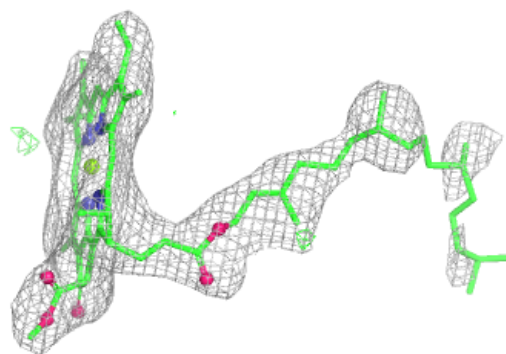


Electron density around CLA D 403:

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

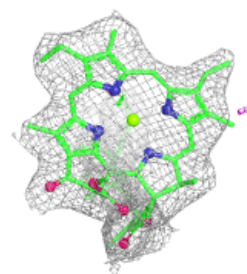
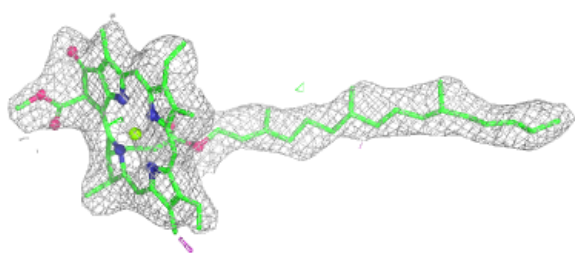
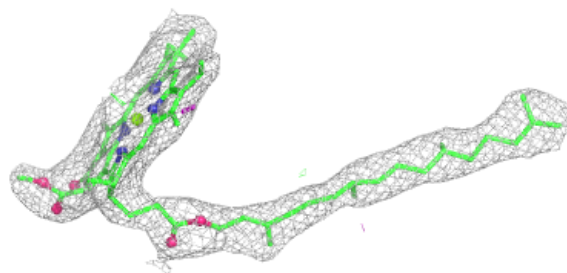
**Electron density around CLA D 404:**

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



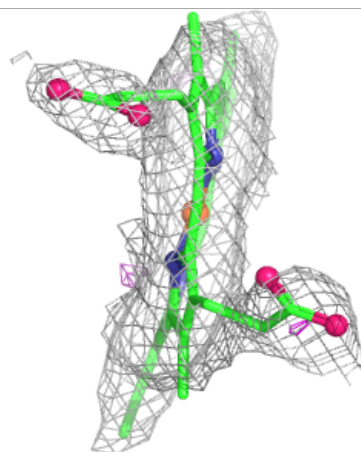
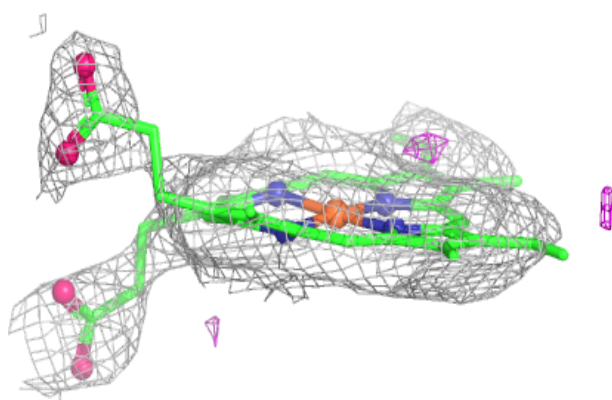
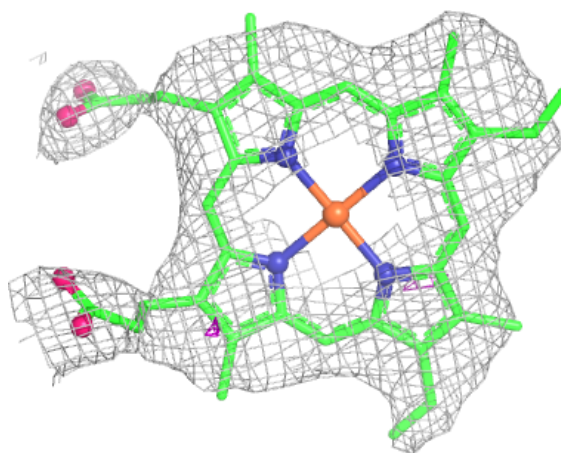
Electron density around CLA B 608:

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



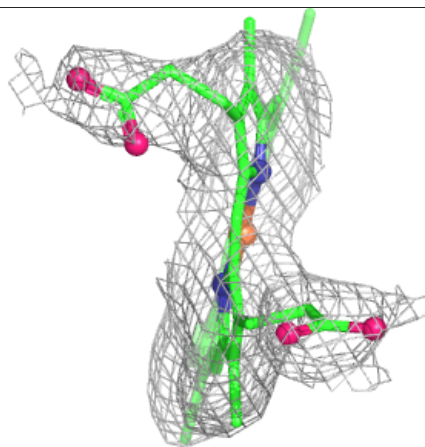
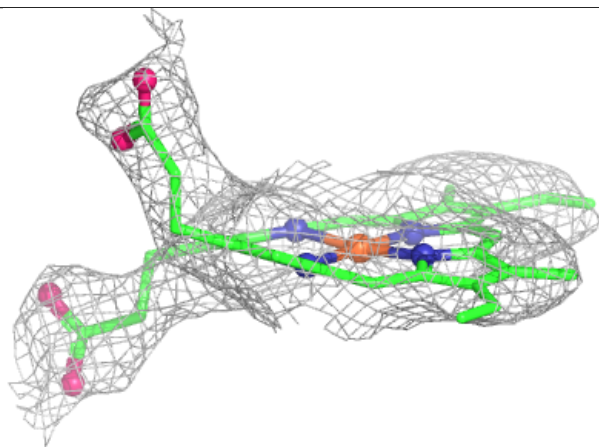
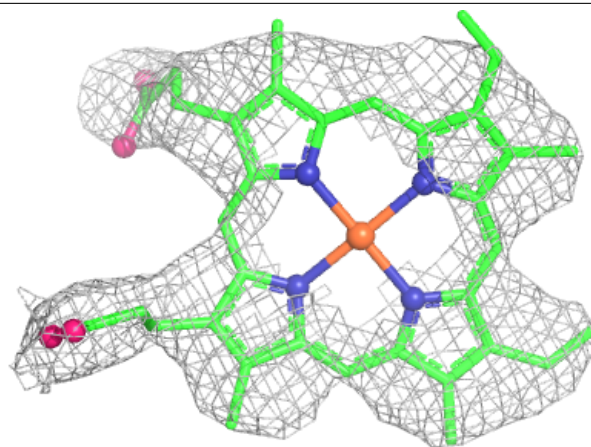
Electron density around HEM E 102:

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



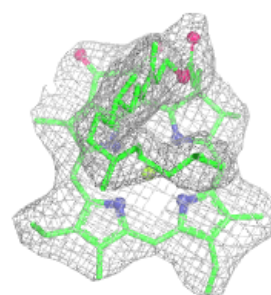
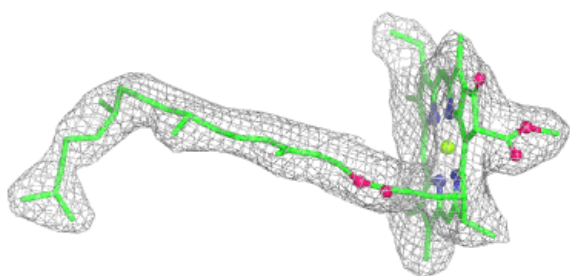
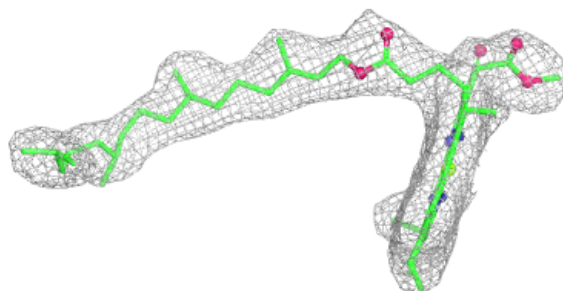
Electron density around HEM e 102:

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

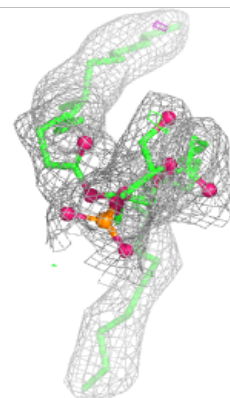
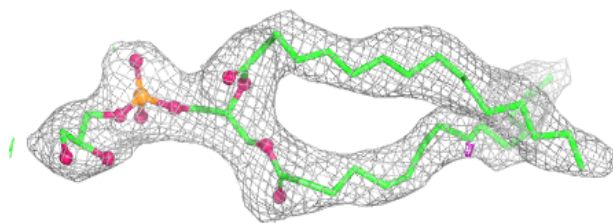
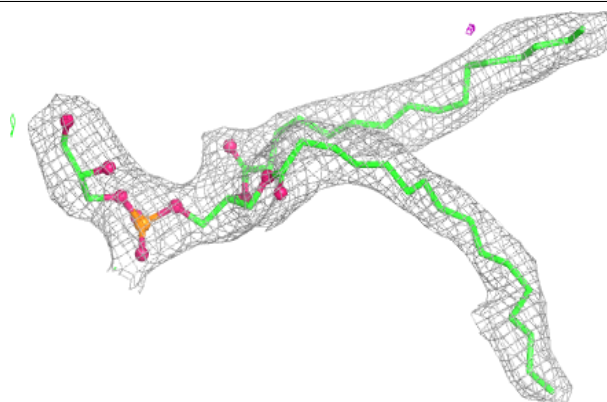


Electron density around CLA b 611:

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

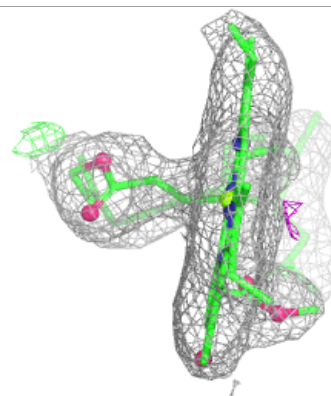
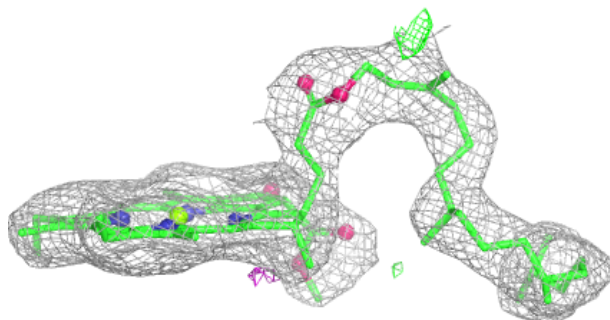
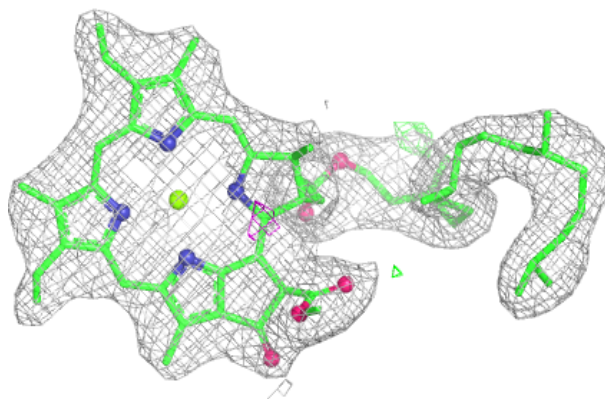
**Electron density around LHG d 407:**

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

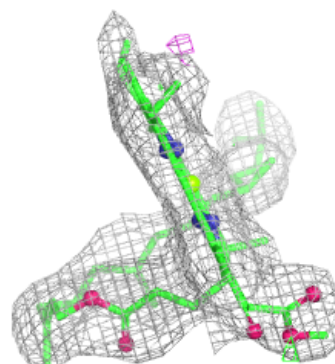
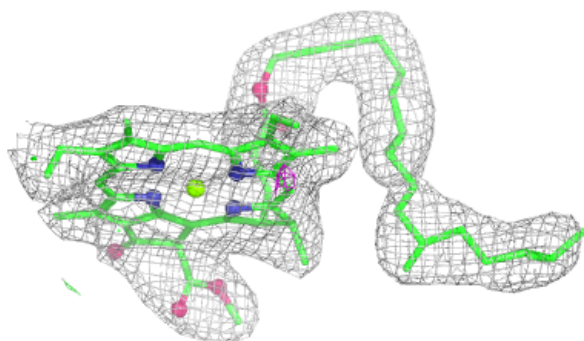
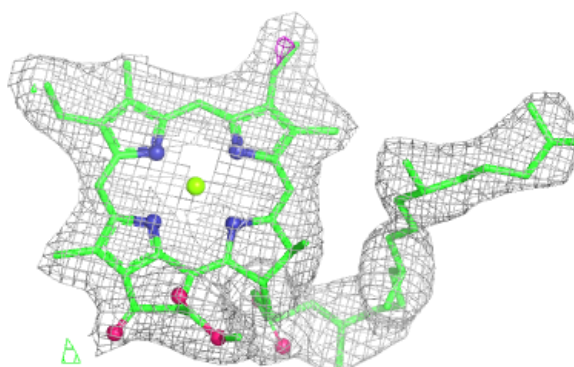


Electron density around CLA b 618:

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

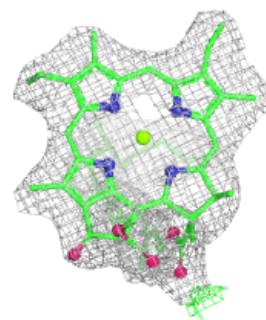
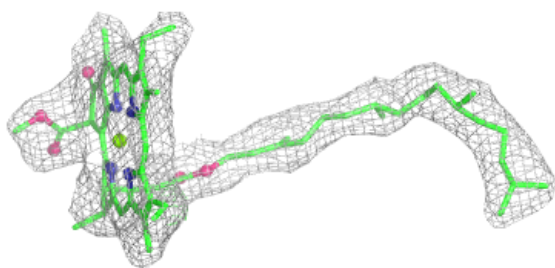
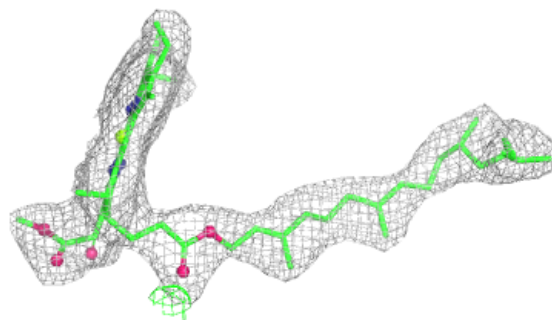
**Electron density around CLA a 719:**

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



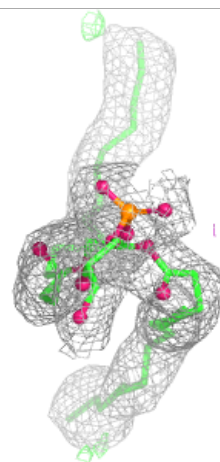
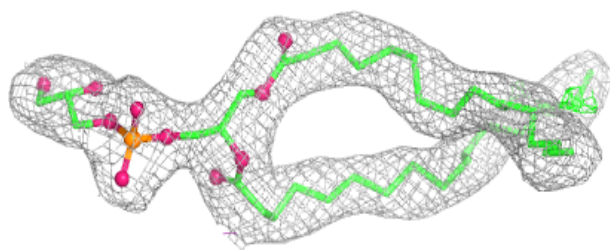
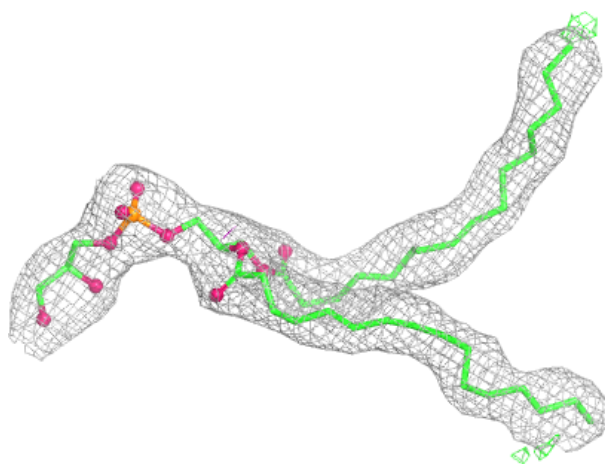
Electron density around CLA B 606:

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



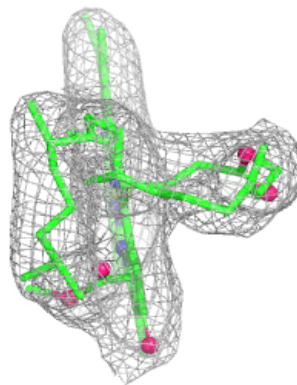
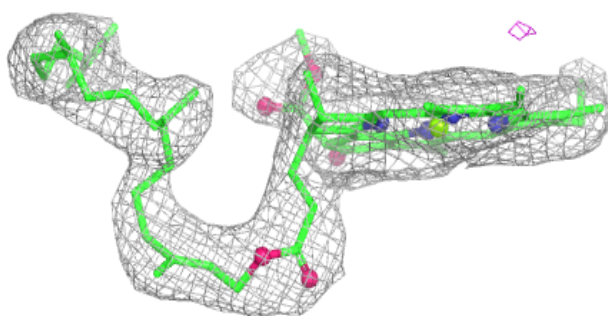
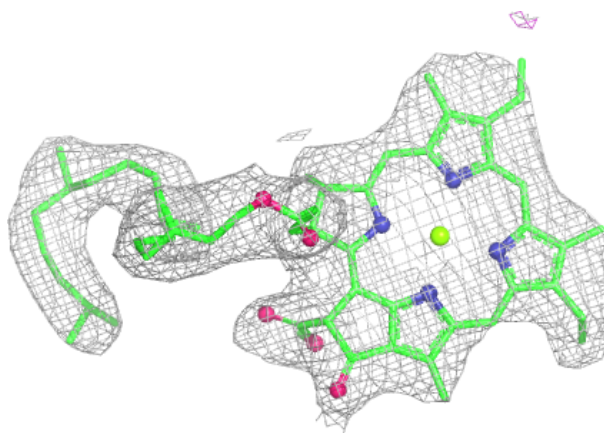
Electron density around LHG D 407:

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

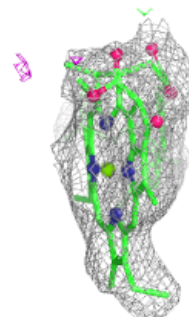
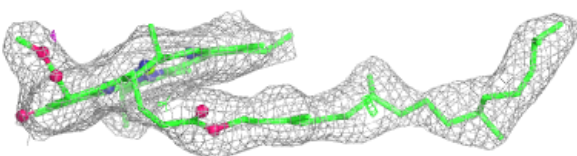
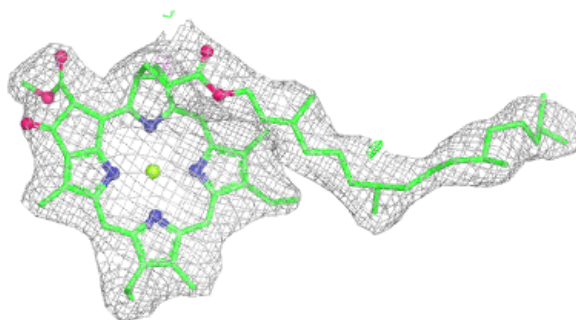


Electron density around CLA B 613:

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

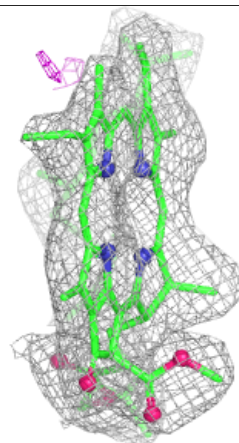
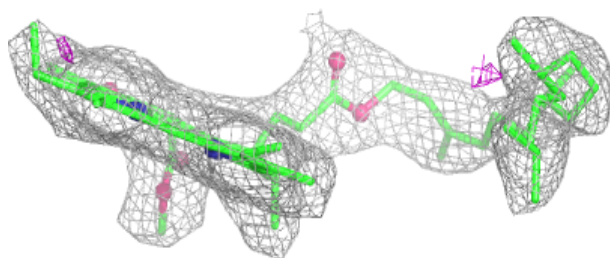
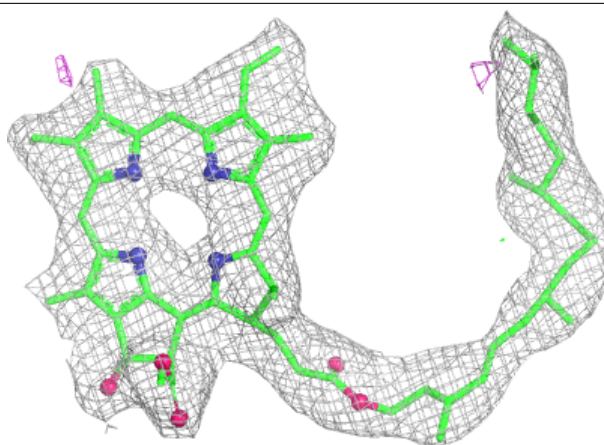
**Electron density around CLA b 609:**

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



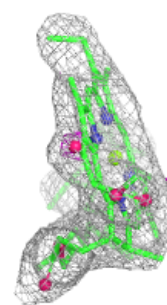
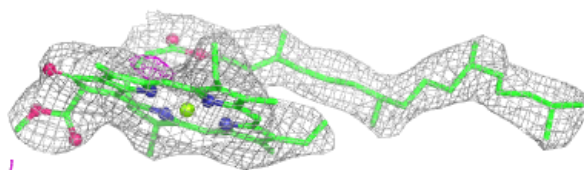
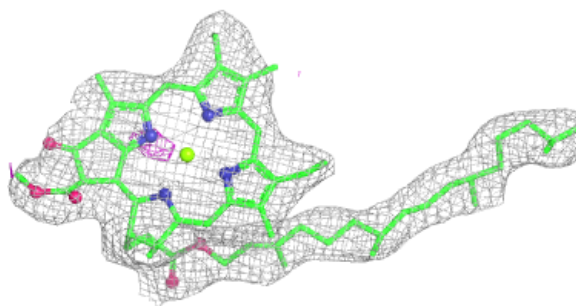
Electron density around PHO a 709:

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

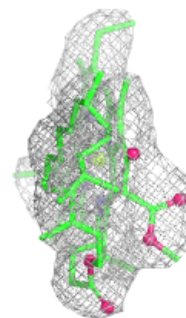
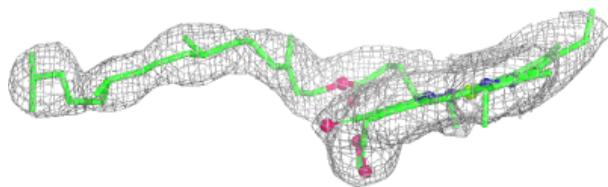
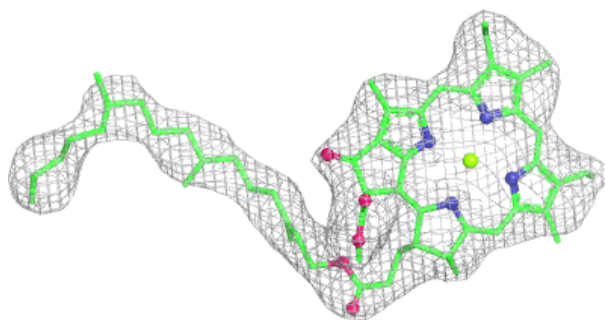


Electron density around CLA c 501:

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

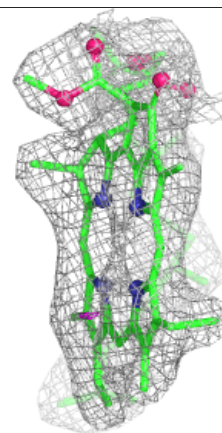
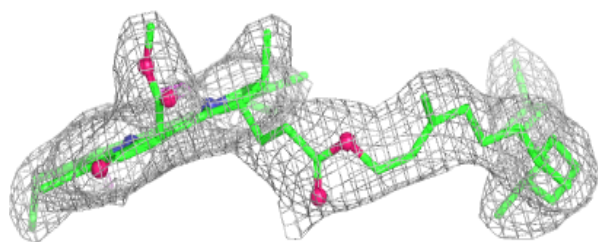
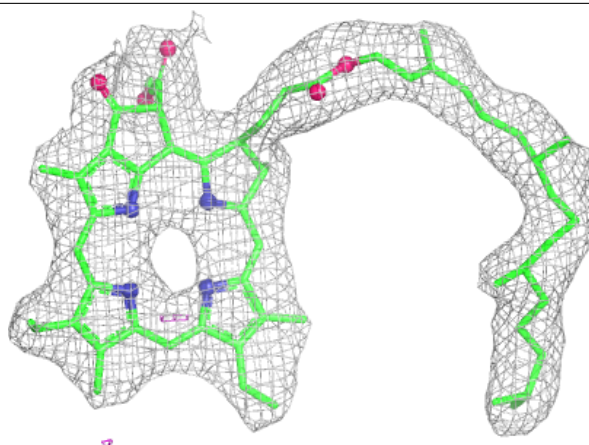
**Electron density around CLA B 603:**

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



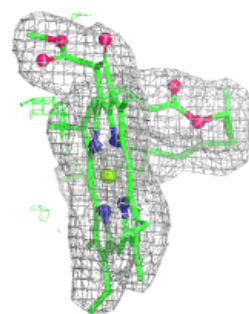
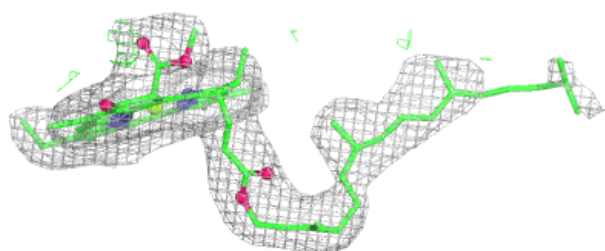
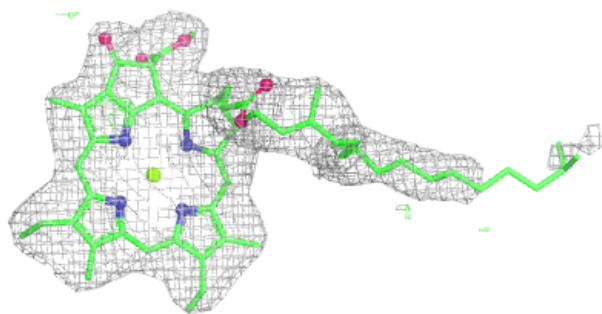
Electron density around PHO A 608:

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



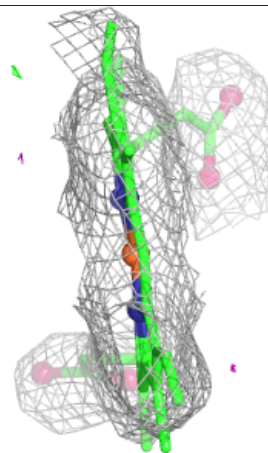
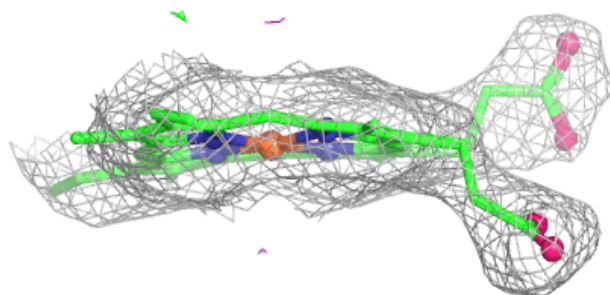
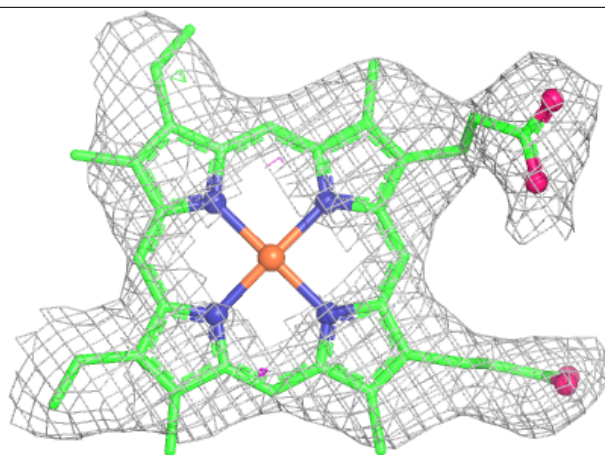
Electron density around CLA a 708:

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



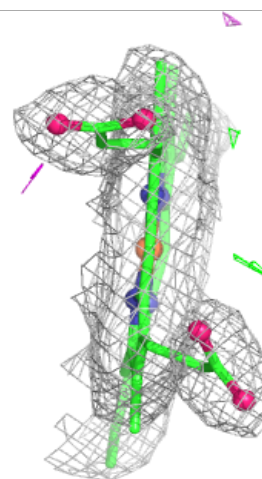
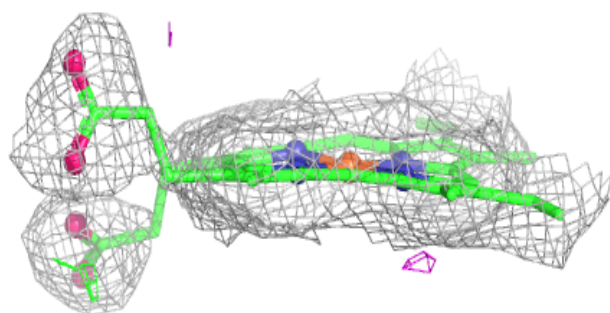
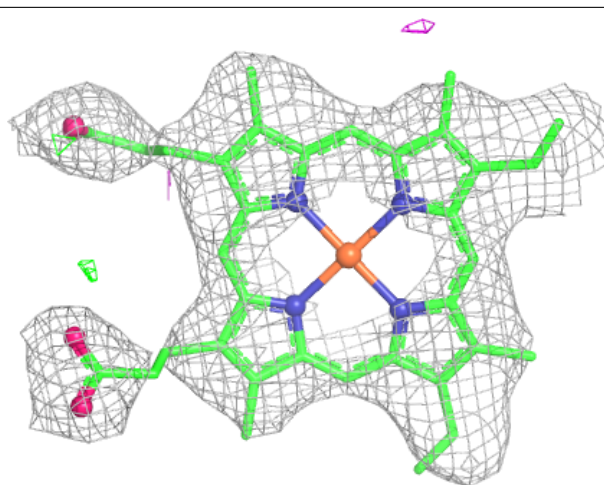
Electron density around HEC V 201:

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



Electron density around HEC v 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.