



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:48 PM EDT

PDB ID : 6DHO / pdb_00006dho
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.07 Angstrom resolution
Authors : Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2018-05-20
Resolution : 2.07 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

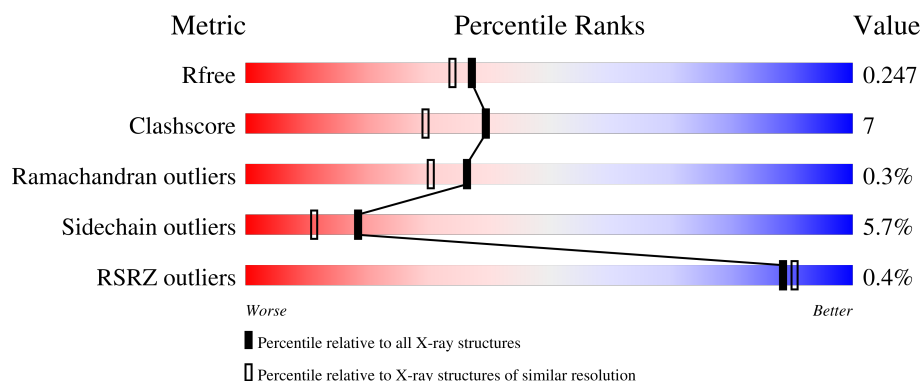
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	334	 88% 11% .

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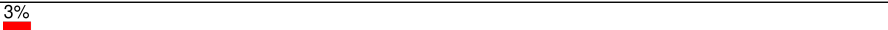
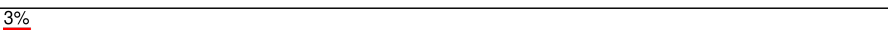
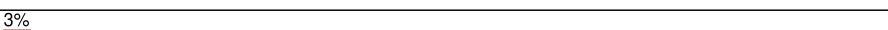
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
 Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
 CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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

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Mol	Chain	Length	Quality of chain
1	a	334	 87% 10% . .
2	B	505	 85% 14% . .
2	b	505	 87% 13% . .
3	C	451	 86% 12% . .
3	c	451	 86% 13% . .
4	D	341	 88% 11% . .
4	d	341	 84% 16% . .
5	E	82	 67% 28% . .
5	e	82	 68% 30% . .
6	F	34	 85% 12% . .
6	f	34	 56% 41% . .
7	H	65	 83% 15% . .
7	h	65	 69% 26% . .
8	I	36	 78% 19% . .
8	i	36	 83% 17% . .
9	J	36	 78% 19% . .
9	j	36	 81% 11% 8% . .
10	K	37	 70% 24% 5% . .
10	k	37	 54% 43% . .
11	L	37	 92% 8% . .
11	l	37	 84% 11% . .
12	M	33	 82% 15% . .
12	m	33	 73% 21% . .
13	O	244	 81% 17% . .
13	o	244	 82% 15% . .

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Mol	Chain	Length	Quality of chain
14	T	30	
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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
36	HEC	V	201	X	-	-	-
36	HEC	v	201	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105756 atoms, of which 52470 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	H	N	O	S	0	59	0
			6018	2010	2937	507	545	19			
1	a	334	Total	C	H	N	O	S	0	59	0
			6006	2007	2928	507	545	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7849	2631	3845	666	694	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7789	2610	3811	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	7	0
			6868	2282	3392	579	601	14			
3	c	451	Total	C	H	N	O	S	0	8	0
			7017	2324	3464	596	619	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1030	338	523	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			516	172	261	40	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	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	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3730	1174	1850	317	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	H	N	O	0	0	0
			519	181	261	36	39			
14	t	30	Total	C	H	N	O	0	0	0
			512	180	256	36	38			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	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	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	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	H	N	O		0	0	0
			593	188	312	45	48				
18	x	38	Total	C	H	N	O		0	0	0
			593	188	312	45	48				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	R	34	Total	C	H	N	O		0	0	0
			569	184	298	47	40				
20	r	31	Total	C	H	N	O		0	0	0
			461	154	234	40	33				

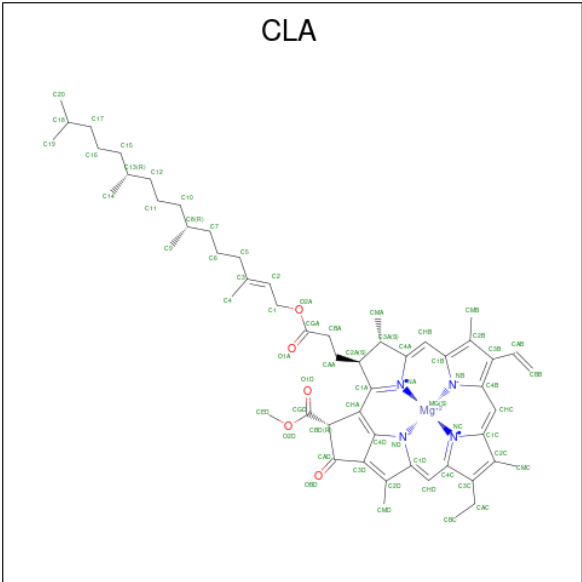
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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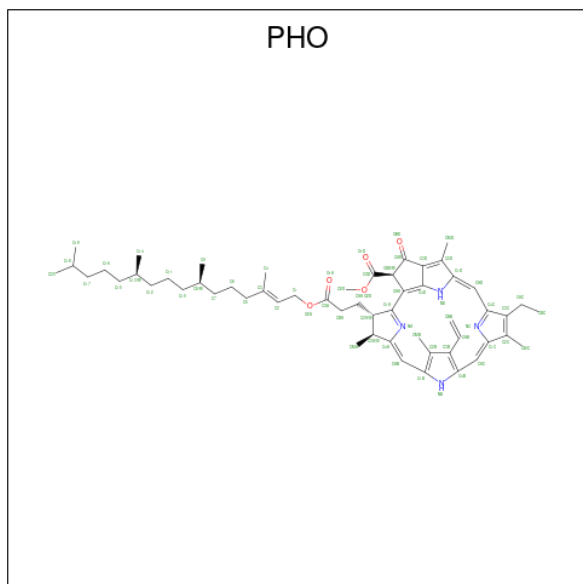
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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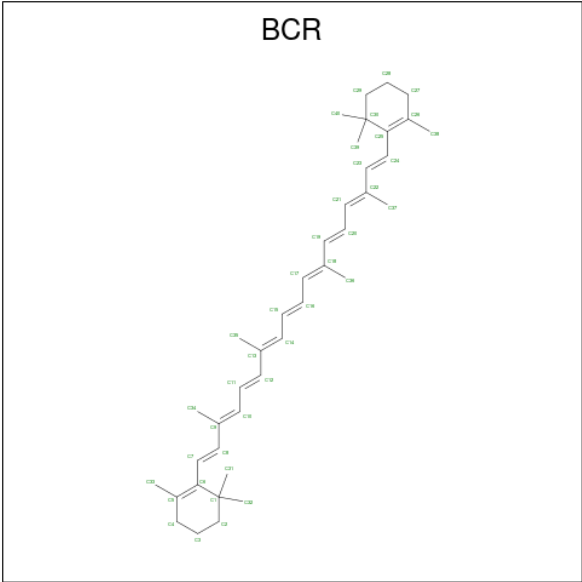
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	h	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	A	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
24	A	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
24	a	1	Total	C	H	N	O		0	0
			138	55	74	4	5			
24	d	1	Total	C	H	N	O		0	0
			138	55	74	4	5			

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



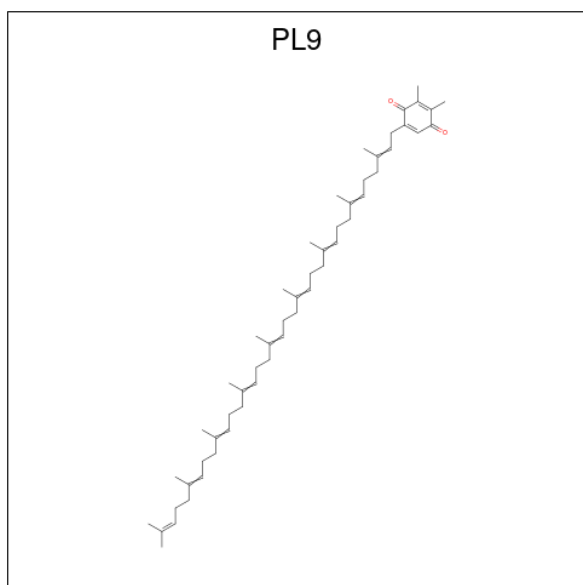
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total	C	H	0	0
			96	40	56		
25	H	1	Total	C	H	0	0
			96	40	56		
25	K	1	Total	C	H	0	0
			96	40	56		
25	K	1	Total	C	H	0	0
			96	40	56		
25	T	1	Total	C	H	0	0
			96	40	56		
25	Z	1	Total	C	H	0	0
			96	40	56		
25	a	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	b	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	d	1	Total	C	H	0	0
			96	40	56		
25	k	1	Total	C	H	0	0
			96	40	56		
25	k	1	Total	C	H	0	0
			96	40	56		
25	t	1	Total	C	H	0	0
			96	40	56		
25	x	1	Total	C	H	0	0
			96	40	56		

- Molecule 26 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).



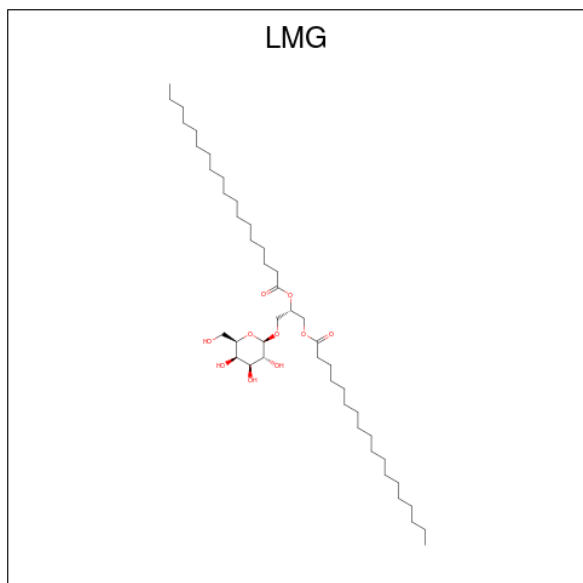
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



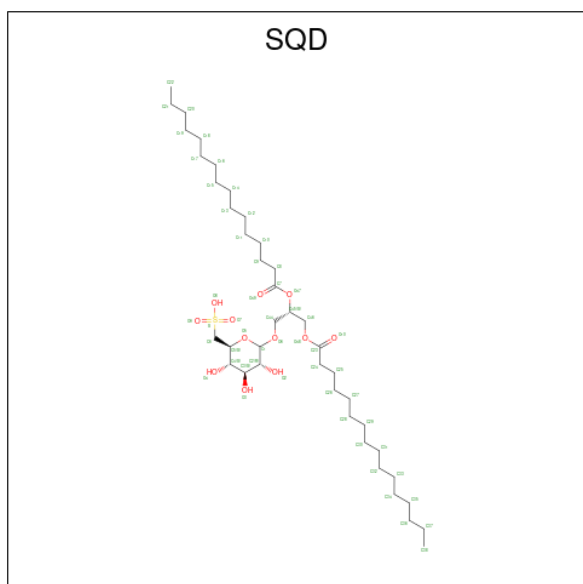
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			57	21	34	2		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

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



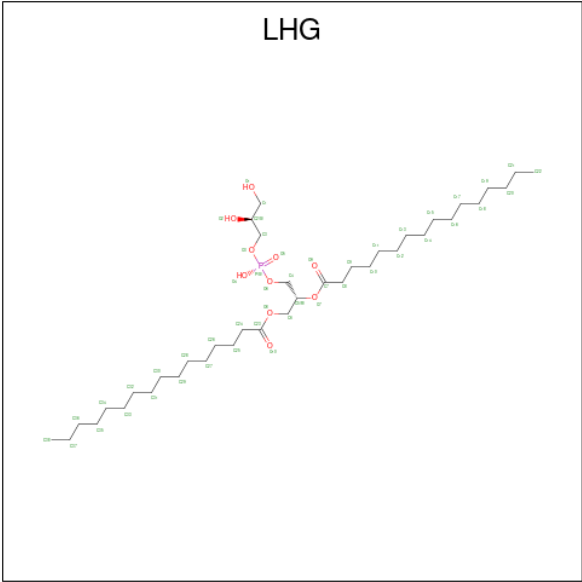
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		

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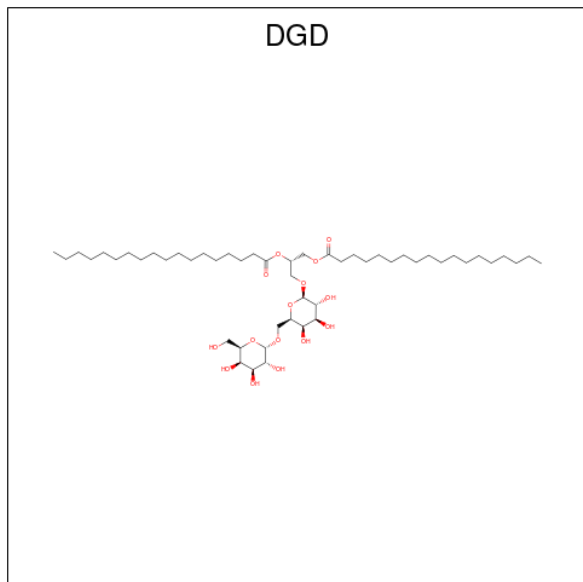
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



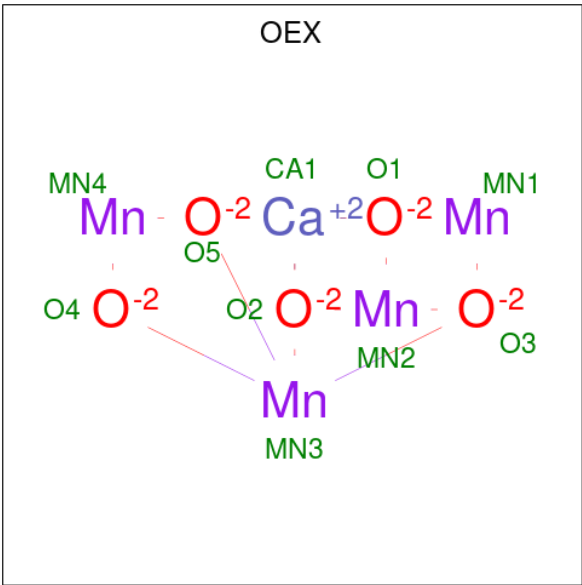
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
29	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
29	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



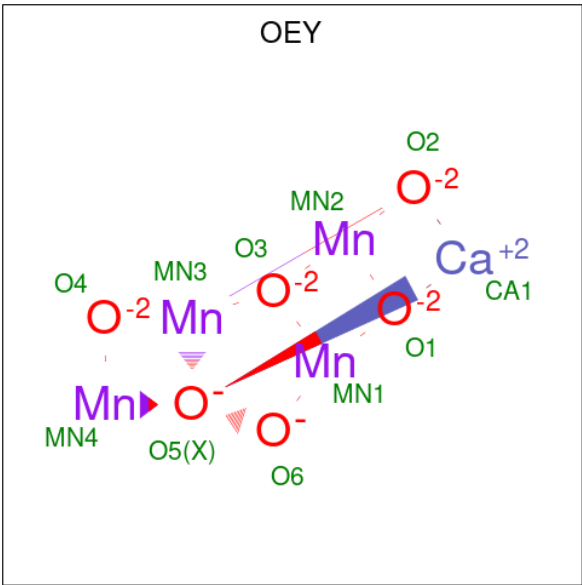
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	a	1	Total	C	H	O	0	0
			119	39	75	5		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



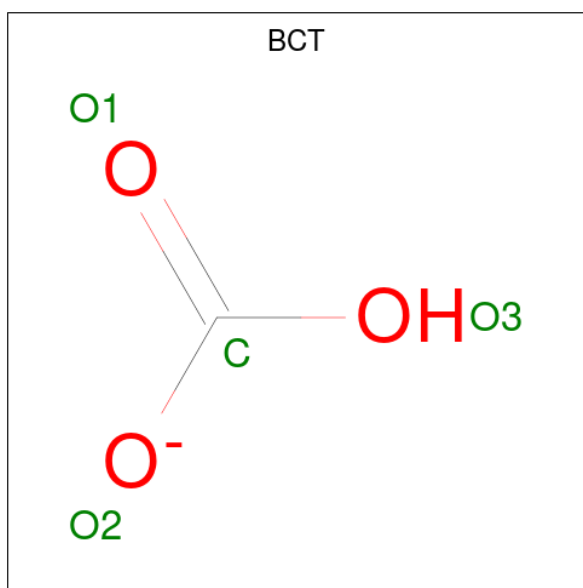
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
32	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 34 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

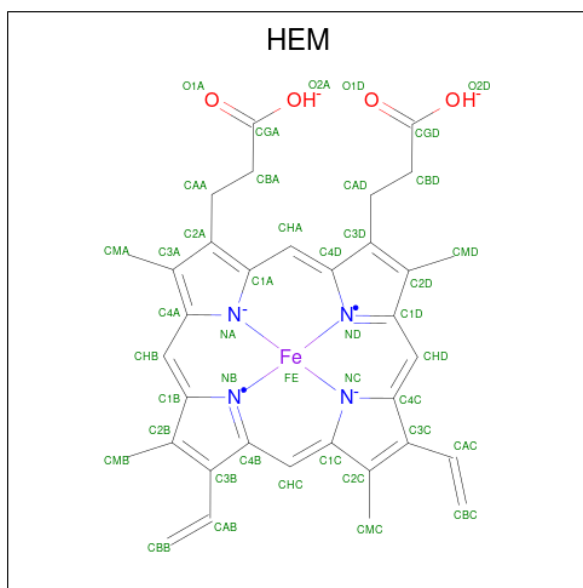
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	5	Total	C	H	O	0	0
			192	67	117	8		
34	C	3	Total	C	H	O	0	0
			103	36	63	4		
34	E	1	Total	C	H	O	0	0
			28	10	16	2		
34	H	1	Total	C	H		0	0
			53	18	35			
34	I	1	Total	C	H		0	0
			41	15	26			
34	J	1	Total	C	H	O	0	0
			28	10	16	2		
34	M	2	Total	C	H	O	0	0
			63	23	38	2		
34	X	1	Total	C	H	O	0	0
			55	18	35	2		
34	a	1	Total	C	H	O	0	0
			28	10	16	2		

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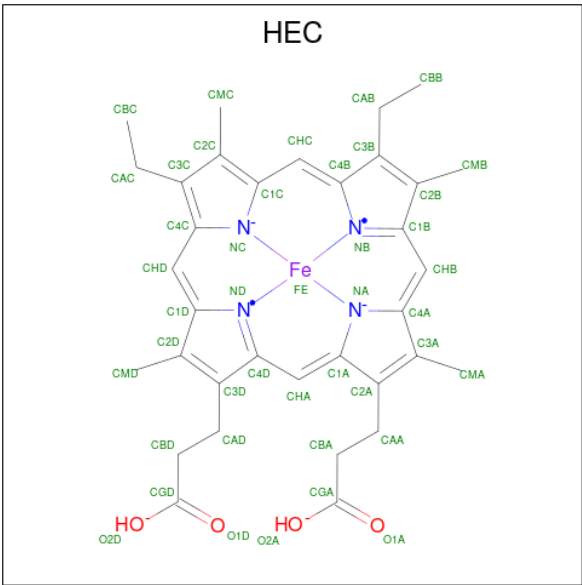
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	b	6	Total	C	H	O	0	0
			267	91	170	6		
34	c	2	Total	C	H	O	0	0
			83	28	51	4		
34	d	2	Total	C	H	O	0	0
			98	33	61	4		
34	j	1	Total	C	H	O	0	0
			28	10	16	2		
34	l	1	Total	C	H		0	0
			53	18	35			
34	m	1	Total	C	H	O	0	0
			28	10	16	2		
34	t	2	Total	C	H	O	0	0
			60	22	36	2		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	e	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
36	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
36	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	146	Total	O	0	8
			146	146		
37	B	213	Total	O	0	0
			213	213		
37	C	193	Total	O	0	0
			193	193		
37	D	129	Total	O	0	0
			129	129		
37	E	29	Total	O	0	0
			29	29		
37	F	14	Total	O	0	0
			14	14		
37	H	29	Total	O	0	0
			29	29		
37	I	14	Total	O	0	0
			14	14		
37	J	12	Total	O	0	0
			12	12		
37	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	8	Total 8	O 8	0	0
37	M	7	Total 7	O 7	0	0
37	O	123	Total 123	O 123	0	0
37	T	14	Total 14	O 14	0	0
37	U	49	Total 49	O 49	0	0
37	V	73	Total 73	O 73	0	0
37	Y	3	Total 3	O 3	0	0
37	X	8	Total 8	O 8	0	0
37	Z	4	Total 4	O 4	0	0
37	R	3	Total 3	O 3	0	0
37	a	125	Total 125	O 125	0	8
37	b	188	Total 188	O 188	0	0
37	c	159	Total 159	O 159	0	0
37	d	123	Total 123	O 123	0	0
37	e	22	Total 22	O 22	0	0
37	f	5	Total 5	O 5	0	0
37	h	20	Total 20	O 20	0	0
37	i	12	Total 12	O 12	0	0
37	j	8	Total 8	O 8	0	0
37	k	4	Total 4	O 4	0	0
37	l	10	Total 10	O 10	0	0

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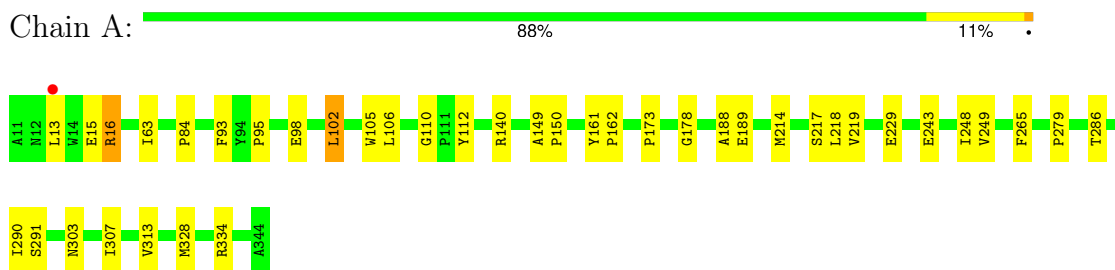
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	6	Total 6	O 6	0	0
37	o	120	Total 120	O 120	0	0
37	t	12	Total 12	O 12	0	0
37	u	50	Total 50	O 50	0	0
37	v	68	Total 68	O 68	0	0
37	y	4	Total 4	O 4	0	0
37	x	11	Total 11	O 11	0	0
37	z	1	Total 1	O 1	0	0
37	r	6	Total 6	O 6	0	0

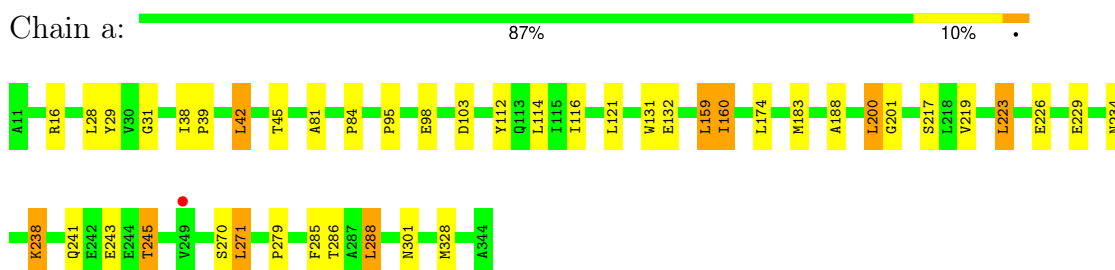
3 Residue-property plots [i](#)

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.

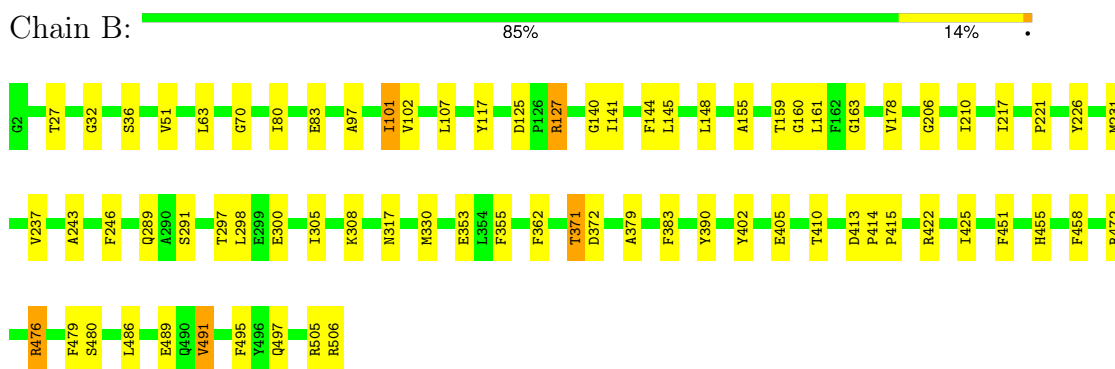
- Molecule 1: Photosystem II protein D1 1



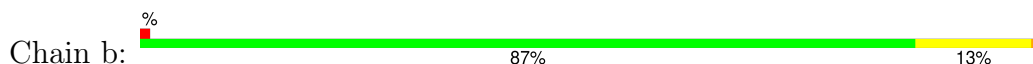
- Molecule 1: Photosystem II protein D1 1

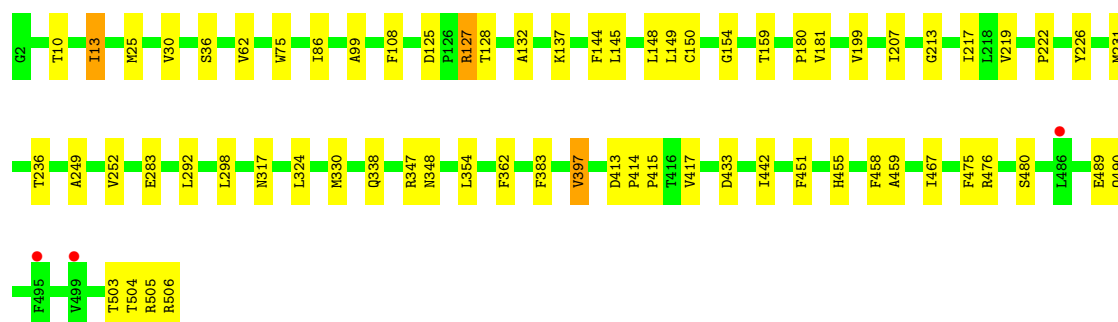


- Molecule 2: Photosystem II CP47 reaction center protein



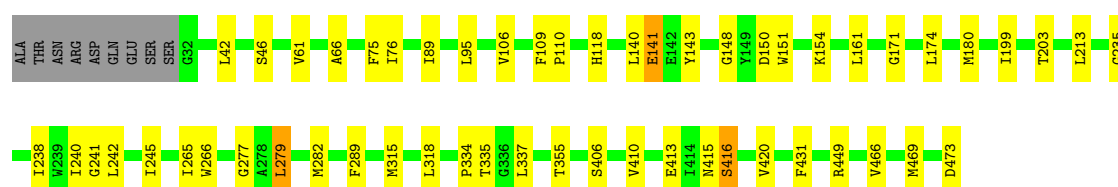
- Molecule 2: Photosystem II CP47 reaction center protein





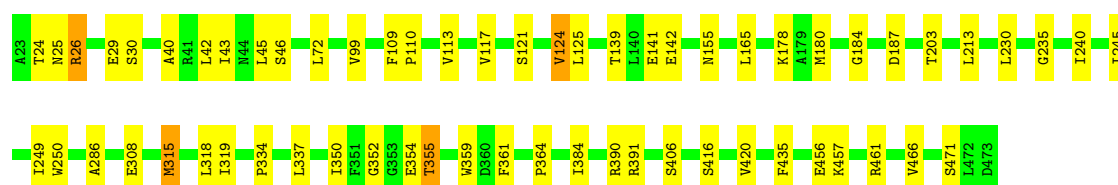
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 12% ..



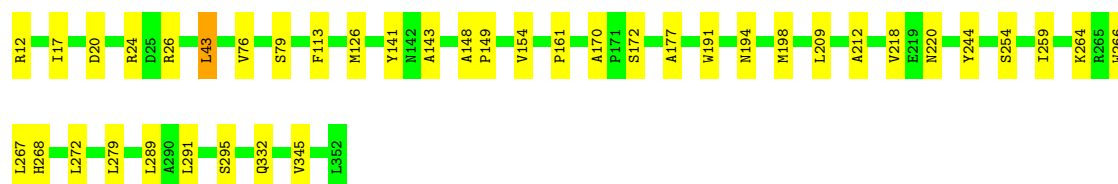
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 86% 13% .



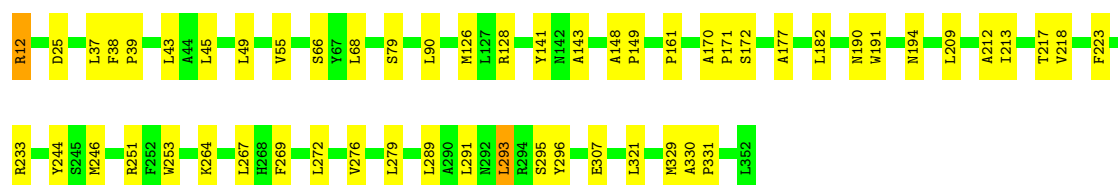
• Molecule 4: Photosystem II D2 protein

Chain D: 88% 11%

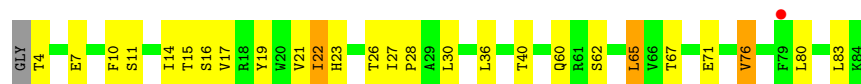


• Molecule 4: Photosystem II D2 protein

Chain d: 84% 16% .



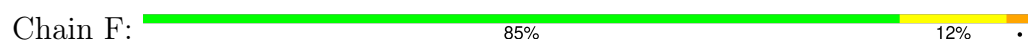
- Molecule 5: Cytochrome b559 subunit alpha



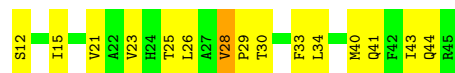
- Molecule 5: Cytochrome b559 subunit alpha



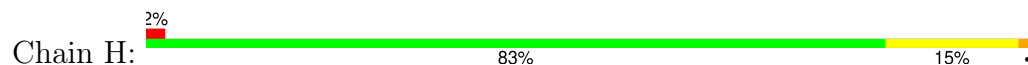
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



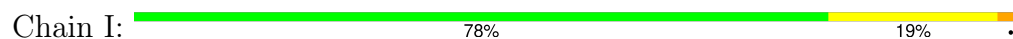
- Molecule 7: Photosystem II reaction center protein H



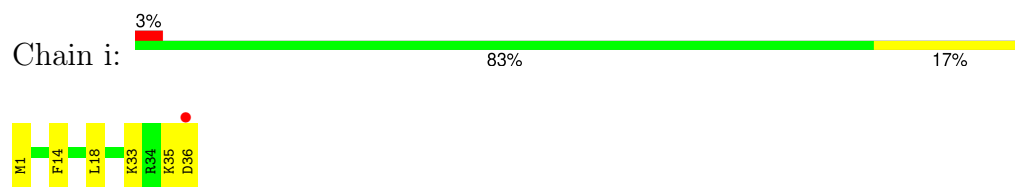
- Molecule 7: Photosystem II reaction center protein H



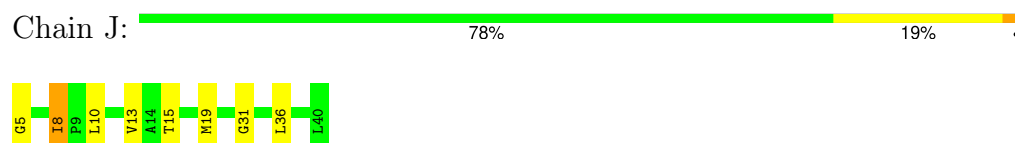
- Molecule 8: Photosystem II reaction center protein I



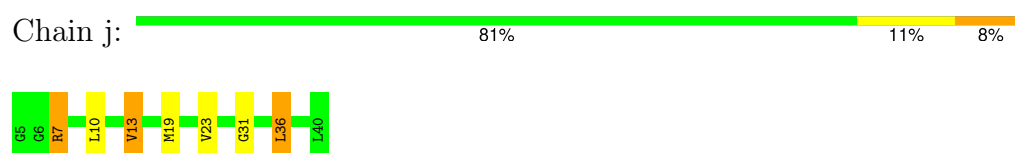
- Molecule 8: Photosystem II reaction center protein I



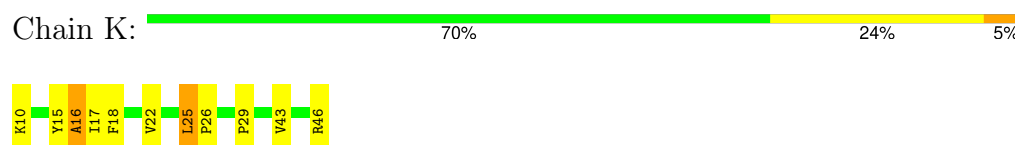
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



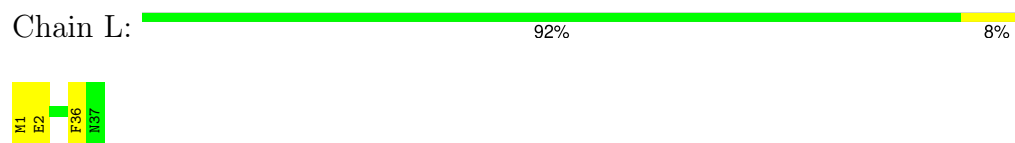
- Molecule 10: Photosystem II reaction center protein K



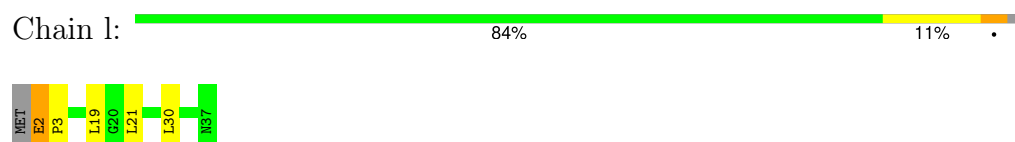
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L

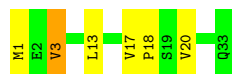


- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

Chain M:  82% 15% .



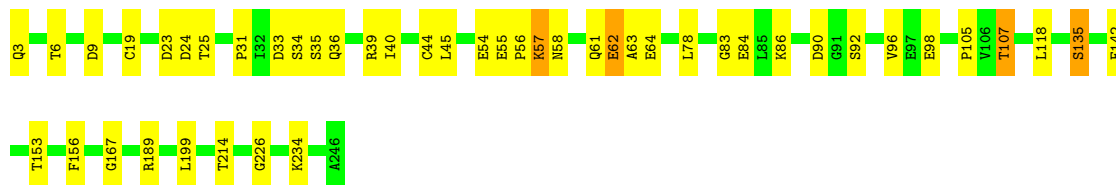
- Molecule 12: Photosystem II reaction center protein M

Chain m:  73% 21% . .



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  81% 17% .



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  82% 15% . .



- Molecule 14: Photosystem II reaction center protein T

Chain T:  83% 13% .



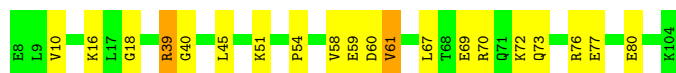
- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 87% 13%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  79% 19%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  89% 10%



- Molecule 16: Cytochrome c-550

Chain V:  80% 19%



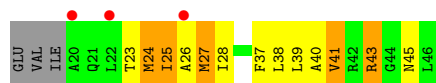
- Molecule 16: Cytochrome c-550

Chain v:  77% 22%

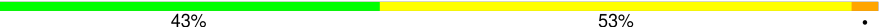


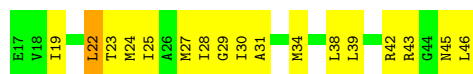
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  10% 47% 27% 17% 10%



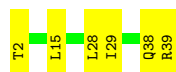
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  43% 53%

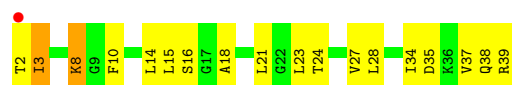


- Molecule 18: Photosystem II reaction center X protein

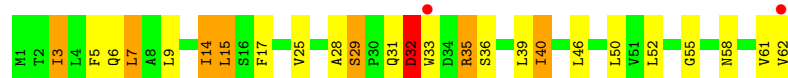
Chain X:  84% 16%



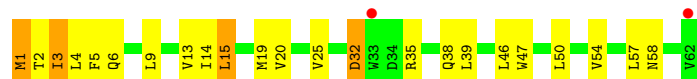
- Molecule 18: Photosystem II reaction center X protein



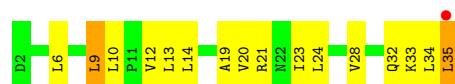
• Molecule 19: Photosystem II reaction center protein Z



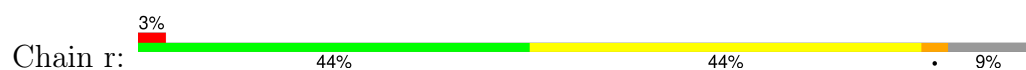
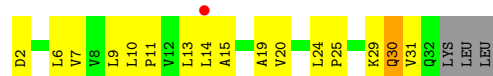
• Molecule 19: Photosystem II reaction center protein Z



• 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	117.01Å 221.54Å 308.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.58 – 2.07 30.58 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.58-2.07) 87.0 (30.58-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 2.06Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.184 , 0.247 0.184 , 0.247	Depositor DCC
R_{free} test set	4294 reflections (0.73%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	105756	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.56	0/3179	0.66	0/4331
1	a	0.52	0/3176	0.63	0/4327
2	B	0.59	1/4160 (0.0%)	0.66	1/5668 (0.0%)
2	b	0.55	0/4118	0.65	0/5611
3	C	0.58	1/3593 (0.0%)	0.63	0/4891
3	c	0.51	0/3673	0.64	0/4998
4	D	0.60	0/2820	0.66	0/3840
4	d	0.57	0/2829	0.65	0/3852
5	E	0.44	0/684	0.62	0/935
5	e	0.42	0/683	0.57	0/932
6	F	0.43	0/284	0.62	0/387
6	f	0.38	0/284	0.65	0/387
7	H	0.55	0/520	0.66	0/709
7	h	0.49	0/511	0.61	0/697
8	I	0.59	0/293	0.61	0/396
8	i	0.60	0/293	0.74	0/396
9	J	0.48	0/263	0.61	0/356
9	j	0.40	0/261	0.52	0/353
10	K	0.43	0/314	0.52	0/427
10	k	0.39	0/303	0.50	0/416
11	L	0.57	0/311	0.69	0/422
11	l	0.59	0/303	0.65	0/412
12	M	0.56	0/249	0.61	0/341
12	m	0.57	0/244	0.66	0/334
13	O	0.55	0/1914	0.65	0/2596
13	o	0.53	0/1905	0.65	0/2583
14	T	0.60	0/257	0.71	0/349
14	t	0.57	0/255	0.62	0/346
15	U	0.47	0/785	0.60	0/1064
15	u	0.54	0/785	0.68	0/1064
16	V	0.52	0/1085	0.61	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.48	0/1085	0.60	0/1473
17	Y	0.37	0/197	0.67	0/264
17	y	0.32	0/219	0.49	0/294
18	X	0.46	0/284	0.54	0/384
18	x	0.34	0/284	0.46	0/384
19	Z	0.40	0/490	0.55	0/669
19	z	0.35	0/488	0.53	0/666
20	R	0.36	0/277	0.55	0/380
20	r	0.27	0/233	0.47	0/323
All	All	0.54	2/43891 (0.0%)	0.64	1/59730 (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
15	u	0	1
19	Z	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	ILE	CA-CB	-11.60	1.48	1.54
2	B	221	PRO	CA-C	-8.10	1.47	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	221	PRO	O-C-N	-5.70	118.69	121.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	Z	32	ASP	Peptide
15	u	53	ALA	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	3081	2937	2950	29	0
1	a	3078	2928	2941	28	0
2	B	4004	3845	3864	43	0
2	b	3978	3811	3836	48	0
3	C	3476	3392	3405	35	0
3	c	3553	3464	3477	37	0
4	D	2726	2624	2632	29	0
4	d	2732	2630	2638	40	0
5	E	662	647	648	17	0
5	e	664	647	648	21	0
6	F	275	281	282	4	0
6	f	275	281	282	8	0
7	H	507	523	523	7	0
7	h	498	518	518	8	0
8	I	296	311	311	3	0
8	i	296	311	311	3	0
9	J	257	268	268	8	0
9	j	255	261	261	7	0
10	K	302	318	318	12	0
10	k	293	305	305	14	0
11	L	304	316	316	3	0
11	l	296	304	304	2	0
12	M	256	269	269	6	0
12	m	251	267	267	7	0
13	O	1880	1850	1852	33	0
13	o	1874	1844	1846	23	0
14	T	258	261	261	2	0
14	t	256	256	256	2	0
15	U	774	772	773	12	0
15	u	774	772	773	7	0
16	V	1064	1070	1073	16	0
16	v	1064	1070	1073	22	0
17	Y	196	208	217	11	0
17	y	218	241	241	10	0
18	X	281	312	312	2	0
18	x	281	312	312	15	0
19	Z	479	509	516	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	477	509	509	25	0
20	R	271	298	298	7	0
20	r	227	234	224	11	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	184	192	192	4	0
23	B	1035	1139	1139	20	0
23	C	839	922	922	11	0
23	D	195	216	216	3	0
23	a	260	288	288	5	0
23	b	970	1067	1067	28	0
23	c	839	919	919	8	0
23	d	130	144	144	1	0
23	h	65	72	72	3	0
24	A	128	148	148	1	0
24	a	64	74	74	0	0
24	d	64	74	74	2	0
25	A	40	56	56	2	0
25	B	120	168	168	8	0
25	C	40	56	56	1	0
25	D	40	56	56	5	0
25	H	40	56	56	2	0
25	K	80	112	112	3	0
25	T	40	56	56	3	0
25	Z	40	56	56	4	0
25	a	40	56	56	2	0
25	b	120	168	168	8	0
25	c	80	112	112	2	0
25	d	40	56	56	3	0
25	k	80	112	112	4	0
25	t	40	56	56	6	0
25	x	40	56	56	2	0
26	A	55	80	80	6	0
26	D	55	80	80	0	0
26	a	55	80	80	6	0
26	d	55	80	80	2	0
27	A	48	66	66	1	0
27	B	28	40	40	0	0
27	C	48	66	66	0	0
27	D	84	117	117	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	M	51	72	72	0	0
27	b	78	120	120	2	0
27	c	134	181	181	4	0
27	d	44	58	58	1	0
27	m	51	72	72	1	0
28	A	91	135	134	2	0
28	B	54	78	78	1	0
28	F	36	45	46	0	0
28	a	90	134	132	4	0
28	b	49	65	65	1	0
28	f	41	49	49	2	0
29	A	49	74	74	4	0
29	B	98	148	148	2	0
29	D	96	141	141	3	0
29	d	137	199	199	9	0
29	e	42	57	57	2	0
29	l	49	74	74	1	0
30	A	66	96	96	3	0
30	C	186	246	244	0	0
30	H	62	82	82	1	0
30	a	44	75	75	3	0
30	c	186	246	243	0	0
30	h	62	82	82	1	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	A	11	0	0	2	0
32	a	11	0	0	1	0
33	A	4	1	1	0	0
33	a	4	1	1	0	0
34	B	75	117	0	0	0
34	C	40	63	0	0	0
34	E	12	16	0	0	0
34	H	18	35	0	0	0
34	I	15	26	0	0	0
34	J	12	16	0	0	0
34	M	25	38	0	0	0
34	X	20	35	0	0	0
34	a	12	16	0	0	0
34	b	97	170	0	0	0
34	c	32	51	0	0	0
34	d	37	61	0	0	0
34	j	12	16	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	l	18	35	0	0	0
34	m	12	16	0	0	0
34	t	24	36	0	0	0
35	E	43	30	30	5	0
35	e	43	30	30	3	0
36	V	43	30	30	1	0
36	v	43	30	30	0	0
37	A	146	0	0	4	0
37	B	213	0	0	8	0
37	C	193	0	0	0	0
37	D	129	0	0	4	0
37	E	29	0	0	2	0
37	F	14	0	0	0	0
37	H	29	0	0	0	0
37	I	14	0	0	1	0
37	J	12	0	0	2	0
37	K	6	0	0	0	0
37	L	8	0	0	0	0
37	M	7	0	0	0	0
37	O	123	0	0	8	0
37	R	3	0	0	0	0
37	T	14	0	0	0	0
37	U	49	0	0	7	0
37	V	73	0	0	2	0
37	X	8	0	0	0	0
37	Y	3	0	0	0	0
37	Z	4	0	0	0	0
37	a	125	0	0	1	0
37	b	188	0	0	6	0
37	c	159	0	0	6	0
37	d	123	0	0	3	0
37	e	22	0	0	0	0
37	f	5	0	0	0	0
37	h	20	0	0	2	0
37	i	12	0	0	0	0
37	j	8	0	0	1	0
37	k	4	0	0	0	0
37	l	10	0	0	0	0
37	m	6	0	0	1	0
37	o	120	0	0	4	0
37	r	6	0	0	2	0
37	t	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	u	50	0	0	2	0
37	v	68	0	0	2	0
37	x	11	0	0	2	0
37	y	4	0	0	0	0
37	z	1	0	0	0	0
All	All	53286	52470	51850	688	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 688 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)
2:B:410:THR:O	37:B:701:HOH:O	1.74	1.04
3:c:391[A]:ARG:NH1	37:c:601:HOH:O	1.98	0.96
13:O:90:ASP:OD1	37:O:301:HOH:O	1.82	0.95
12:m:5:GLN:O	37:m:201:HOH:O	1.87	0.92
2:b:505:ARG:HG3	2:b:506:ARG:HG3	1.49	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/334 (117%)	381 (98%)	9 (2%)	0	100	100
1	a	390/334 (117%)	382 (98%)	8 (2%)	0	100	100
2	B	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
2	b	503/505 (100%)	495 (98%)	7 (1%)	1 (0%)	43	38
3	C	447/451 (99%)	435 (97%)	11 (2%)	1 (0%)	43	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	457/451 (101%)	442 (97%)	14 (3%)	1 (0%)	43	38
4	D	339/341 (99%)	330 (97%)	9 (3%)	0	100	100
4	d	340/341 (100%)	329 (97%)	11 (3%)	0	100	100
5	E	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
5	e	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	55 (90%)	6 (10%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
9	J	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	j	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	0	1 (3%)	3	0
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/33 (94%)	31 (100%)	0	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	226 (93%)	16 (7%)	1 (0%)	30	23
13	o	242/244 (99%)	230 (95%)	8 (3%)	4 (2%)	7	2
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	28 (100%)	0	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
15	u	95/97 (98%)	90 (95%)	4 (4%)	1 (1%)	11	4
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	19 (76%)	4 (16%)	2 (8%)	1	0
17	y	28/30 (93%)	24 (86%)	4 (14%)	0	100	100
18	X	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Z	60/62 (97%)	50 (83%)	7 (12%)	3 (5%)	1	0
19	z	60/62 (97%)	50 (83%)	9 (15%)	1 (2%)	7	2
20	R	32/34 (94%)	30 (94%)	1 (3%)	1 (3%)	3	0
20	r	29/34 (85%)	22 (76%)	6 (21%)	1 (3%)	3	0
All	All	5365/5326 (101%)	5164 (96%)	183 (3%)	18 (0%)	36	30

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	62	GLU
3	c	416	SER
13	o	60	ARG
13	o	61	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/270 (118%)	311 (98%)	8 (2%)	42	38
1	a	318/270 (118%)	303 (95%)	15 (5%)	23	16
2	B	407/403 (101%)	388 (95%)	19 (5%)	23	16
2	b	402/403 (100%)	389 (97%)	13 (3%)	34	29
3	C	351/352 (100%)	341 (97%)	10 (3%)	38	34
3	c	360/352 (102%)	341 (95%)	19 (5%)	20	13
4	D	277/276 (100%)	271 (98%)	6 (2%)	45	43
4	d	278/276 (101%)	269 (97%)	9 (3%)	34	29
5	E	72/72 (100%)	62 (86%)	10 (14%)	3	1
5	e	71/72 (99%)	68 (96%)	3 (4%)	26	20
6	F	28/28 (100%)	27 (96%)	1 (4%)	31	25
6	f	28/28 (100%)	23 (82%)	5 (18%)	2	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	53/54 (98%)	50 (94%)	3 (6%)	18	11
7	h	53/54 (98%)	48 (91%)	5 (9%)	8	3
8	I	32/32 (100%)	28 (88%)	4 (12%)	4	1
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	24/24 (100%)	23 (96%)	1 (4%)	26	20
9	j	23/24 (96%)	20 (87%)	3 (13%)	4	1
10	K	31/30 (103%)	26 (84%)	5 (16%)	2	0
10	k	30/30 (100%)	25 (83%)	5 (17%)	2	0
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	33
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	4
12	M	28/29 (97%)	26 (93%)	2 (7%)	13	7
12	m	28/29 (97%)	27 (96%)	1 (4%)	31	25
13	O	208/207 (100%)	194 (93%)	14 (7%)	15	8
13	o	207/207 (100%)	191 (92%)	16 (8%)	12	5
14	T	26/26 (100%)	22 (85%)	4 (15%)	2	0
14	t	25/26 (96%)	24 (96%)	1 (4%)	28	22
15	U	84/84 (100%)	78 (93%)	6 (7%)	13	7
15	u	84/84 (100%)	84 (100%)	0	100	100
16	V	117/117 (100%)	112 (96%)	5 (4%)	26	20
16	v	117/117 (100%)	110 (94%)	7 (6%)	17	10
17	Y	19/23 (83%)	13 (68%)	6 (32%)	0	0
17	y	22/23 (96%)	17 (77%)	5 (23%)	1	0
18	X	31/31 (100%)	28 (90%)	3 (10%)	8	3
18	x	31/31 (100%)	25 (81%)	6 (19%)	1	0
19	Z	52/52 (100%)	41 (79%)	11 (21%)	1	0
19	z	51/52 (98%)	44 (86%)	7 (14%)	3	1
20	R	28/29 (97%)	19 (68%)	9 (32%)	0	0
20	r	19/29 (66%)	16 (84%)	3 (16%)	2	0
All	All	4435/4348 (102%)	4181 (94%)	254 (6%)	18	11

5 of 254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Z	46	LEU
13	o	135	SER
2	b	13	ILE
13	o	133	VAL
17	y	45	ASN

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

Mol	Chain	Res	Type
2	b	338	GLN
3	c	25	ASN
2	b	497	GLN
3	c	201	ASN
4	D	334	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	$\# Z > 2$
12	FME	M	1	12	8,9,10	0.96	1 (12%)	8,9,11	1.01	0
14	FME	T	1	14	8,9,10	1.13	1 (12%)	8,9,11	1.73	3 (37%)
8	FME	i	1	8	8,9,10	1.02	0	8,9,11	1.11	1 (12%)
8	FME	I	1	8	8,9,10	0.90	1 (12%)	8,9,11	1.61	3 (37%)
14	FME	t	1	14	8,9,10	1.10	1 (12%)	8,9,11	1.97	1 (12%)
12	FME	m	1	12	8,9,10	1.06	1 (12%)	8,9,11	0.97	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.79	1.42	1.46
14	T	1	FME	CA-N	-2.43	1.43	1.46
12	m	1	FME	CA-N	-2.19	1.43	1.46
8	I	1	FME	CA-N	-2.03	1.43	1.46
12	M	1	FME	CA-N	-2.02	1.43	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-4.32	116.18	122.82
8	I	1	FME	CA-N-CN	-3.12	118.02	122.82
14	T	1	FME	CA-N-CN	-2.62	118.79	122.82
14	T	1	FME	CB-CA-N	2.45	114.97	110.52
8	I	1	FME	CB-CA-N	2.40	114.88	110.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
12	M	1	FME	CB-CA-N-CN
8	i	1	FME	CB-CA-N-CN
12	M	1	FME	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic and 31 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	BCR	d	404	-	41,41,41	1.21	3 (7%)	56,56,56	1.22	6 (10%)
23	CLA	b	610	2	69,73,73	1.34	10 (14%)	82,113,113	1.13	4 (4%)
30	DGD	c	518	-	63,63,67	1.11	6 (9%)	77,77,81	1.46	15 (19%)
35	HEM	E	101	6,5	50,50,50	1.43	8 (16%)	67,82,82	1.13	4 (5%)
23	CLA	c	506	3	69,73,73	1.88	9 (13%)	82,113,113	1.34	15 (18%)
25	BCR	A	409	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	8 (14%)
33	BCT	A	418	21	3,3,3	1.03	0	2,3,3	3.51	2 (100%)
29	LHG	D	407	-	48,48,48	1.02	3 (6%)	51,54,54	1.33	7 (13%)
23	CLA	B	612	2	69,73,73	1.23	8 (11%)	82,113,113	1.39	8 (9%)
25	BCR	B	617	-	41,41,41	1.23	4 (9%)	56,56,56	1.37	6 (10%)
23	CLA	B	610	37	69,73,73	1.35	9 (13%)	82,113,113	1.40	10 (12%)
23	CLA	h	101	37	69,73,73	1.49	10 (14%)	82,113,113	1.39	10 (12%)
23	CLA	c	507	37	69,73,73	1.26	9 (13%)	82,113,113	1.34	8 (9%)
23	CLA	D	402	4	69,73,73	1.15	9 (13%)	82,113,113	1.26	6 (7%)
24	PHO	A	407	-	58,69,69	1.96	10 (17%)	55,99,99	1.43	9 (16%)
24	PHO	d	401	-	58,69,69	2.14	13 (22%)	55,99,99	1.73	10 (18%)
28	SQD	a	413	-	35,35,54	1.13	2 (5%)	37,37,65	1.40	5 (13%)
25	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.44	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	B	623	-	48,48,48	0.90	2 (4%)	51,54,54	1.45	6 (11%)
25	BCR	k	102	-	41,41,41	0.93	1 (2%)	56,56,56	1.18	4 (7%)
25	BCR	x	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.30	6 (10%)
23	CLA	b	614	2	69,73,73	1.43	10 (14%)	82,113,113	1.35	12 (14%)
23	CLA	C	505	3	69,73,73	1.24	6 (8%)	82,113,113	1.14	5 (6%)
23	CLA	b	615	2	69,73,73	1.26	7 (10%)	82,113,113	1.43	9 (10%)
33	BCT	a	404	21	3,3,3	1.24	0	2,3,3	3.17	2 (100%)
31	OEX	A	416[A]	3,37,1	0,14,14	-	-	-		
28	SQD	B	624	-	52,54,54	0.93	2 (3%)	62,65,65	1.78	12 (19%)
25	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	12 (21%)
27	LMG	M	101	-	51,51,55	0.99	3 (5%)	59,59,63	1.50	11 (18%)
28	SQD	f	101	-	39,41,54	1.16	4 (10%)	49,52,65	1.66	8 (16%)
23	CLA	c	501	3	69,73,73	1.41	11 (15%)	82,113,113	1.56	10 (12%)
23	CLA	a	406	37	69,73,73	1.51	10 (14%)	82,113,113	1.41	7 (8%)
23	CLA	B	607	37	69,73,73	1.34	9 (13%)	82,113,113	1.35	8 (9%)
23	CLA	B	601	37	69,73,73	1.39	8 (11%)	82,113,113	1.69	10 (12%)
29	LHG	l	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.24	5 (9%)
27	LMG	c	519	-	37,37,55	1.14	4 (10%)	45,45,63	1.27	6 (13%)
23	CLA	b	608	37	69,73,73	1.43	9 (13%)	82,113,113	1.24	8 (9%)
28	SQD	A	414	-	38,38,54	1.05	3 (7%)	40,40,65	1.26	3 (7%)
29	LHG	d	406	-	48,48,48	0.74	1 (2%)	51,54,54	1.31	6 (11%)
23	CLA	c	502	3	69,73,73	1.40	10 (14%)	82,113,113	1.35	8 (9%)
29	LHG	A	413	-	48,48,48	1.01	4 (8%)	51,54,54	1.23	4 (7%)
23	CLA	B	606	2	69,73,73	1.58	10 (14%)	82,113,113	1.57	13 (15%)
23	CLA	C	501	3	69,73,73	1.48	12 (17%)	82,113,113	1.38	8 (9%)
29	LHG	e	101	-	41,41,48	0.93	3 (7%)	44,47,54	1.40	5 (11%)
24	PHO	a	407	-	58,69,69	2.26	13 (22%)	55,99,99	1.34	6 (10%)
25	BCR	B	619	-	41,41,41	1.27	4 (9%)	56,56,56	1.34	9 (16%)
27	LMG	D	409	-	31,31,55	1.02	3 (9%)	33,33,63	1.26	3 (9%)
23	CLA	B	603	2	69,73,73	1.27	10 (14%)	82,113,113	1.27	10 (12%)
23	CLA	C	510	3	69,73,73	1.34	10 (14%)	82,113,113	1.31	7 (8%)
32	OEY	A	417[B]	3,37,1	0,16,16	-	-	-		
23	CLA	b	604	2	69,73,73	1.19	6 (8%)	82,113,113	1.45	12 (14%)
25	BCR	H	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.42	6 (10%)
29	LHG	D	408	-	46,46,48	1.10	4 (8%)	49,52,54	1.33	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	508	3	69,73,73	1.20	8 (11%)	82,113,113	1.34	11 (13%)
25	BCR	b	618	-	41,41,41	1.19	3 (7%)	56,56,56	1.43	10 (17%)
30	DGD	H	102	-	63,63,67	1.33	8 (12%)	77,77,81	1.45	10 (12%)
35	HEM	e	102	6,5	50,50,50	1.51	7 (14%)	67,82,82	1.19	6 (8%)
23	CLA	C	507	37	69,73,73	1.30	8 (11%)	82,113,113	1.42	8 (9%)
29	LHG	d	407	-	48,48,48	0.82	1 (2%)	51,54,54	1.31	6 (11%)
27	LMG	b	623	-	21,21,55	0.88	1 (4%)	20,20,63	0.96	1 (5%)
23	CLA	b	606	2	69,73,73	1.16	10 (14%)	82,113,113	1.48	15 (18%)
23	CLA	b	607	2	69,73,73	1.43	7 (10%)	82,113,113	1.57	8 (9%)
23	CLA	c	505	3	69,73,73	1.21	8 (11%)	82,113,113	1.38	10 (12%)
27	LMG	d	409	-	44,44,55	1.04	3 (6%)	52,52,63	1.33	7 (13%)
23	CLA	c	508	3	68,72,73	1.43	9 (13%)	80,111,113	1.34	8 (10%)
23	CLA	b	603	2	69,73,73	1.19	8 (11%)	82,113,113	1.35	8 (9%)
27	LMG	C	518	-	48,48,55	1.04	3 (6%)	56,56,63	1.34	8 (14%)
23	CLA	D	401	37	69,73,73	1.15	7 (10%)	82,113,113	1.25	8 (9%)
25	BCR	b	619	-	41,41,41	1.25	2 (4%)	56,56,56	1.23	6 (10%)
23	CLA	b	613	2	69,73,73	1.34	8 (11%)	82,113,113	1.34	13 (15%)
23	CLA	B	611	2	69,73,73	1.17	6 (8%)	82,113,113	1.39	10 (12%)
23	CLA	C	512	3	69,73,73	1.42	9 (13%)	82,113,113	1.31	11 (13%)
25	BCR	T	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.54	11 (19%)
23	CLA	B	614	2	69,73,73	1.13	9 (13%)	82,113,113	1.39	10 (12%)
30	DGD	C	516	-	63,63,67	1.08	4 (6%)	77,77,81	1.44	11 (14%)
23	CLA	b	616	2	69,73,73	1.42	12 (17%)	82,113,113	1.27	4 (4%)
27	LMG	B	621	-	26,26,55	0.79	0	26,26,63	1.12	2 (7%)
23	CLA	C	513	3	69,73,73	1.38	10 (14%)	82,113,113	1.40	6 (7%)
25	BCR	K	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	6 (10%)
23	CLA	C	506	3	69,73,73	1.76	11 (15%)	82,113,113	1.24	7 (8%)
32	OHEY	a	417[B]	3,37,1	0,16,16	-	-	-	-	-
25	BCR	k	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.26	6 (10%)
23	CLA	c	509	3	69,73,73	1.28	8 (11%)	82,113,113	1.40	9 (10%)
28	SQD	F	101	-	34,36,54	1.01	3 (8%)	42,45,65	1.68	9 (21%)
25	BCR	t	101	-	41,41,41	1.02	3 (7%)	56,56,56	1.43	9 (16%)
23	CLA	B	616	2	64,68,73	1.36	7 (10%)	76,107,113	1.45	12 (15%)
23	CLA	a	411	37	69,73,73	1.54	9 (13%)	82,113,113	1.65	9 (10%)
27	LMG	D	406	-	51,51,55	1.00	2 (3%)	59,59,63	1.28	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	608	2	69,73,73	1.18	7 (10%)	82,113,113	1.29	8 (9%)
23	CLA	d	403	4	69,73,73	1.23	9 (13%)	82,113,113	1.23	9 (10%)
23	CLA	c	503	3	69,73,73	1.43	10 (14%)	82,113,113	1.55	9 (10%)
23	CLA	B	605	2	69,73,73	1.30	8 (11%)	82,113,113	1.39	15 (18%)
25	BCR	c	515	-	41,41,41	1.33	3 (7%)	56,56,56	1.41	9 (16%)
23	CLA	B	604	2	69,73,73	1.30	6 (8%)	82,113,113	1.45	12 (14%)
25	BCR	C	514	-	41,41,41	1.21	4 (9%)	56,56,56	1.32	6 (10%)
27	LMG	A	411	-	48,48,55	0.95	2 (4%)	56,56,63	1.40	9 (16%)
23	CLA	C	502	3	69,73,73	1.19	7 (10%)	82,113,113	1.31	10 (12%)
24	PHO	A	406	-	58,69,69	1.66	8 (13%)	55,99,99	1.50	8 (14%)
23	CLA	A	405	37	69,73,73	1.39	8 (11%)	82,113,113	1.32	10 (12%)
23	CLA	C	504	37	63,67,73	1.25	9 (14%)	74,105,113	1.21	7 (9%)
30	DGD	C	517	-	63,63,67	1.14	7 (11%)	77,77,81	1.36	8 (10%)
23	CLA	B	615	2	69,73,73	1.42	12 (17%)	82,113,113	1.25	7 (8%)
29	LHG	d	408	-	38,38,48	0.89	1 (2%)	41,44,54	1.23	3 (7%)
26	PL9	A	410	-	55,55,55	1.08	2 (3%)	68,69,69	1.66	13 (19%)
36	HEC	v	201	16	50,50,50	1.44	5 (10%)	68,82,82	1.23	7 (10%)
30	DGD	h	102	-	63,63,67	1.02	5 (7%)	77,77,81	1.54	14 (18%)
25	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	9 (16%)
23	CLA	c	512	3	69,73,73	1.25	10 (14%)	82,113,113	1.34	8 (9%)
23	CLA	C	511	3	69,73,73	1.48	10 (14%)	82,113,113	1.54	5 (6%)
28	SQD	a	412	-	52,54,54	0.97	4 (7%)	62,65,65	1.87	11 (17%)
36	HEC	V	201	16	50,50,50	1.45	5 (10%)	68,82,82	1.20	6 (8%)
25	BCR	D	404	-	41,41,41	1.21	2 (4%)	56,56,56	1.28	5 (8%)
23	CLA	c	511	3	69,73,73	1.50	9 (13%)	82,113,113	1.34	7 (8%)
23	CLA	B	613	2	69,73,73	1.31	8 (11%)	82,113,113	1.34	5 (6%)
23	CLA	b	612	2	69,73,73	1.29	8 (11%)	82,113,113	1.37	12 (14%)
30	DGD	C	515	-	63,63,67	1.41	9 (14%)	77,77,81	1.33	9 (11%)
30	DGD	c	516	-	63,63,67	1.29	6 (9%)	77,77,81	1.38	11 (14%)
30	DGD	c	517	-	63,63,67	1.10	6 (9%)	77,77,81	1.41	9 (11%)
23	CLA	A	404	1	69,73,73	1.49	12 (17%)	82,113,113	1.37	11 (13%)
23	CLA	c	504	37	64,68,73	1.21	10 (15%)	76,107,113	1.35	11 (14%)
23	CLA	d	402	4	69,73,73	1.34	9 (13%)	82,113,113	1.58	7 (8%)
27	LMG	c	521	-	48,48,55	1.12	6 (12%)	56,56,63	1.37	9 (16%)
28	SQD	b	601	-	47,49,54	0.94	3 (6%)	57,60,65	1.92	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	OEX	a	416[A]	3,37,1	0,14,14	-	-	-		
28	SQD	A	412	-	50,52,54	1.06	3 (6%)	60,63,65	2.21	15 (25%)
23	CLA	C	503	3	69,73,73	1.61	11 (15%)	82,113,113	1.76	14 (17%)
23	CLA	C	509	3	69,73,73	1.33	9 (13%)	82,113,113	1.20	6 (7%)
27	LMG	m	101	-	51,51,55	0.83	2 (3%)	59,59,63	1.56	12 (20%)
23	CLA	a	405	1	69,73,73	1.33	6 (8%)	82,113,113	1.45	8 (9%)
23	CLA	D	403	4	69,73,73	1.62	10 (14%)	82,113,113	1.14	7 (8%)
23	CLA	b	617	2	64,68,73	1.05	6 (9%)	76,107,113	1.39	11 (14%)
23	CLA	B	609	2	69,73,73	1.40	12 (17%)	82,113,113	1.43	12 (14%)
25	BCR	b	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	8 (14%)
27	LMG	c	523	-	49,49,55	0.90	2 (4%)	57,57,63	1.31	7 (12%)
25	BCR	Z	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.30	8 (14%)
26	PL9	a	410	-	55,55,55	1.12	4 (7%)	68,69,69	1.72	11 (16%)
26	PL9	d	405	-	55,55,55	1.40	9 (16%)	68,69,69	1.74	18 (26%)
30	DGD	A	415	-	67,67,67	1.25	8 (11%)	81,81,81	1.48	9 (11%)
25	BCR	a	409	-	41,41,41	1.02	2 (4%)	56,56,56	1.33	10 (17%)
23	CLA	c	513	3	69,73,73	1.21	9 (13%)	82,113,113	1.18	7 (8%)
23	CLA	b	611	37	69,73,73	1.20	7 (10%)	82,113,113	1.28	8 (9%)
29	LHG	B	622	-	48,48,48	0.71	1 (2%)	51,54,54	1.13	4 (7%)
23	CLA	a	408	1	69,73,73	1.48	11 (15%)	82,113,113	1.32	9 (10%)
23	CLA	b	605	2	69,73,73	1.23	7 (10%)	82,113,113	1.46	10 (12%)
23	CLA	B	602	2	69,73,73	1.55	11 (15%)	82,113,113	1.35	9 (10%)
27	LMG	b	622	-	55,55,55	1.05	3 (5%)	63,63,63	1.46	7 (11%)
23	CLA	b	609	2	69,73,73	1.34	9 (13%)	82,113,113	1.49	14 (17%)
26	PL9	D	405	-	55,55,55	1.61	10 (18%)	68,69,69	1.44	11 (16%)
23	CLA	c	510	3	69,73,73	1.26	9 (13%)	82,113,113	1.42	8 (9%)
23	CLA	A	408	1	58,62,73	1.66	9 (15%)	68,99,113	1.39	12 (17%)
30	DGD	a	414	-	43,43,67	1.49	6 (13%)	45,45,81	1.51	7 (15%)

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	BCR	d	404	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	610	2	-	10/39/115/115	-
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2
35	HEM	E	101	6,5	-	3/14/54/54	-
23	CLA	c	506	3	-	14/39/115/115	-
25	BCR	A	409	-	-	11/29/63/63	0/2/2/2
29	LHG	D	407	-	-	25/53/53/53	-
23	CLA	B	612	2	-	4/39/115/115	-
25	BCR	B	617	-	-	11/29/63/63	0/2/2/2
23	CLA	B	610	37	-	6/39/115/115	-
23	CLA	h	101	37	-	19/39/115/115	-
23	CLA	c	507	37	-	12/39/115/115	-
23	CLA	D	402	4	-	7/39/115/115	-
24	PHO	A	407	-	-	1/37/103/103	0/5/6/6
24	PHO	d	401	-	-	5/37/103/103	0/5/6/6
28	SQD	a	413	-	-	19/37/37/69	-
25	BCR	K	101	-	-	5/29/63/63	0/2/2/2
29	LHG	B	623	-	-	21/53/53/53	-
25	BCR	k	102	-	-	4/29/63/63	0/2/2/2
25	BCR	x	101	-	-	5/29/63/63	0/2/2/2
23	CLA	b	614	2	-	3/39/115/115	-
23	CLA	C	505	3	-	12/39/115/115	-
23	CLA	b	615	2	-	14/39/115/115	-
28	SQD	B	624	-	-	24/49/69/69	0/1/1/1
25	BCR	c	514	-	-	16/29/63/63	0/2/2/2
27	LMG	M	101	-	-	19/46/66/70	0/1/1/1
28	SQD	f	101	-	-	13/36/56/69	0/1/1/1
23	CLA	c	501	3	-	5/39/115/115	-
23	CLA	a	406	37	-	11/39/115/115	-
23	CLA	B	607	37	-	11/39/115/115	-
23	CLA	B	601	37	-	16/39/115/115	-
29	LHG	l	101	-	-	18/53/53/53	-
27	LMG	c	519	-	-	12/31/51/70	0/1/1/1
23	CLA	b	608	37	-	11/39/115/115	-
28	SQD	A	414	-	-	18/39/39/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	d	406	-	-	22/53/53/53	-
23	CLA	c	502	3	-	4/39/115/115	-
29	LHG	A	413	-	-	27/53/53/53	-
23	CLA	B	606	2	-	11/39/115/115	-
23	CLA	C	501	3	-	6/39/115/115	-
29	LHG	e	101	-	-	27/46/46/53	-
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
25	BCR	B	619	-	-	7/29/63/63	0/2/2/2
27	LMG	D	409	-	-	13/33/33/70	-
23	CLA	B	603	2	-	16/39/115/115	-
23	CLA	C	510	3	-	10/39/115/115	-
23	CLA	b	604	2	-	9/39/115/115	-
25	BCR	H	101	-	-	4/29/63/63	0/2/2/2
29	LHG	D	408	-	-	20/51/51/53	-
23	CLA	C	508	3	-	3/39/115/115	-
25	BCR	b	618	-	-	6/29/63/63	0/2/2/2
30	DGD	H	102	-	-	13/51/91/95	0/2/2/2
35	HEM	e	102	6,5	-	5/14/54/54	-
23	CLA	C	507	37	-	8/39/115/115	-
29	LHG	d	407	-	-	24/53/53/53	-
27	LMG	b	623	-	-	9/17/17/70	-
23	CLA	b	606	2	-	8/39/115/115	-
23	CLA	b	607	2	-	10/39/115/115	-
23	CLA	c	505	3	-	12/39/115/115	-
27	LMG	d	409	-	-	13/39/59/70	0/1/1/1
23	CLA	c	508	3	-	10/38/114/115	-
23	CLA	b	603	2	-	8/39/115/115	-
27	LMG	C	518	-	-	15/43/63/70	0/1/1/1
23	CLA	D	401	37	-	3/39/115/115	-
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
23	CLA	b	613	2	-	9/39/115/115	-
23	CLA	B	611	2	-	8/39/115/115	-
23	CLA	C	512	3	-	10/39/115/115	-
25	BCR	T	101	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	614	2	-	12/39/115/115	-
30	DGD	C	516	-	-	21/51/91/95	0/2/2/2
23	CLA	b	616	2	-	6/39/115/115	-
27	LMG	B	621	-	-	11/22/22/70	-
23	CLA	C	513	3	-	9/39/115/115	-
25	BCR	K	102	-	-	10/29/63/63	0/2/2/2
23	CLA	C	506	3	-	10/39/115/115	-
25	BCR	k	101	-	-	11/29/63/63	0/2/2/2
23	CLA	c	509	3	-	12/39/115/115	-
28	SQD	F	101	-	-	16/28/48/69	0/1/1/1
25	BCR	t	101	-	-	5/29/63/63	0/2/2/2
23	CLA	B	616	2	-	8/33/109/115	-
23	CLA	a	411	37	-	3/39/115/115	-
27	LMG	D	406	-	-	14/46/66/70	0/1/1/1
23	CLA	B	608	2	-	0/39/115/115	-
23	CLA	d	403	4	-	6/39/115/115	-
23	CLA	c	503	3	-	7/39/115/115	-
23	CLA	B	605	2	-	11/39/115/115	-
25	BCR	c	515	-	-	9/29/63/63	0/2/2/2
23	CLA	B	604	2	-	10/39/115/115	-
25	BCR	C	514	-	-	2/29/63/63	0/2/2/2
27	LMG	A	411	-	-	20/43/63/70	0/1/1/1
23	CLA	C	502	3	-	8/39/115/115	-
24	PHO	A	406	-	-	5/37/103/103	0/5/6/6
23	CLA	A	405	37	-	5/39/115/115	-
23	CLA	C	504	37	-	8/32/108/115	-
30	DGD	C	517	-	-	15/51/91/95	0/2/2/2
23	CLA	B	615	2	-	10/39/115/115	-
29	LHG	d	408	-	-	12/43/43/53	-
26	PL9	A	410	-	-	27/53/73/73	0/1/1/1
36	HEC	v	201	16	1/1/7/7	2/14/54/54	-
30	DGD	h	102	-	-	17/51/91/95	0/2/2/2
25	BCR	B	618	-	-	4/29/63/63	0/2/2/2
23	CLA	c	512	3	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	511	3	-	3/39/115/115	-
28	SQD	a	412	-	-	24/49/69/69	0/1/1/1
36	HEC	V	201	16	1/1/7/7	6/14/54/54	-
25	BCR	D	404	-	-	5/29/63/63	0/2/2/2
23	CLA	c	511	3	-	9/39/115/115	-
23	CLA	B	613	2	-	8/39/115/115	-
23	CLA	b	612	2	-	8/39/115/115	-
30	DGD	C	515	-	-	21/51/91/95	0/2/2/2
30	DGD	c	516	-	-	26/51/91/95	0/2/2/2
30	DGD	c	517	-	-	18/51/91/95	0/2/2/2
23	CLA	A	404	1	-	5/39/115/115	-
23	CLA	c	504	37	-	5/33/109/115	-
23	CLA	d	402	4	-	10/39/115/115	-
27	LMG	c	521	-	-	20/43/63/70	0/1/1/1
28	SQD	b	601	-	-	18/44/64/69	0/1/1/1
28	SQD	A	412	-	-	20/47/67/69	0/1/1/1
23	CLA	C	503	3	-	6/39/115/115	-
23	CLA	C	509	3	-	10/39/115/115	-
27	LMG	m	101	-	-	18/46/66/70	0/1/1/1
23	CLA	a	405	1	-	3/39/115/115	-
23	CLA	D	403	4	-	12/39/115/115	-
23	CLA	b	617	2	-	9/33/109/115	-
23	CLA	B	609	2	-	3/39/115/115	-
25	BCR	b	620	-	-	5/29/63/63	0/2/2/2
27	LMG	c	523	-	-	27/44/64/70	0/1/1/1
25	BCR	Z	101	-	-	9/29/63/63	0/2/2/2
26	PL9	a	410	-	-	24/53/73/73	0/1/1/1
26	PL9	d	405	-	-	17/53/73/73	0/1/1/1
30	DGD	A	415	-	-	25/55/95/95	0/2/2/2
25	BCR	a	409	-	-	6/29/63/63	0/2/2/2
23	CLA	c	513	3	-	7/39/115/115	-
23	CLA	b	611	37	-	11/39/115/115	-
29	LHG	B	622	-	-	20/53/53/53	-
23	CLA	a	408	1	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	605	2	-	11/39/115/115	-
23	CLA	B	602	2	-	4/39/115/115	-
27	LMG	b	622	-	-	25/50/70/70	0/1/1/1
23	CLA	b	609	2	-	6/39/115/115	-
26	PL9	D	405	-	-	11/53/73/73	0/1/1/1
23	CLA	c	510	3	-	14/39/115/115	-
23	CLA	A	408	1	-	3/26/102/115	-
30	DGD	a	414	-	-	24/45/45/95	-

The worst 5 of 917 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	MG-ND	-11.97	1.82	2.05
24	a	407	PHO	C1B-C2B	10.42	1.50	1.39
24	d	401	PHO	C1B-C2B	9.72	1.50	1.39
23	D	403	CLA	MG-NB	-9.15	1.87	2.05
24	a	407	PHO	C3B-C4B	8.51	1.50	1.41

The worst 5 of 1246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C4A-NA-C1A	9.80	111.15	106.68
23	C	511	CLA	C4A-NA-C1A	9.77	111.14	106.68
23	d	402	CLA	C4A-NA-C1A	9.76	111.13	106.68
23	C	503	CLA	C4A-NA-C1A	9.64	111.08	106.68
23	a	411	CLA	C4A-NA-C1A	9.54	111.03	106.68

All (2) chirality outliers are listed below:

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

5 of 1648 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	C4B-C3B-CAB-CBB
23	B	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

106 monomers are involved in 194 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	d	404	BCR	3	0
35	E	101	HEM	5	0
23	c	506	CLA	1	0
25	A	409	BCR	2	0
29	D	407	LHG	1	0
23	B	612	CLA	2	0
23	h	101	CLA	3	0
23	c	507	CLA	1	0
24	A	407	PHO	1	0
24	d	401	PHO	2	0
28	a	413	SQD	3	0
25	K	101	BCR	2	0
29	B	623	LHG	2	0
25	k	102	BCR	2	0
25	x	101	BCR	2	0
23	b	614	CLA	4	0
23	C	505	CLA	2	0
23	b	615	CLA	3	0
28	B	624	SQD	1	0
25	c	514	BCR	1	0
28	f	101	SQD	2	0
23	c	501	CLA	1	0
23	B	601	CLA	2	0
29	l	101	LHG	1	0
23	b	608	CLA	2	0
28	A	414	SQD	1	0
29	d	406	LHG	5	0
23	c	502	CLA	1	0
29	A	413	LHG	4	0
23	B	606	CLA	3	0
23	C	501	CLA	1	0
29	e	101	LHG	2	0
25	B	619	BCR	3	0
23	B	603	CLA	1	0
32	A	417[B]	OEY	2	0
23	b	604	CLA	3	0

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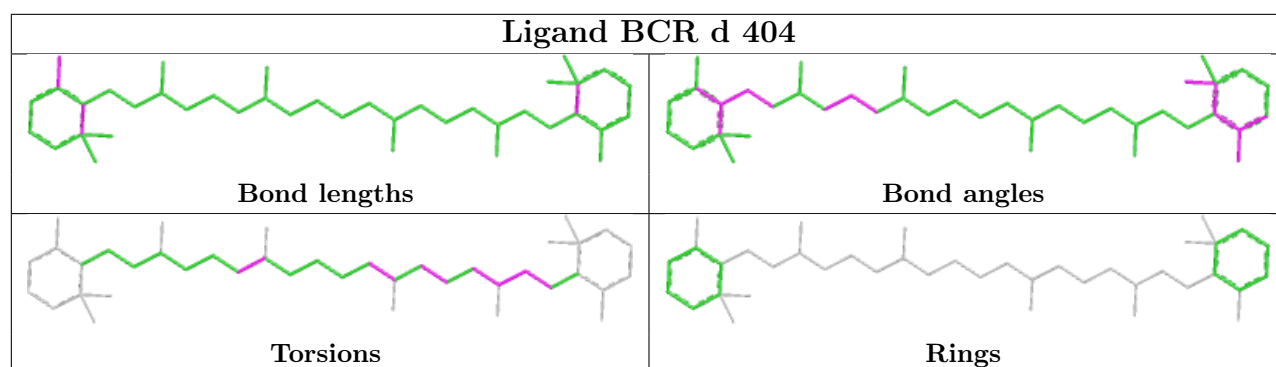
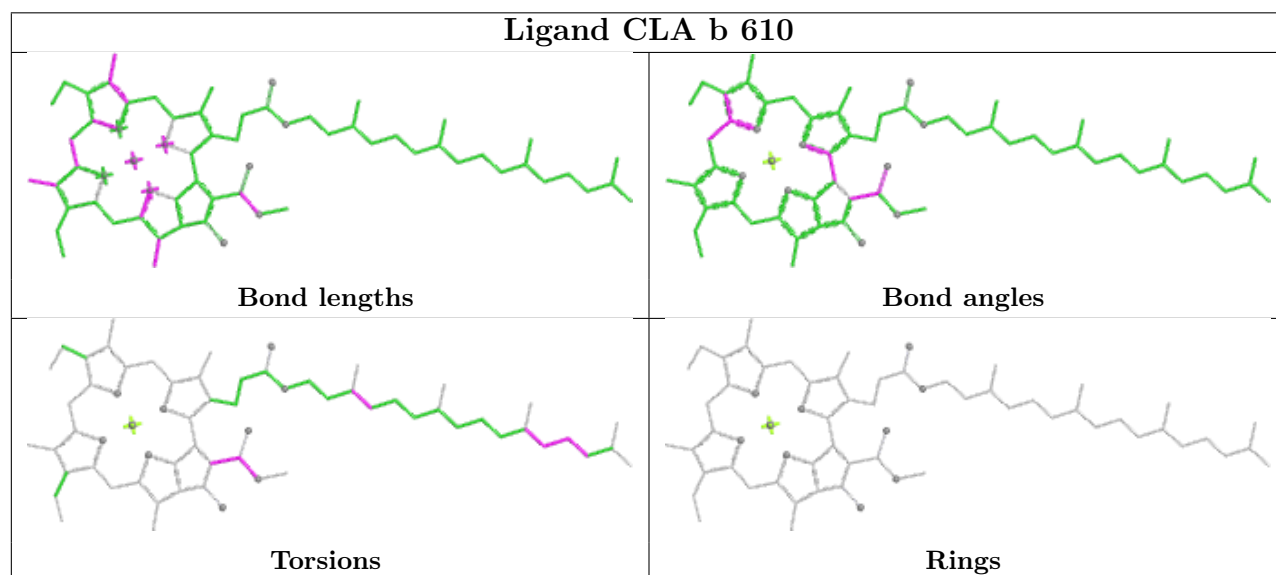
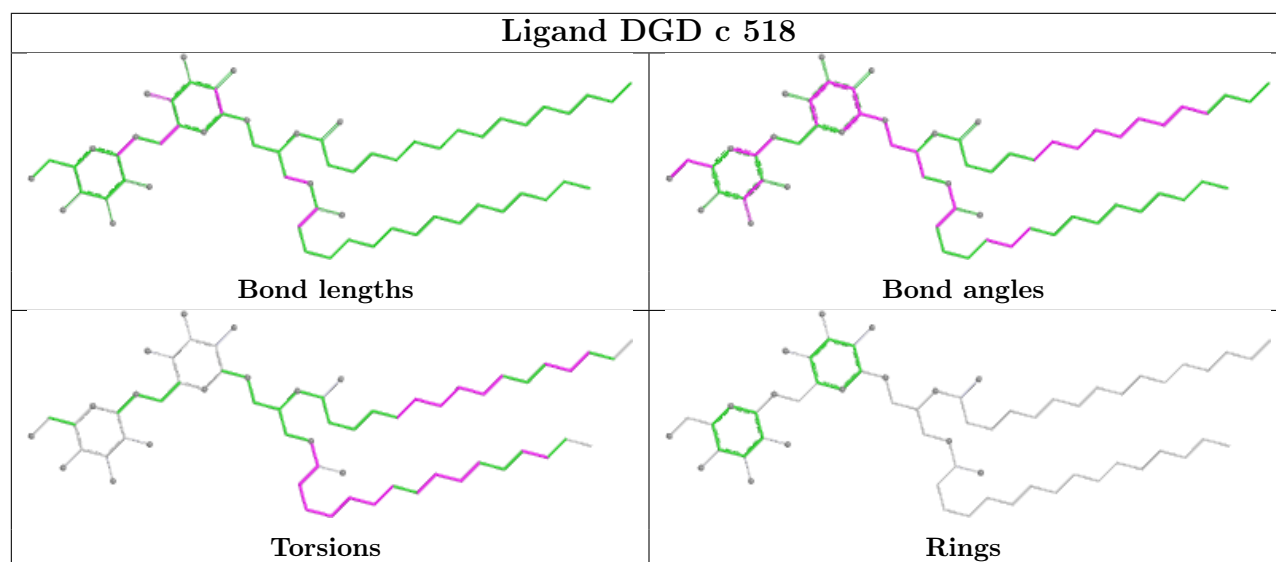
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	H	101	BCR	2	0
29	D	408	LHG	2	0
23	C	508	CLA	2	0
25	b	618	BCR	4	0
30	H	102	DGD	1	0
35	e	102	HEM	3	0
29	d	407	LHG	3	0
23	b	606	CLA	6	0
23	b	607	CLA	5	0
27	d	409	LMG	1	0
23	c	508	CLA	1	0
23	b	603	CLA	2	0
23	D	401	CLA	2	0
25	b	619	BCR	3	0
23	b	613	CLA	2	0
25	T	101	BCR	3	0
23	B	614	CLA	1	0
23	b	616	CLA	3	0
23	C	513	CLA	3	0
25	K	102	BCR	1	0
23	C	506	CLA	1	0
32	a	417[B]	OEY	1	0
25	k	101	BCR	2	0
23	c	509	CLA	1	0
25	t	101	BCR	6	0
23	a	411	CLA	4	0
27	D	406	LMG	1	0
23	B	608	CLA	1	0
23	d	403	CLA	1	0
23	B	605	CLA	2	0
25	c	515	BCR	1	0
23	B	604	CLA	3	0
25	C	514	BCR	1	0
27	A	411	LMG	1	0
23	A	405	CLA	1	0
23	C	504	CLA	2	0
23	B	615	CLA	2	0
29	d	408	LHG	1	0
26	A	410	PL9	6	0
30	h	102	DGD	1	0
25	B	618	BCR	5	0
23	C	511	CLA	1	0

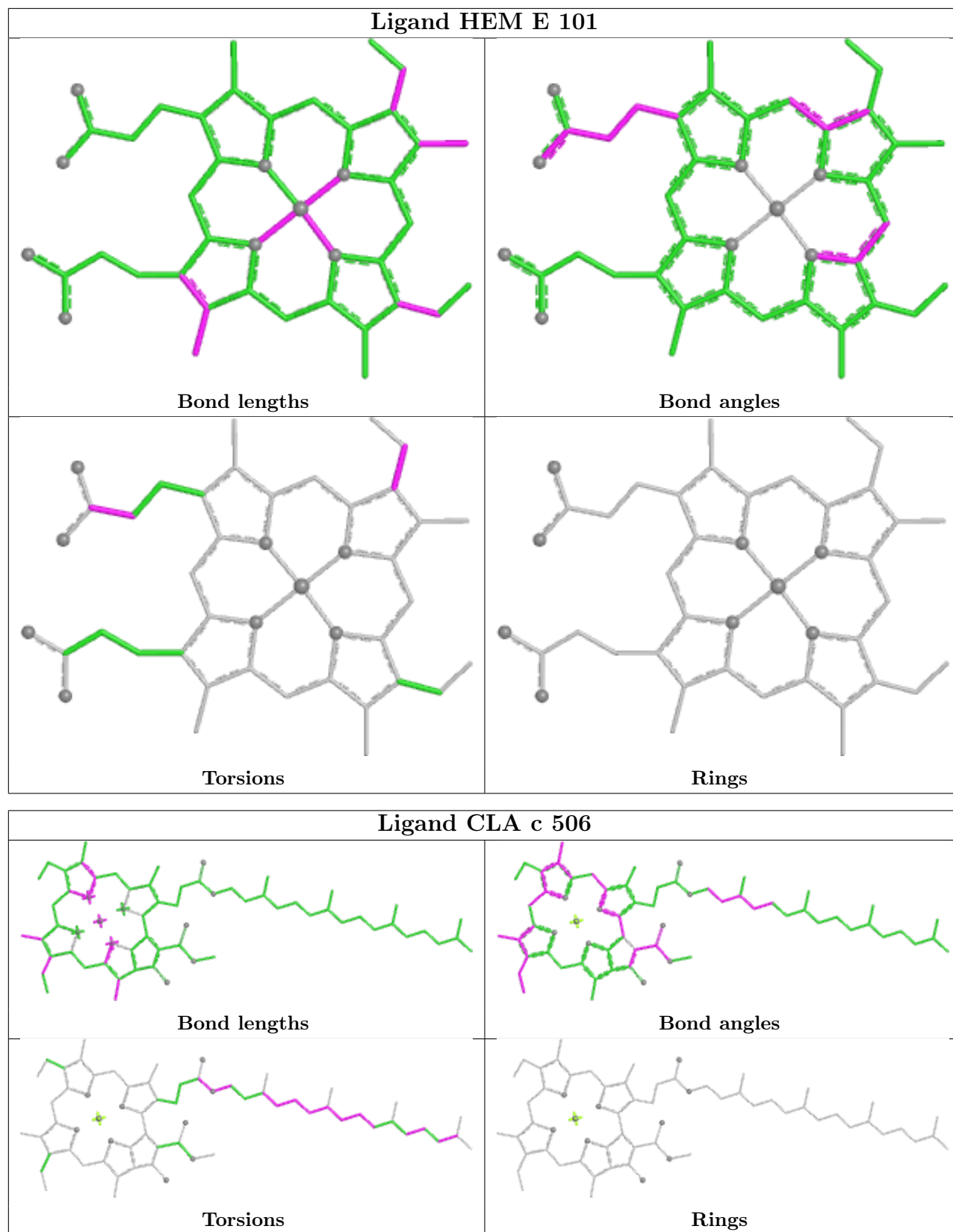
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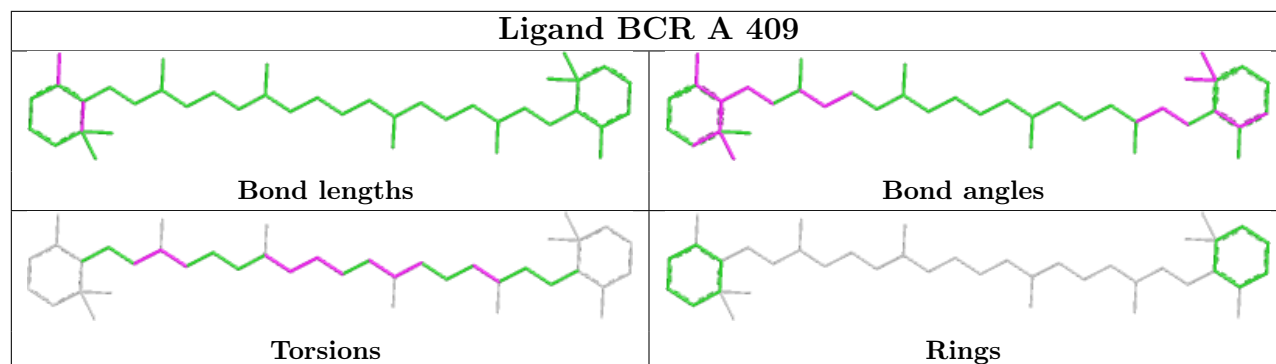
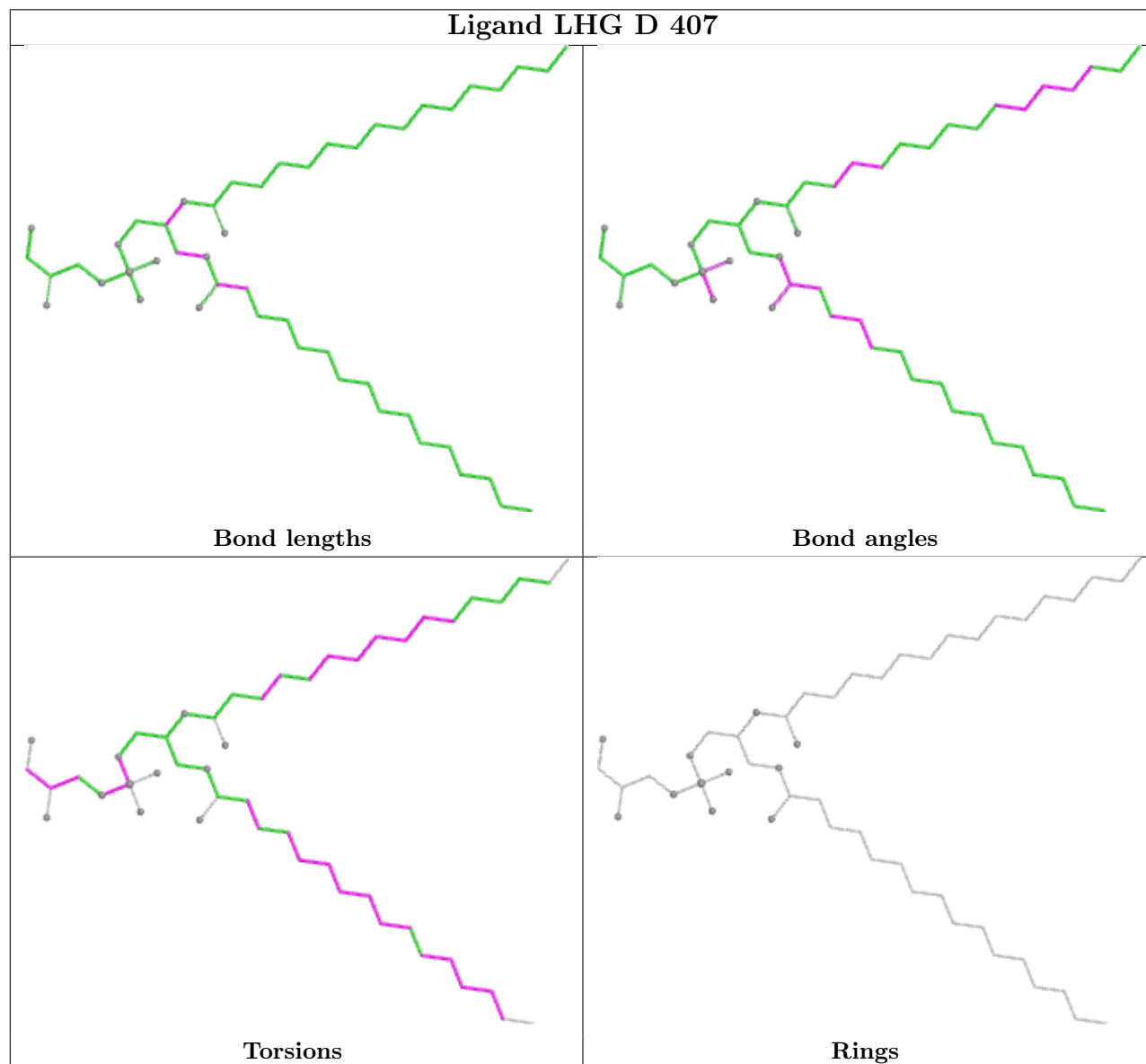
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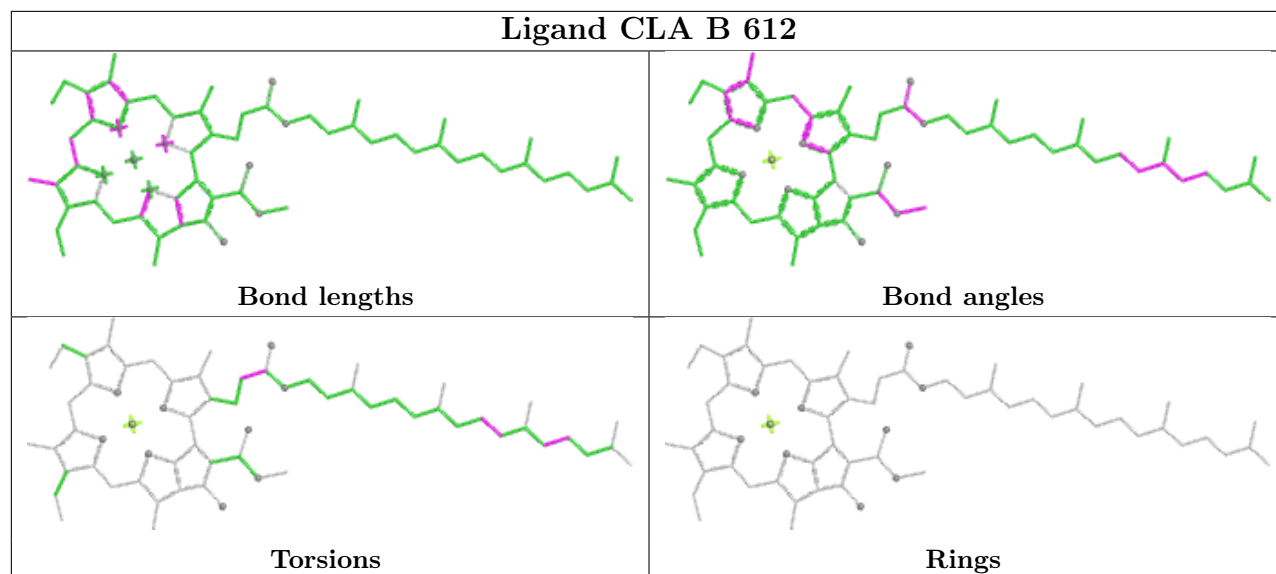
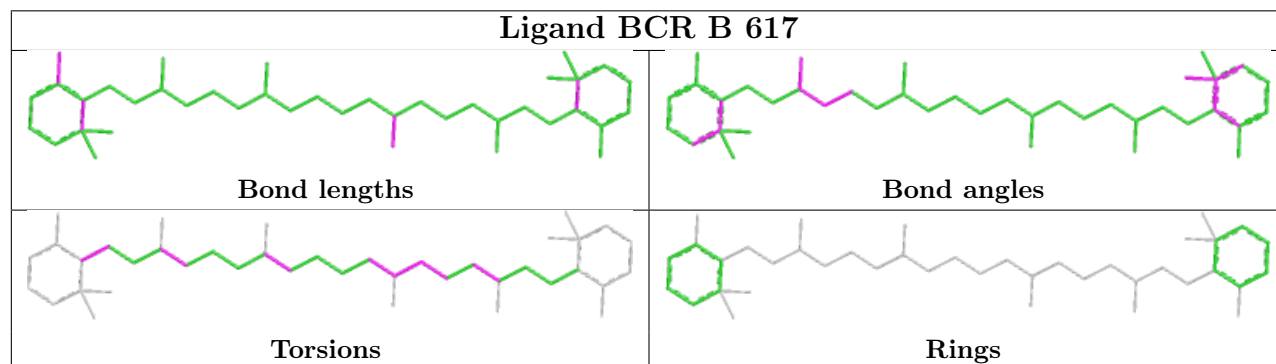
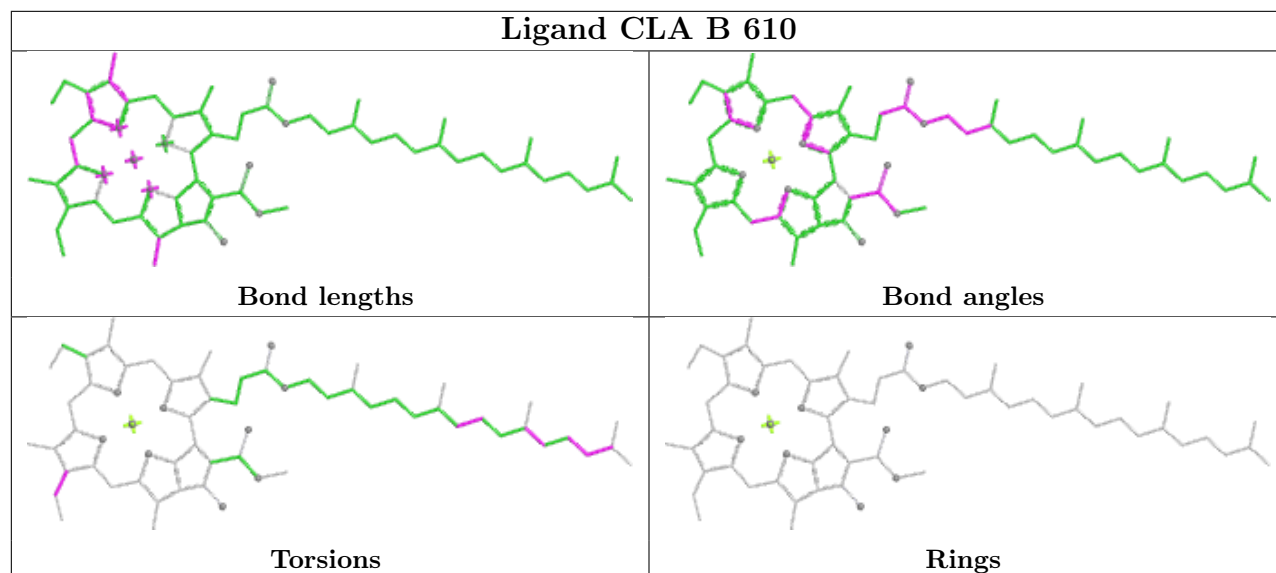
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	412	SQD	1	0
36	V	201	HEC	1	0
25	D	404	BCR	5	0
23	c	511	CLA	1	0
23	B	613	CLA	2	0
23	A	404	CLA	3	0
23	c	504	CLA	1	0
27	c	521	LMG	2	0
28	b	601	SQD	1	0
28	A	412	SQD	1	0
23	C	509	CLA	1	0
27	m	101	LMG	1	0
23	a	405	CLA	1	0
23	D	403	CLA	1	0
23	B	609	CLA	2	0
25	b	620	BCR	1	0
27	c	523	LMG	2	0
25	Z	101	BCR	4	0
26	a	410	PL9	6	0
26	d	405	PL9	2	0
30	A	415	DGD	3	0
25	a	409	BCR	2	0
23	b	611	CLA	4	0
23	b	605	CLA	2	0
23	B	602	CLA	3	0
27	b	622	LMG	2	0
23	c	510	CLA	2	0
30	a	414	DGD	3	0

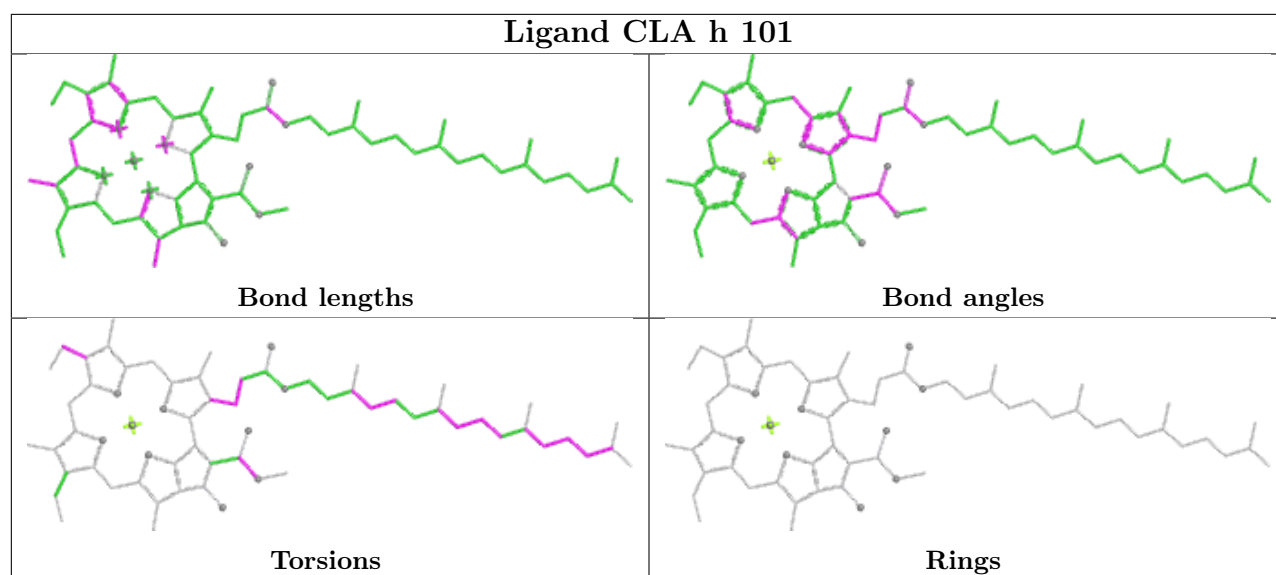
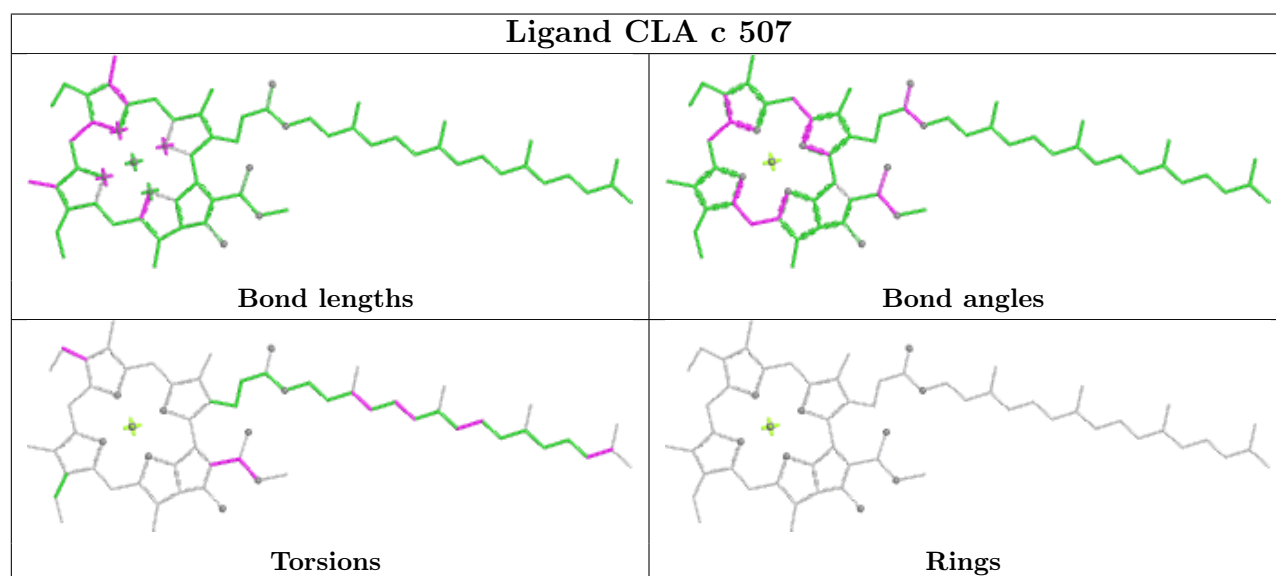
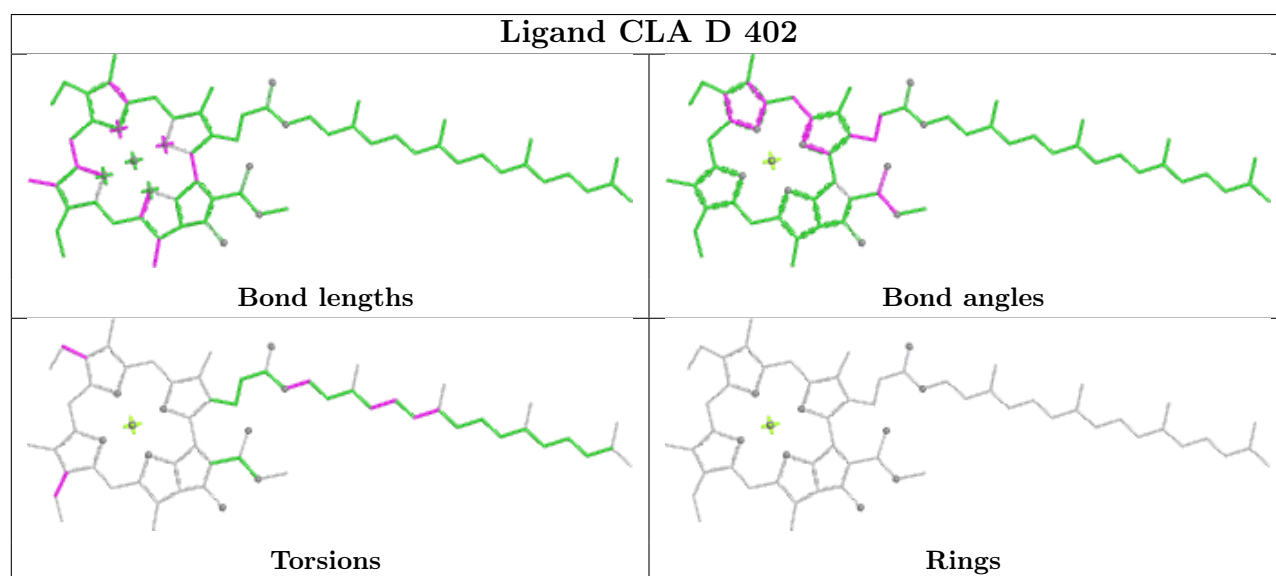
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

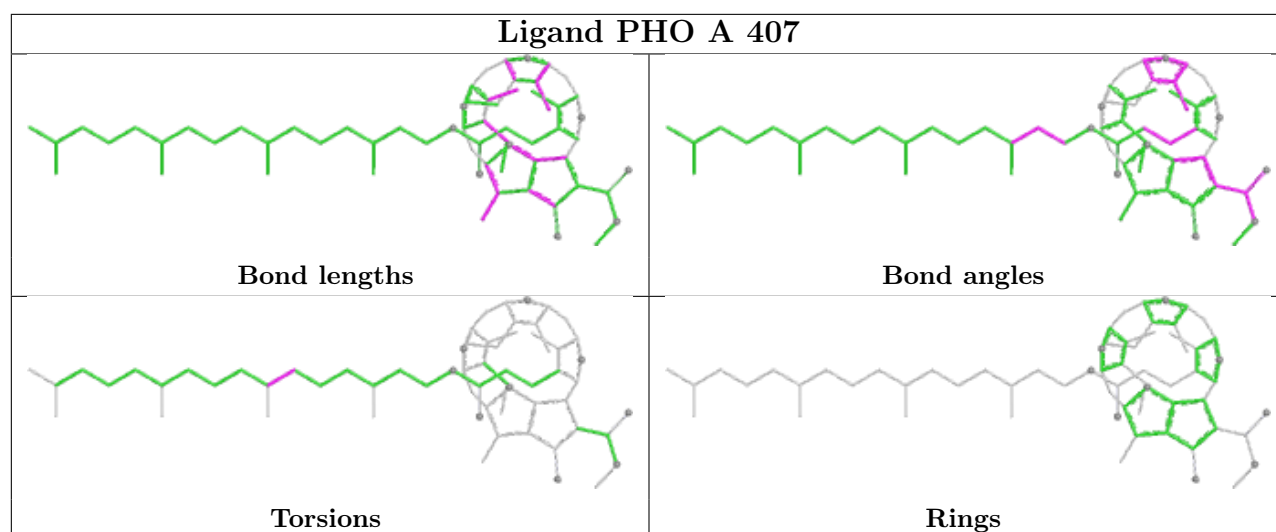
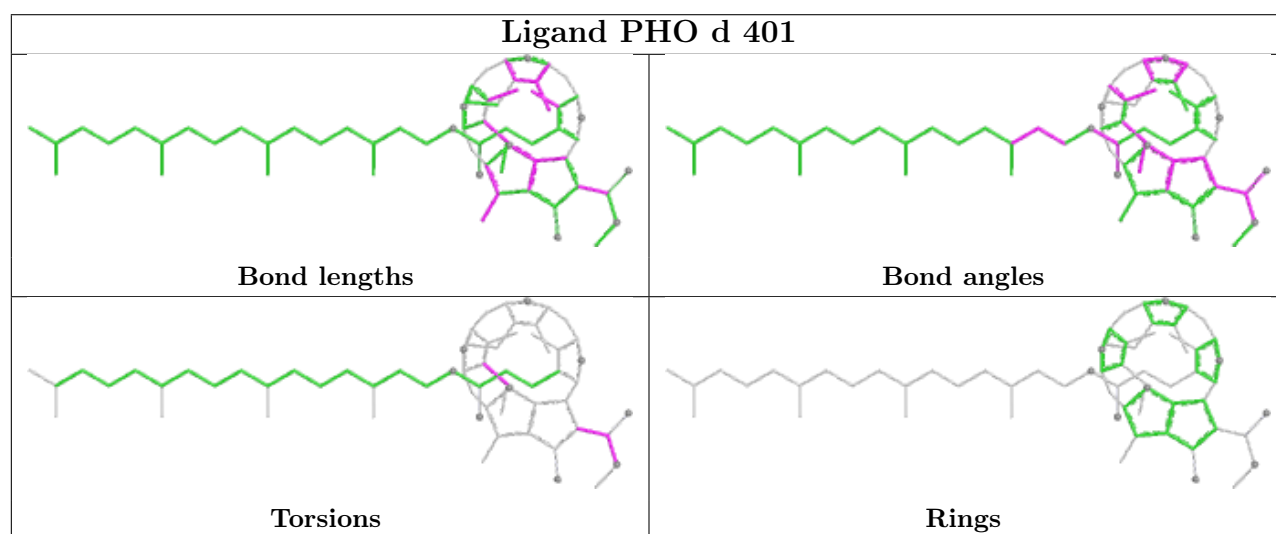
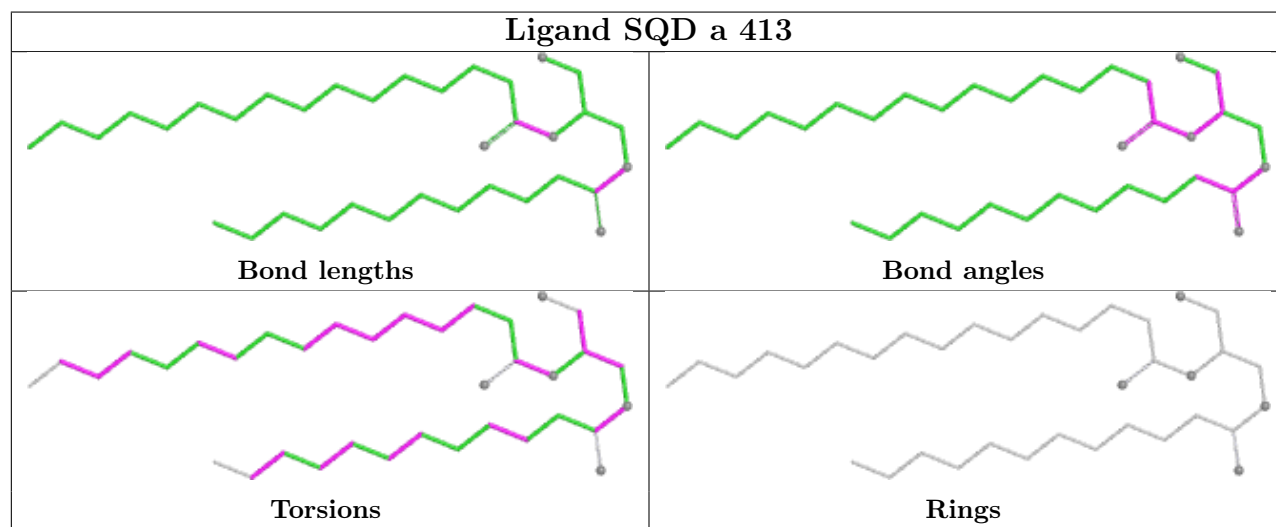


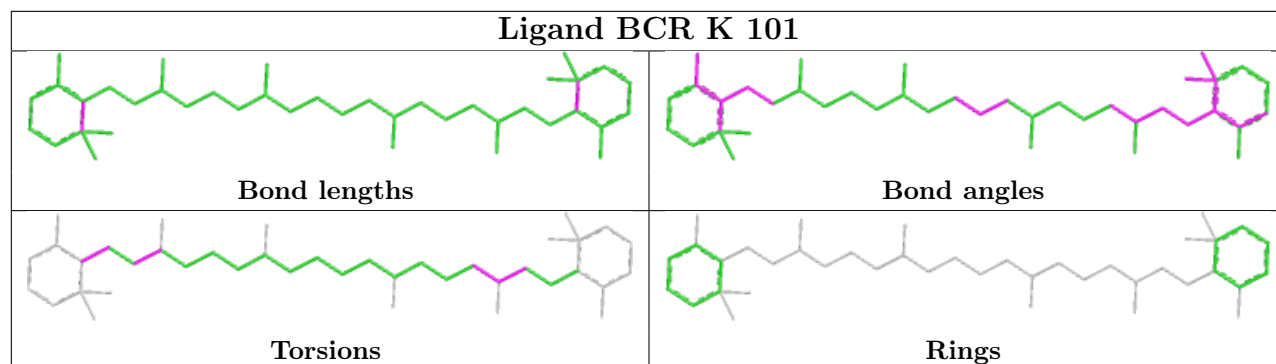
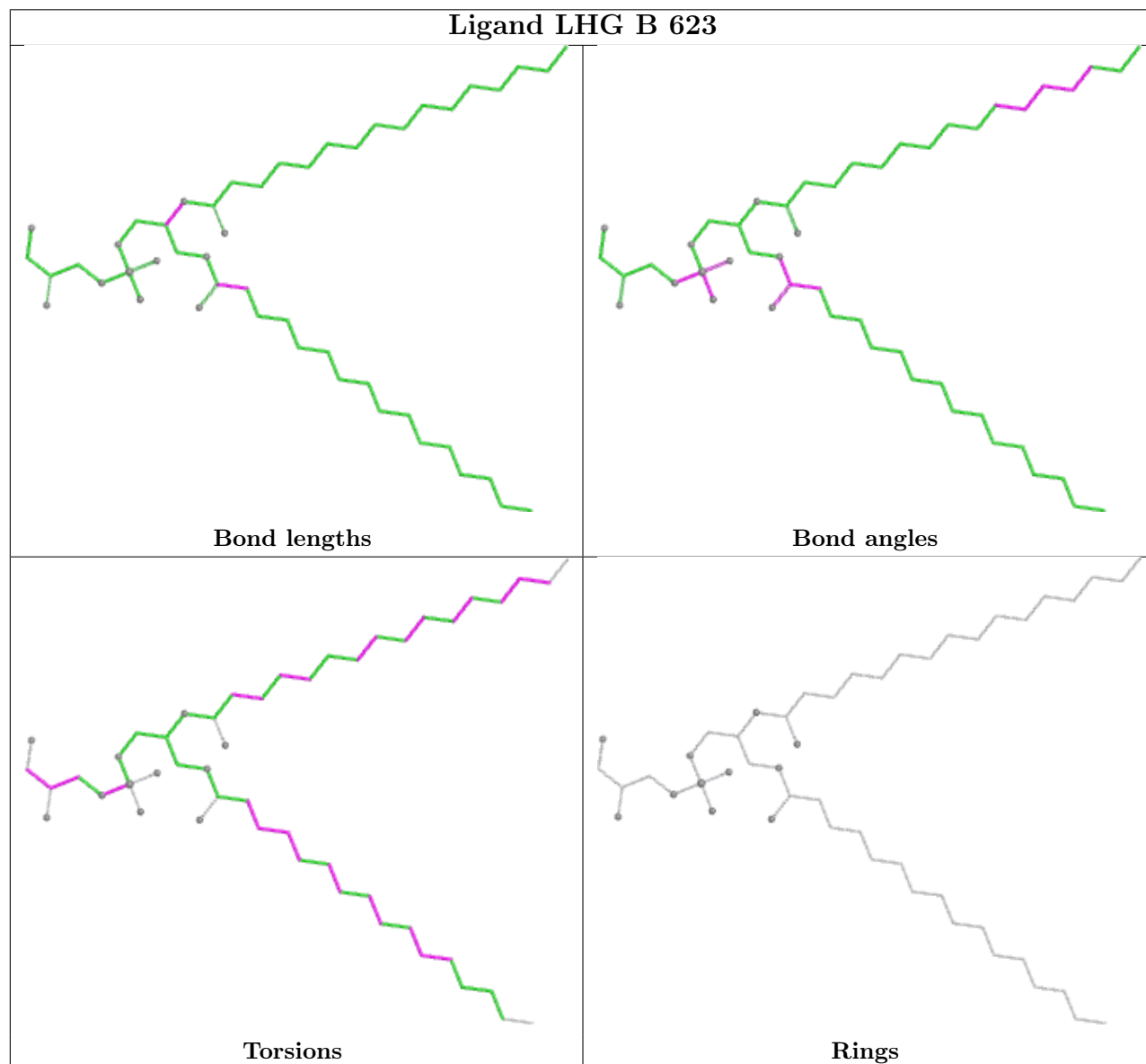


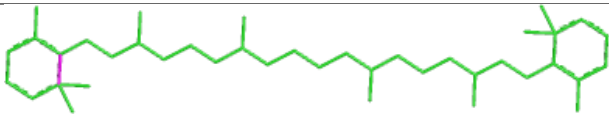
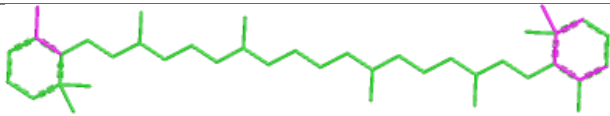
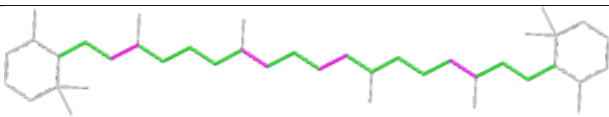
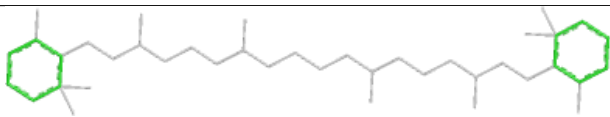


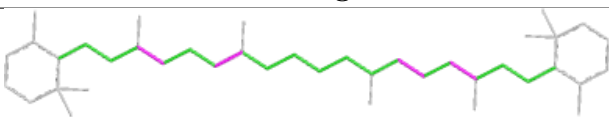
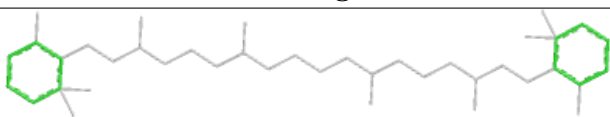


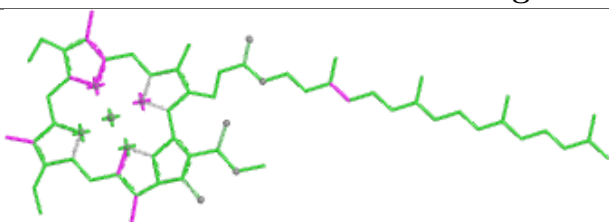
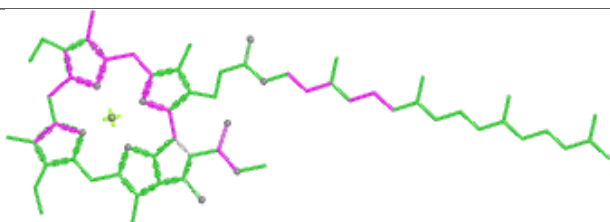
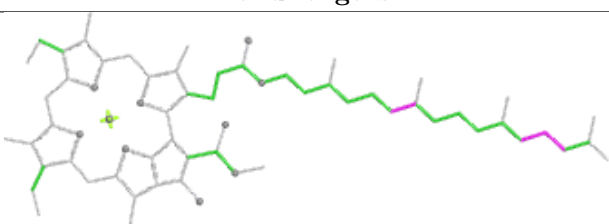
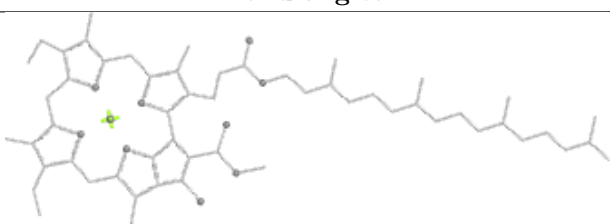


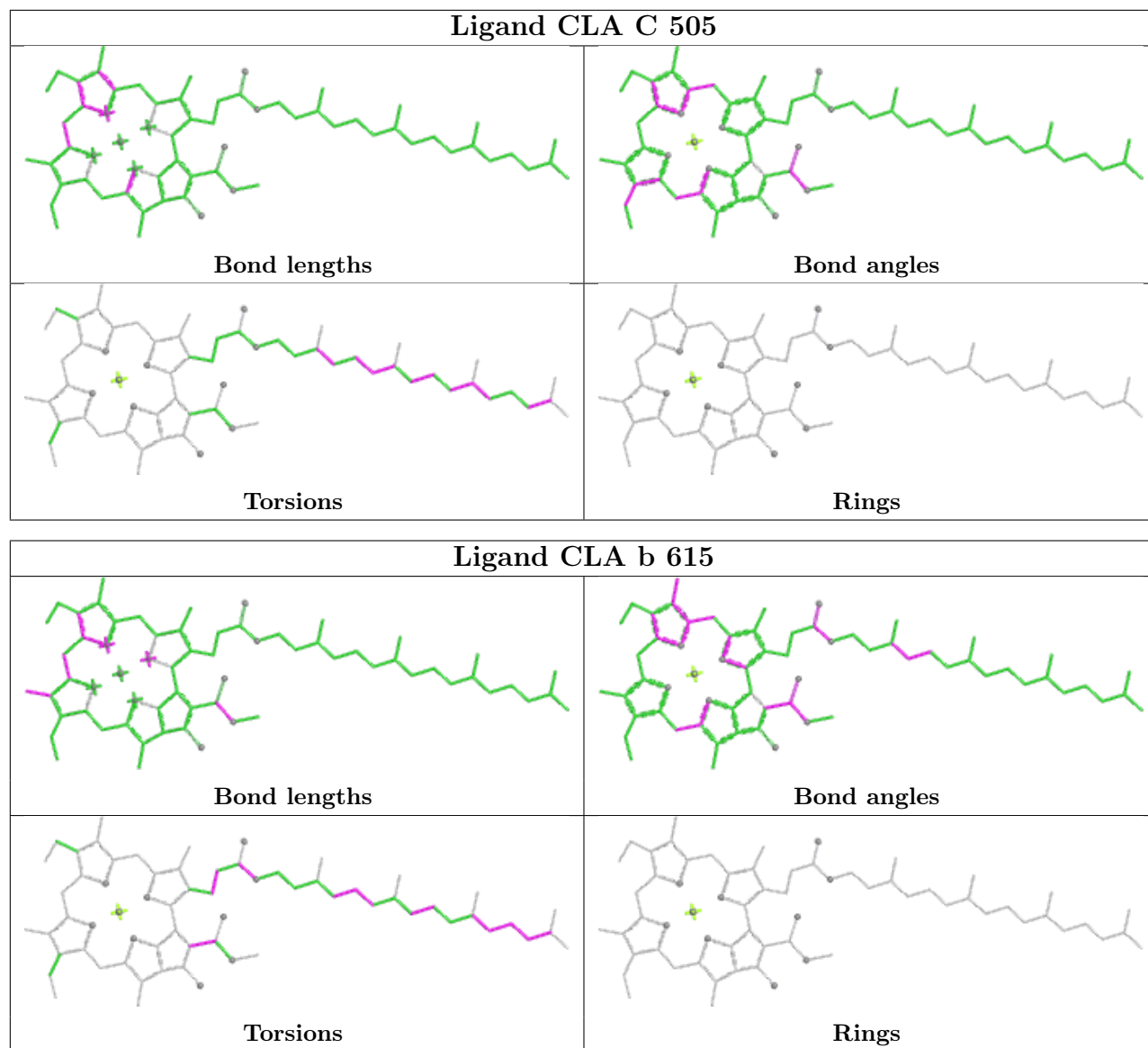


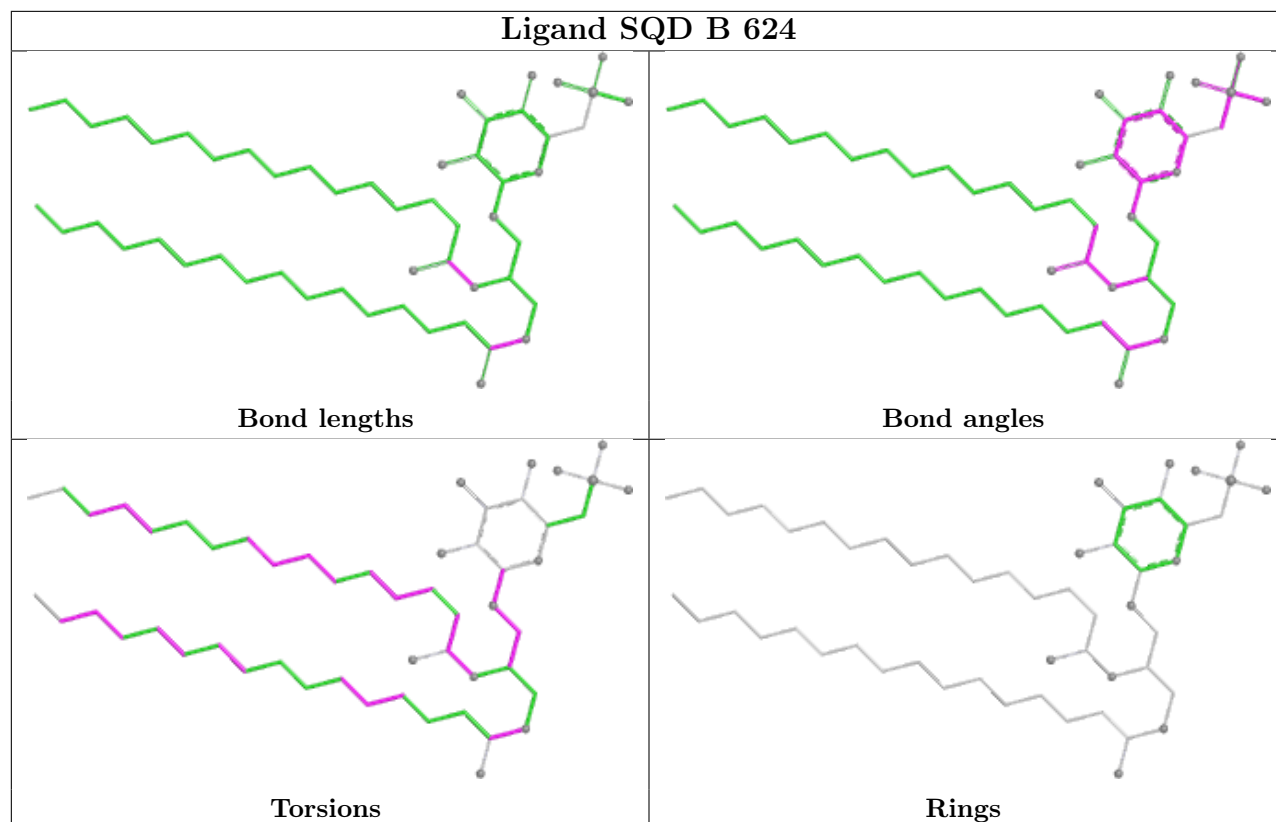
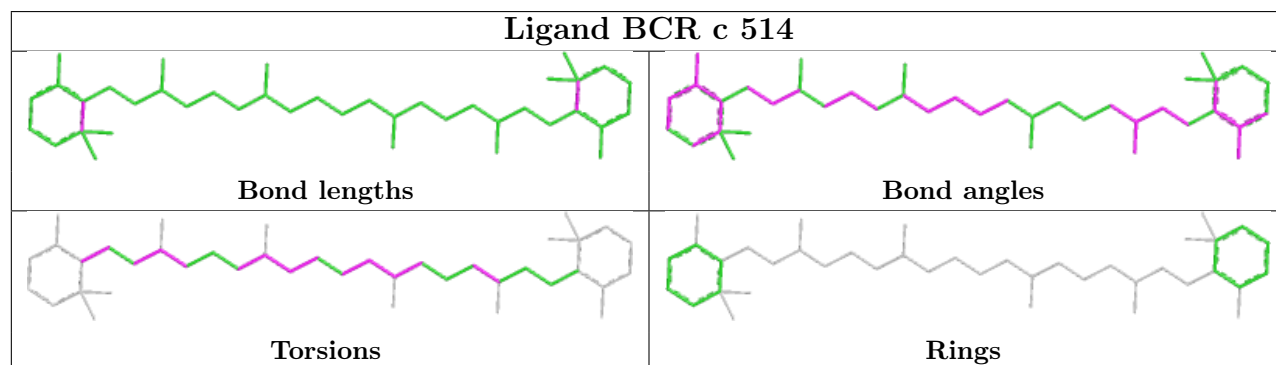
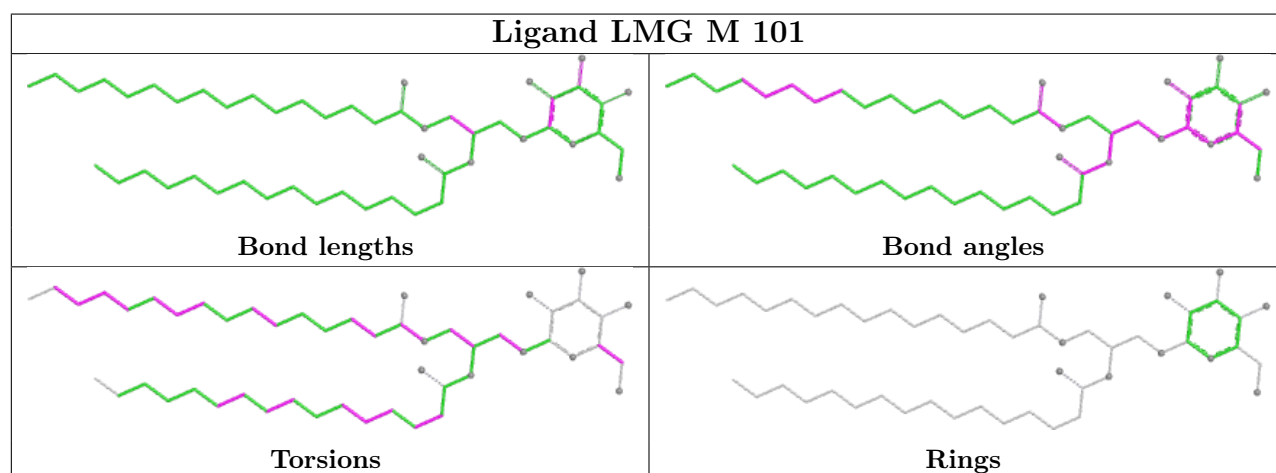


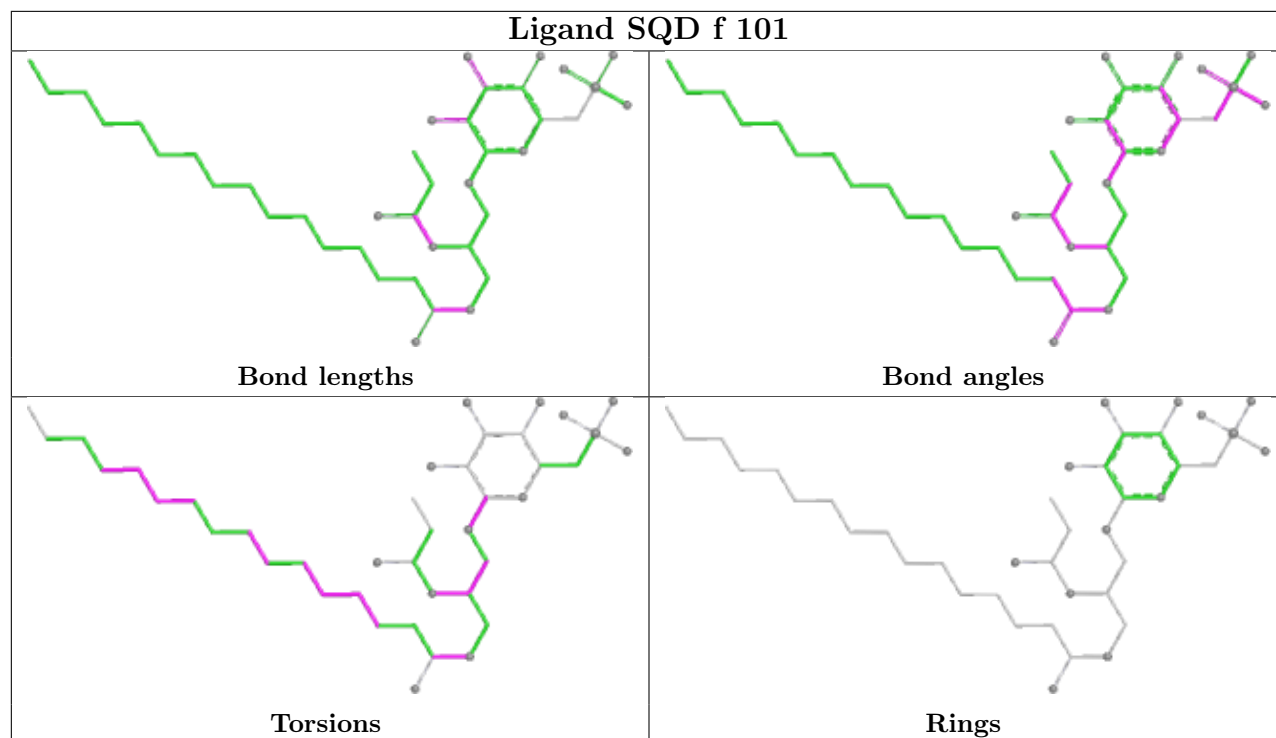
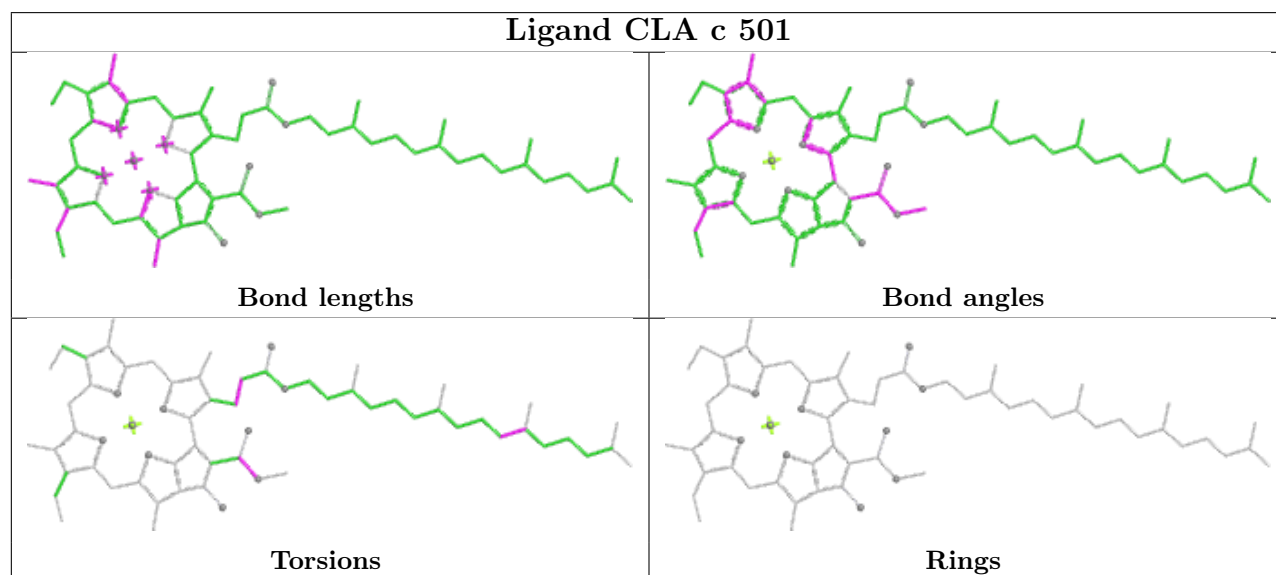
Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR x 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

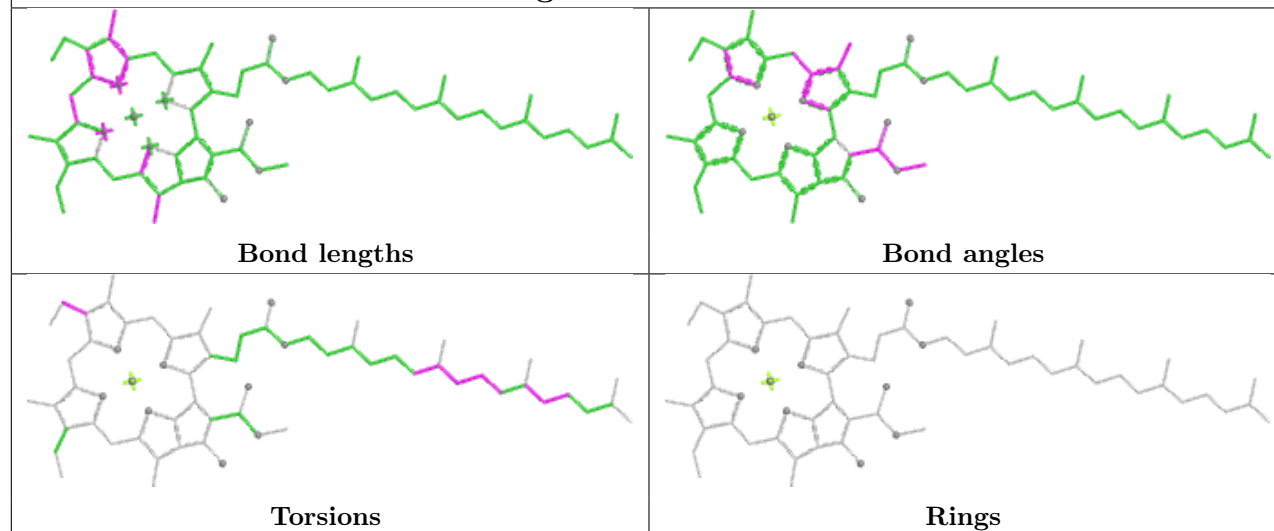
Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings



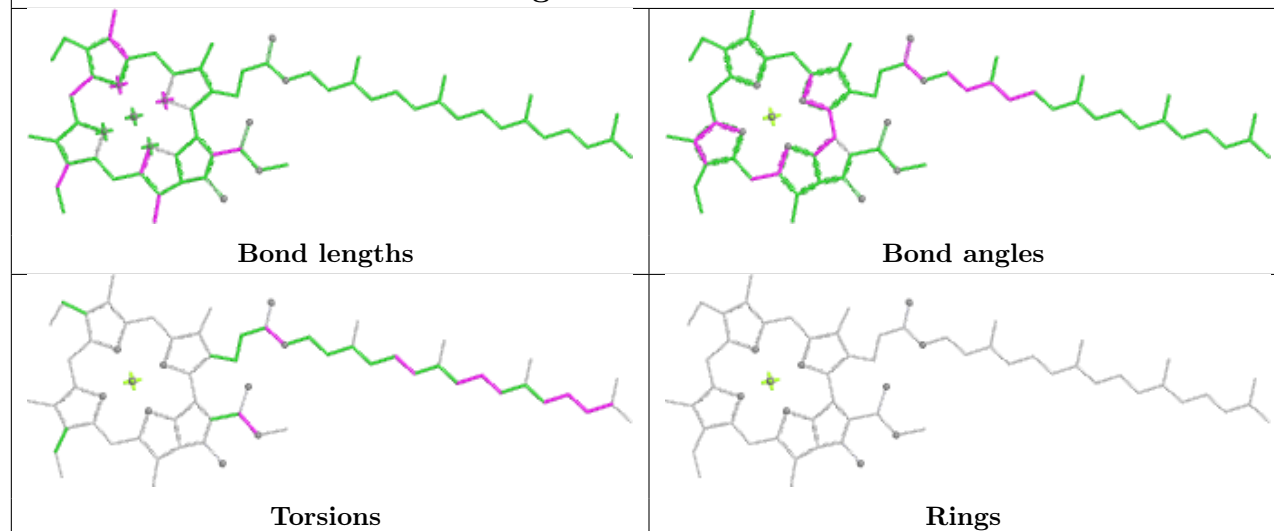




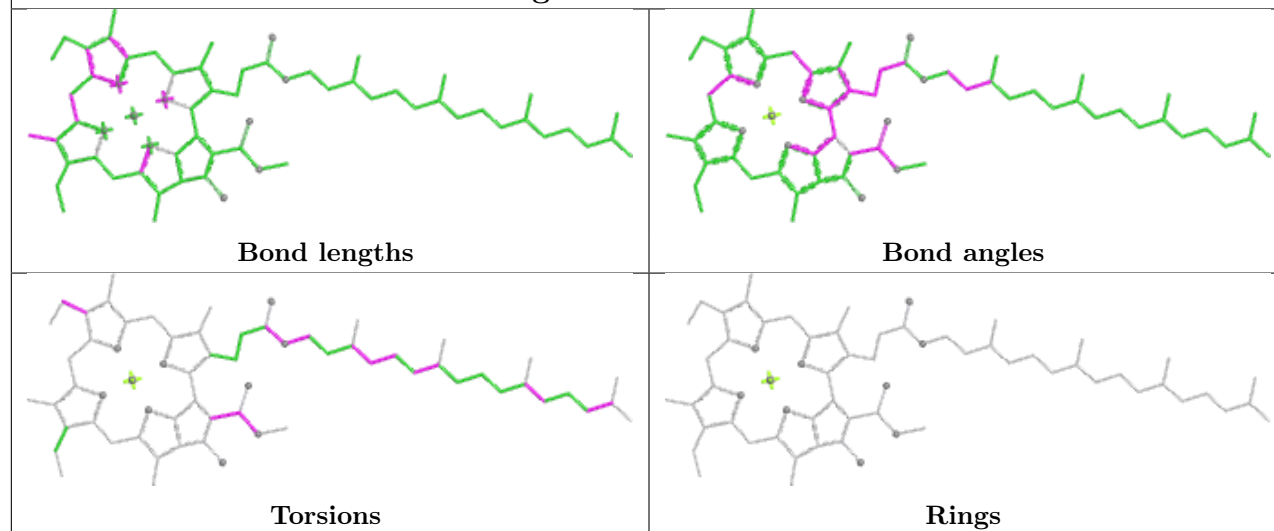
Ligand CLA a 406

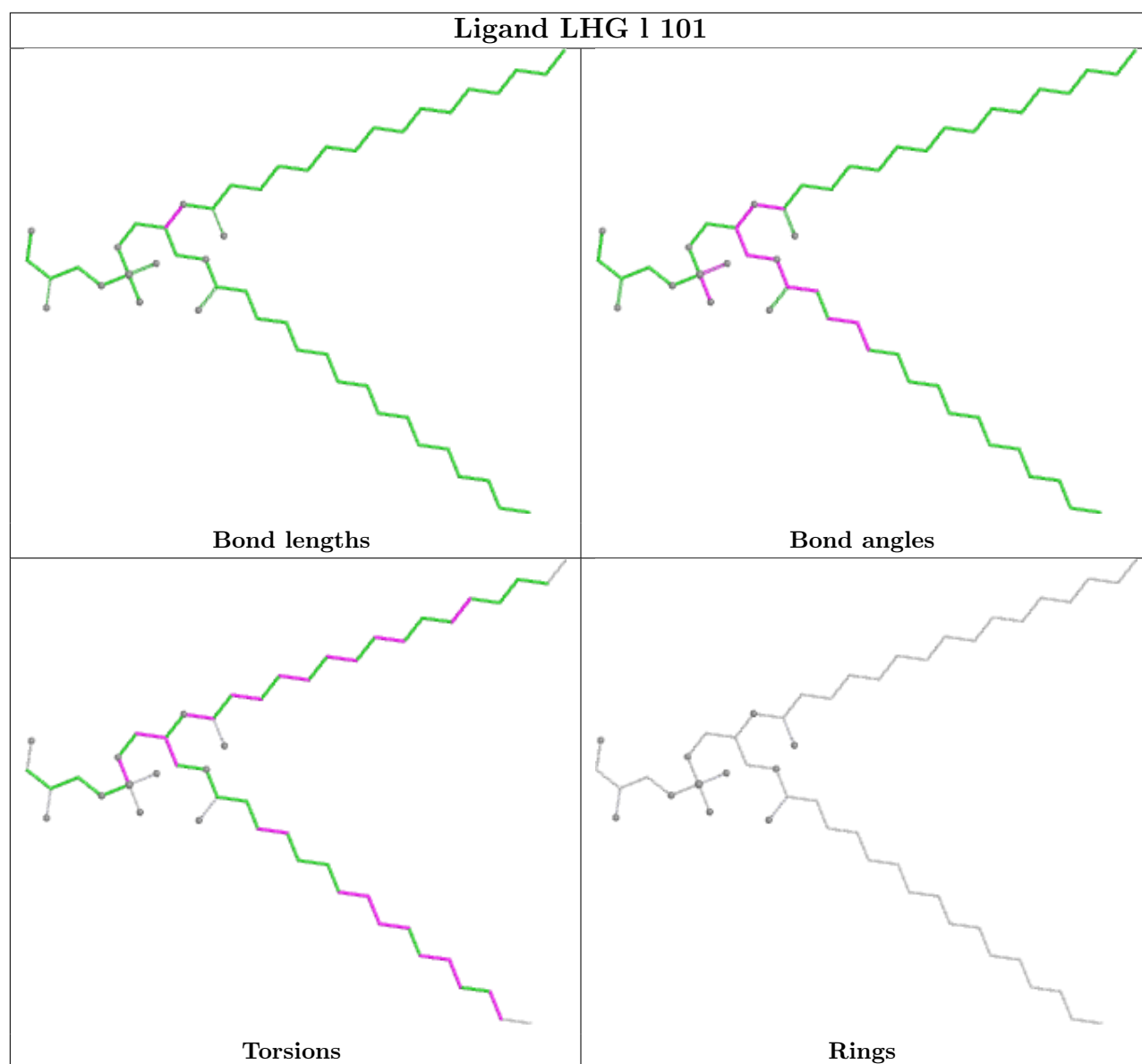
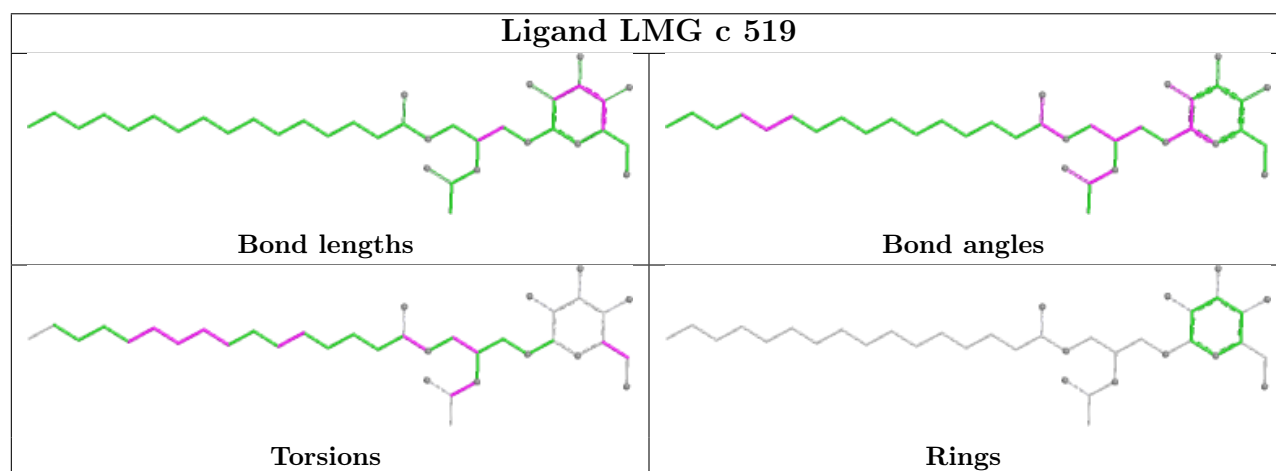


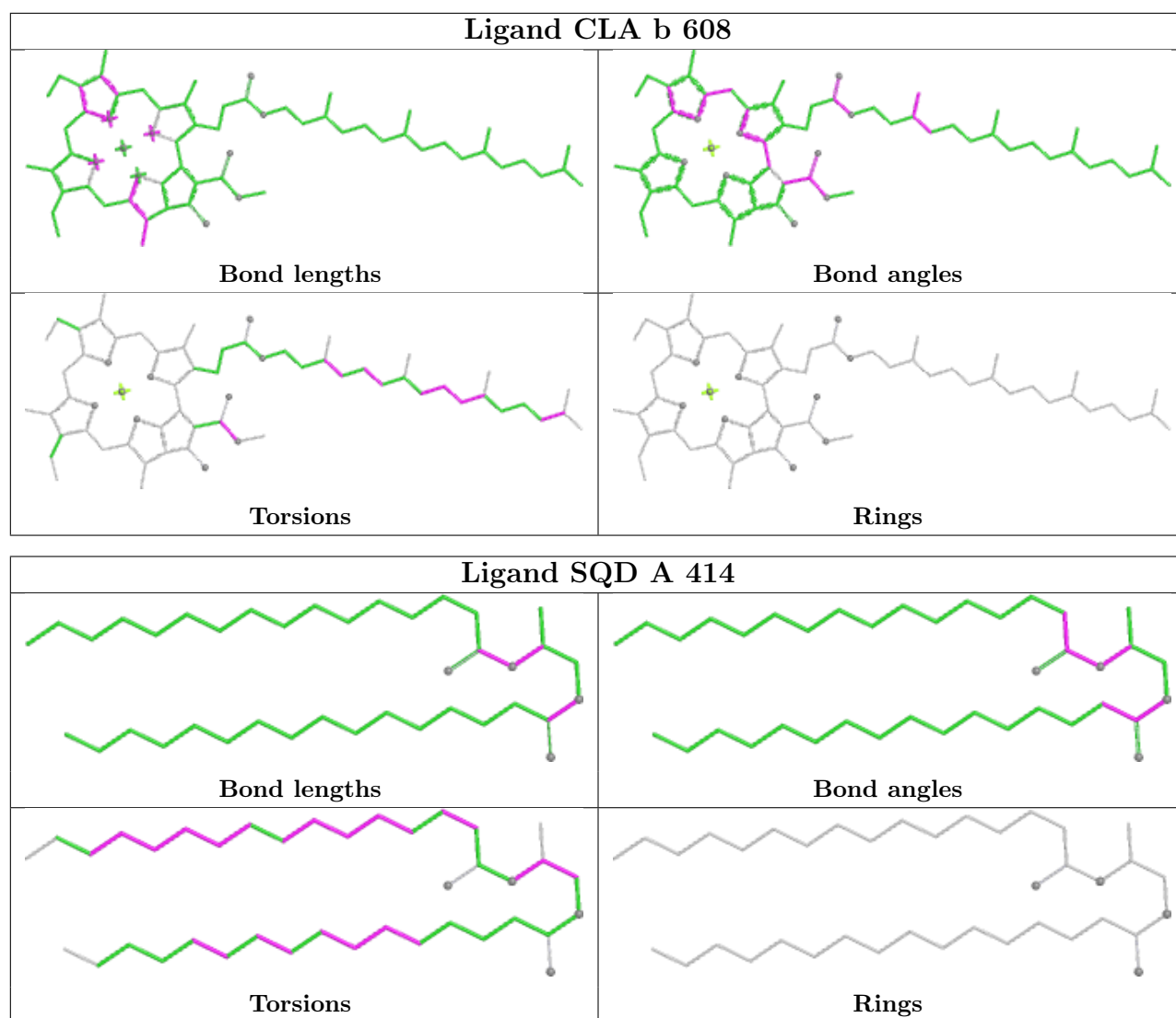
Ligand CLA B 607

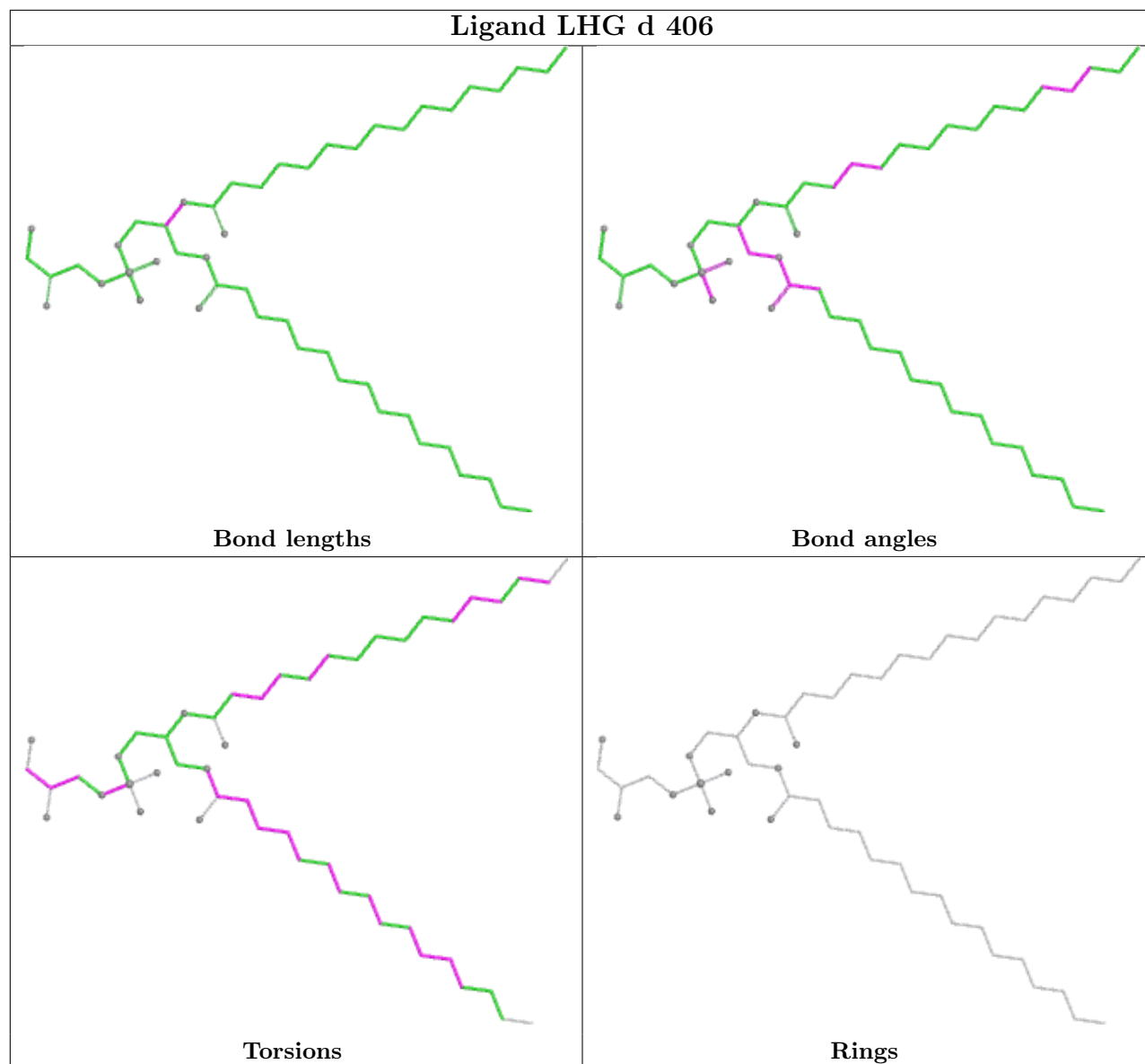
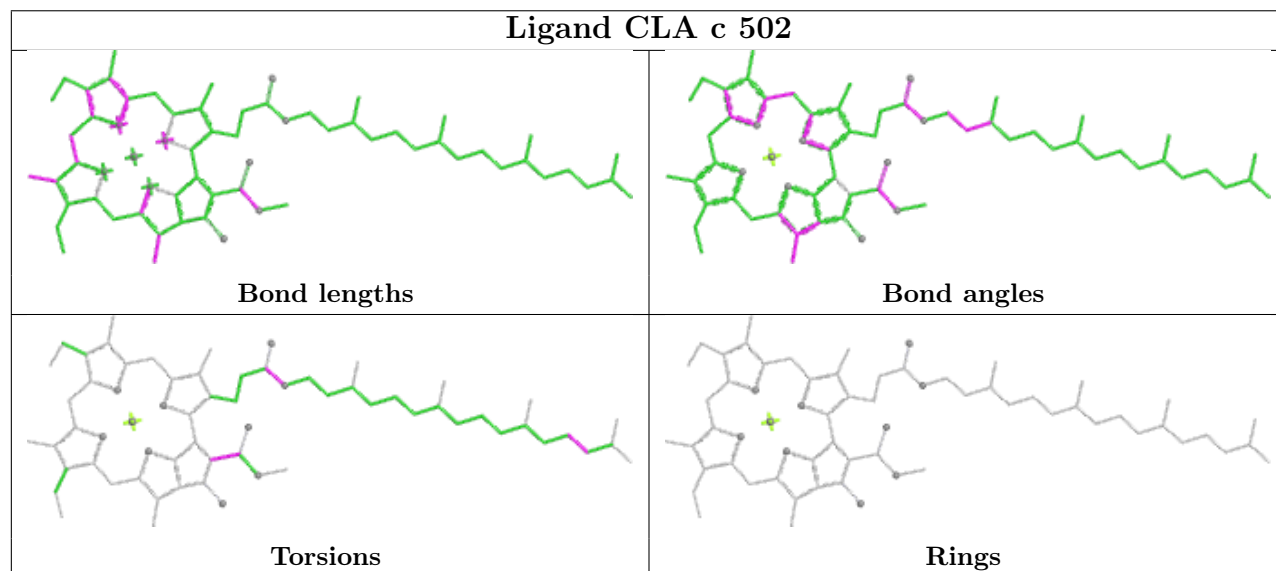


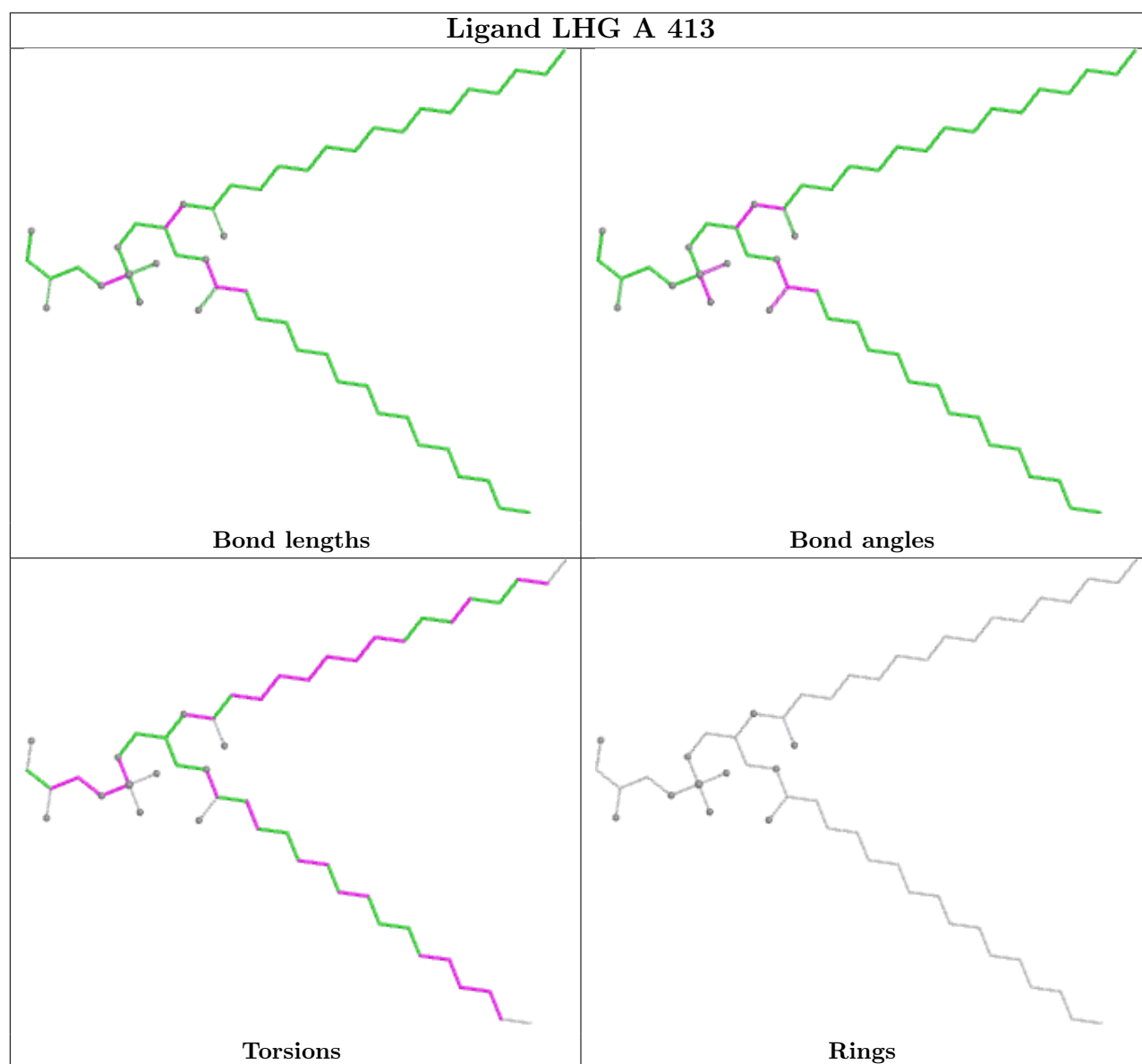
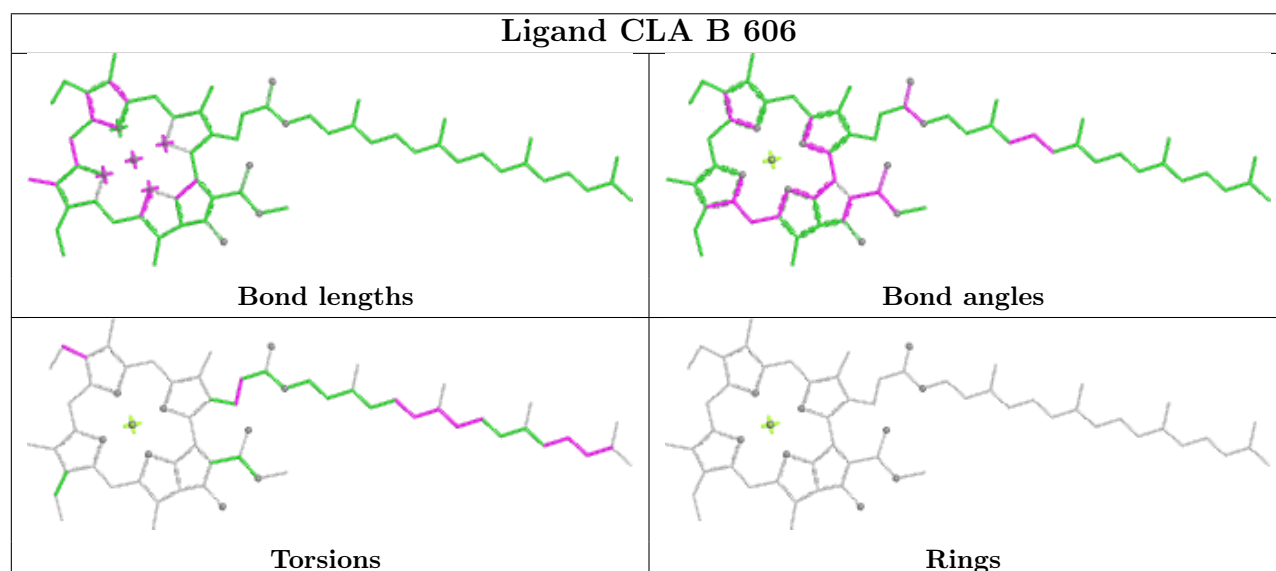
Ligand CLA B 601

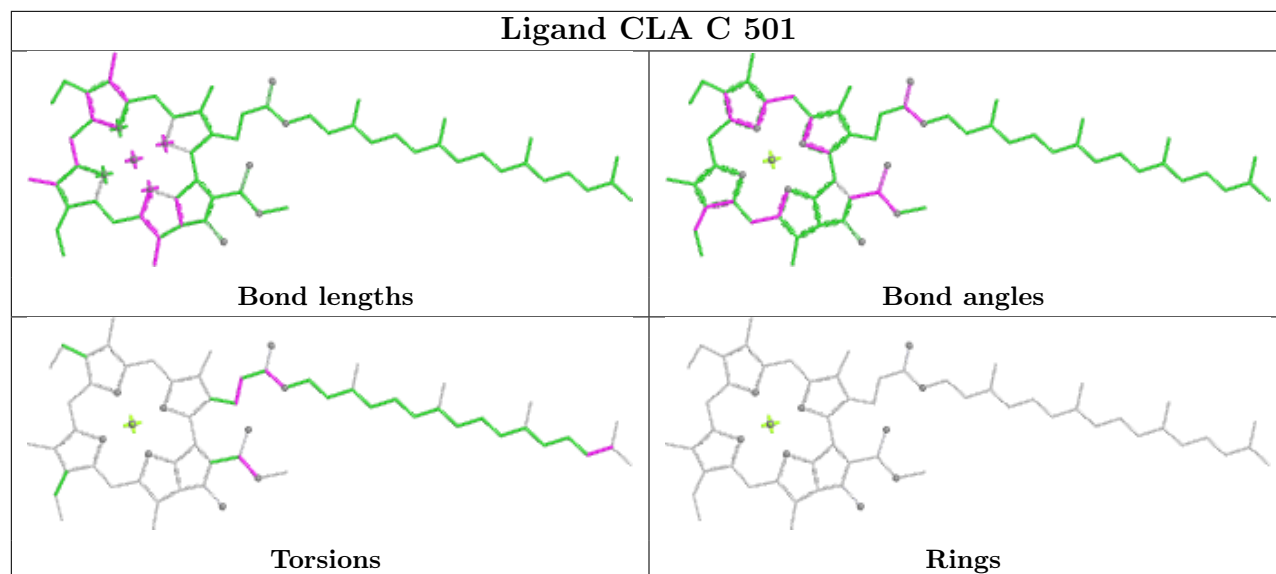
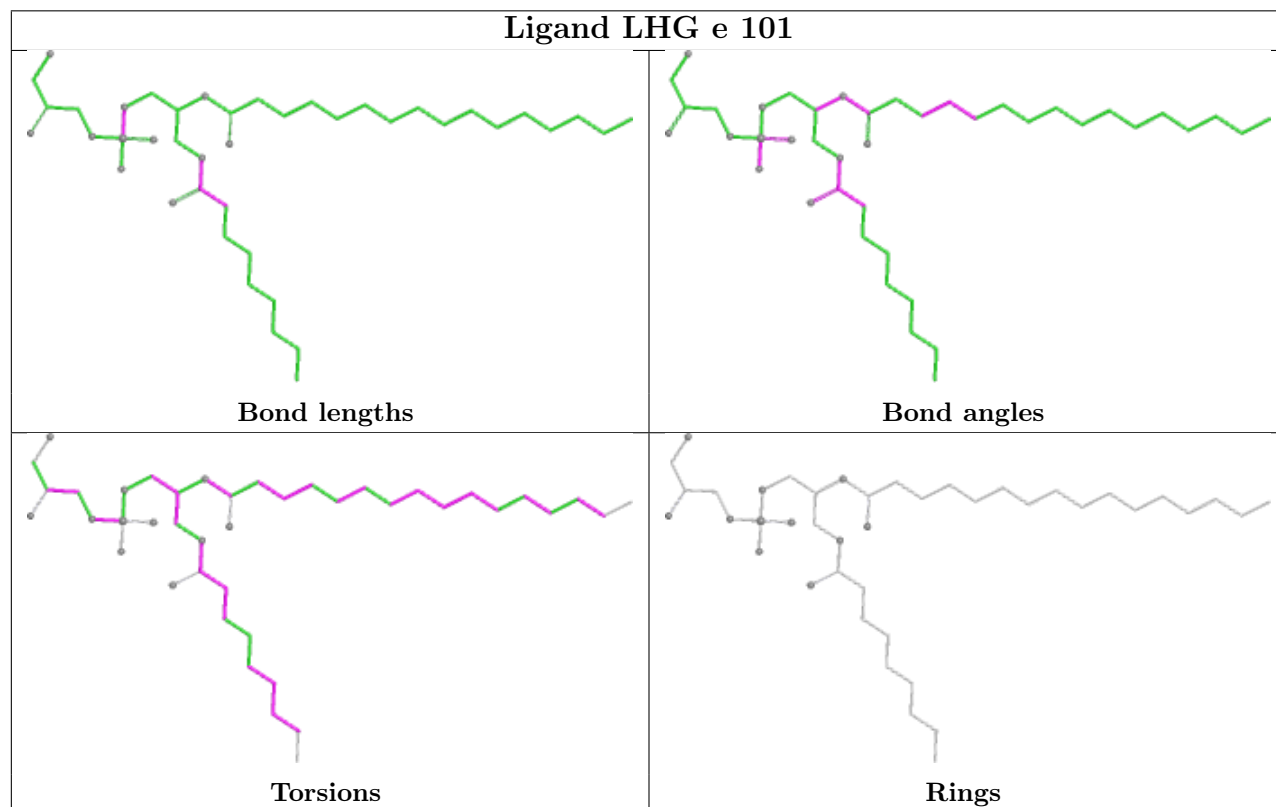


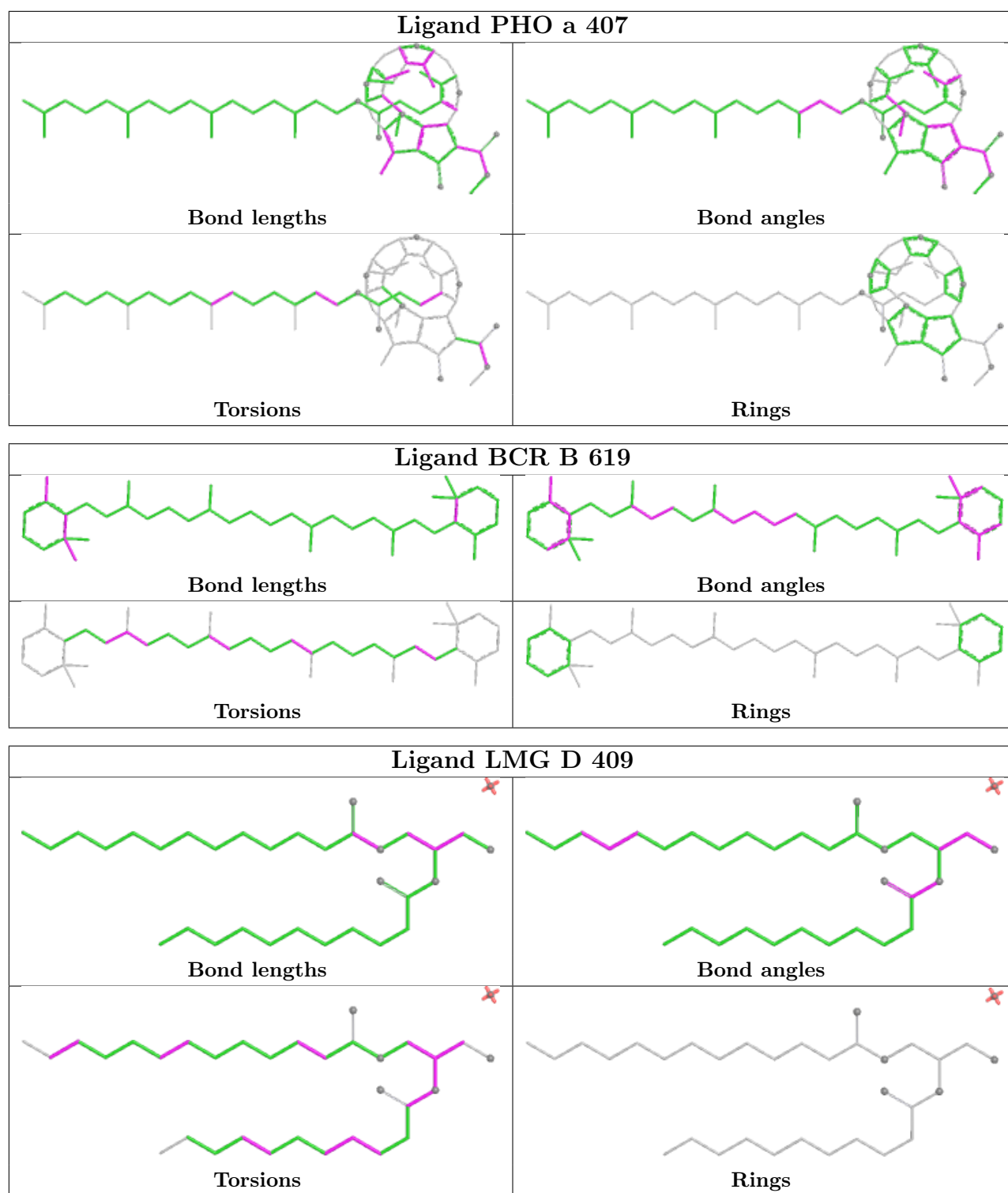


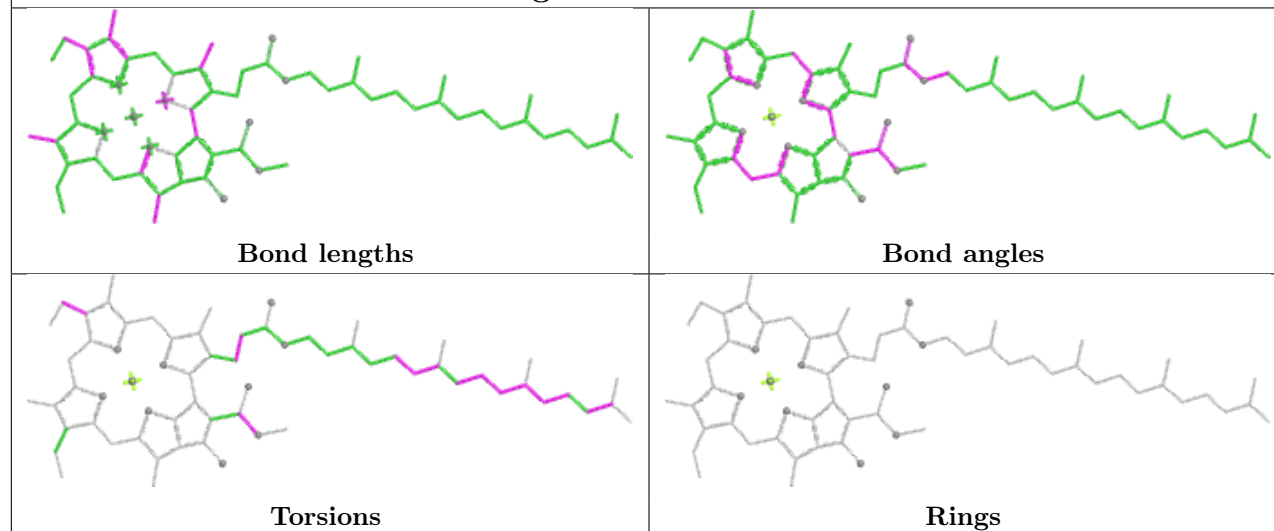
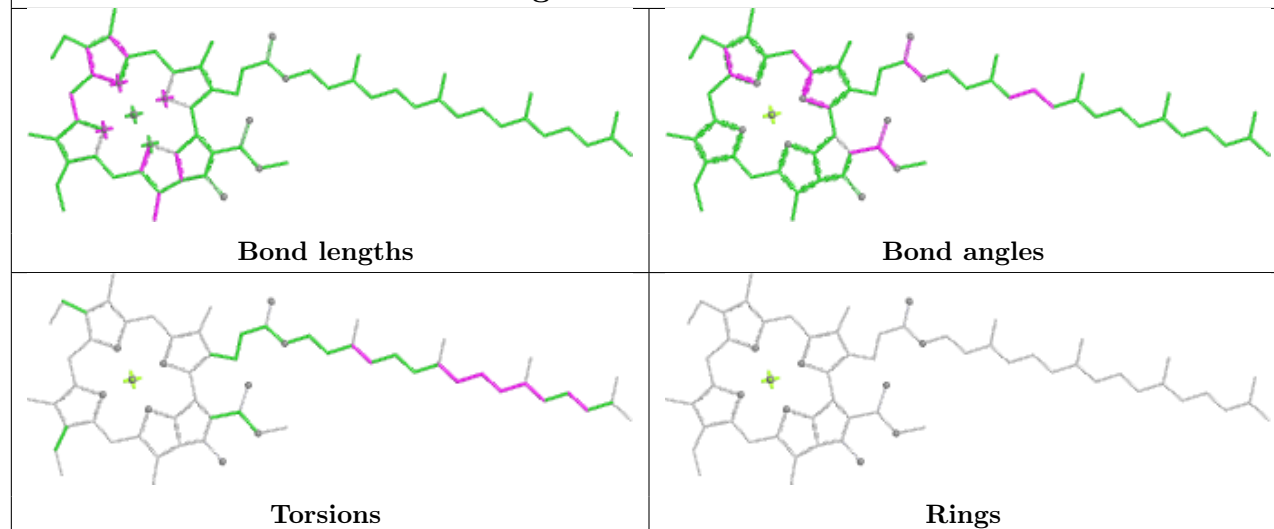
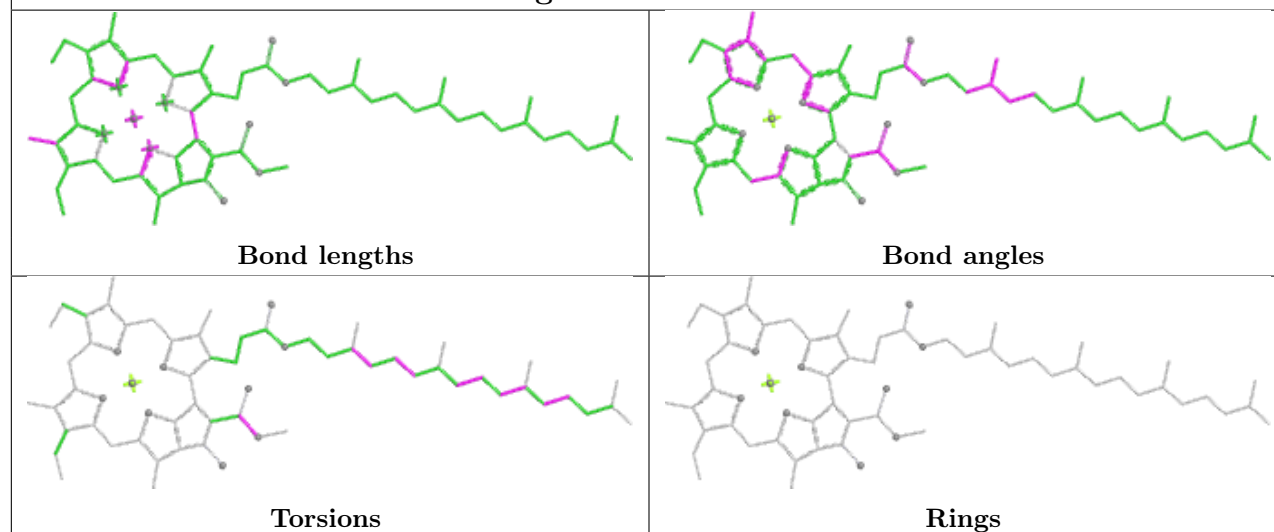


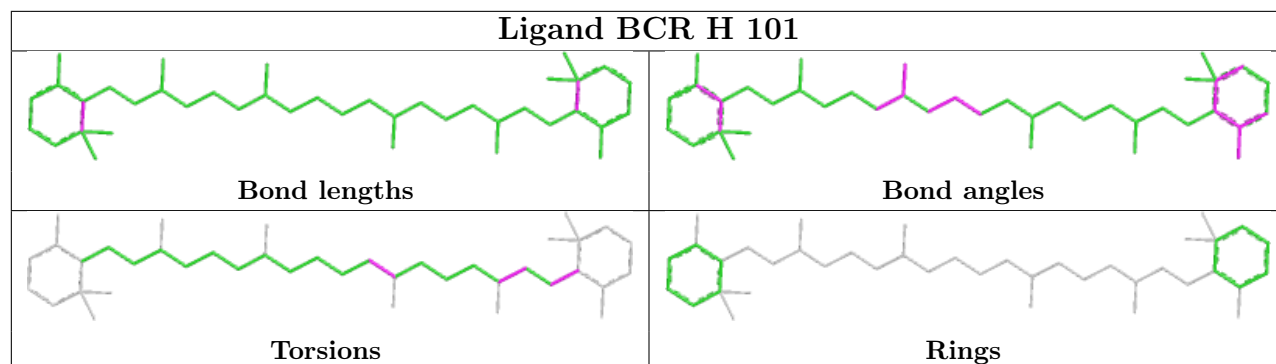
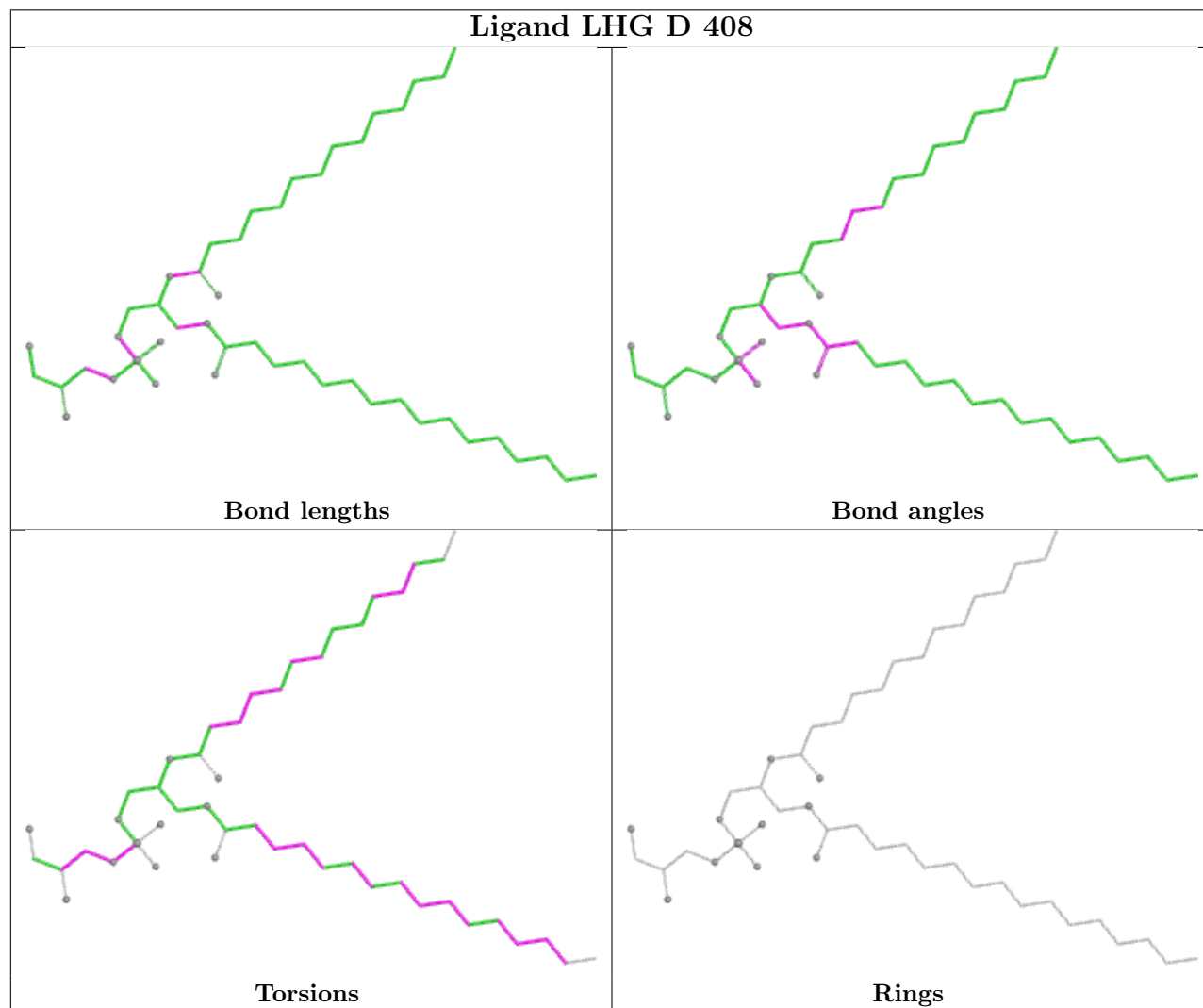


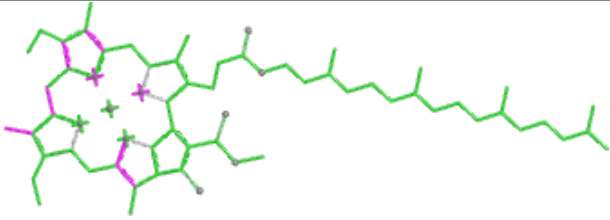
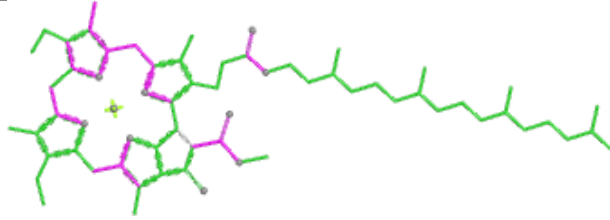
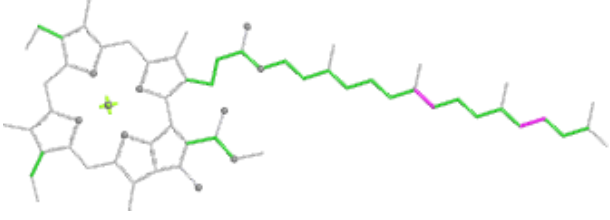
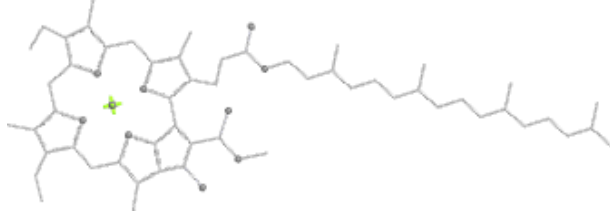
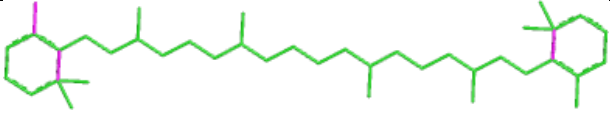
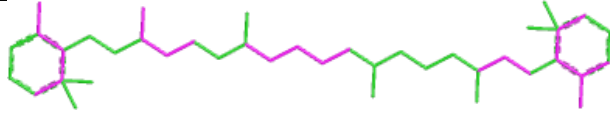
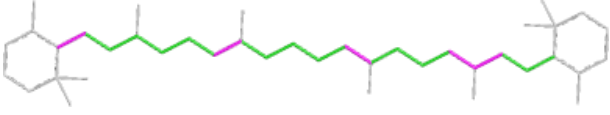
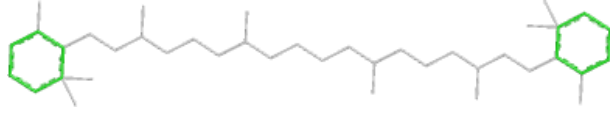
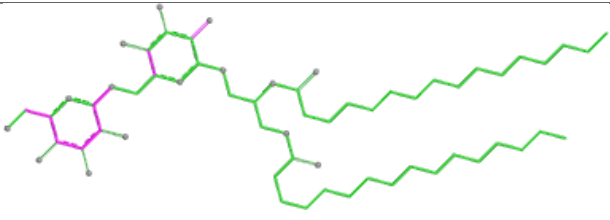
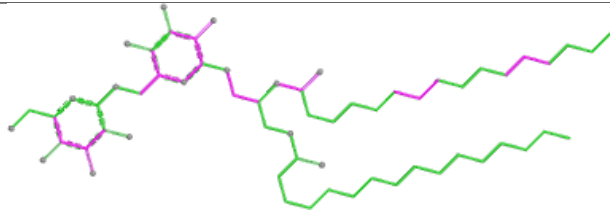
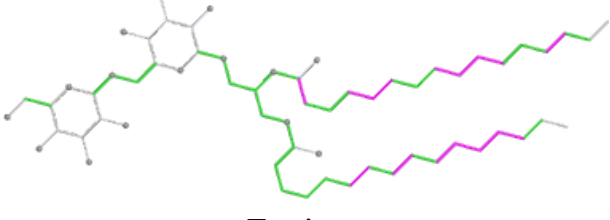
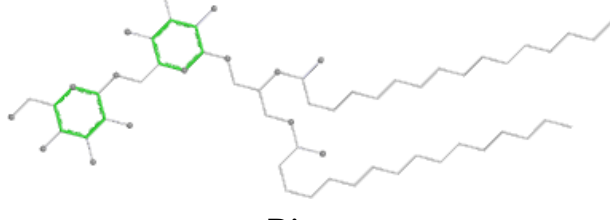




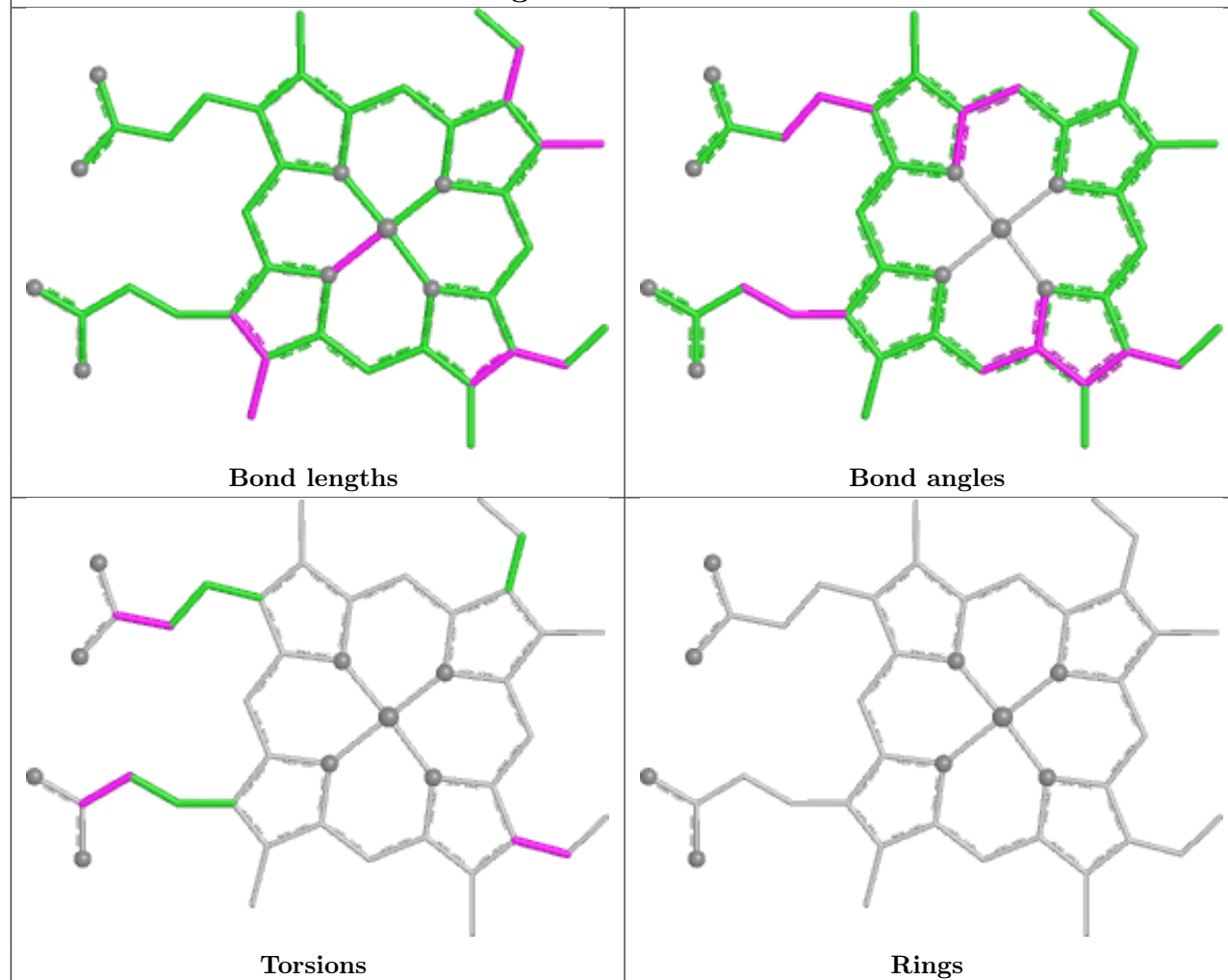


Ligand CLA B 603**Ligand CLA C 510****Ligand CLA b 604**

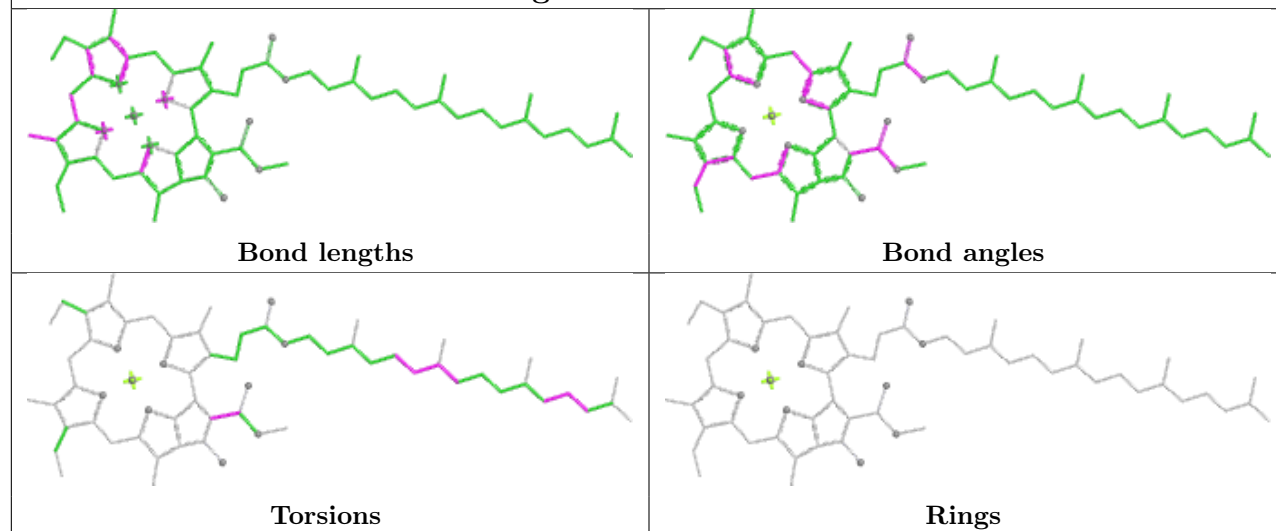


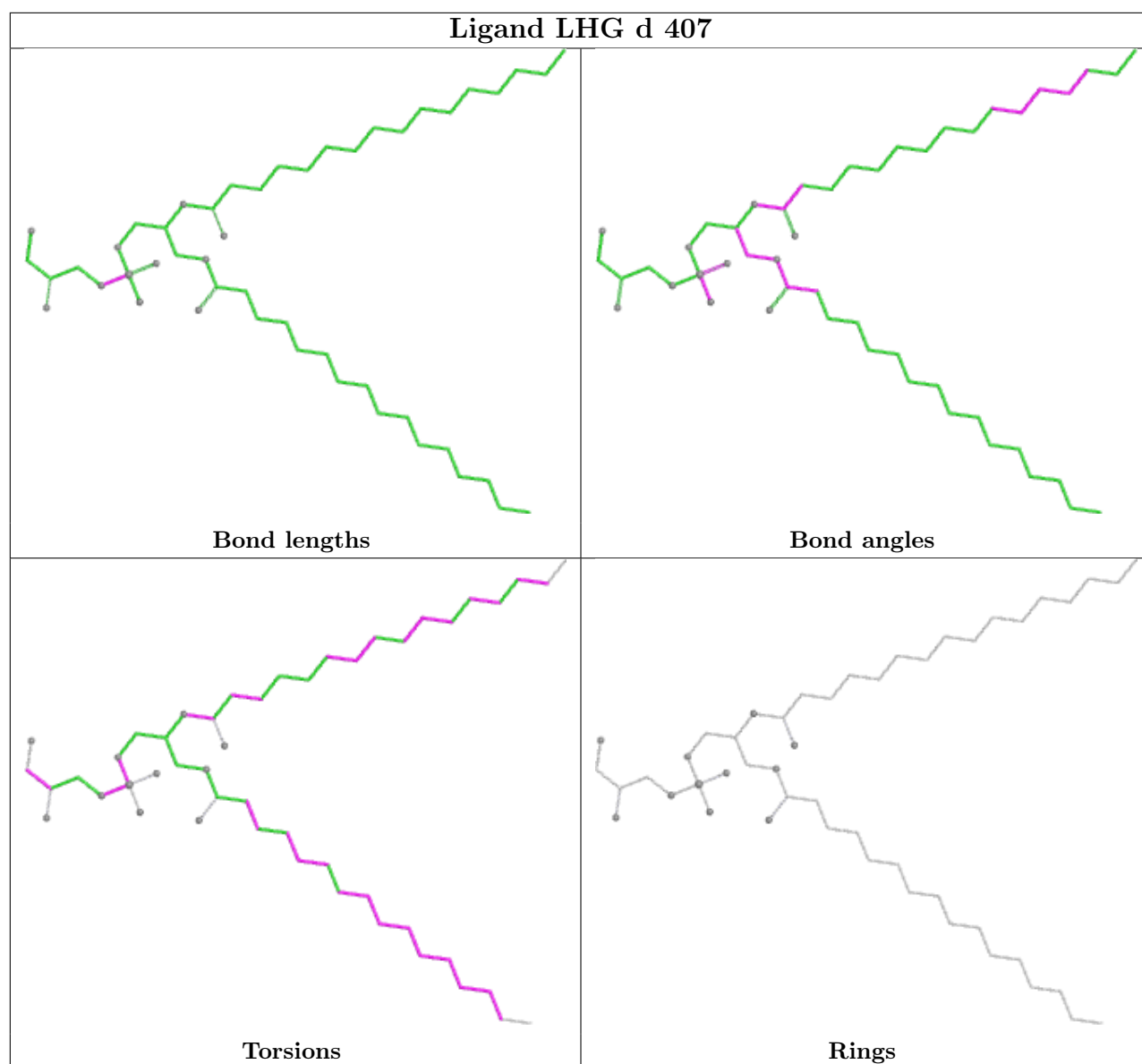
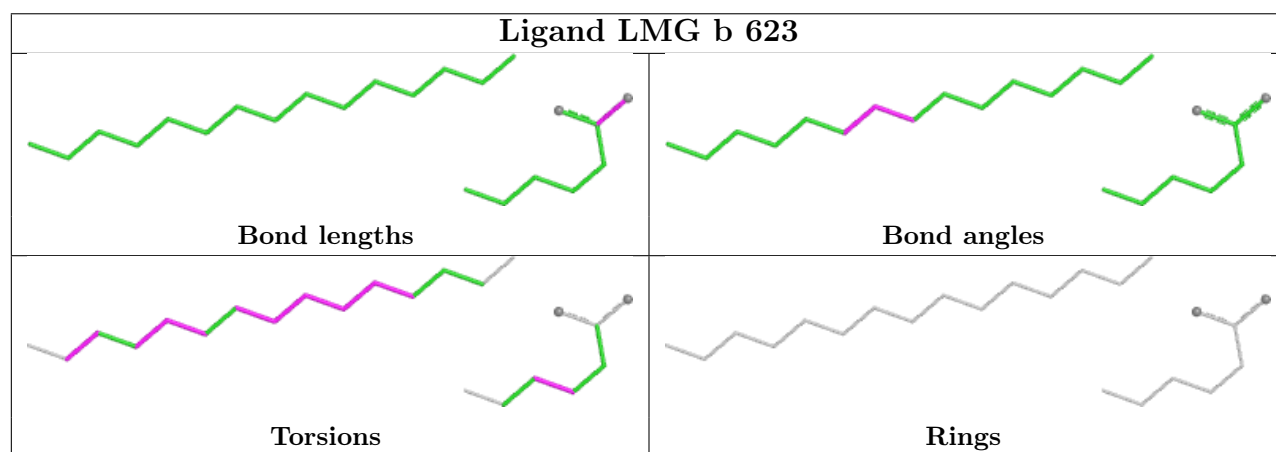
Ligand CLA C 508	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 618	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGD H 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

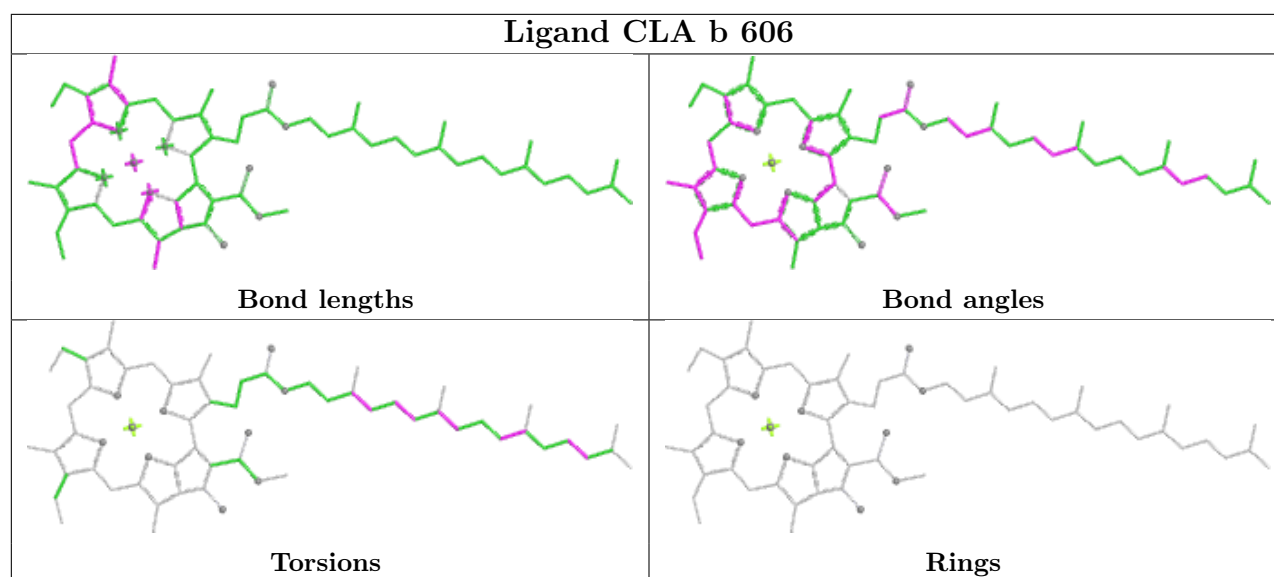
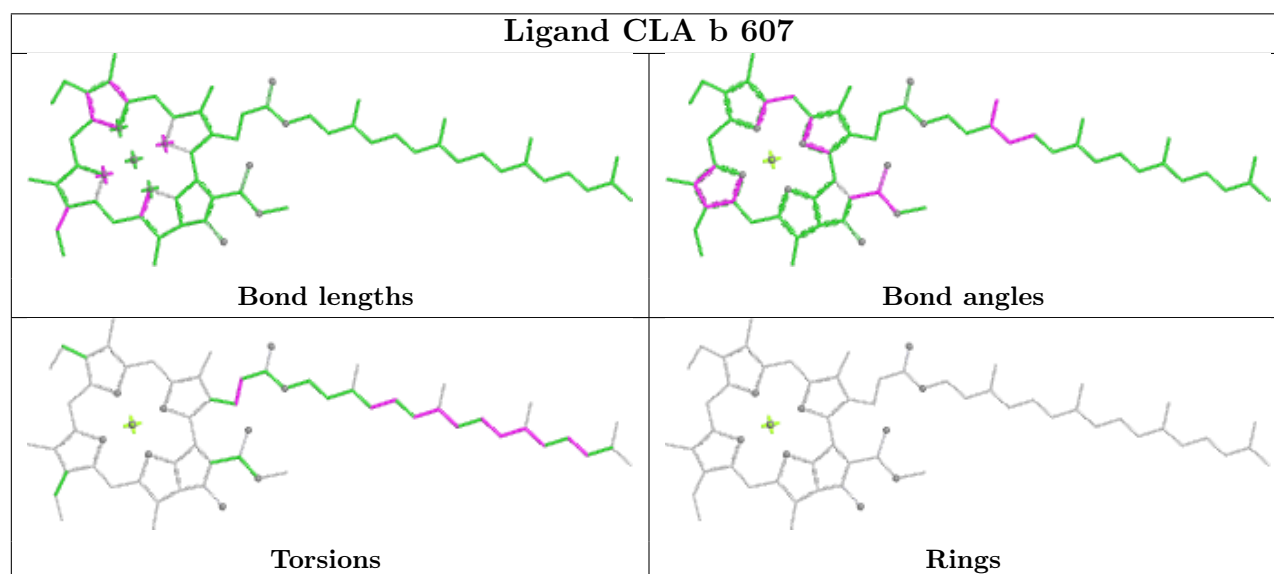
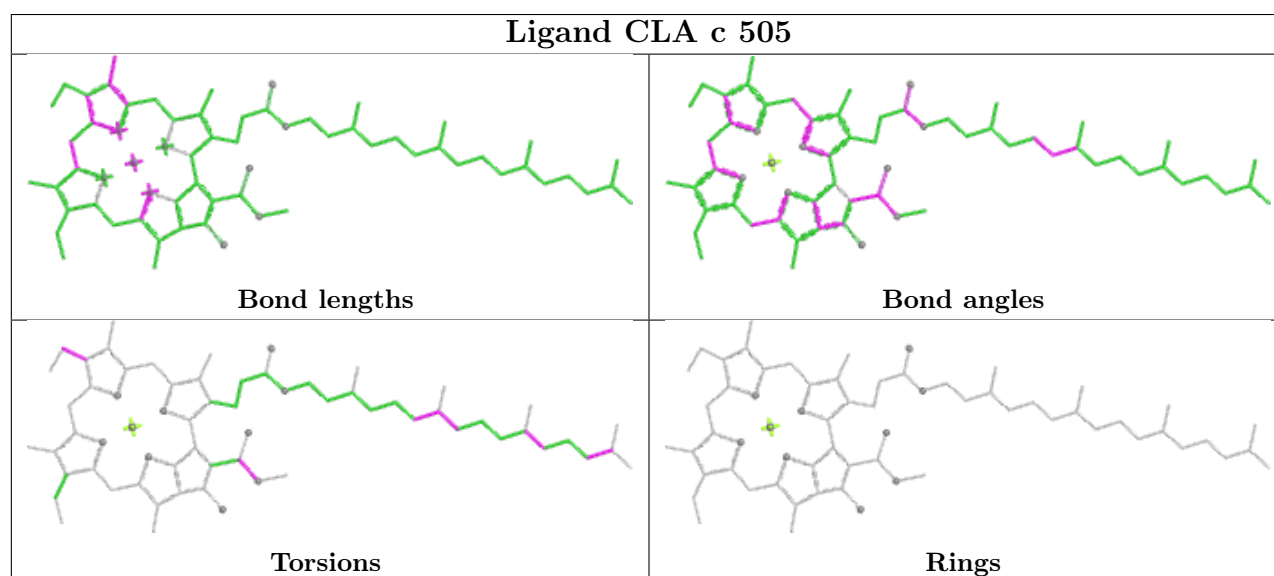
Ligand HEM e 102

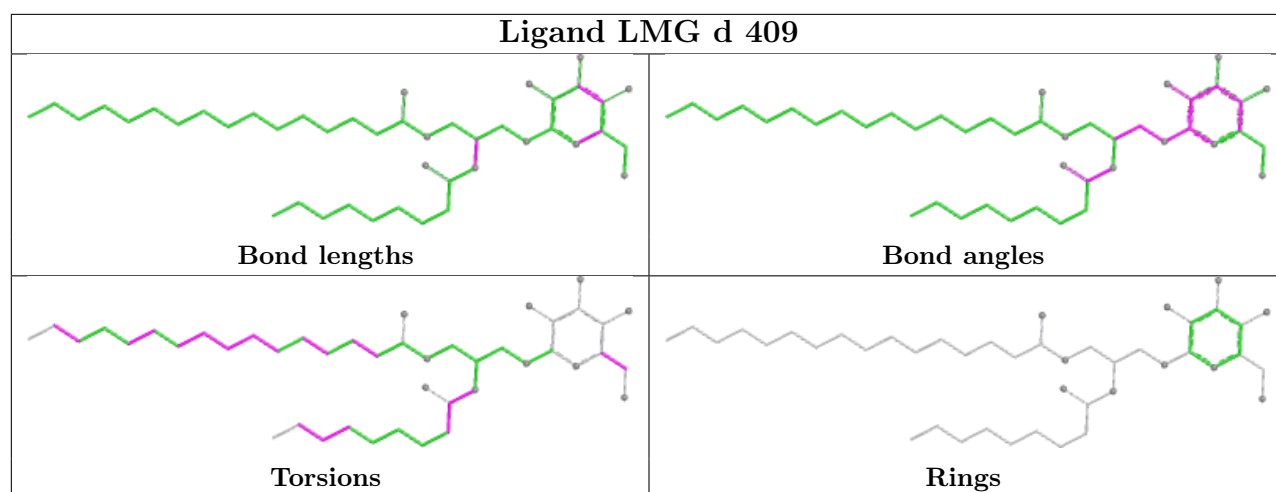
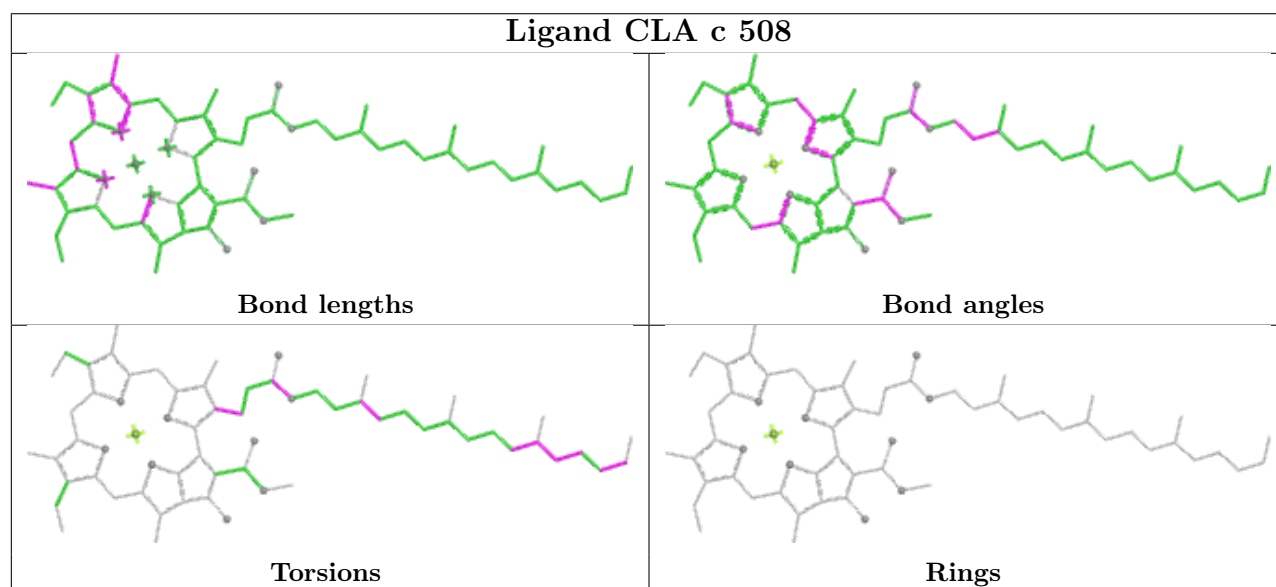
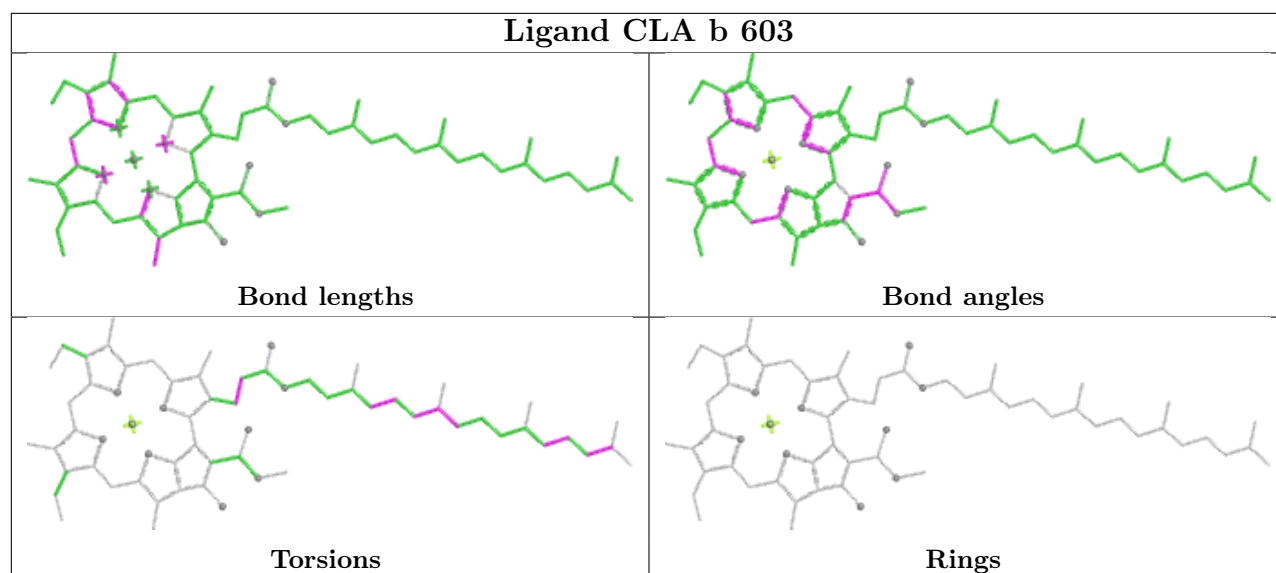


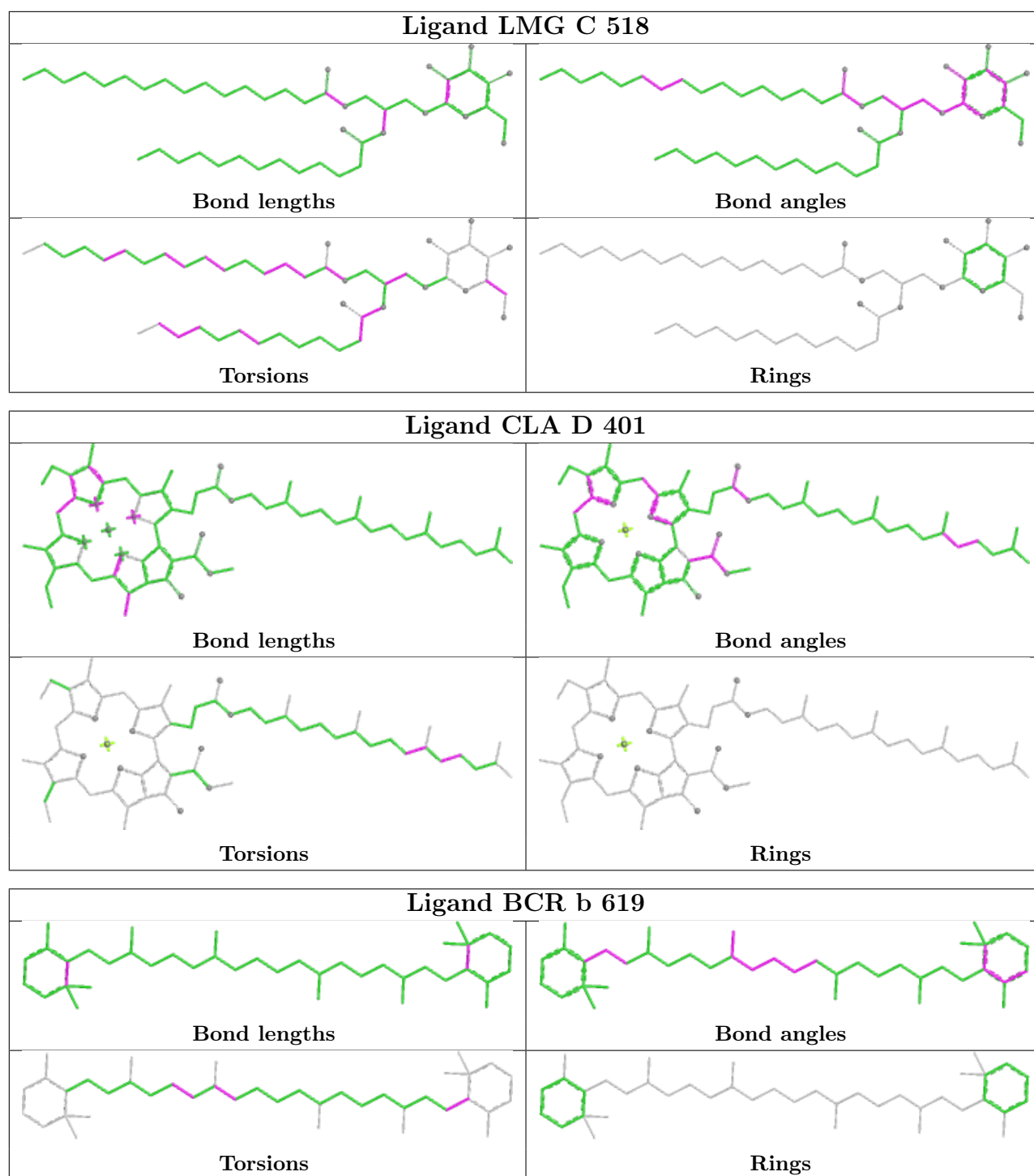
Ligand CLA C 507

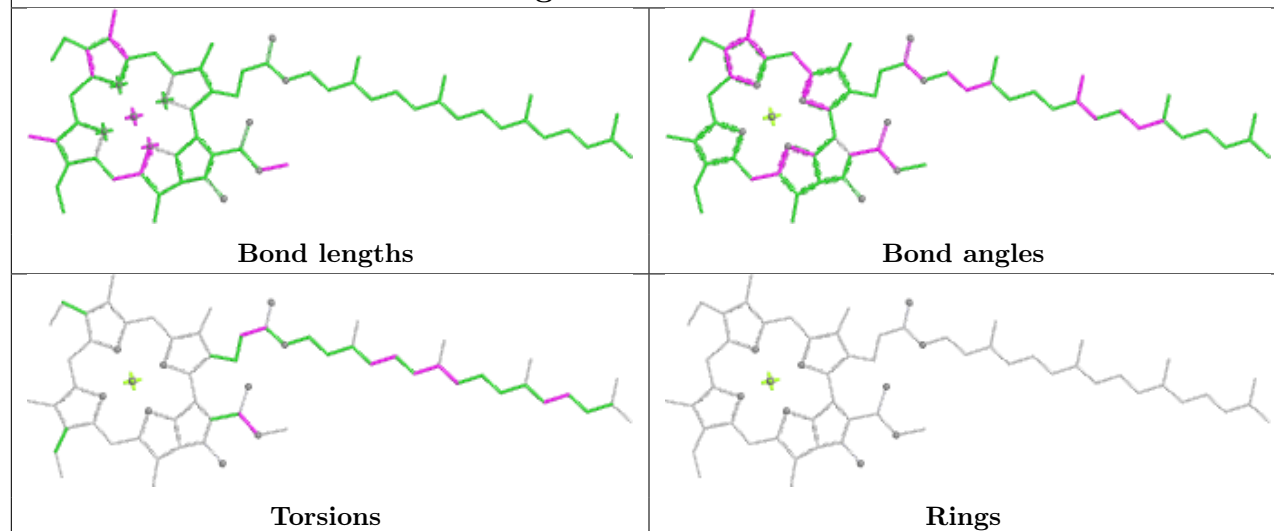
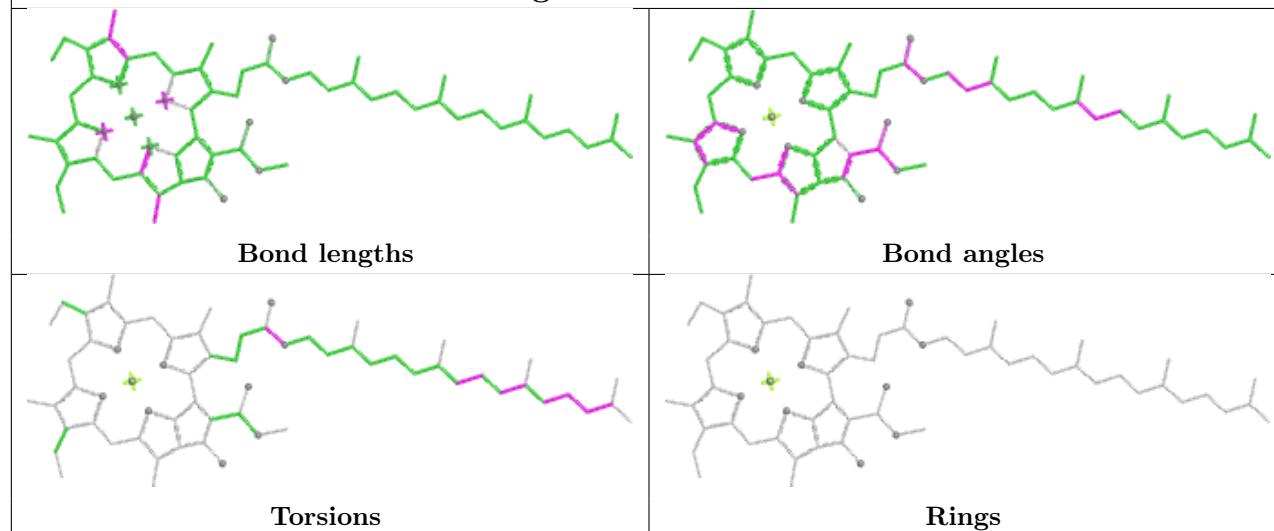
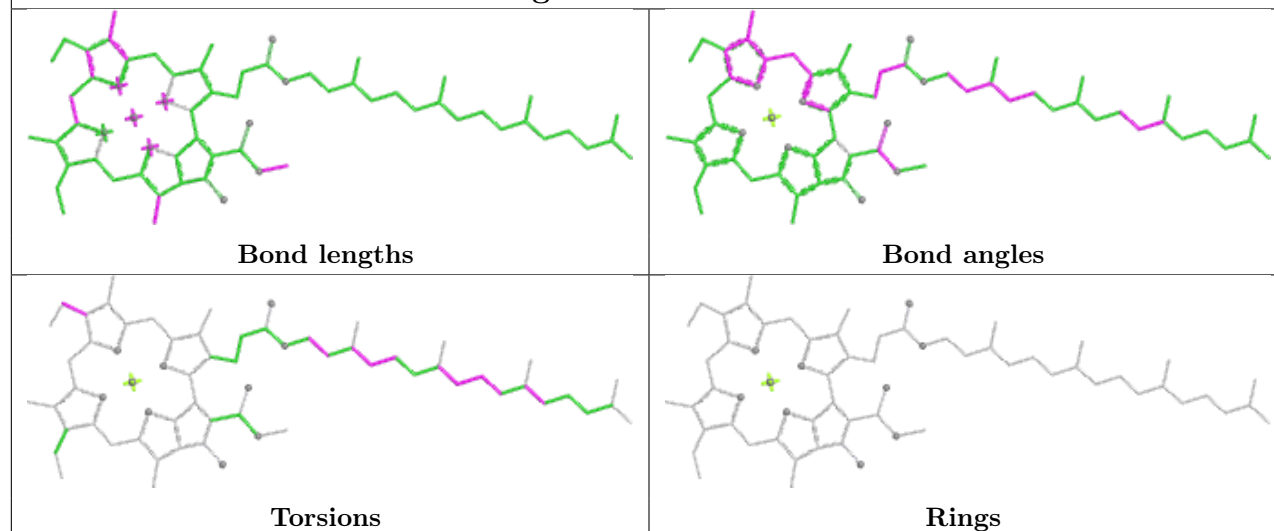


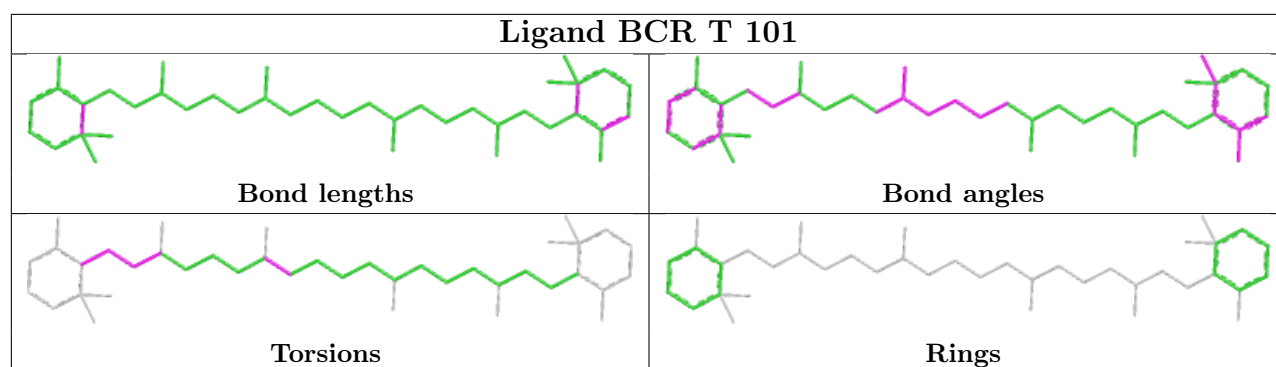
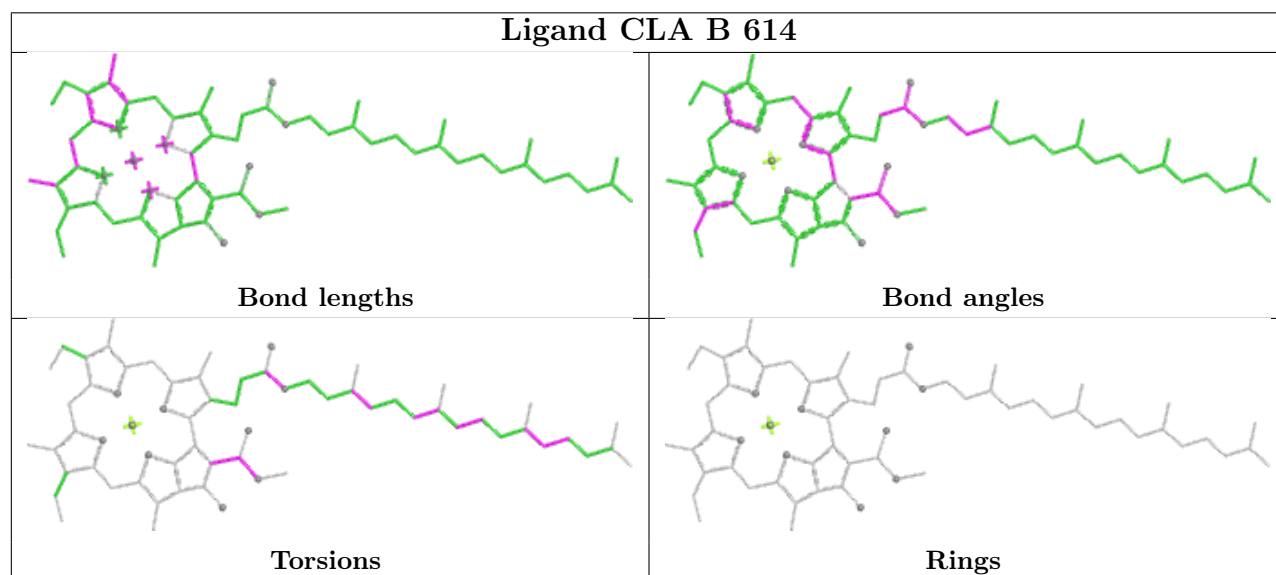
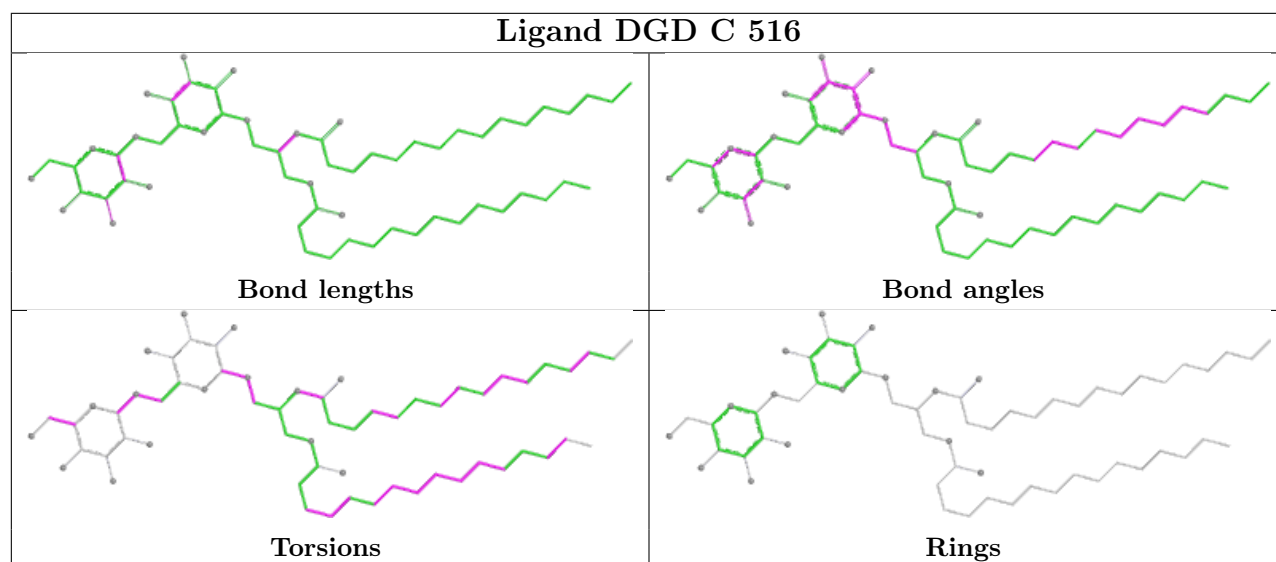




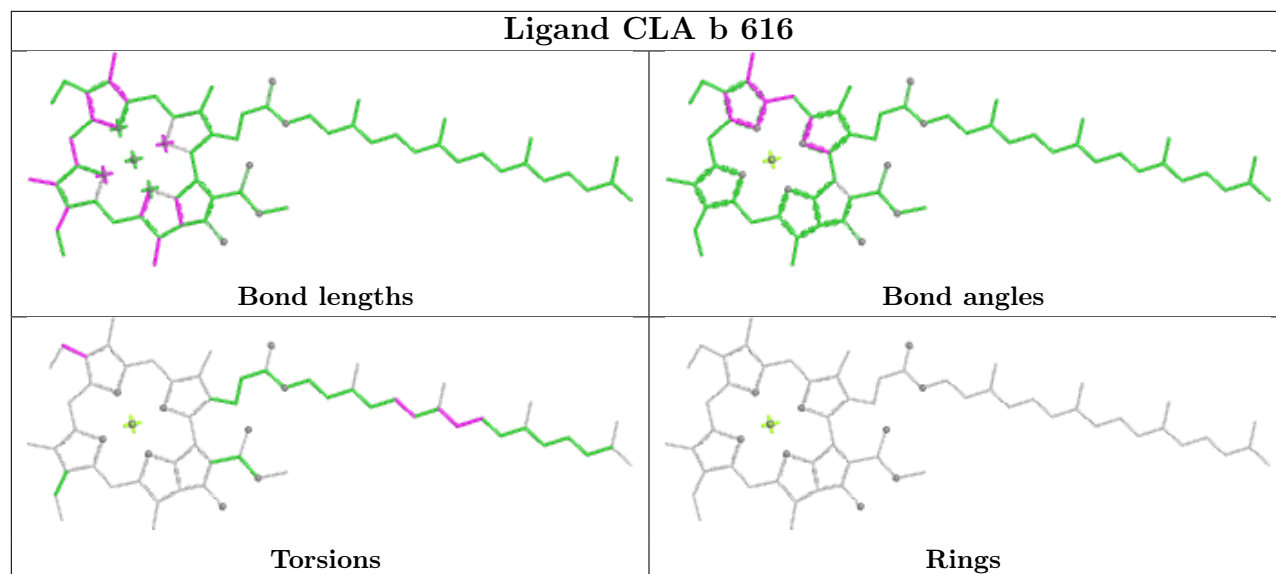




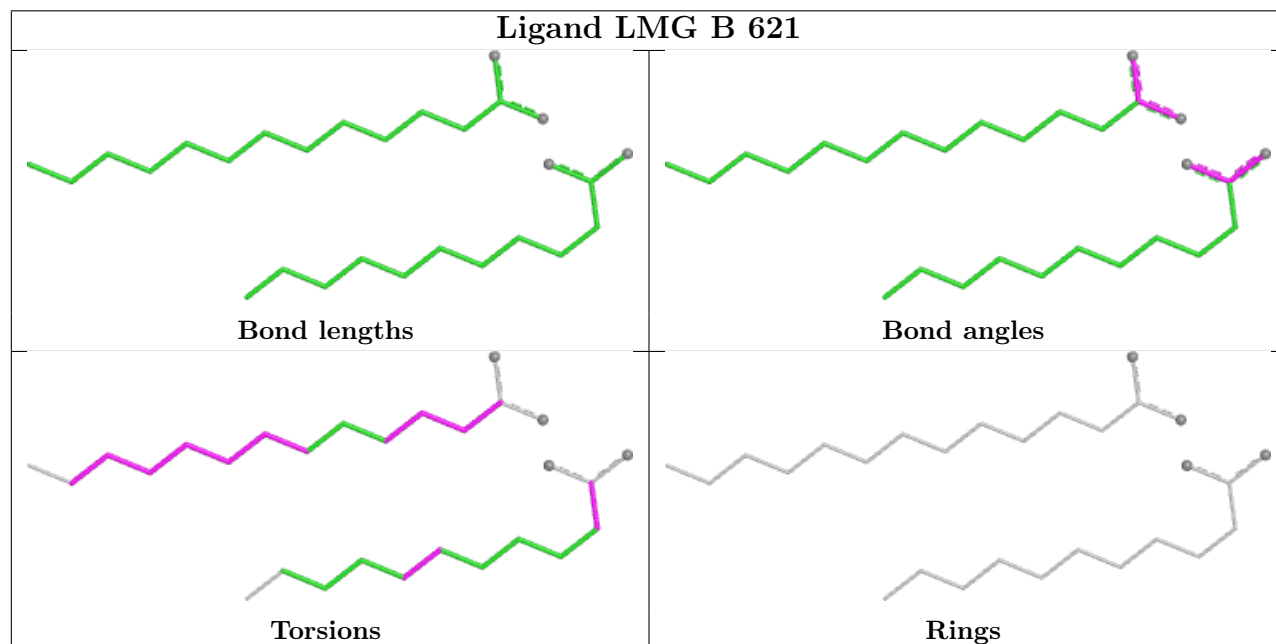
Ligand CLA b 613**Ligand CLA B 611****Ligand CLA C 512**

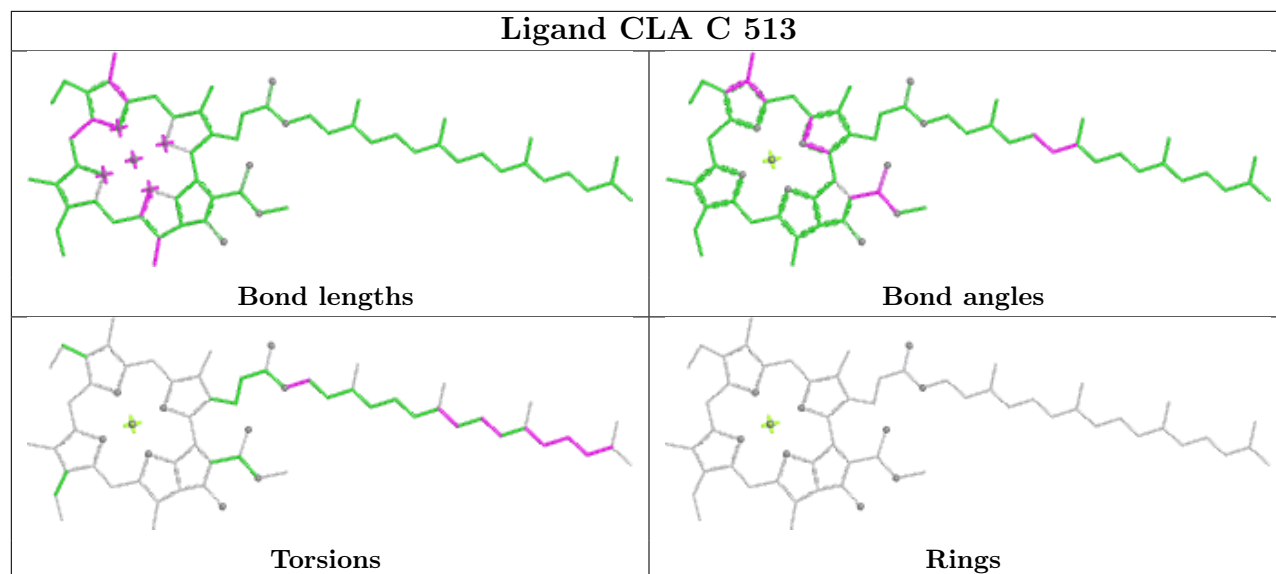
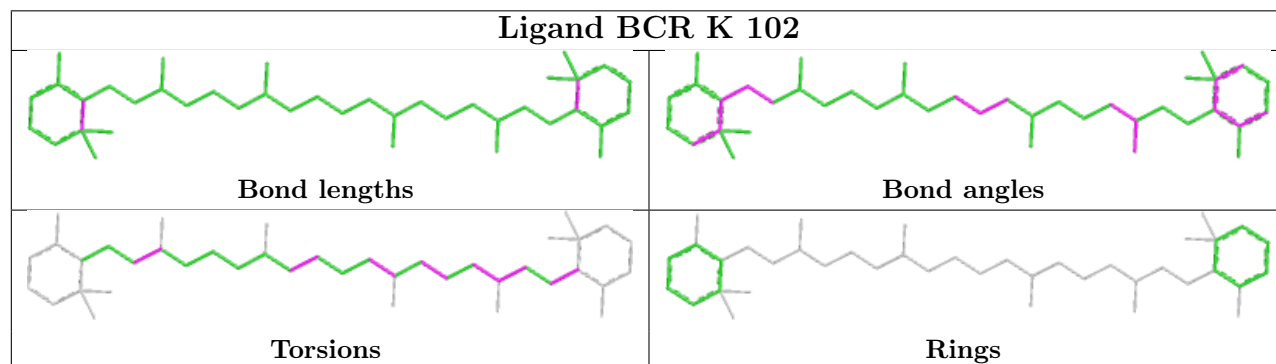
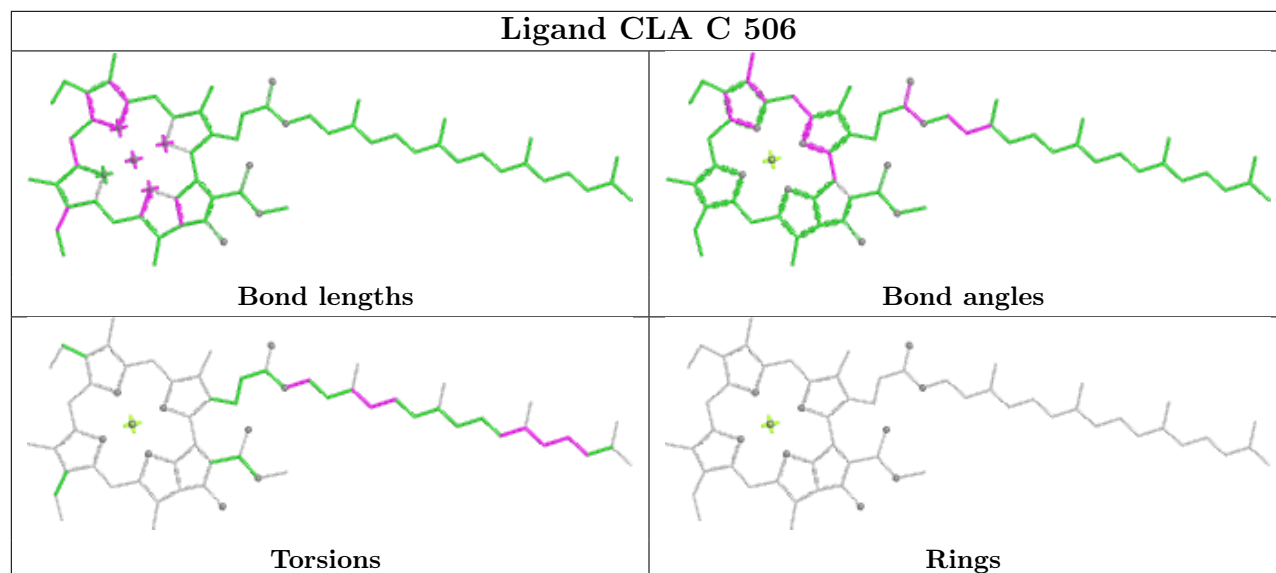


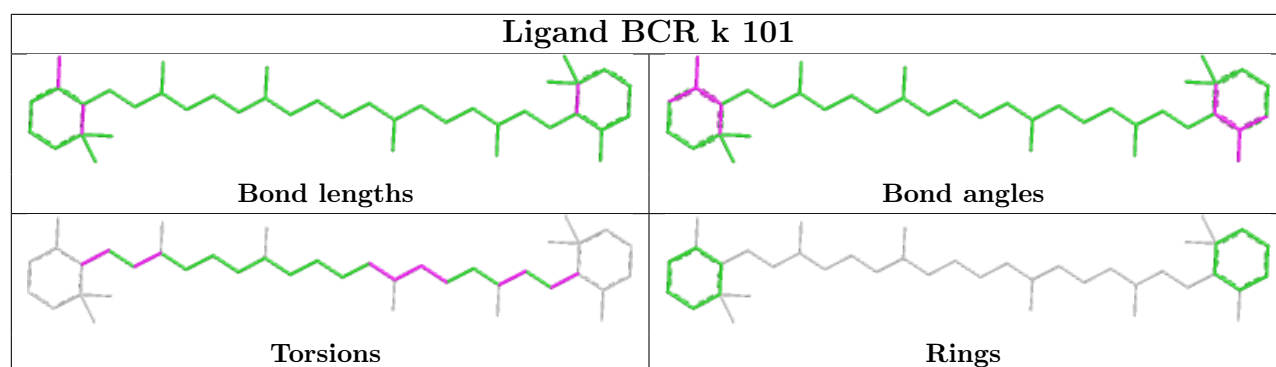
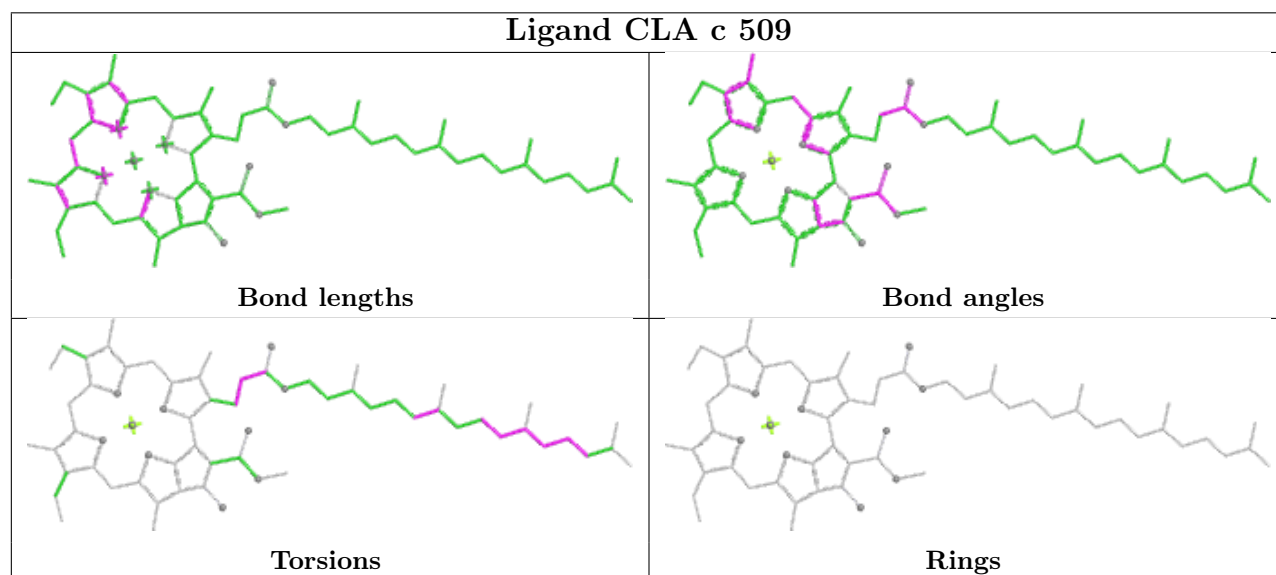
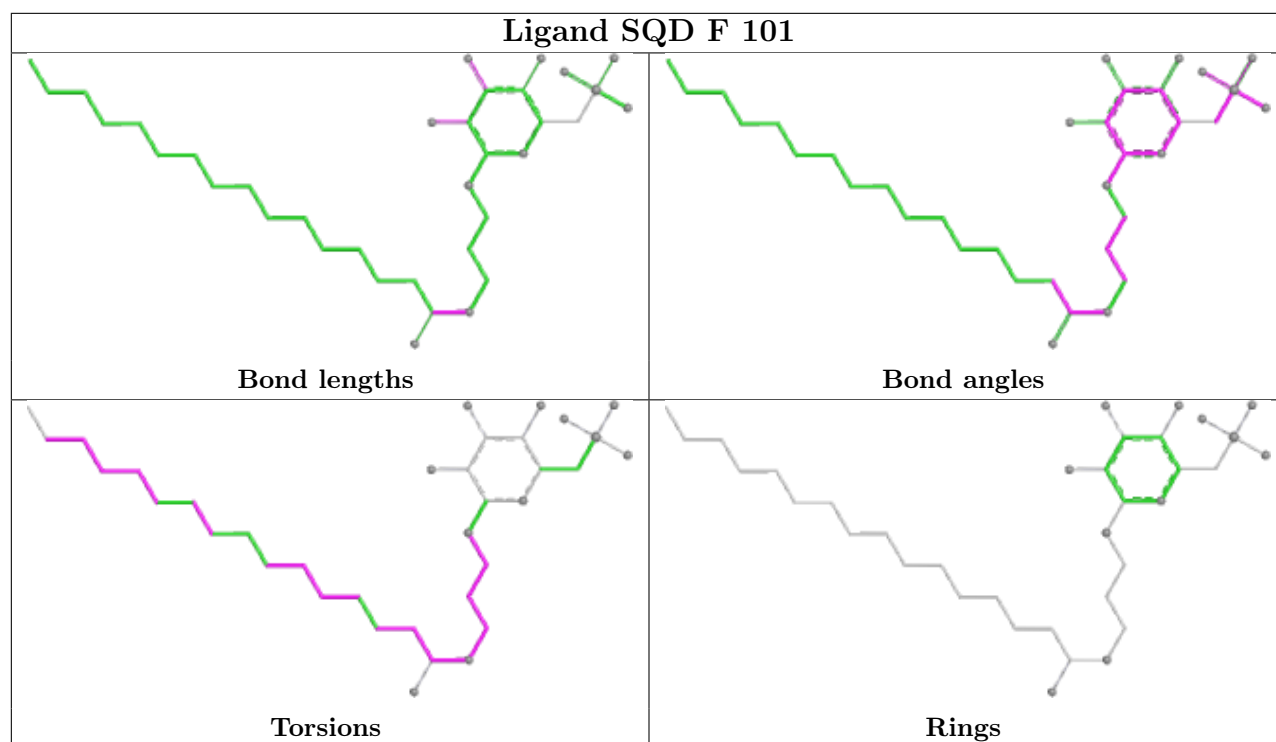
Ligand CLA b 616

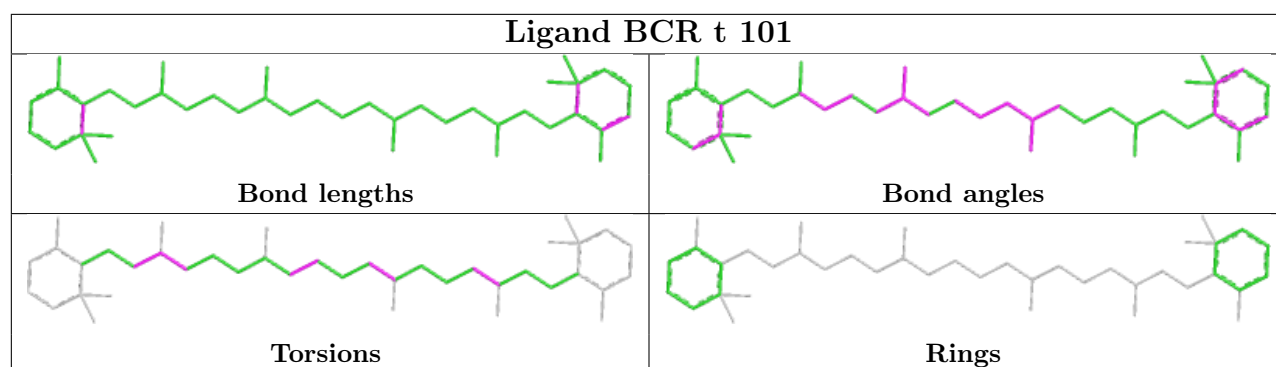
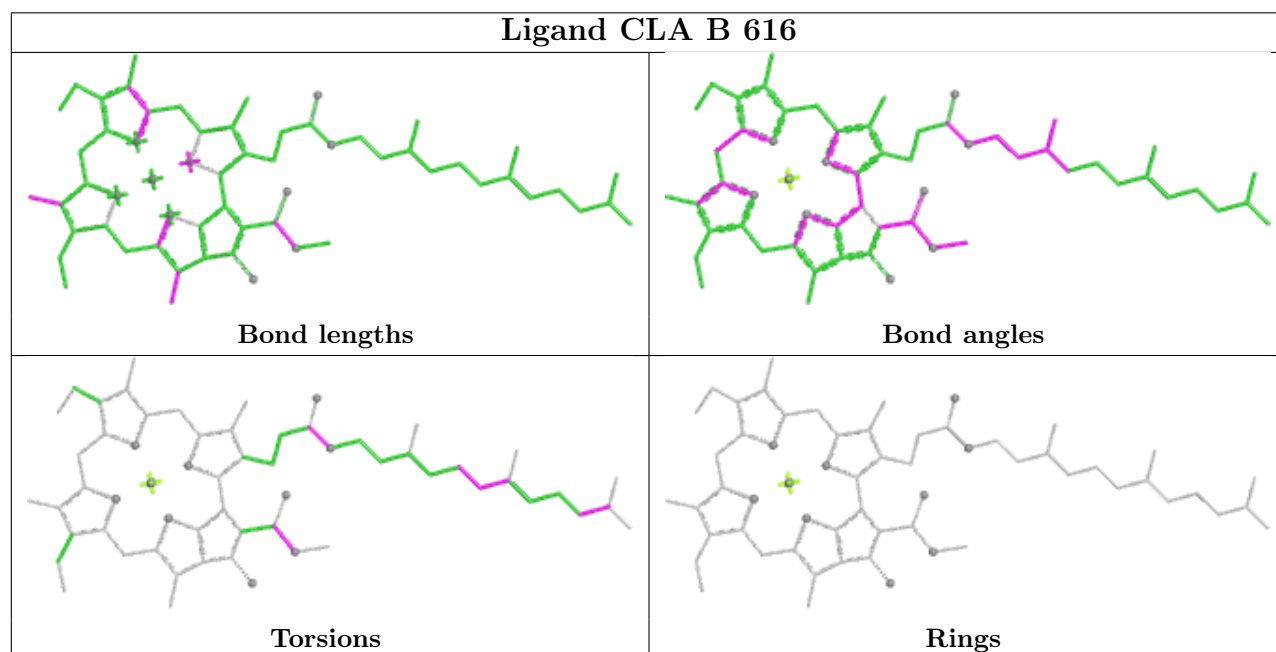
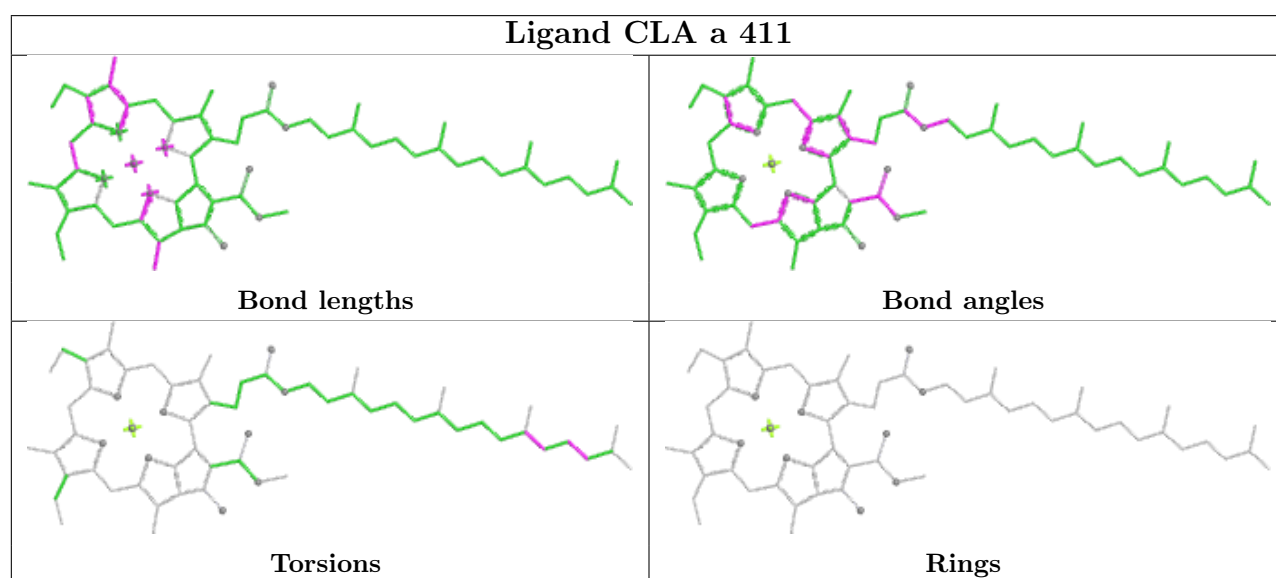


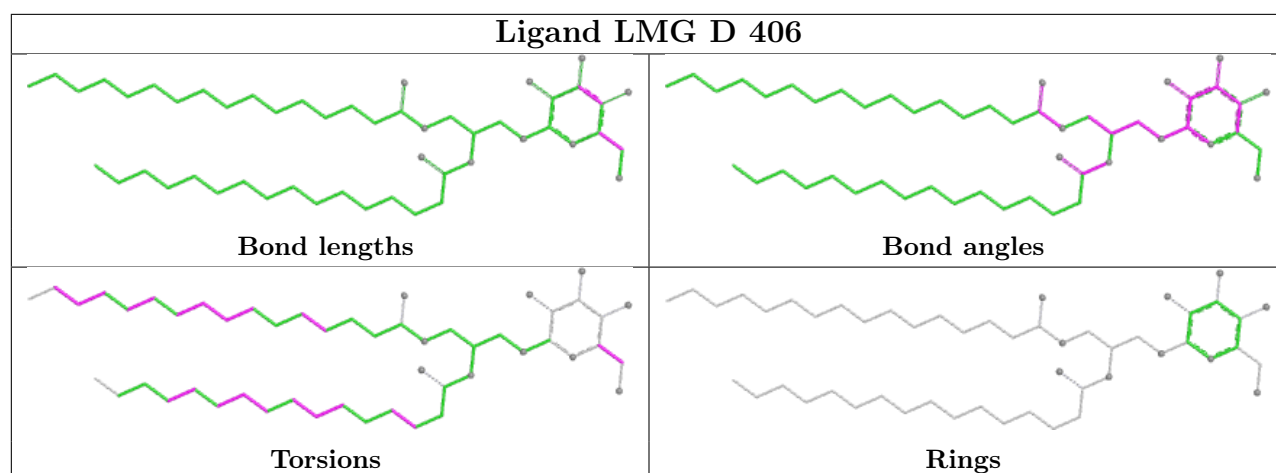
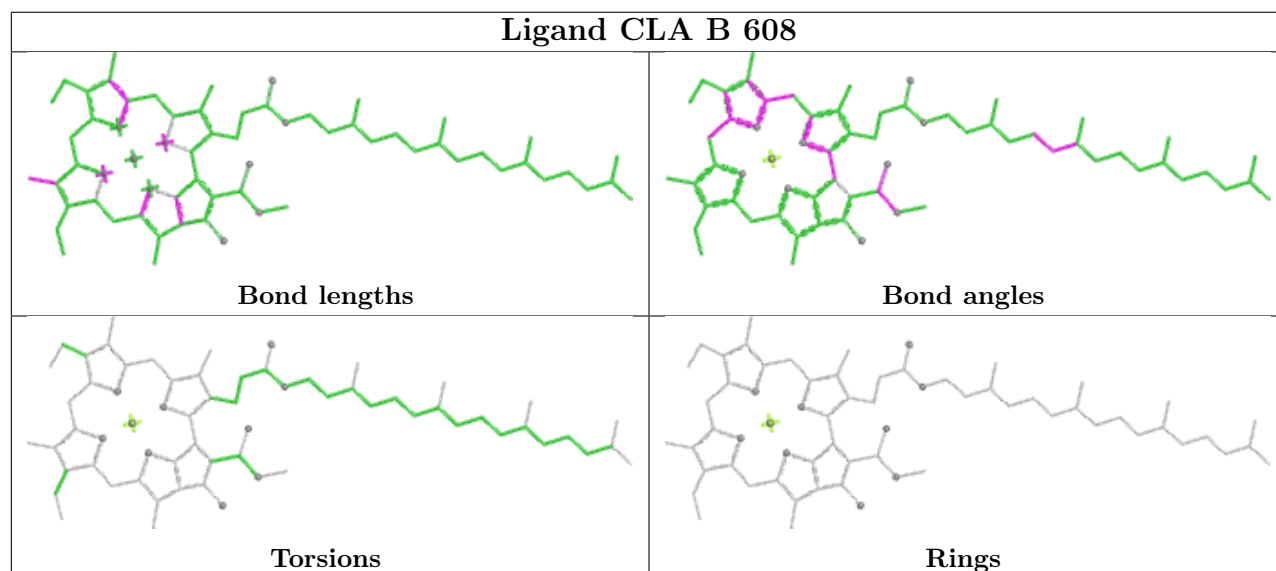
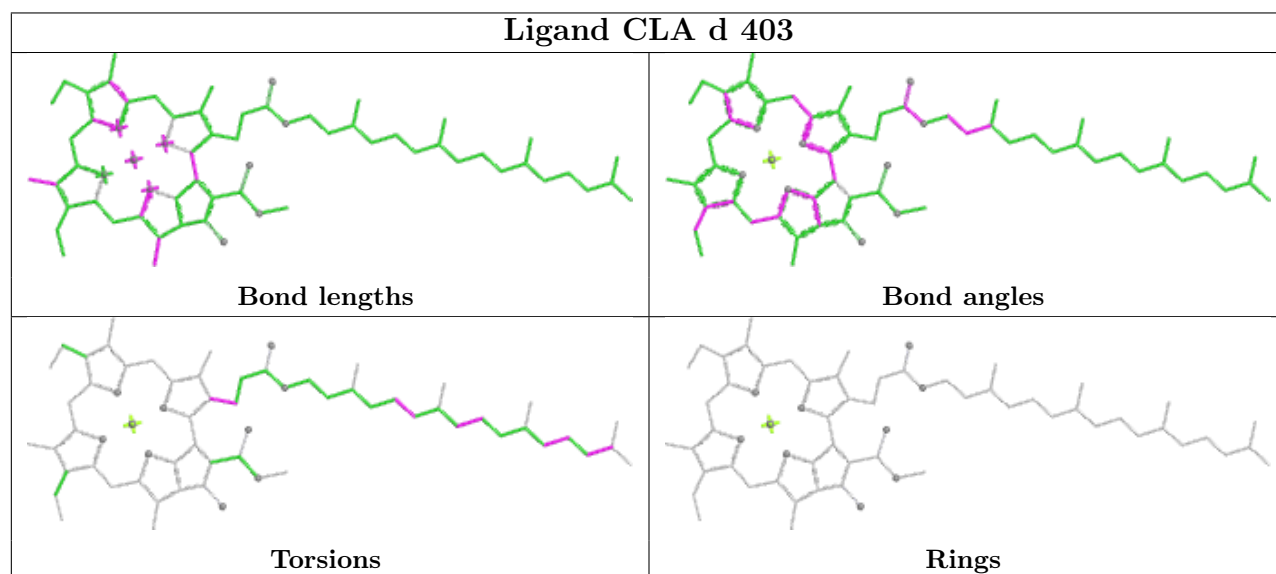
Ligand LMG B 621

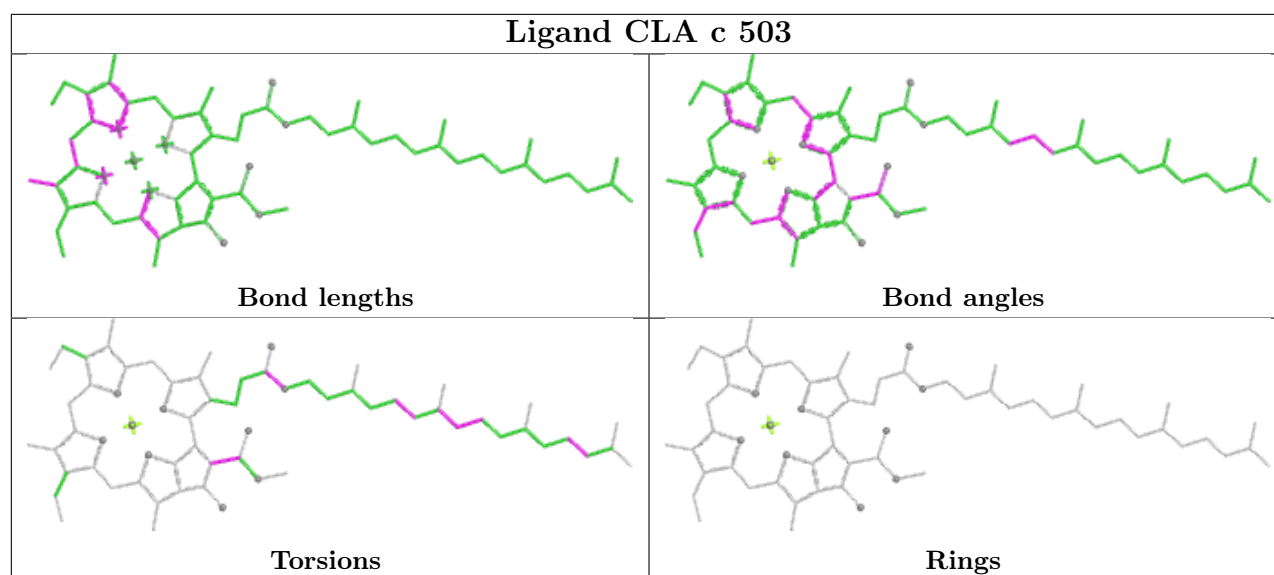
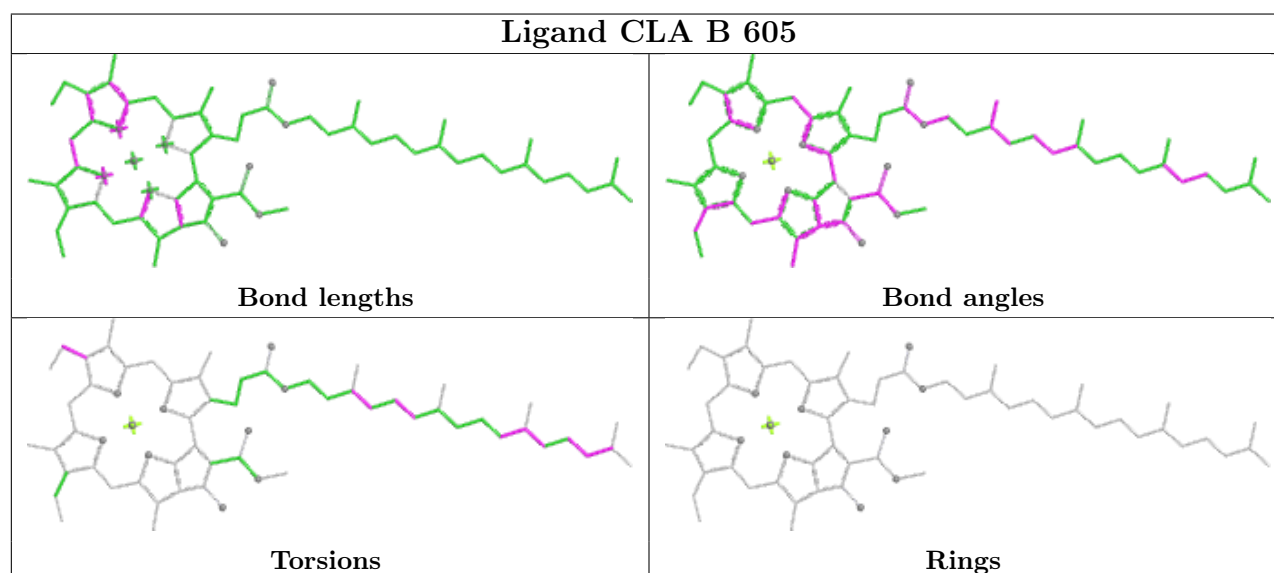
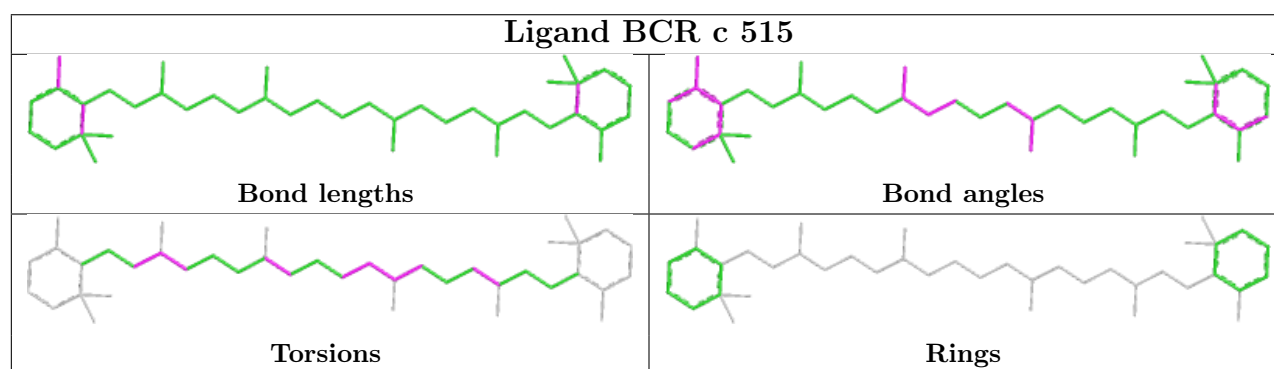


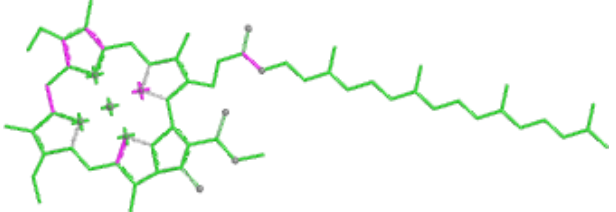
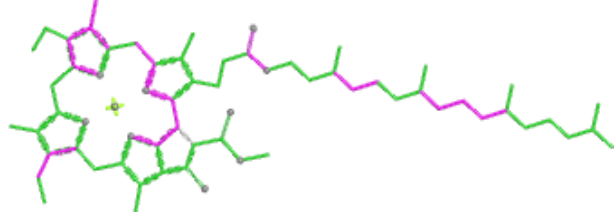
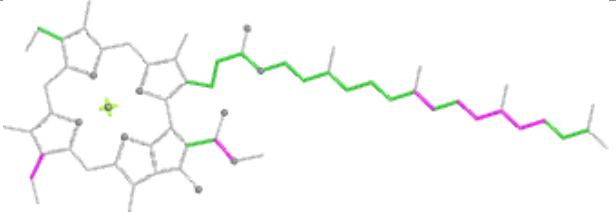
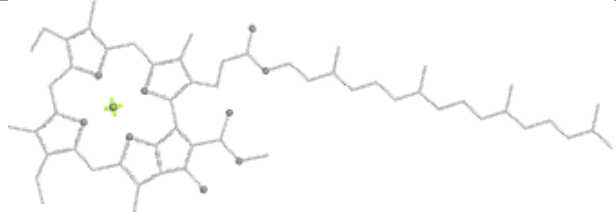
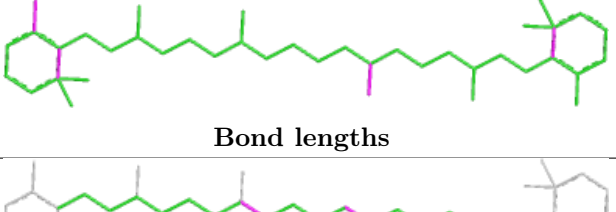
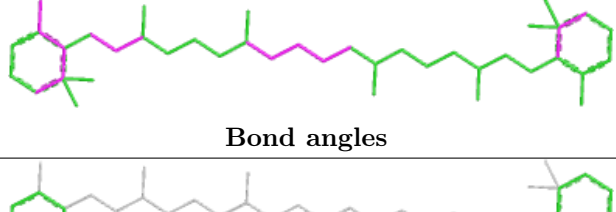
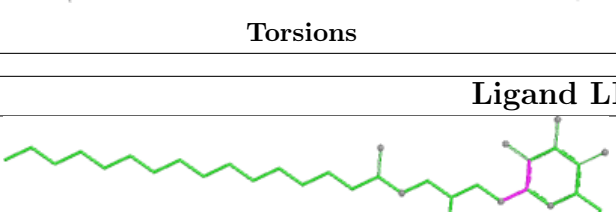
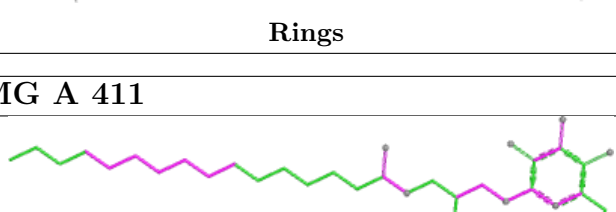
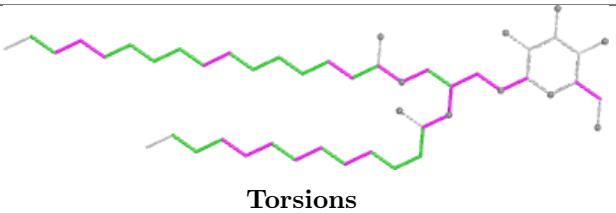
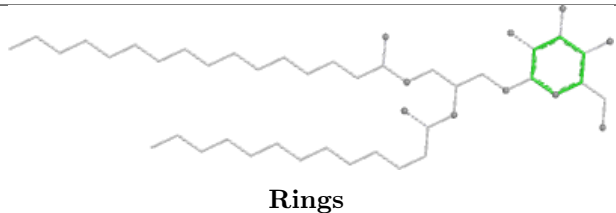


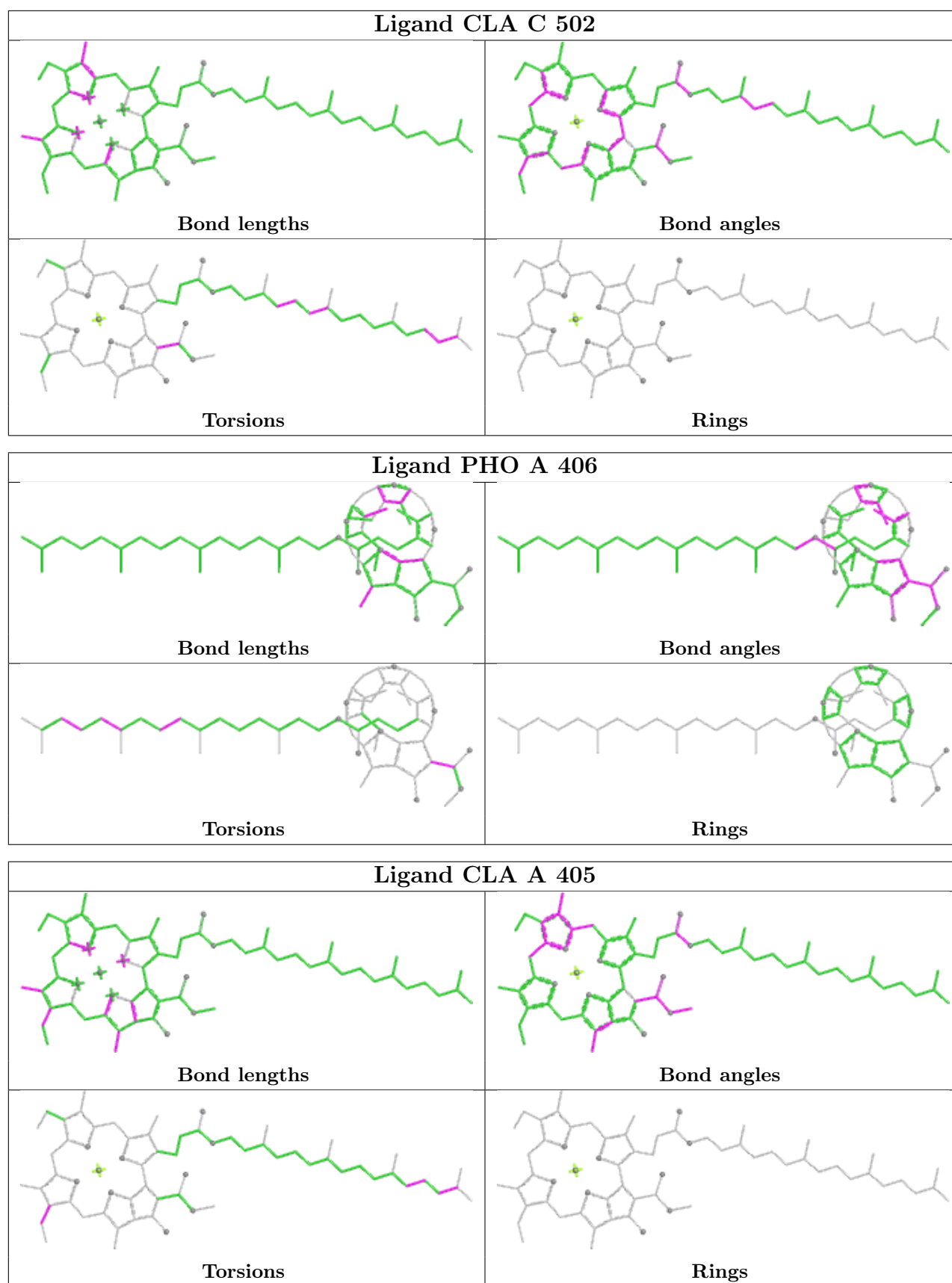


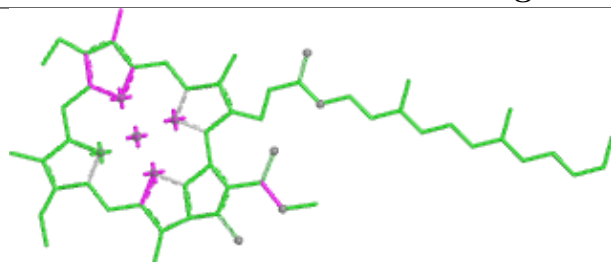




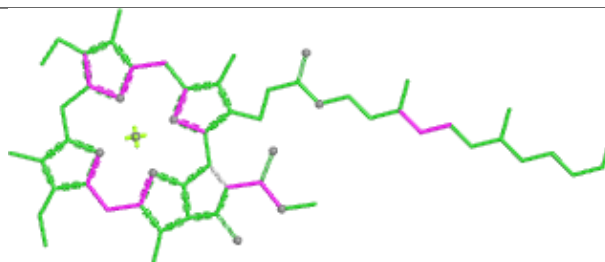


Ligand CLA B 604	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR C 514	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG A 411	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

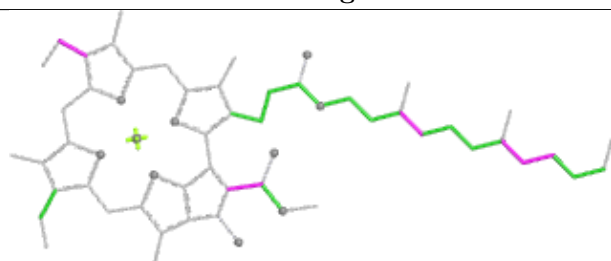


Ligand CLA C 504

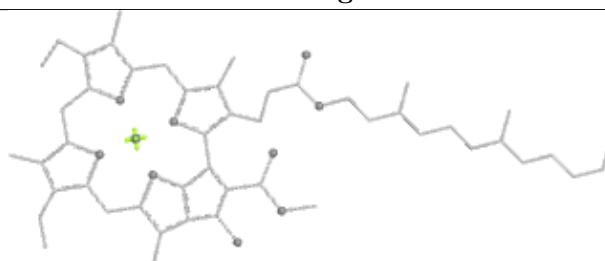
Bond lengths



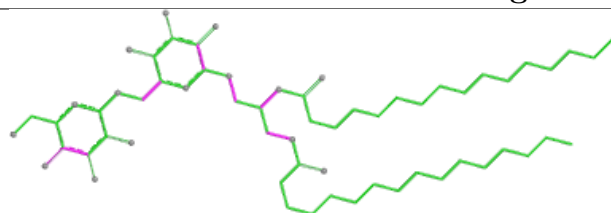
Bond angles



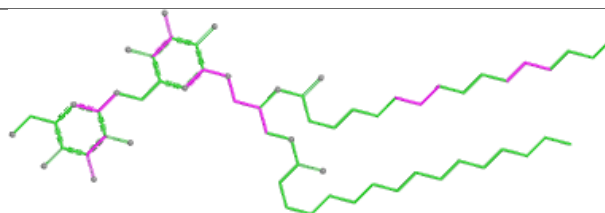
Torsions



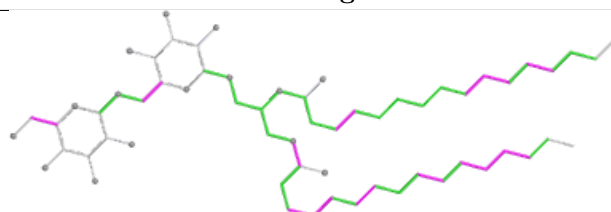
Rings

Ligand DGD C 517

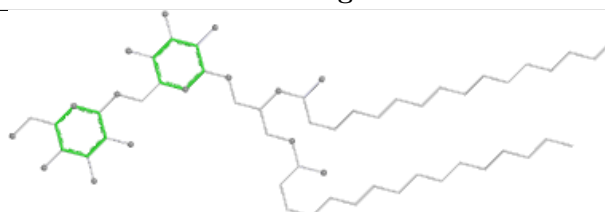
Bond lengths



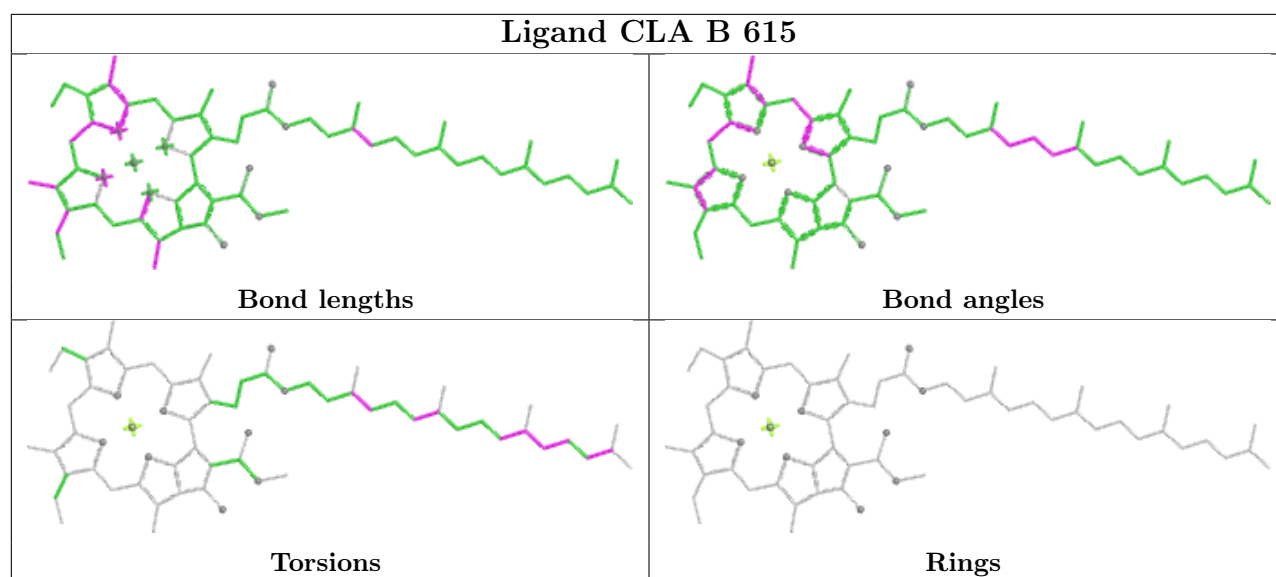
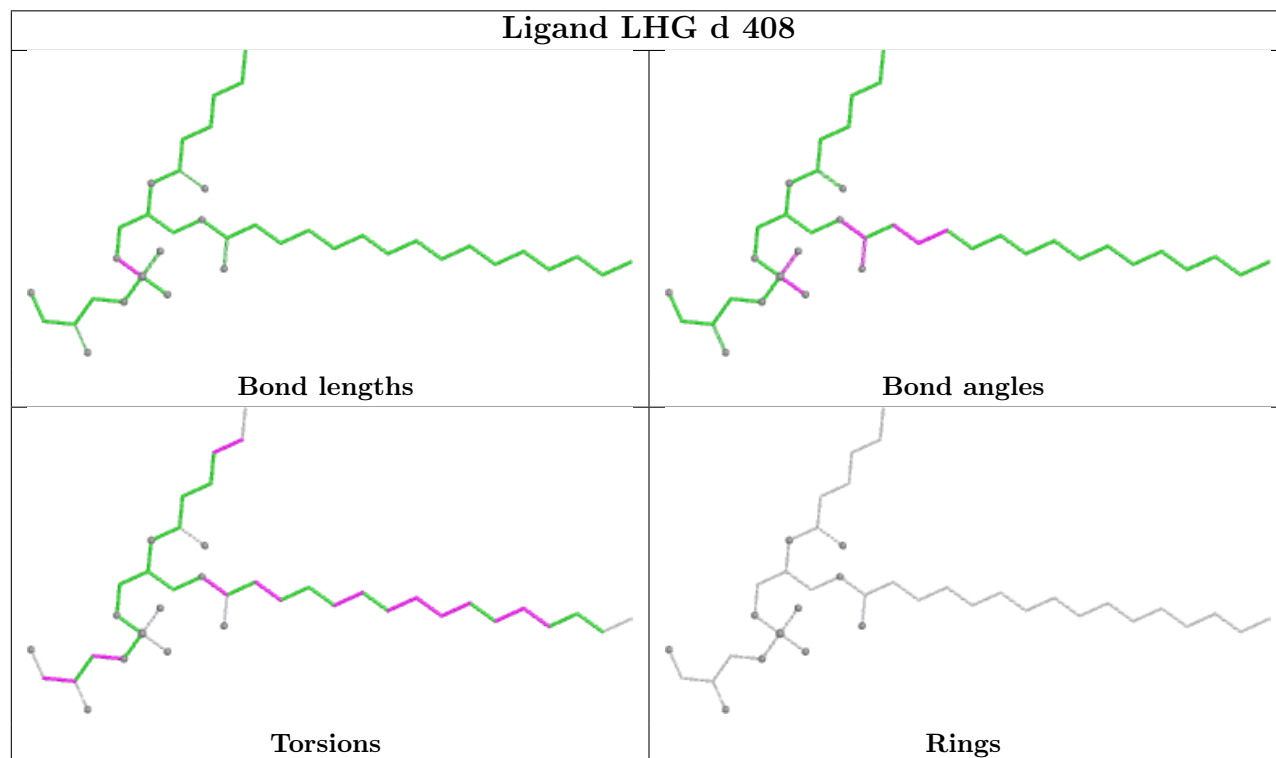
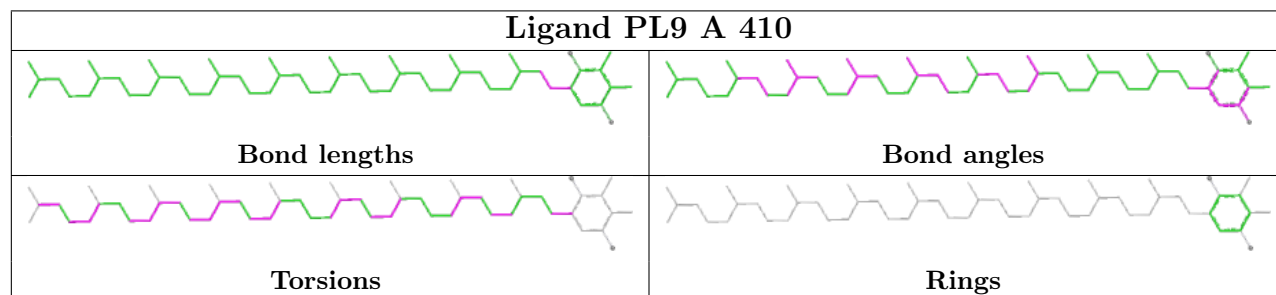
Bond angles



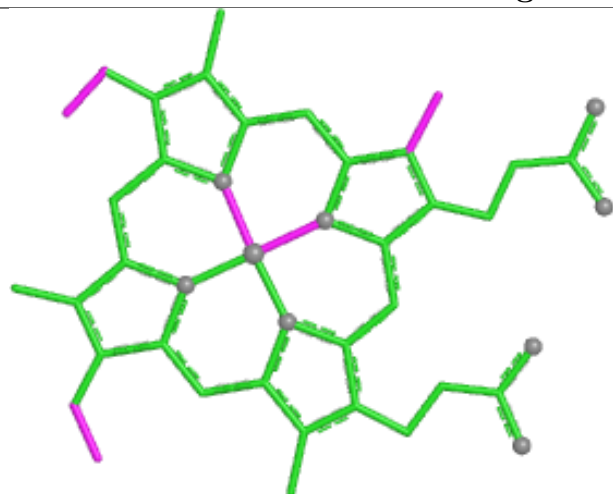
Torsions



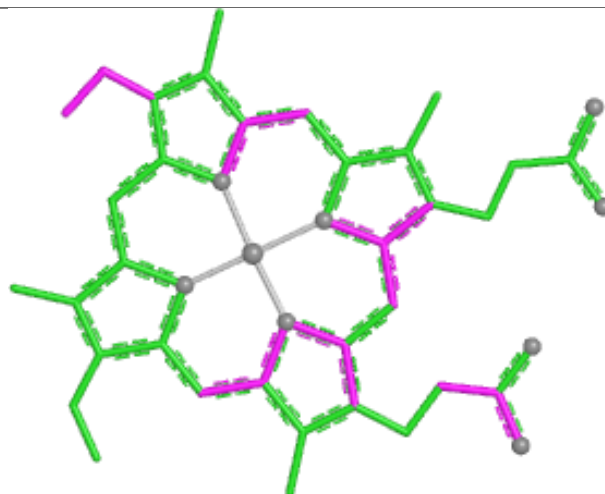
Rings



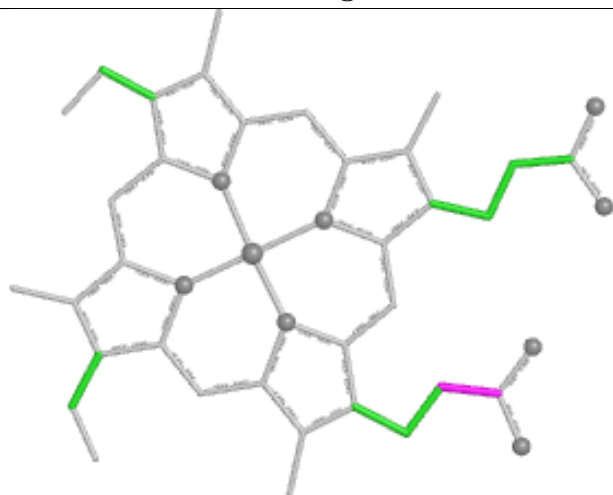
Ligand HEC v 201



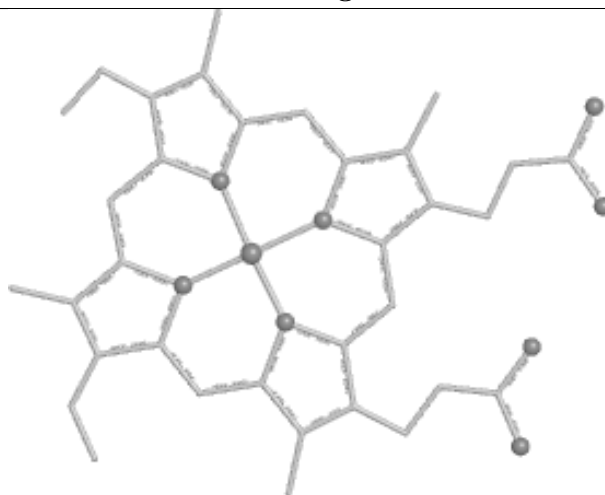
Bond lengths



Bond angles

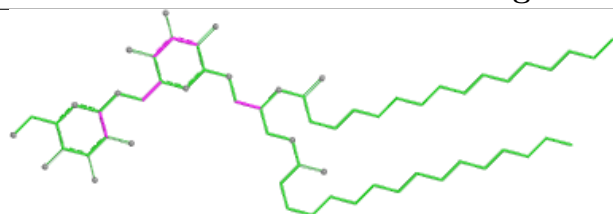


Torsions

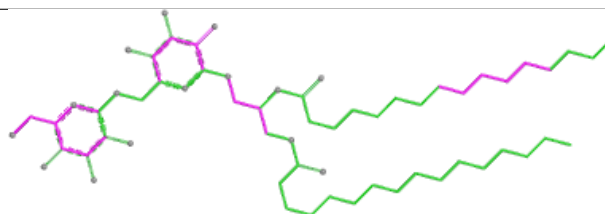


Rings

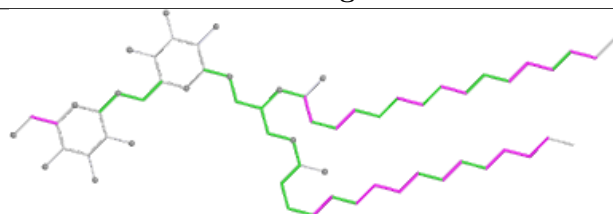
Ligand DGD h 102



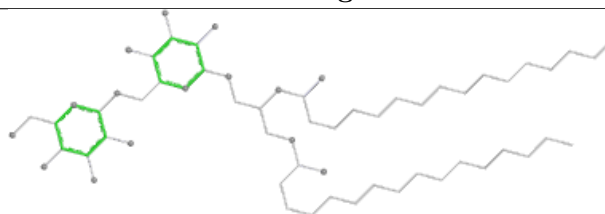
Bond lengths



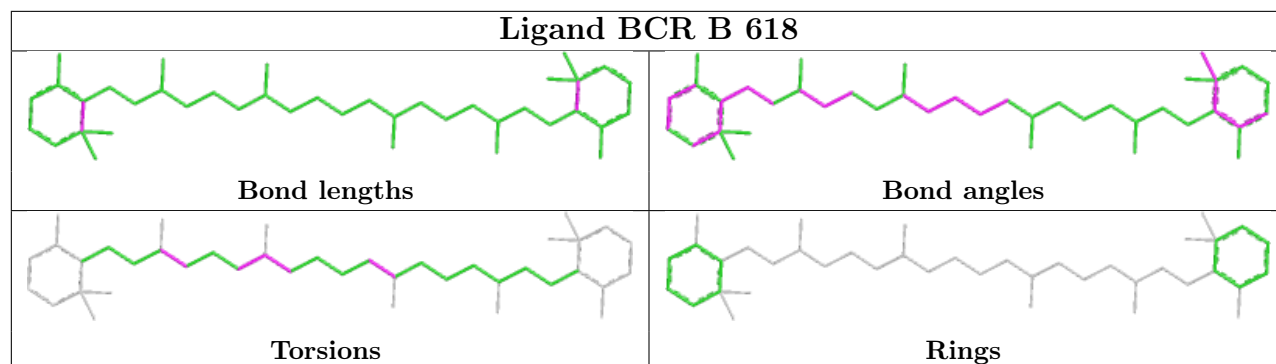
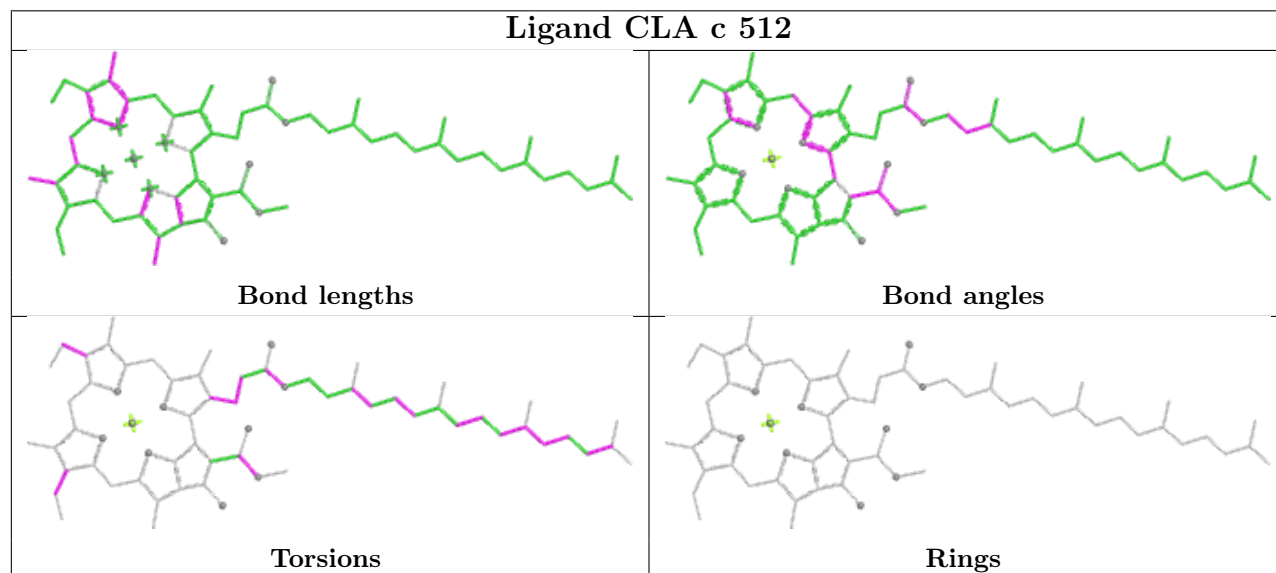
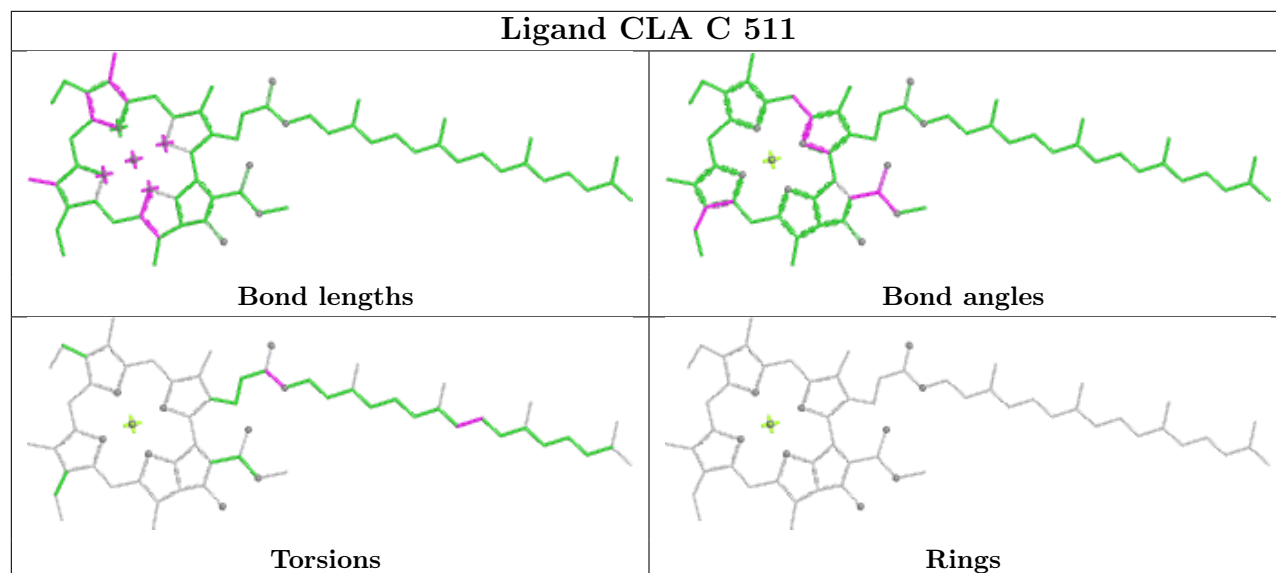
Bond angles

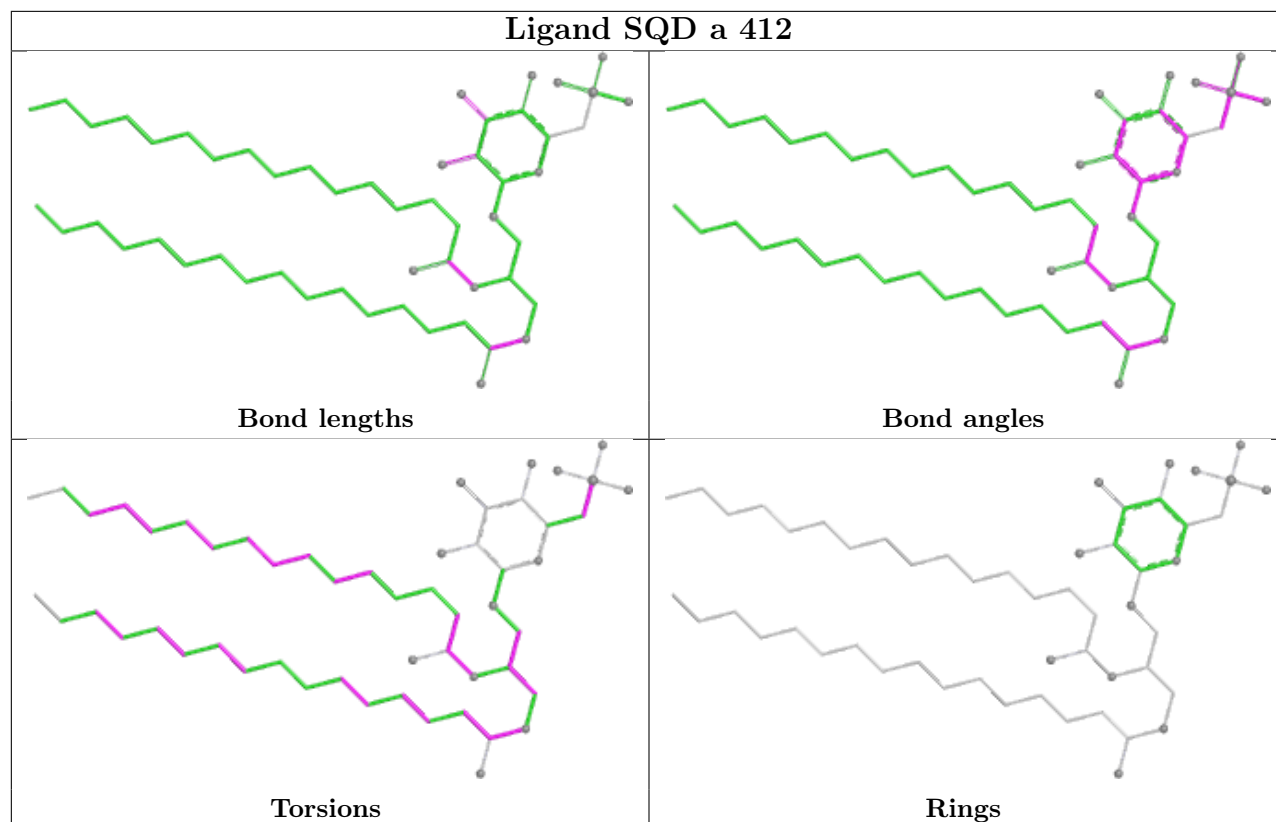


Torsions

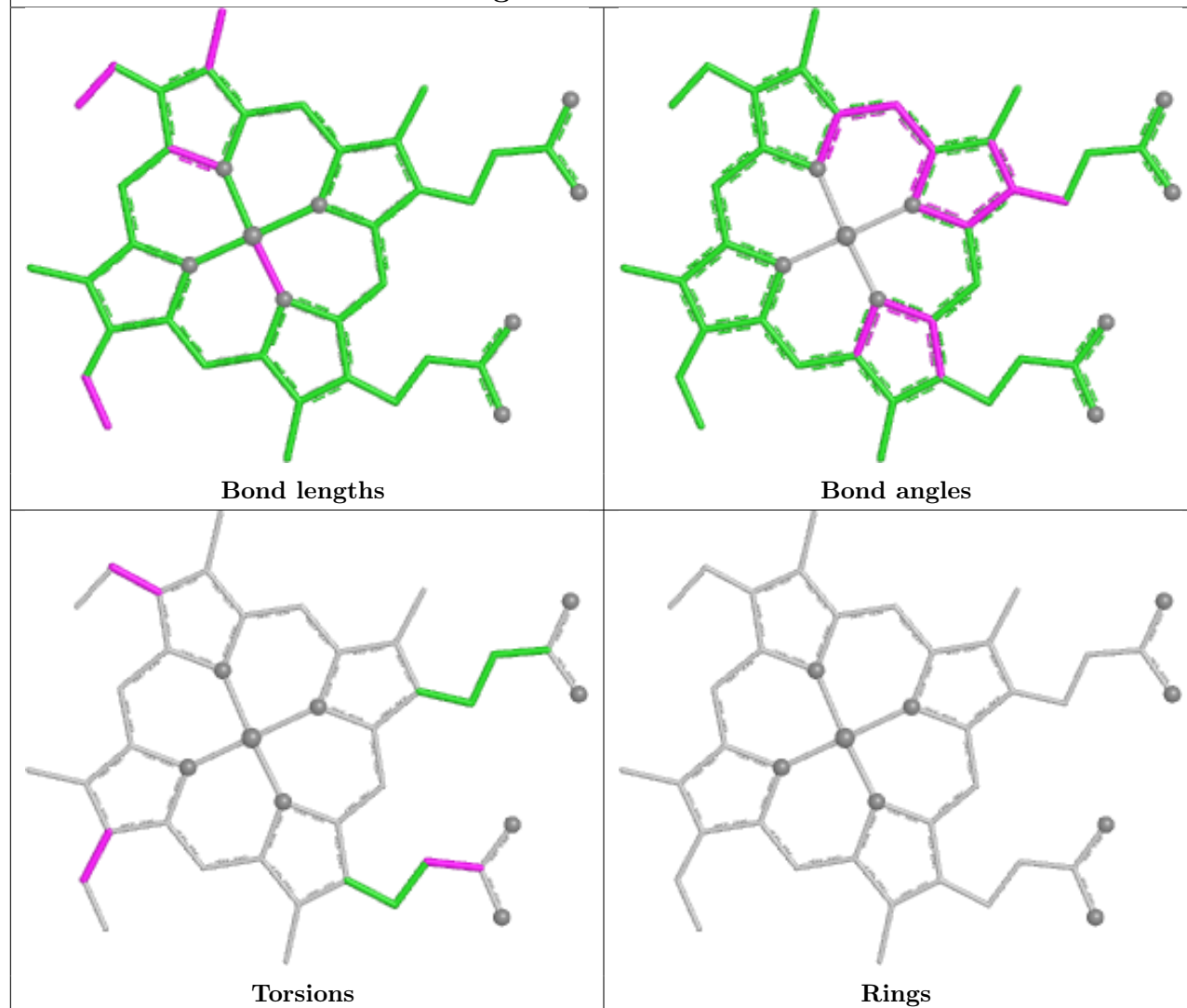


Rings

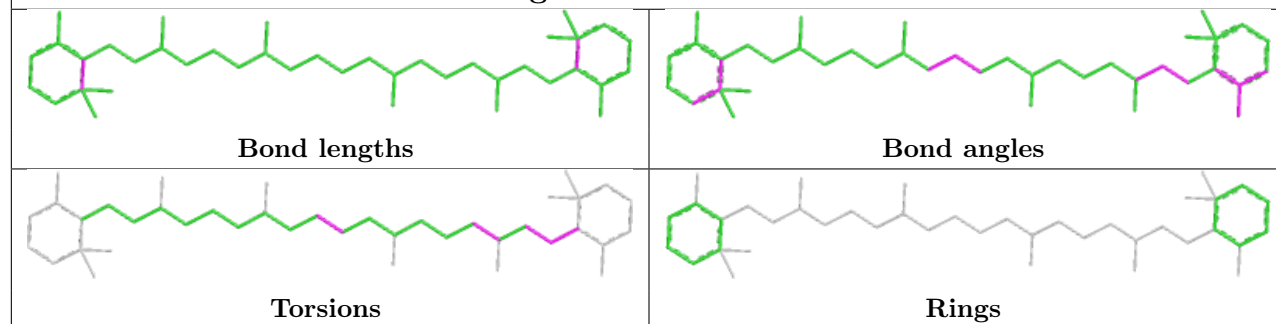


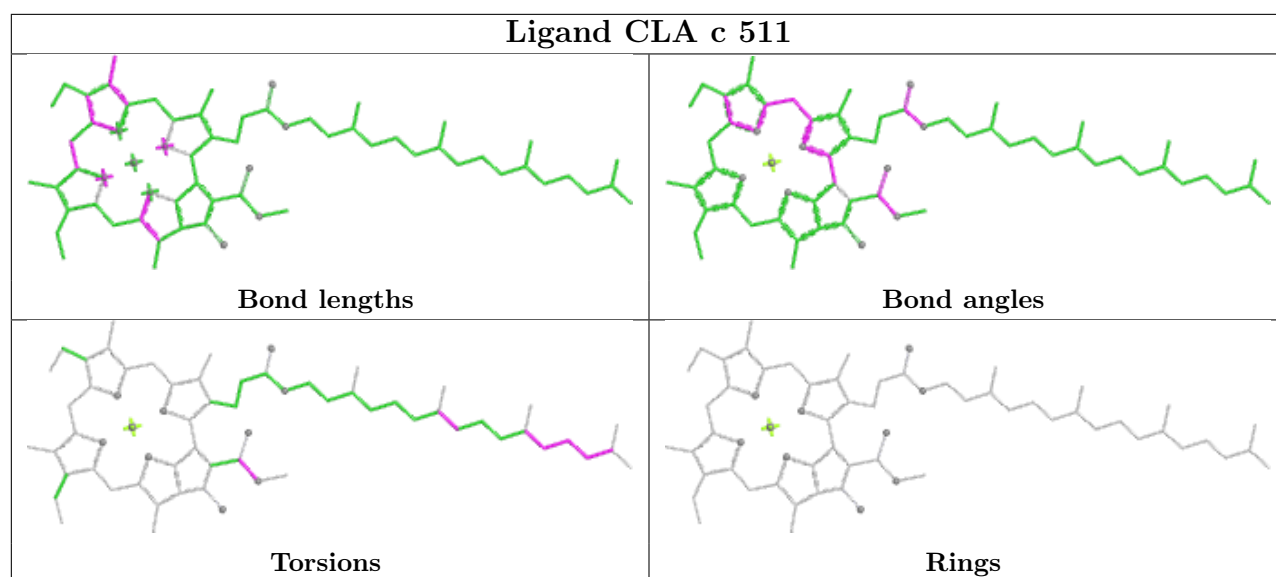
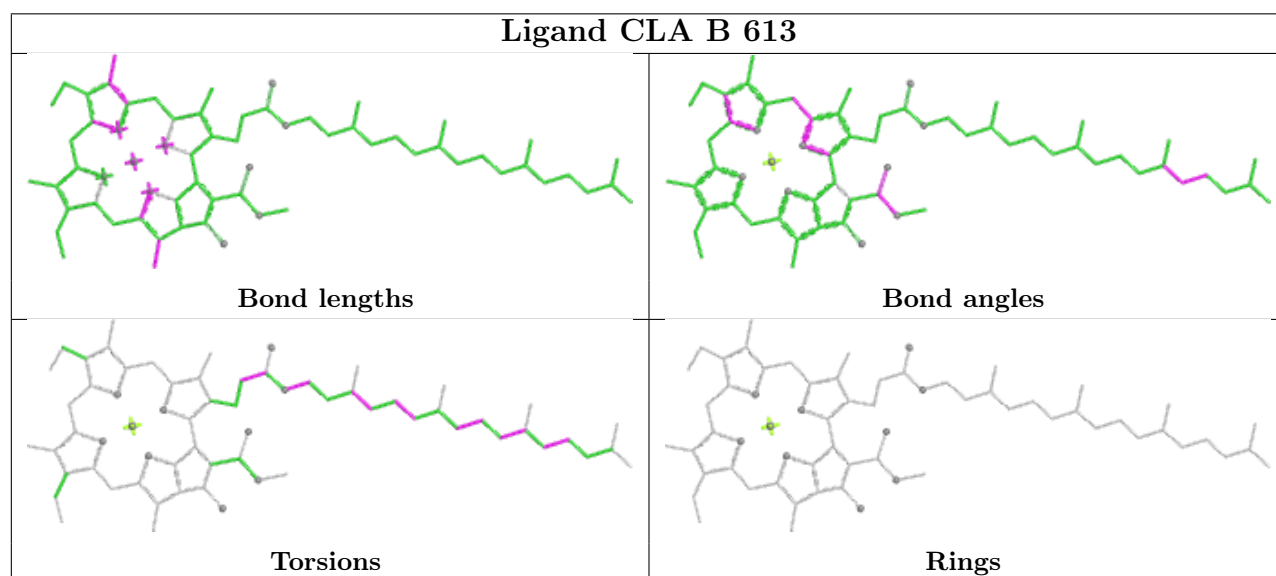
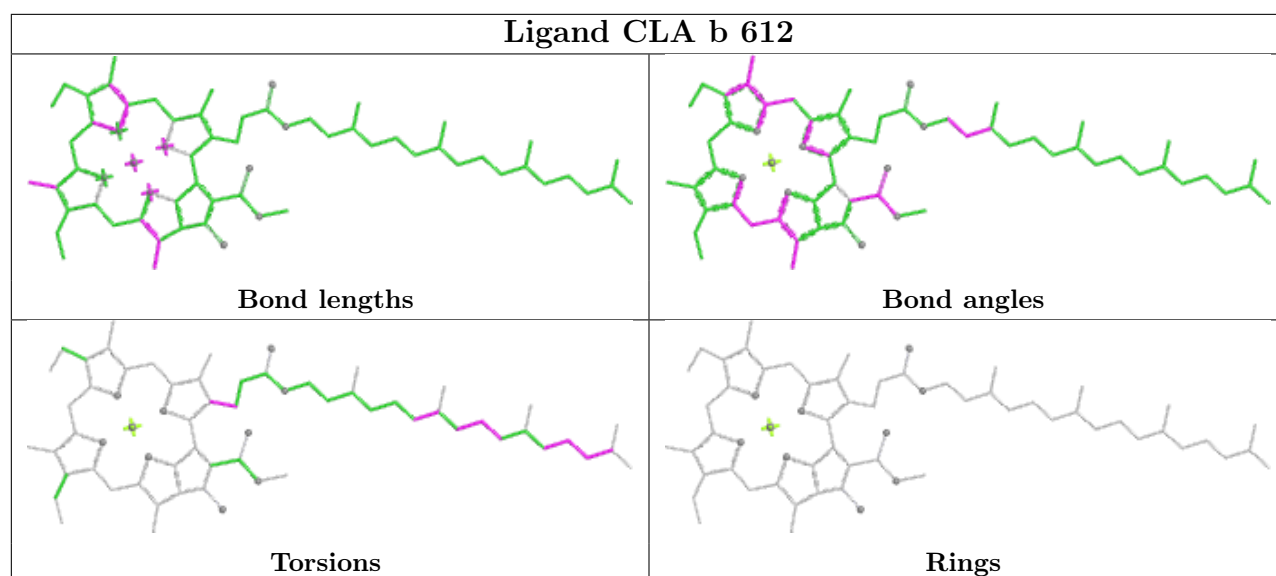


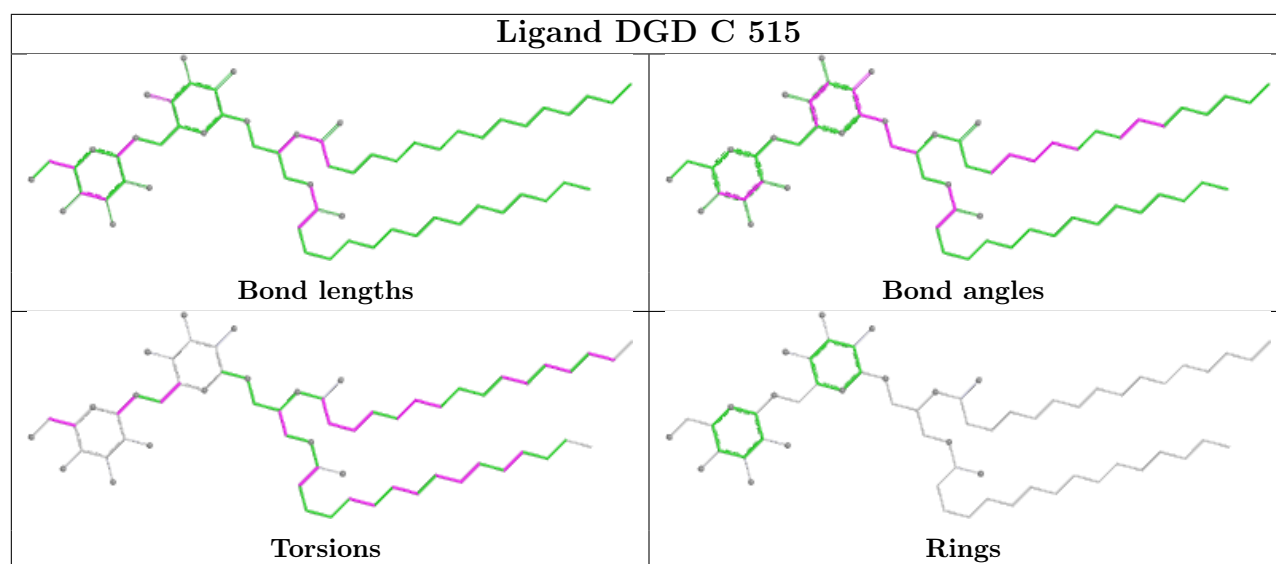
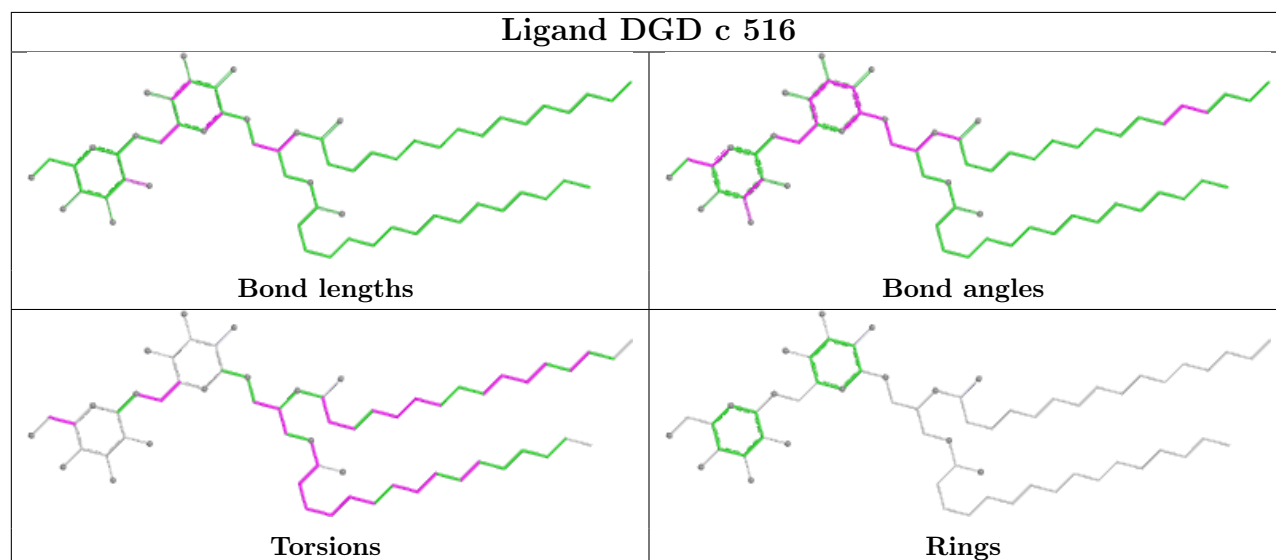
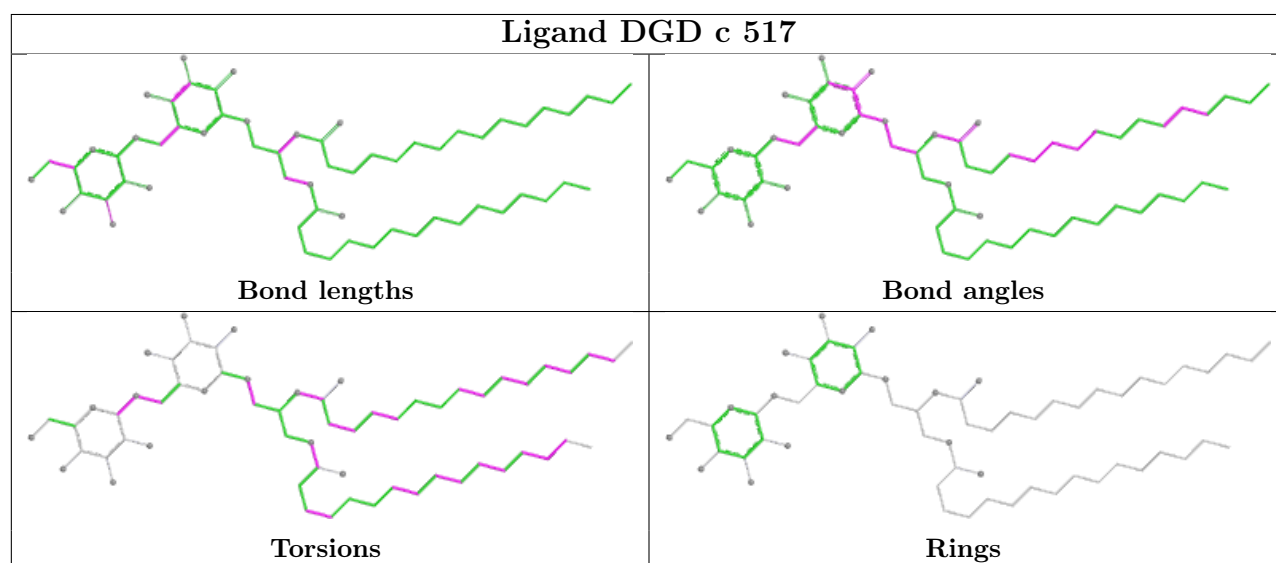
Ligand HEC V 201

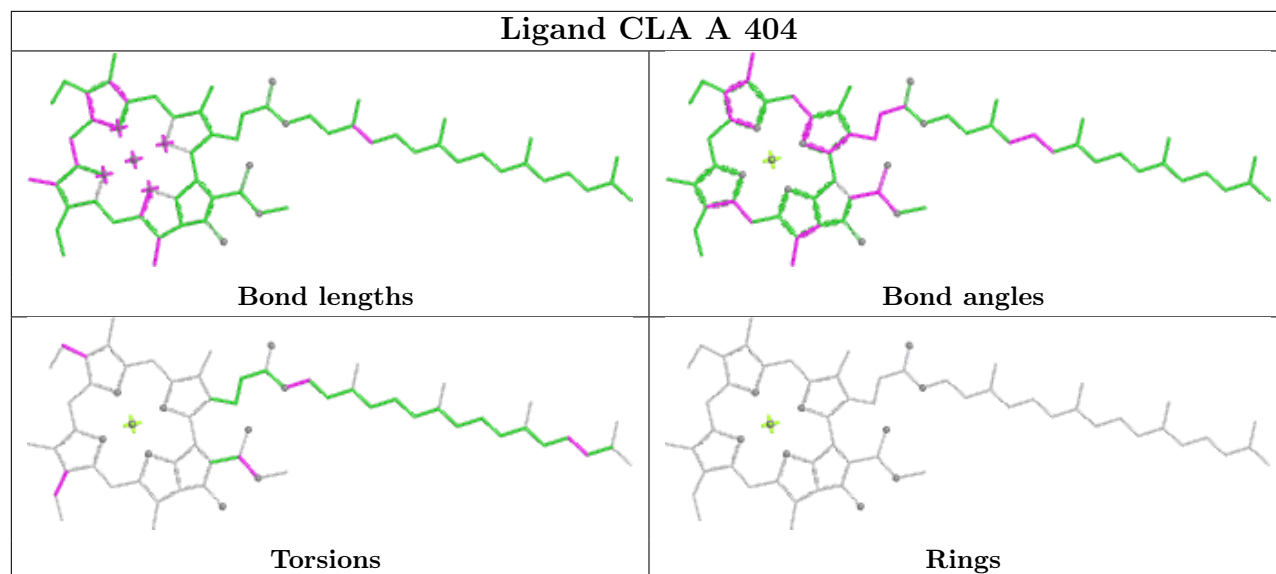
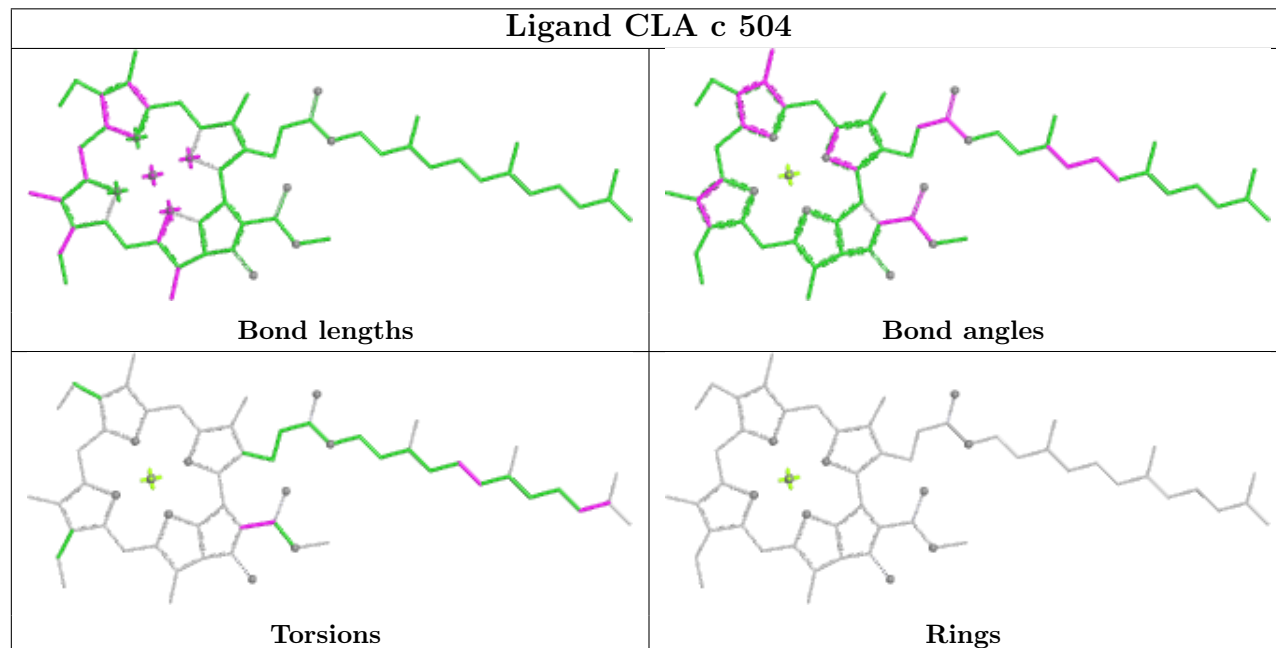


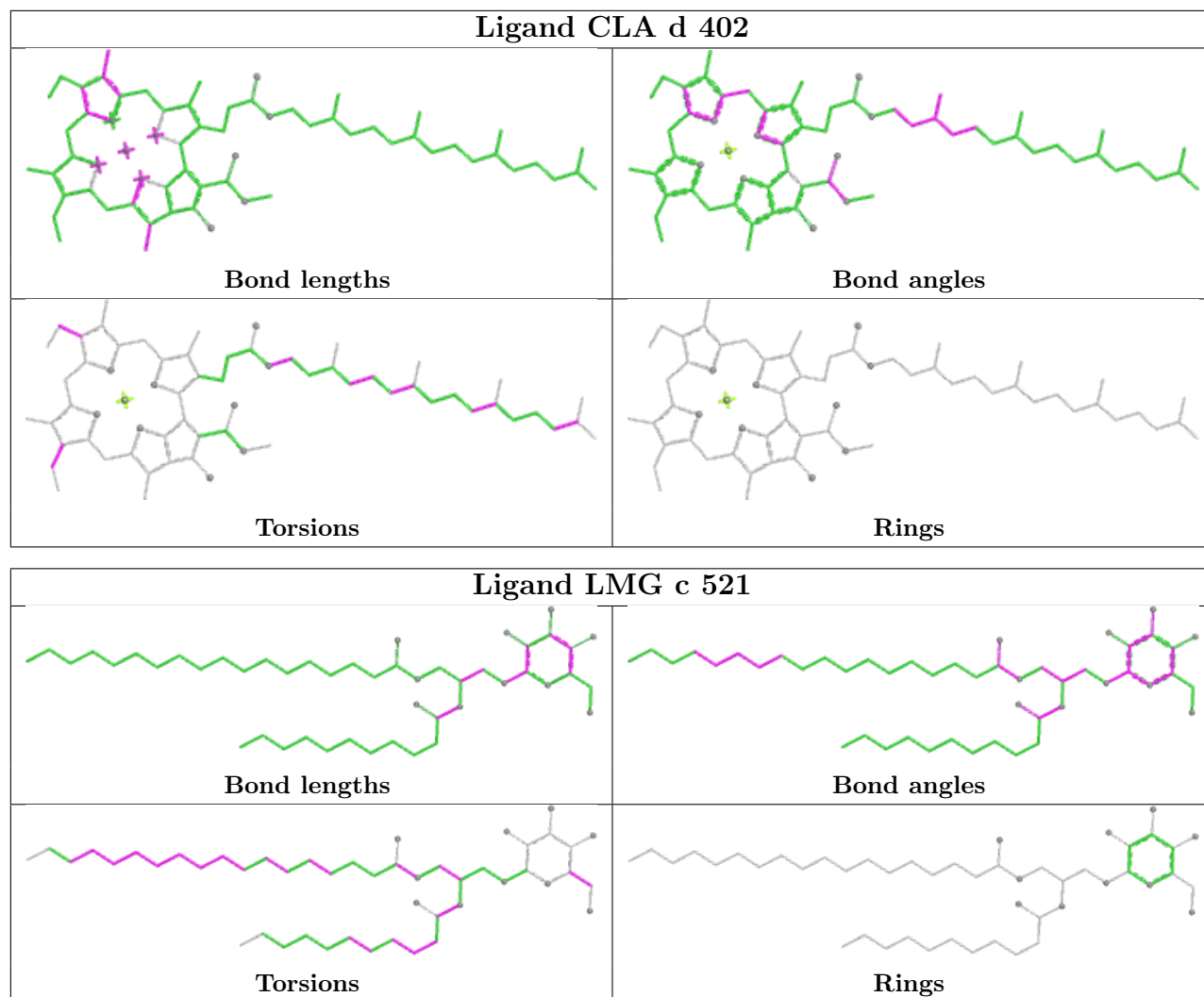
Ligand BCR D 404

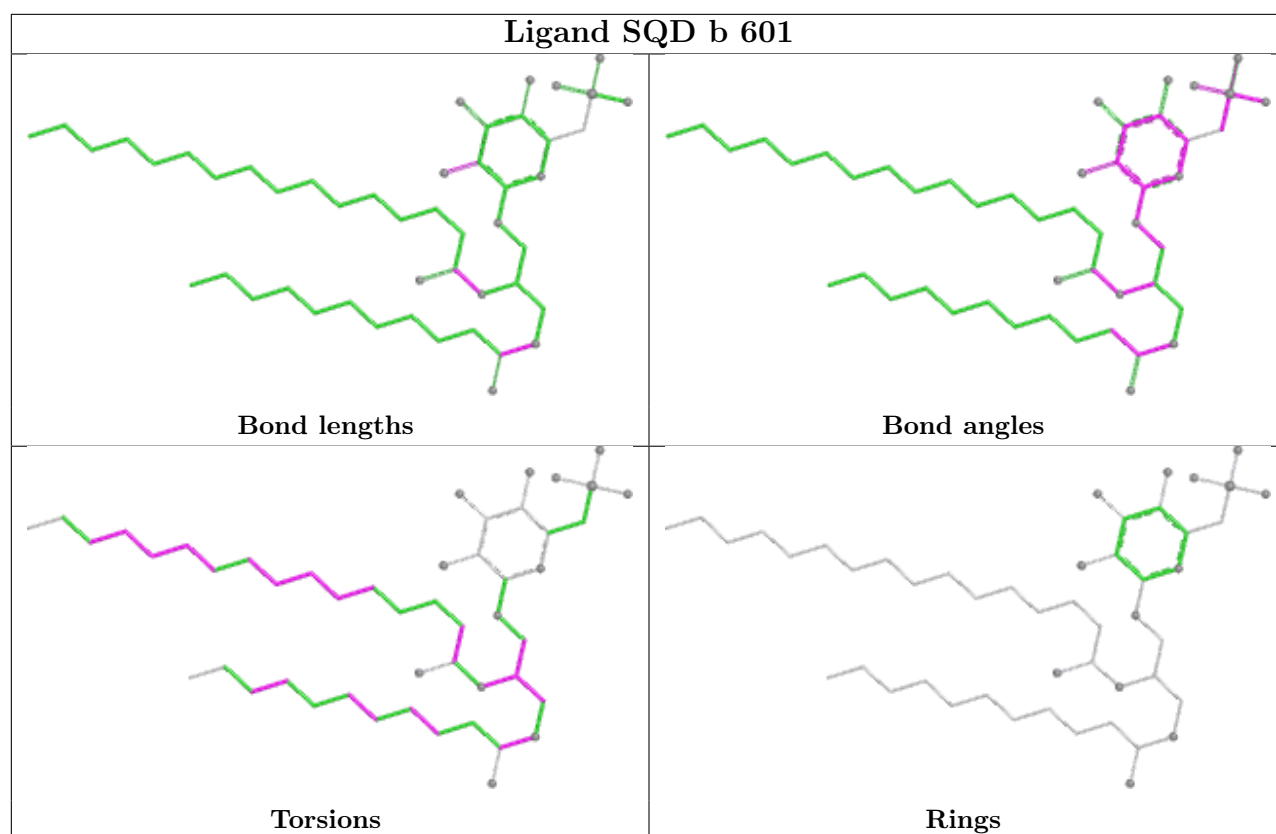
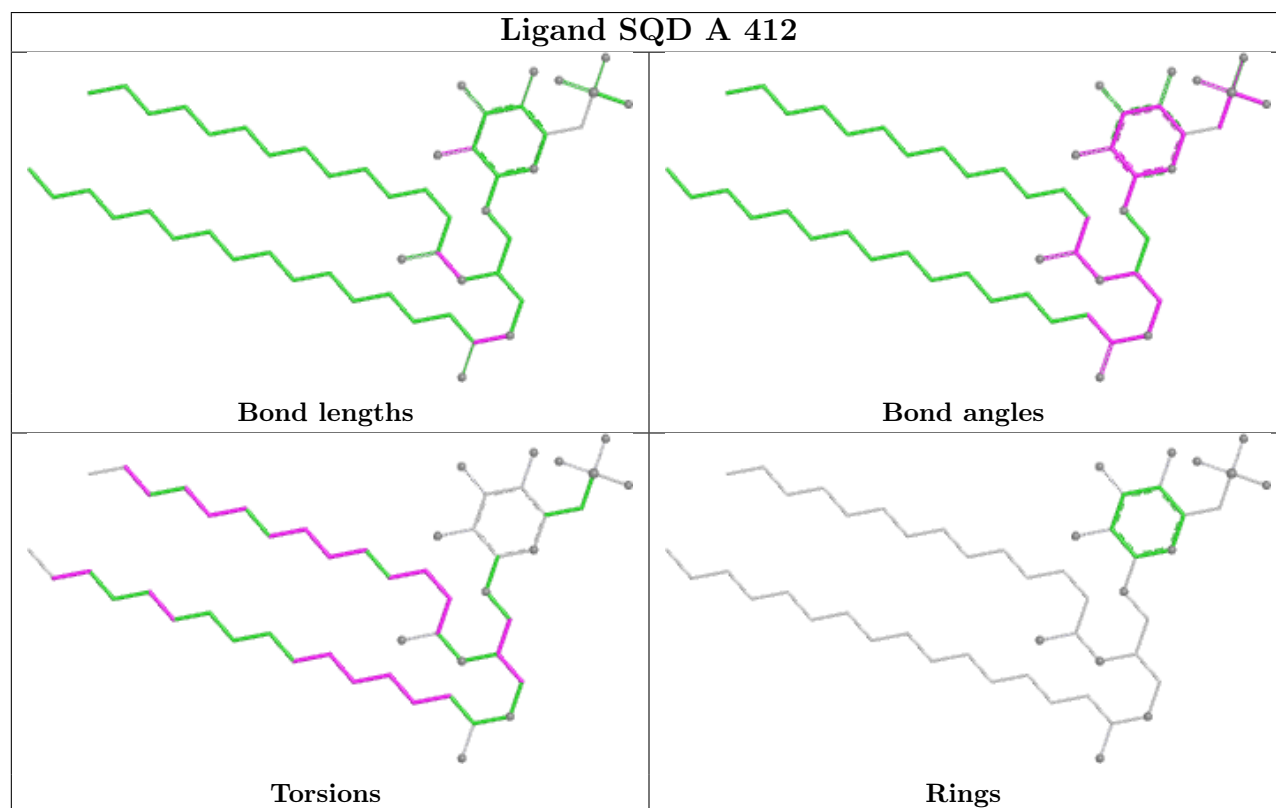


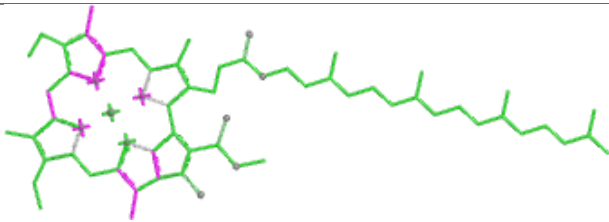
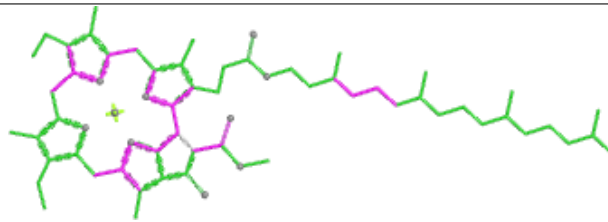
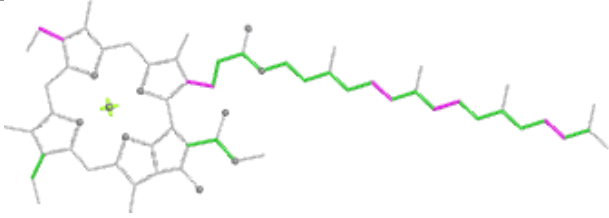
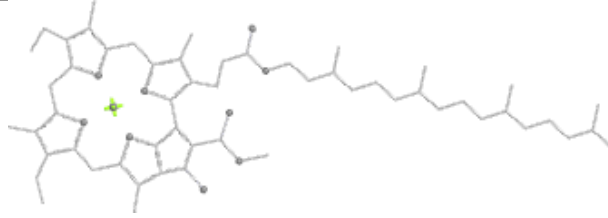


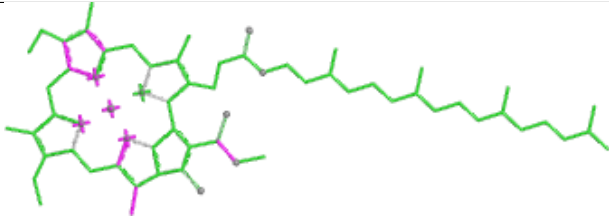
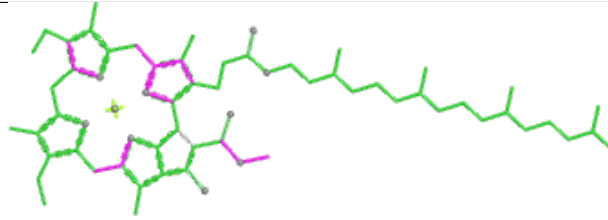
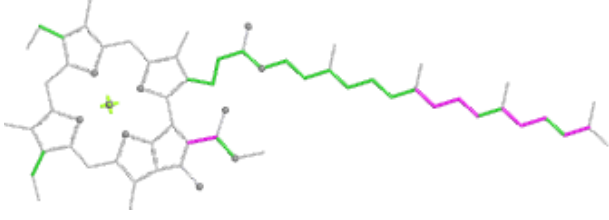
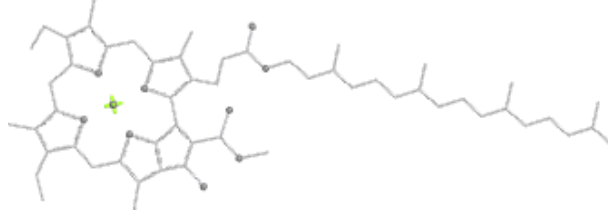


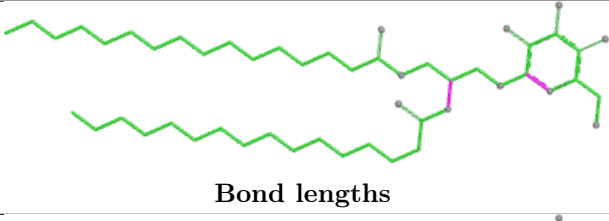
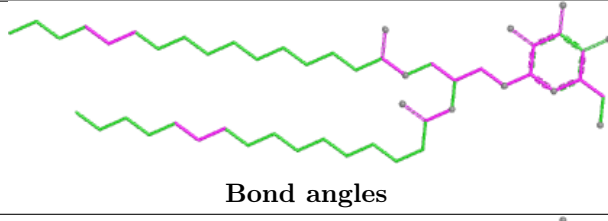
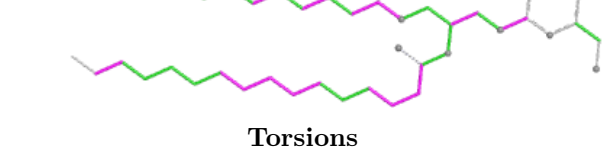
Ligand CLA A 404**Ligand CLA c 504**

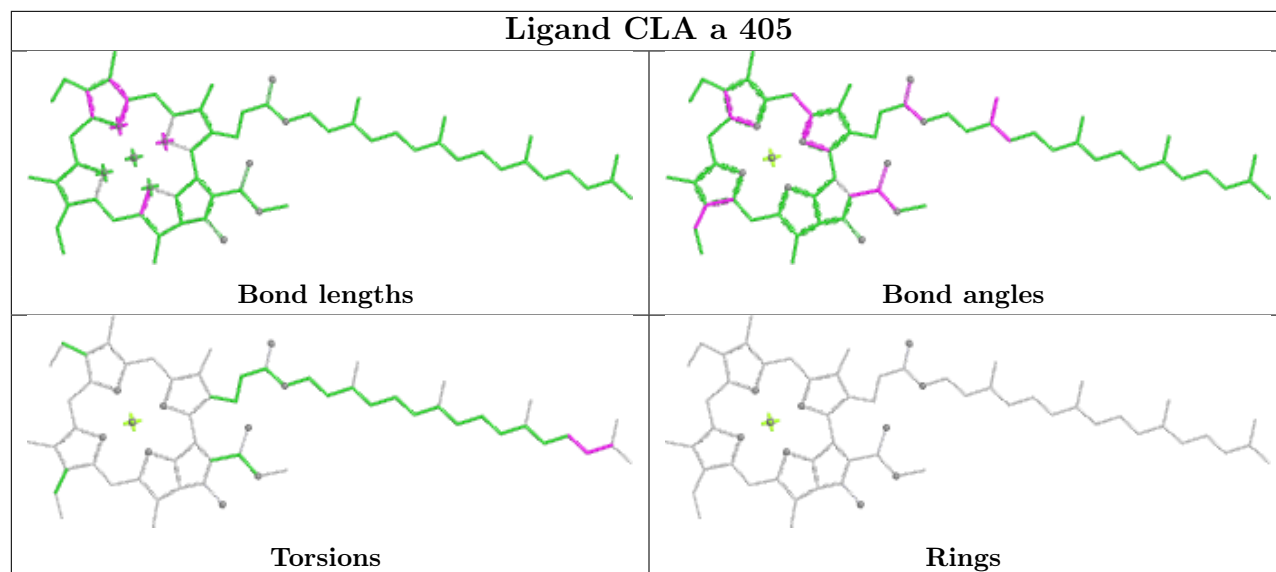
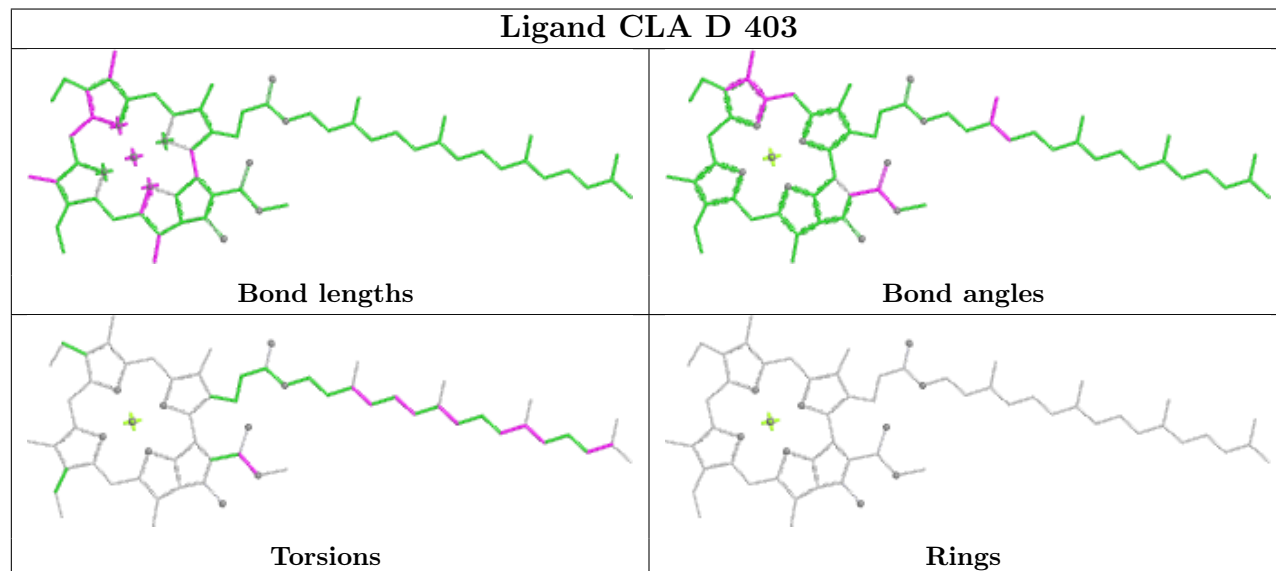


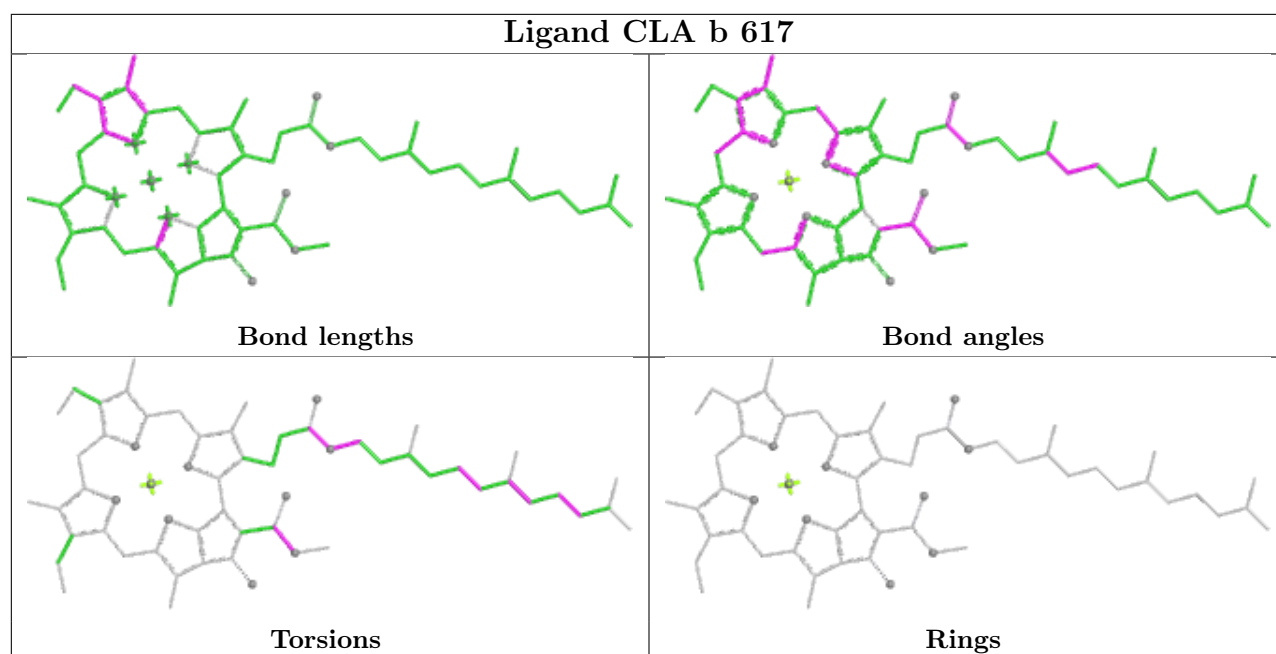
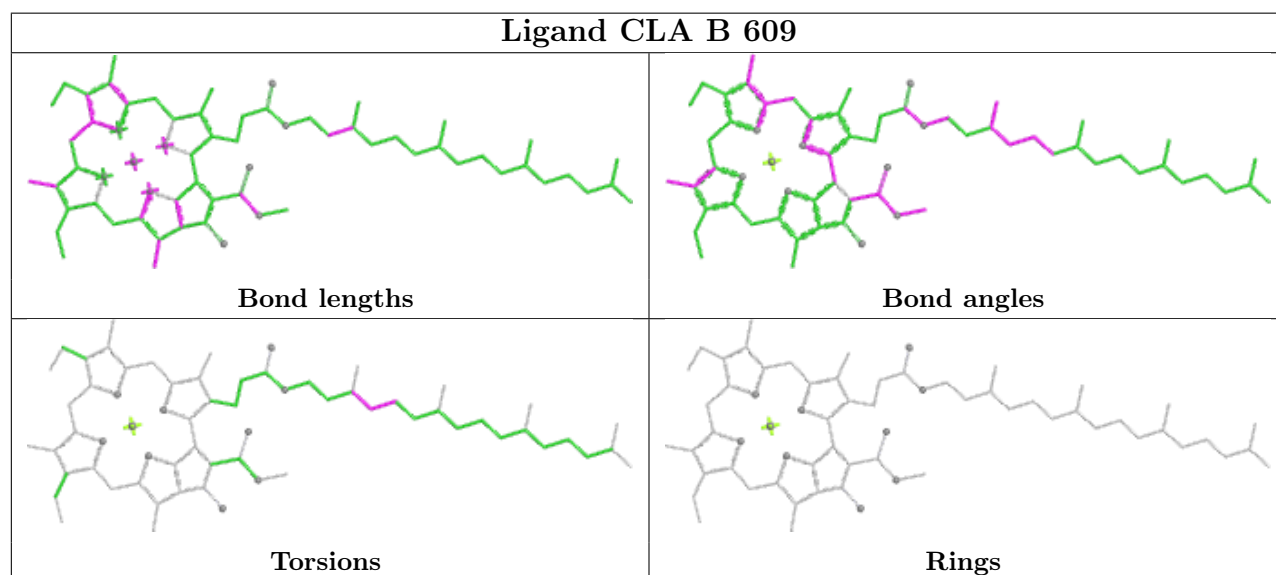
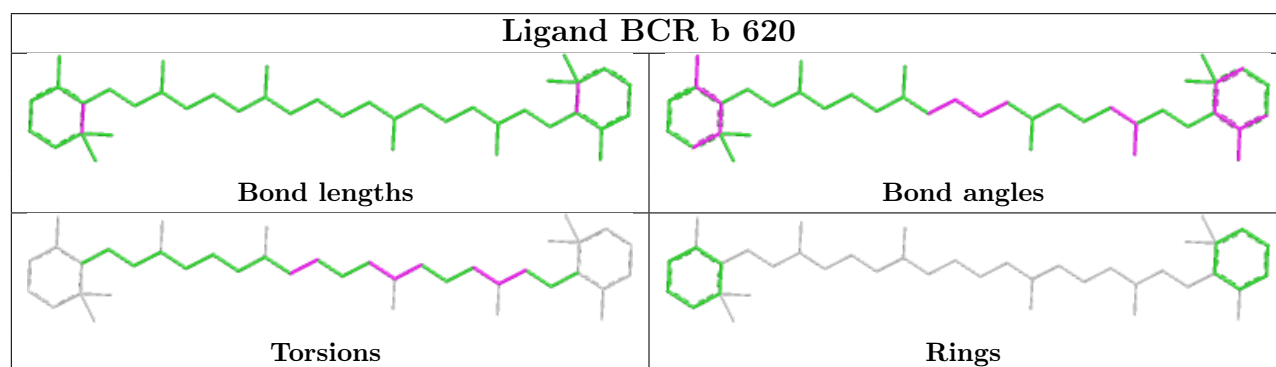


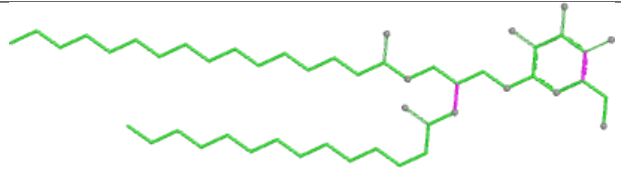
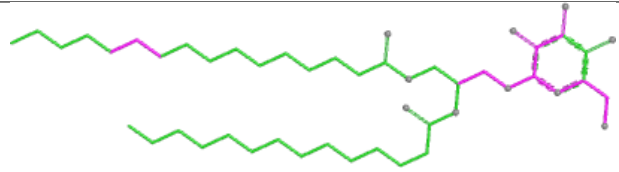
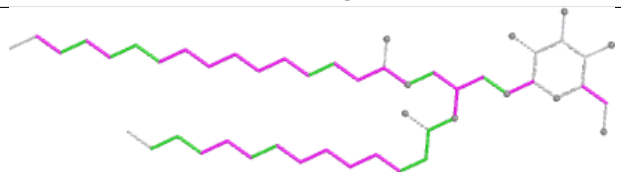
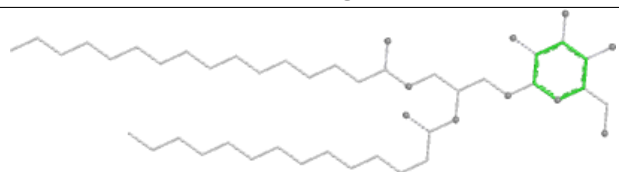
Ligand CLA C 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

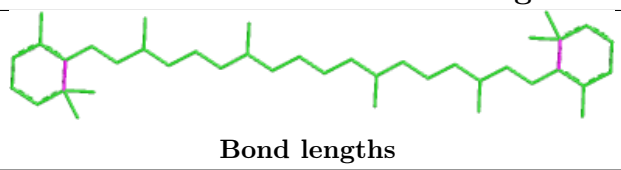
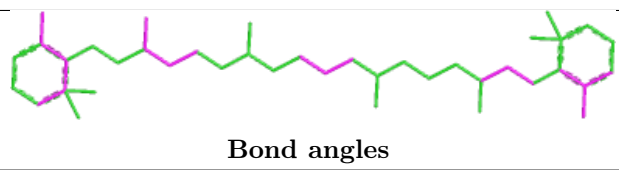
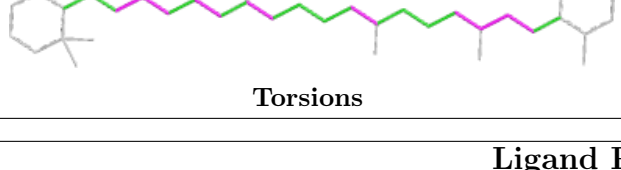
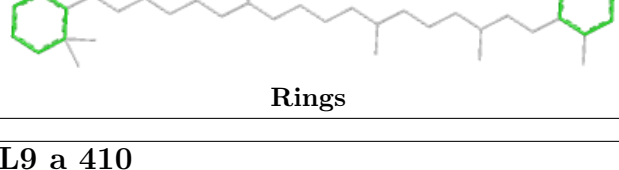
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

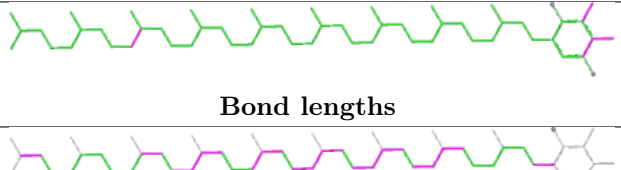
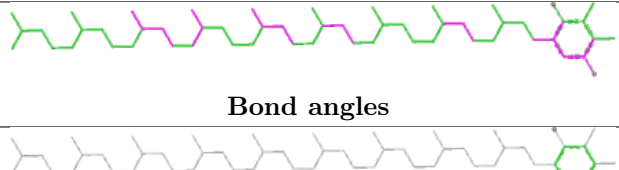
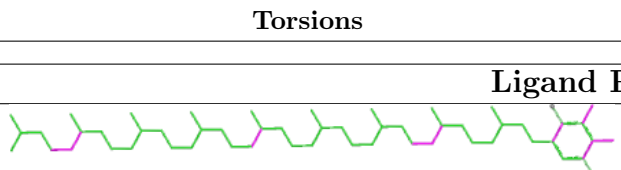
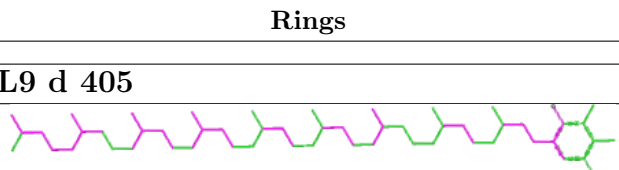
Ligand LMG m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

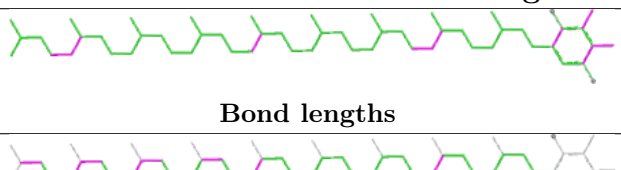
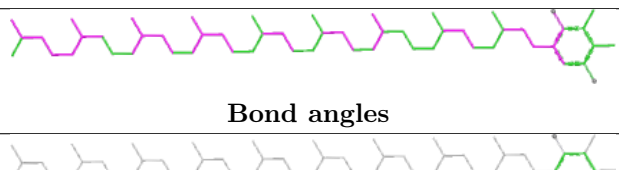
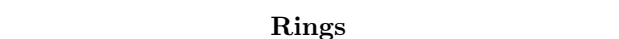
Ligand CLA a 405**Ligand CLA D 403**

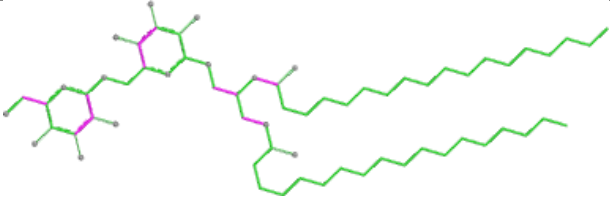
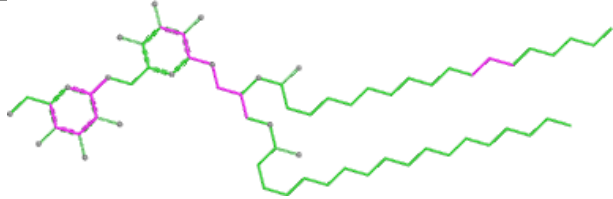
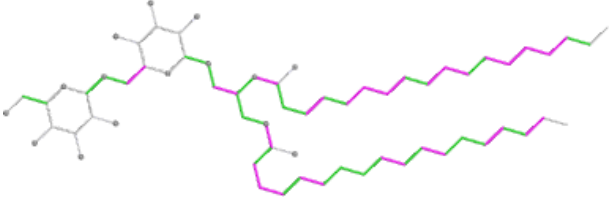
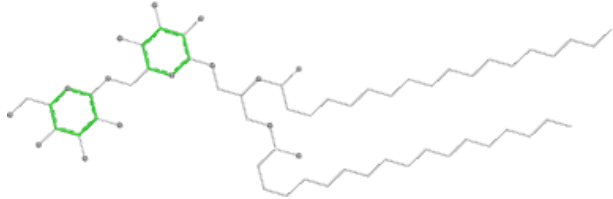
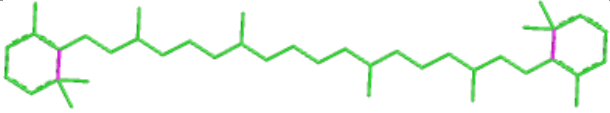
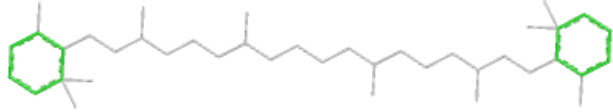
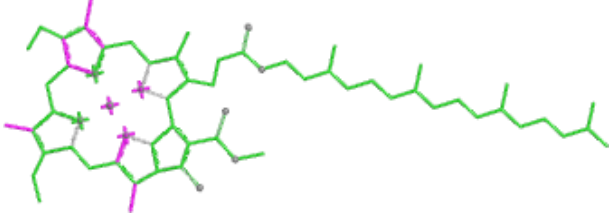
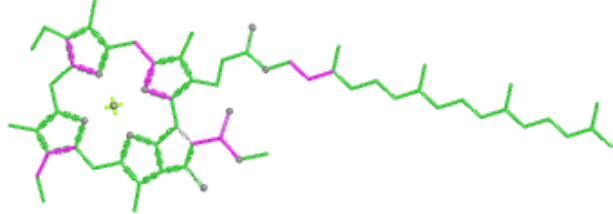
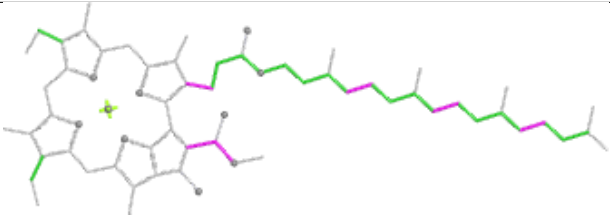
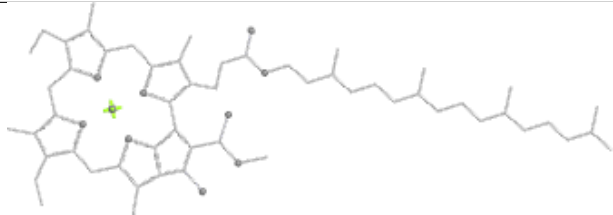


Ligand LMG c 523	
	
Bond lengths	Bond angles
	
Torsions	Rings

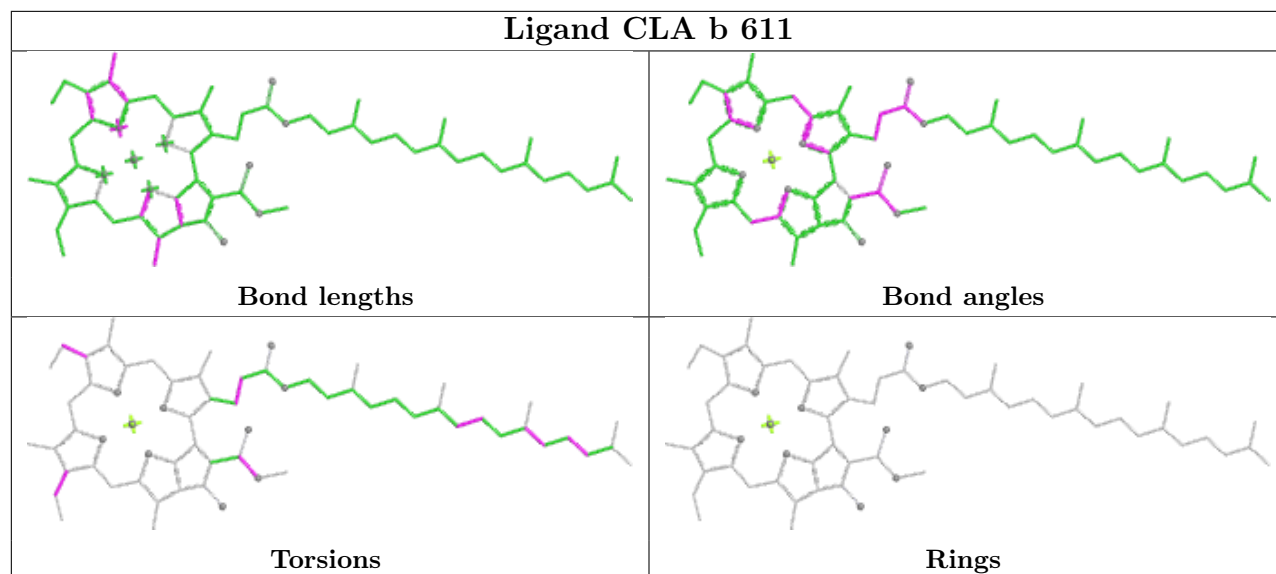
Ligand BCR Z 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

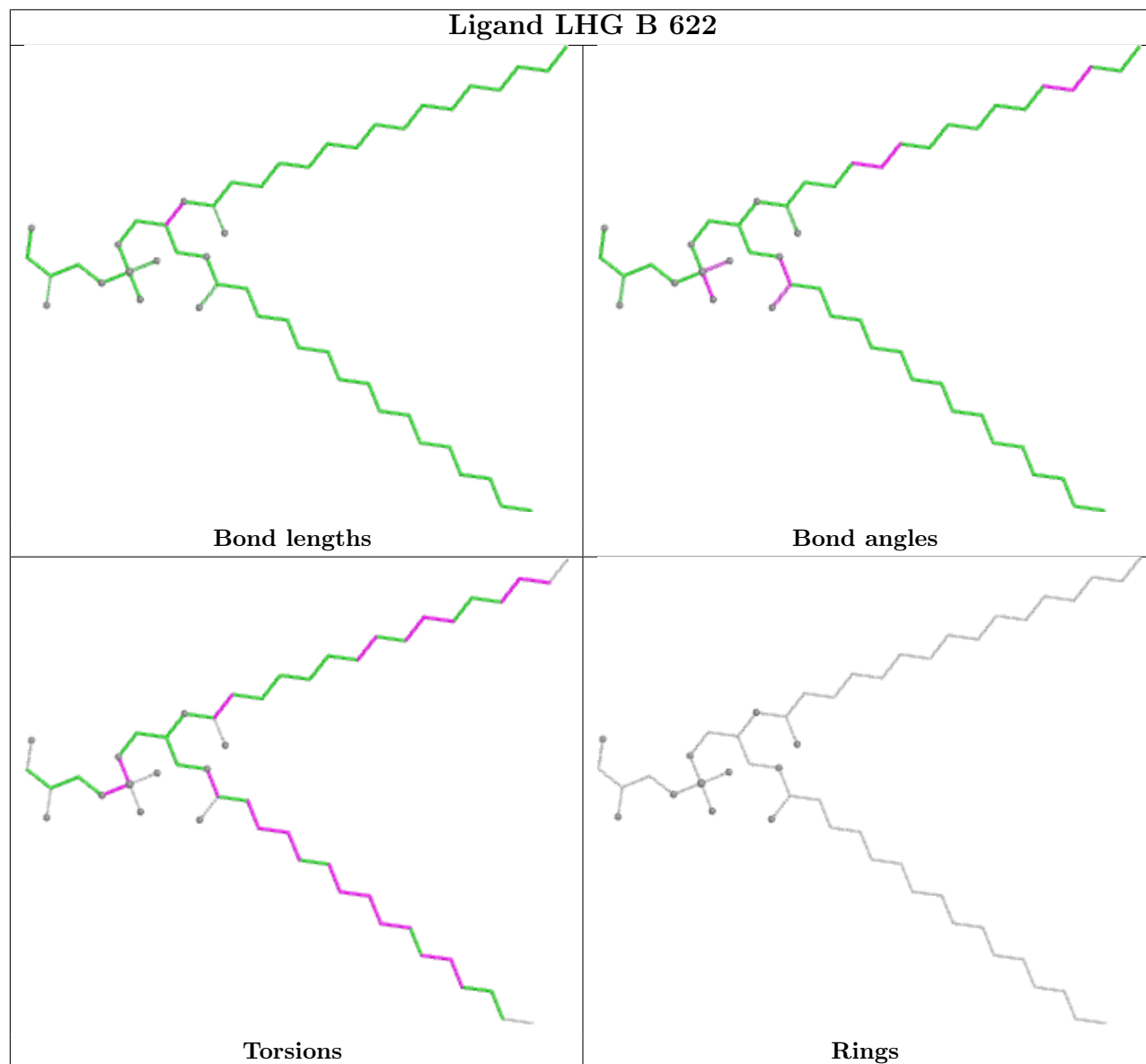
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD A 415	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR a 409	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA c 513	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

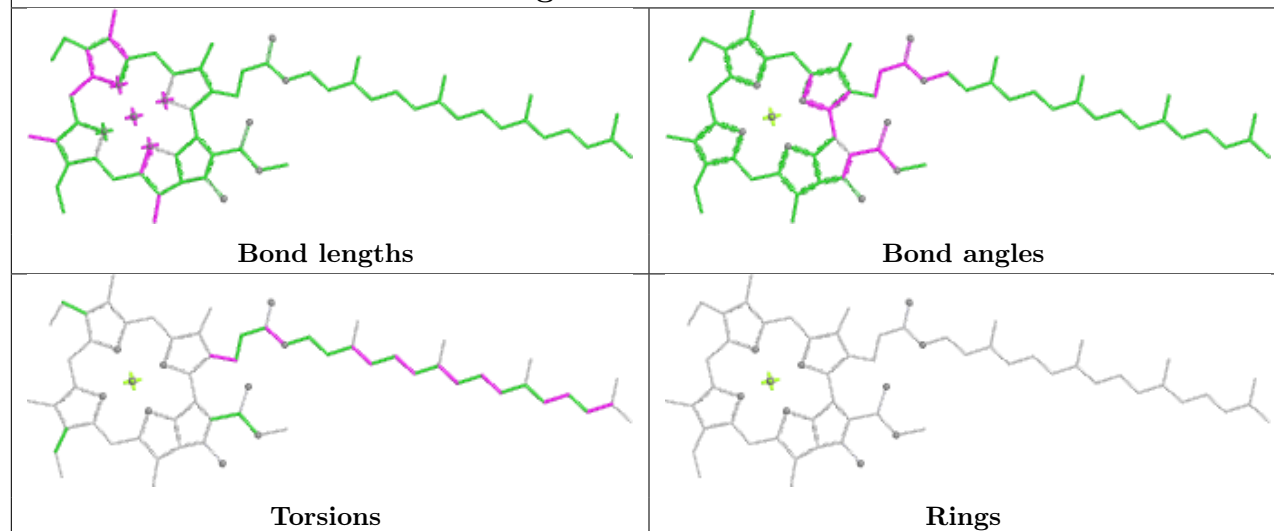
Ligand CLA b 611



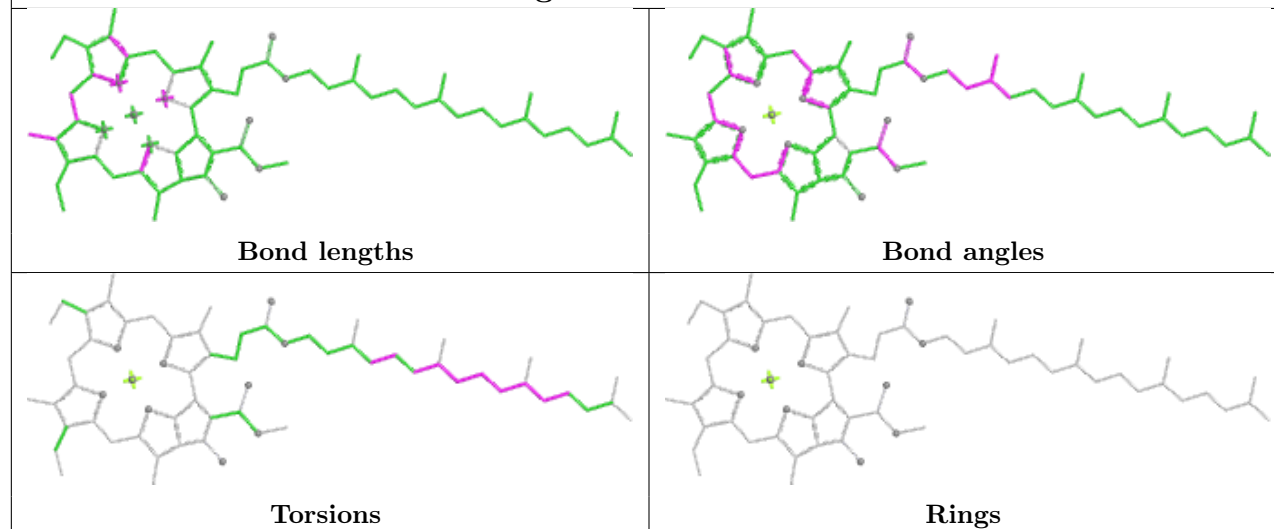
Ligand LHG B 622



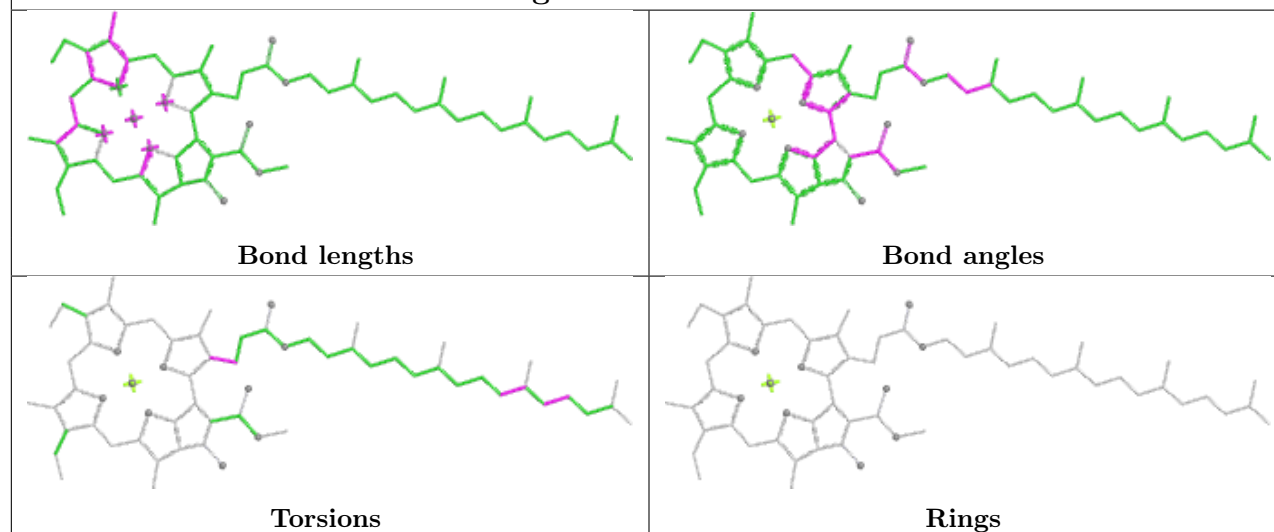
Ligand CLA a 408

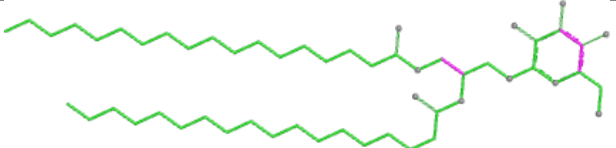
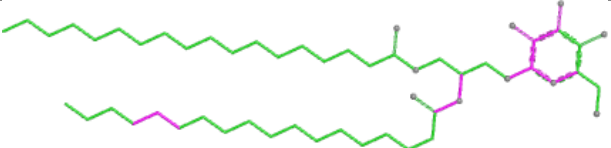
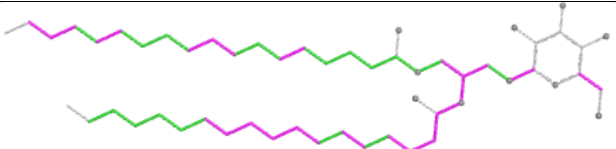
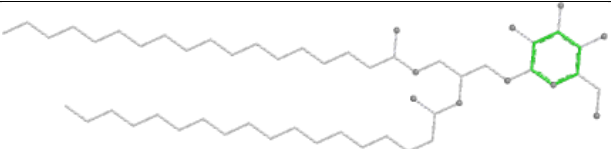


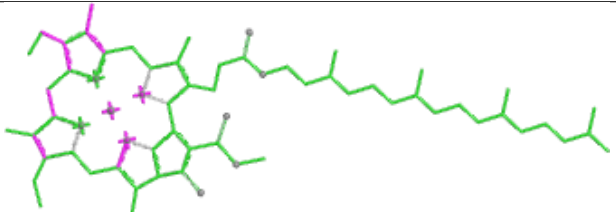
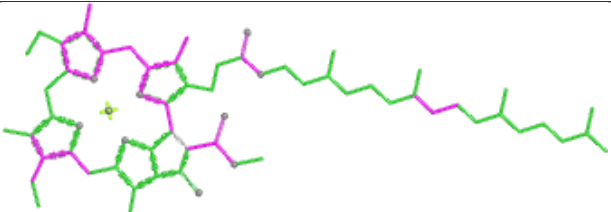
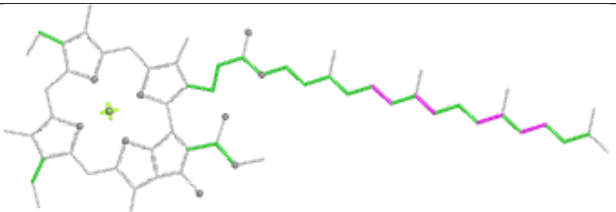
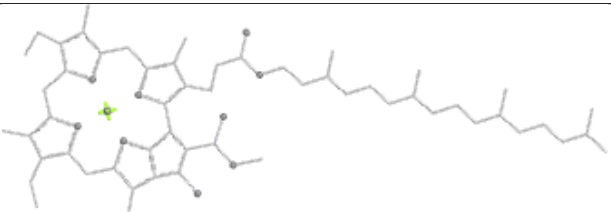
Ligand CLA b 605

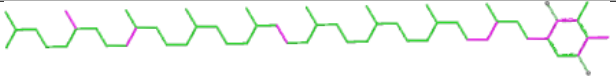
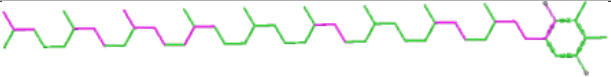
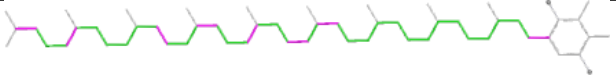
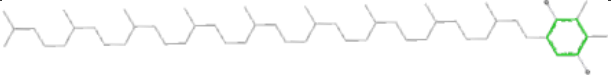


Ligand CLA B 602

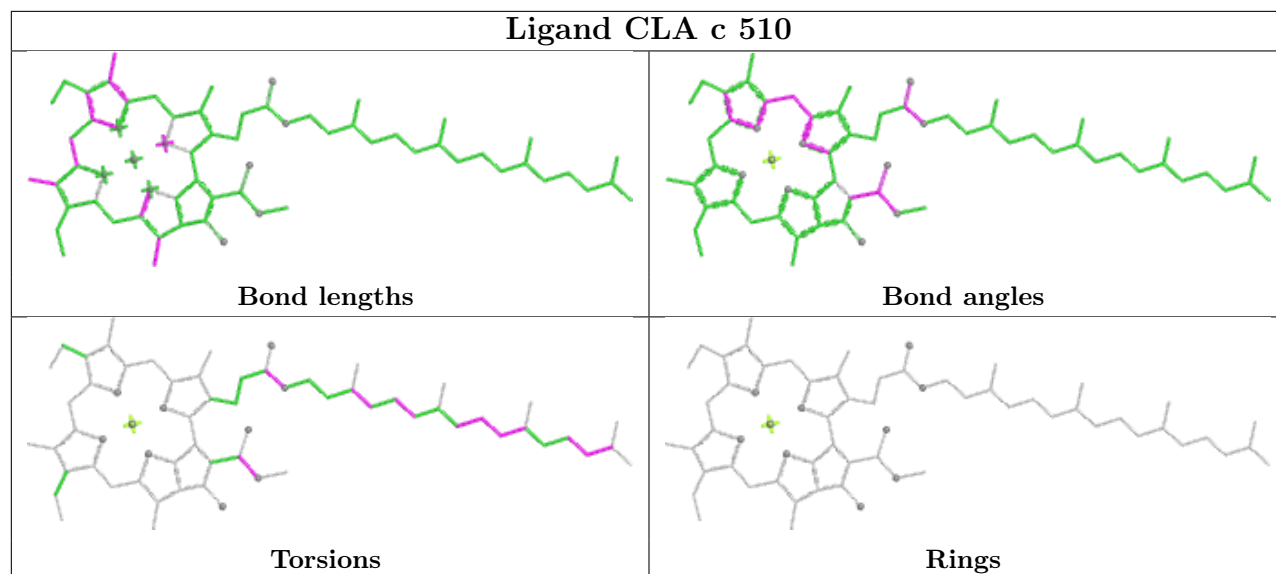


Ligand LMG b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

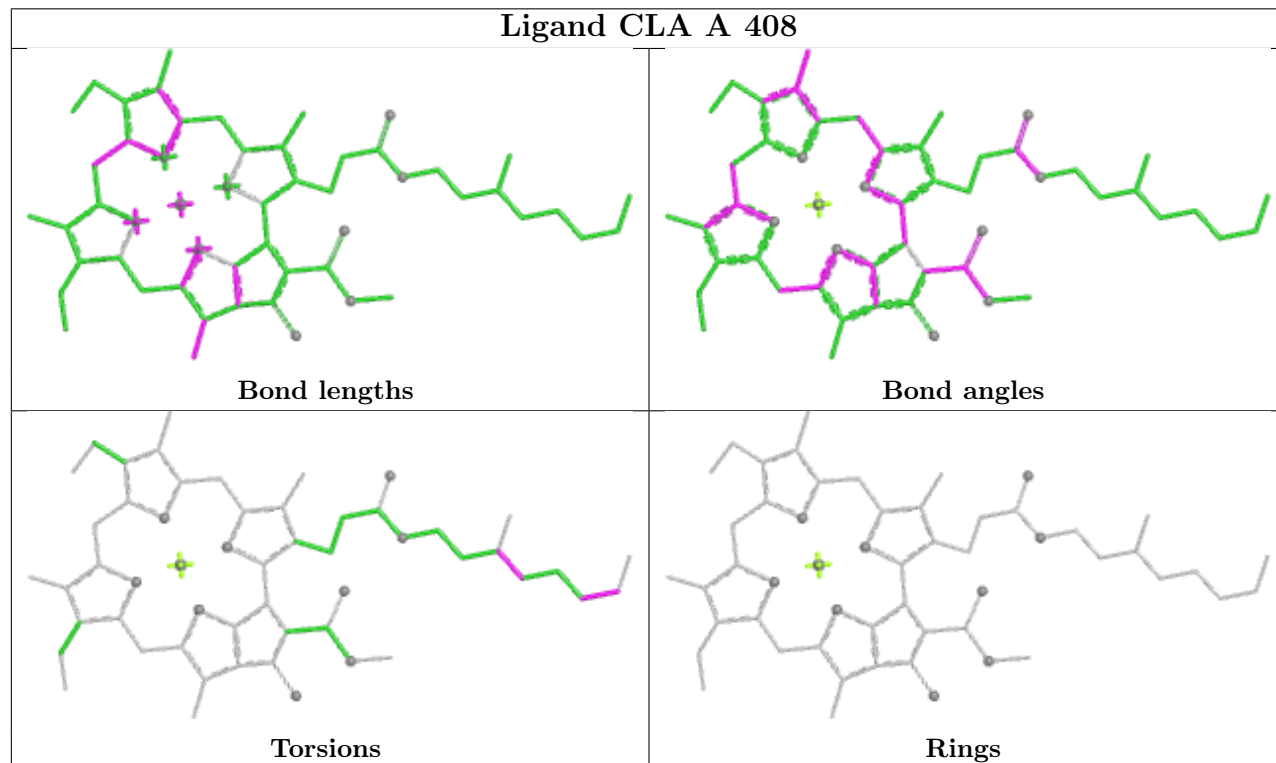
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

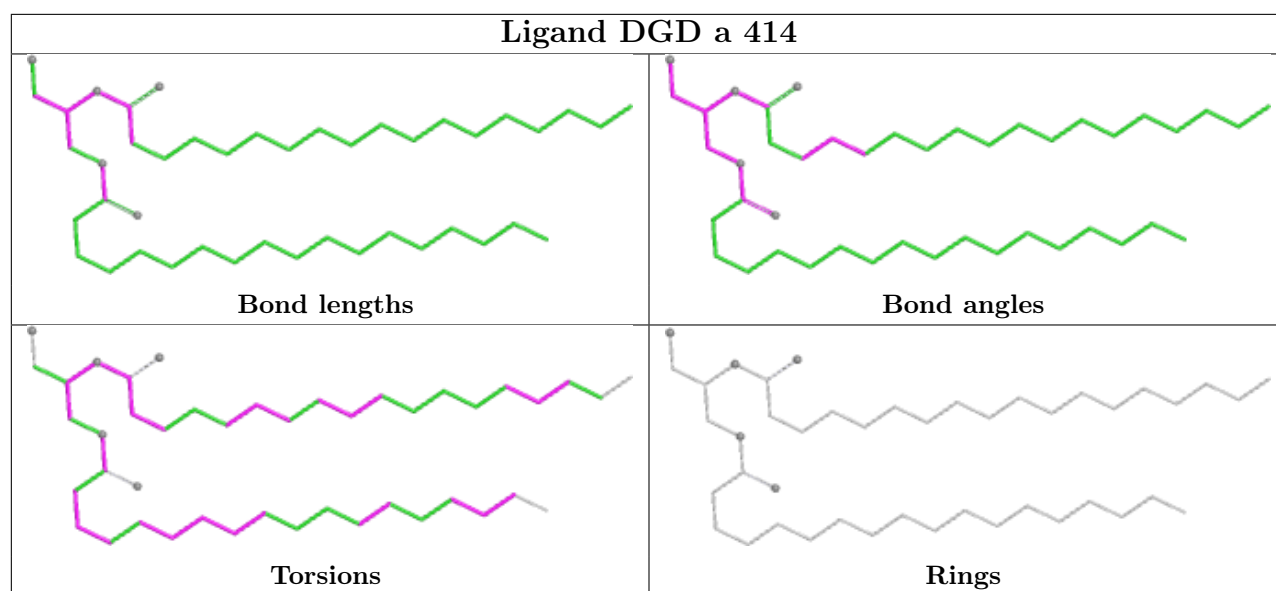
Ligand PL9 D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 510



Ligand CLA A 408





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	334/334 (100%)	-0.64	1 (0%) 90 92	12, 30, 52, 79	59 (17%)
1	a	334/334 (100%)	-0.53	1 (0%) 90 92	12, 32, 65, 89	59 (17%)
2	B	505/505 (100%)	-0.55	0 100 100	17, 35, 68, 108	4 (0%)
2	b	505/505 (100%)	-0.43	3 (0%) 85 88	21, 39, 79, 114	0
3	C	442/451 (98%)	-0.52	0 100 100	14, 39, 58, 83	7 (1%)
3	c	451/451 (100%)	-0.39	0 100 100	14, 43, 68, 105	8 (1%)
4	D	341/341 (100%)	-0.69	0 100 100	15, 32, 52, 99	1 (0%)
4	d	341/341 (100%)	-0.52	0 100 100	17, 36, 62, 92	2 (0%)
5	E	81/82 (98%)	0.07	1 (1%) 76 78	30, 55, 75, 92	1 (1%)
5	e	82/82 (100%)	0.19	0 100 100	40, 65, 90, 102	0
6	F	34/34 (100%)	-0.23	0 100 100	38, 46, 68, 86	0
6	f	34/34 (100%)	0.16	0 100 100	45, 55, 82, 95	0
7	H	65/65 (100%)	-0.33	1 (1%) 72 74	35, 44, 65, 86	0
7	h	63/65 (96%)	-0.02	0 100 100	42, 52, 70, 81	0
8	I	35/36 (97%)	-0.45	0 100 100	33, 41, 72, 88	0
8	i	35/36 (97%)	-0.22	1 (2%) 53 55	34, 43, 78, 88	0
9	J	36/36 (100%)	-0.23	0 100 100	39, 54, 81, 104	0
9	j	36/36 (100%)	0.13	0 100 100	43, 57, 94, 98	0
10	K	37/37 (100%)	-0.06	0 100 100	31, 57, 76, 78	1 (2%)
10	k	37/37 (100%)	0.20	0 100 100	48, 62, 79, 89	0
11	L	37/37 (100%)	-0.68	0 100 100	26, 32, 71, 77	0
11	l	36/37 (97%)	-0.59	0 100 100	27, 33, 82, 92	0
12	M	32/33 (96%)	-0.53	0 100 100	30, 35, 62, 80	0
12	m	31/33 (93%)	-0.54	0 100 100	28, 37, 53, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.34	0 100 100	22, 44, 91, 155	1 (0%)
13	o	244/244 (100%)	-0.34	1 (0%) 88 90	26, 43, 86, 142	0
14	T	29/30 (96%)	-0.65	0 100 100	26, 35, 64, 78	0
14	t	29/30 (96%)	-0.52	1 (3%) 48 48	26, 34, 87, 99	0
15	U	97/97 (100%)	-0.34	0 100 100	33, 47, 73, 105	0
15	u	97/97 (100%)	-0.38	1 (1%) 79 82	30, 43, 62, 97	0
16	V	137/137 (100%)	-0.49	0 100 100	29, 43, 60, 87	0
16	v	137/137 (100%)	-0.23	0 100 100	34, 51, 74, 89	0
17	Y	27/30 (90%)	0.97	3 (11%) 10 10	58, 84, 125, 131	0
17	y	30/30 (100%)	0.57	0 100 100	65, 81, 97, 118	0
18	X	38/38 (100%)	-0.03	0 100 100	42, 54, 83, 86	0
18	x	38/38 (100%)	0.09	1 (2%) 57 59	50, 63, 95, 108	0
19	Z	62/62 (100%)	0.57	2 (3%) 50 50	53, 71, 122, 140	0
19	z	62/62 (100%)	0.71	2 (3%) 50 50	59, 76, 119, 136	0
20	R	34/34 (100%)	0.75	1 (2%) 53 55	65, 77, 100, 106	0
20	r	31/34 (91%)	1.08	1 (3%) 50 50	75, 93, 109, 117	0
All	All	5300/5326 (99%)	-0.38	21 (0%) 88 90	12, 40, 81, 155	143 (2%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	35	LEU	3.6
19	z	33	TRP	3.4
1	A	13	LEU	3.0
15	u	53	ALA	2.9
13	o	58	ASN	2.9

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
12	FME	M	1	10/11	0.95	0.08	34,48,63,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	FME	t	1	10/11	0.95	0.08	29,37,64,69	0
8	FME	i	1	10/11	0.96	0.07	35,48,60,64	0
12	FME	m	1	10/11	0.96	0.08	31,46,65,72	0
8	FME	I	1	10/11	0.96	0.07	35,54,65,68	0
14	FME	T	1	10/11	0.97	0.07	27,44,65,71	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
34	UNL	H	103	53/-	0.78	0.15	43,73,86,90	0
34	UNL	b	627	26/-	0.80	0.16	42,58,69,74	0
27	LMG	b	623	23/55	0.81	0.17	43,70,95,98	0
29	LHG	e	101	42/49	0.82	0.12	57,87,116,139	0
27	LMG	c	521	48/55	0.82	0.14	44,77,121,128	0
29	LHG	A	413	49/49	0.82	0.14	51,85,125,130	0
27	LMG	b	622	55/55	0.83	0.15	35,73,101,104	0
34	UNL	c	522	28/-	0.83	0.12	46,66,88,93	0
34	UNL	a	415	28/-	0.84	0.11	39,66,77,79	0
34	UNL	b	626	55/-	0.84	0.12	44,61,77,81	0
34	UNL	E	102	28/-	0.84	0.13	52,79,91,94	0
30	DGD	A	415	66/66	0.84	0.12	45,68,93,108	0
34	UNL	t	103	26/-	0.84	0.13	42,64,76,81	0
26	PL9	a	410	55/55	0.85	0.14	36,67,91,98	0
34	UNL	b	625	44/-	0.85	0.14	34,58,80,84	0
30	DGD	a	414	44/66	0.86	0.13	36,58,84,92	0
34	UNL	B	626	46/-	0.86	0.12	44,64,84,93	0
34	UNL	B	627	28/-	0.86	0.14	42,64,86,91	0
34	UNL	B	628	47/-	0.86	0.13	47,65,78,89	0
28	SQD	a	413	36/54	0.86	0.12	31,67,87,96	0
34	UNL	d	411	55/-	0.86	0.11	42,58,72,73	0
34	UNL	m	102	28/-	0.86	0.12	42,59,73,78	0
23	CLA	h	101	65/65	0.86	0.11	45,69,93,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	LMG	D	409	33/55	0.87	0.12	32,54,107,111	0
27	LMG	c	519	37/55	0.87	0.11	44,70,88,97	0
26	PL9	A	410	55/55	0.87	0.14	39,62,83,94	135
34	UNL	b	602	47/-	0.87	0.12	35,50,64,73	0
34	UNL	b	624	40/-	0.87	0.12	46,63,83,85	0
28	SQD	A	414	39/54	0.87	0.12	36,69,93,99	0
27	LMG	C	518	48/55	0.88	0.11	43,72,96,103	0
34	UNL	b	621	55/-	0.88	0.10	39,57,86,91	0
27	LMG	c	523	49/55	0.88	0.10	32,56,87,111	0
34	UNL	c	520	55/-	0.88	0.11	39,61,79,86	0
34	UNL	B	620	43/-	0.89	0.10	34,51,68,74	0
28	SQD	b	601	49/54	0.89	0.10	38,60,102,112	0
28	SQD	f	101	41/54	0.89	0.12	54,87,117,125	0
25	BCR	x	101	40/40	0.89	0.10	35,57,76,82	0
34	UNL	C	521	47/-	0.89	0.10	37,56,73,74	0
27	LMG	A	411	48/55	0.89	0.10	37,62,78,103	0
28	SQD	B	624	54/54	0.89	0.10	39,58,90,100	0
34	UNL	I	101	41/-	0.89	0.12	37,53,75,79	0
34	UNL	d	410	43/-	0.89	0.13	39,58,70,78	0
34	UNL	J	101	28/-	0.89	0.11	52,64,78,86	0
34	UNL	X	101	55/-	0.89	0.10	34,49,75,79	0
27	LMG	B	621	28/55	0.89	0.11	31,47,60,70	0
27	LMG	m	101	51/55	0.90	0.09	30,51,81,97	0
34	UNL	j	101	28/-	0.90	0.10	42,56,67,67	0
25	BCR	K	101	40/40	0.91	0.09	36,53,73,79	0
34	UNL	B	625	28/-	0.91	0.10	31,46,69,70	0
25	BCR	c	514	40/40	0.91	0.09	40,59,77,79	0
28	SQD	a	412	54/54	0.91	0.10	34,69,91,95	0
25	BCR	k	101	40/40	0.91	0.09	39,65,81,83	0
34	UNL	C	519	28/-	0.91	0.10	34,46,55,56	0
34	UNL	C	520	28/-	0.91	0.09	42,51,64,65	0
34	UNL	l	102	53/-	0.91	0.11	33,50,87,91	0
23	CLA	B	601	65/65	0.91	0.10	32,61,99,105	0
34	UNL	t	102	34/-	0.91	0.09	35,50,58,65	0
30	DGD	h	102	62/66	0.91	0.09	33,52,65,70	0
25	BCR	d	404	40/40	0.92	0.08	36,54,90,102	0
25	BCR	D	404	40/40	0.92	0.10	25,46,103,108	0
25	BCR	k	102	40/40	0.92	0.10	37,57,66,73	0
30	DGD	C	516	62/66	0.92	0.09	30,54,108,129	0
23	CLA	c	512	65/65	0.92	0.10	40,58,97,107	0
23	CLA	C	513	65/65	0.92	0.10	45,68,95,101	0
27	LMG	M	101	51/55	0.92	0.08	25,47,72,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	SQD	A	412	52/54	0.93	0.09	32,61,93,101	0
25	BCR	b	619	40/40	0.93	0.07	27,39,55,58	0
23	CLA	c	513	65/65	0.93	0.09	47,72,109,114	0
34	UNL	M	102	37/-	0.93	0.09	26,45,54,69	0
34	UNL	M	103	26/-	0.93	0.10	24,49,57,63	0
28	SQD	F	101	36/54	0.93	0.10	41,71,87,95	0
25	BCR	c	515	40/40	0.93	0.09	31,48,64,72	0
30	DGD	H	102	62/66	0.93	0.08	30,49,61,74	0
27	LMG	d	409	44/55	0.93	0.09	31,58,89,105	0
30	DGD	c	517	62/66	0.93	0.08	31,52,86,96	0
25	BCR	Z	101	40/40	0.93	0.09	34,57,72,75	0
23	CLA	C	503	65/65	0.94	0.07	29,42,52,55	0
25	BCR	b	618	40/40	0.94	0.07	22,43,54,58	0
23	CLA	c	503	65/65	0.94	0.07	32,45,56,62	0
27	LMG	D	406	51/55	0.94	0.09	26,56,89,97	0
25	BCR	b	620	40/40	0.94	0.07	28,47,61,67	0
25	BCR	B	618	40/40	0.94	0.06	23,39,54,56	0
25	BCR	B	619	40/40	0.94	0.07	27,42,65,78	0
25	BCR	C	514	40/40	0.94	0.08	27,39,54,59	0
29	LHG	d	406	49/49	0.94	0.10	36,52,82,94	0
29	LHG	d	408	39/49	0.94	0.08	26,47,73,78	0
23	CLA	c	511	65/65	0.94	0.09	34,57,74,76	0
25	BCR	H	101	40/40	0.94	0.07	31,47,57,62	0
25	BCR	t	101	40/40	0.94	0.06	25,36,53,61	0
23	CLA	C	512	65/65	0.94	0.09	33,56,102,109	0
25	BCR	K	102	40/40	0.94	0.10	34,58,73,76	0
25	BCR	T	101	40/40	0.94	0.06	27,40,60,62	0
23	CLA	c	504	60/65	0.95	0.08	30,44,86,93	0
23	CLA	c	505	65/65	0.95	0.07	23,43,68,72	0
23	CLA	c	506	65/65	0.95	0.09	28,51,111,120	0
29	LHG	B	623	49/49	0.95	0.08	25,44,76,87	0
29	LHG	D	408	47/49	0.95	0.09	26,46,84,100	0
23	CLA	c	508	64/65	0.95	0.08	30,45,93,113	0
23	CLA	c	509	65/65	0.95	0.08	30,48,67,68	0
25	BCR	a	409	40/40	0.95	0.06	22,33,42,46	0
29	LHG	l	101	49/49	0.95	0.08	29,48,59,64	0
23	CLA	c	510	65/65	0.95	0.07	33,50,69,76	0
30	DGD	C	515	62/66	0.95	0.08	21,40,86,103	0
23	CLA	C	508	65/65	0.95	0.08	23,41,119,127	0
23	CLA	C	509	65/65	0.95	0.08	26,45,65,79	0
23	CLA	C	510	65/65	0.95	0.07	29,46,75,87	0
23	CLA	C	511	65/65	0.95	0.08	35,51,67,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	DGD	c	518	62/66	0.95	0.07	29,52,82,94	0
24	PHO	d	401	64/64	0.95	0.06	27,38,50,59	0
25	BCR	A	409	40/40	0.95	0.06	24,34,43,47	0
25	BCR	B	617	40/40	0.95	0.07	26,40,54,56	0
23	CLA	B	609	65/65	0.95	0.07	24,35,57,66	0
23	CLA	C	502	65/65	0.95	0.07	24,44,56,64	0
23	CLA	b	617	60/65	0.95	0.08	28,44,105,113	0
23	CLA	B	606	65/65	0.95	0.07	21,35,73,83	0
26	PL9	d	405	55/55	0.95	0.06	21,35,44,47	0
23	CLA	B	612	65/65	0.96	0.06	21,32,46,51	0
23	CLA	C	504	59/65	0.96	0.07	24,44,83,93	0
23	CLA	a	405	65/65	0.96	0.06	17,29,50,61	0
23	CLA	a	406	65/65	0.96	0.07	24,40,100,112	0
23	CLA	a	408	65/65	0.96	0.08	16,36,95,107	0
23	CLA	d	403	65/65	0.96	0.07	29,49,97,109	0
23	CLA	b	607	65/65	0.96	0.07	24,40,74,83	0
24	PHO	A	407	64/64	0.96	0.05	22,32,44,50	0
24	PHO	a	407	64/64	0.96	0.06	22,31,40,48	0
29	LHG	B	622	49/49	0.96	0.07	26,42,57,74	0
26	PL9	D	405	55/55	0.96	0.06	17,32,48,52	0
23	CLA	b	609	65/65	0.96	0.07	24,41,70,74	0
23	CLA	b	610	65/65	0.96	0.07	30,46,71,89	0
29	LHG	d	407	49/49	0.96	0.07	24,44,61,72	0
23	CLA	b	611	65/65	0.96	0.07	24,38,51,57	0
23	CLA	b	613	65/65	0.96	0.07	20,34,49,55	0
23	CLA	b	615	65/65	0.96	0.08	20,37,81,97	0
23	CLA	b	616	65/65	0.96	0.07	26,39,62,68	0
23	CLA	C	505	65/65	0.96	0.08	25,43,73,83	0
23	CLA	c	501	65/65	0.96	0.06	25,39,52,59	0
30	DGD	C	517	62/66	0.96	0.07	23,45,82,93	0
23	CLA	c	502	65/65	0.96	0.07	27,43,65,69	0
23	CLA	C	506	65/65	0.96	0.07	27,42,95,110	0
30	DGD	c	516	62/66	0.96	0.07	21,43,78,84	0
23	CLA	B	614	65/65	0.96	0.07	21,38,83,95	0
23	CLA	B	615	65/65	0.96	0.06	24,36,70,87	0
23	CLA	B	616	60/65	0.96	0.09	23,41,93,102	0
23	CLA	c	507	65/65	0.96	0.07	21,43,62,66	0
23	CLA	B	603	65/65	0.96	0.06	16,32,70,72	0
23	CLA	B	611	65/65	0.97	0.05	17,30,46,53	0
24	PHO	A	406	64/64	0.97	0.05	15,28,37,41	0
23	CLA	C	507	65/65	0.97	0.06	23,40,57,62	0
23	CLA	A	405	65/65	0.97	0.08	18,34,99,118	0

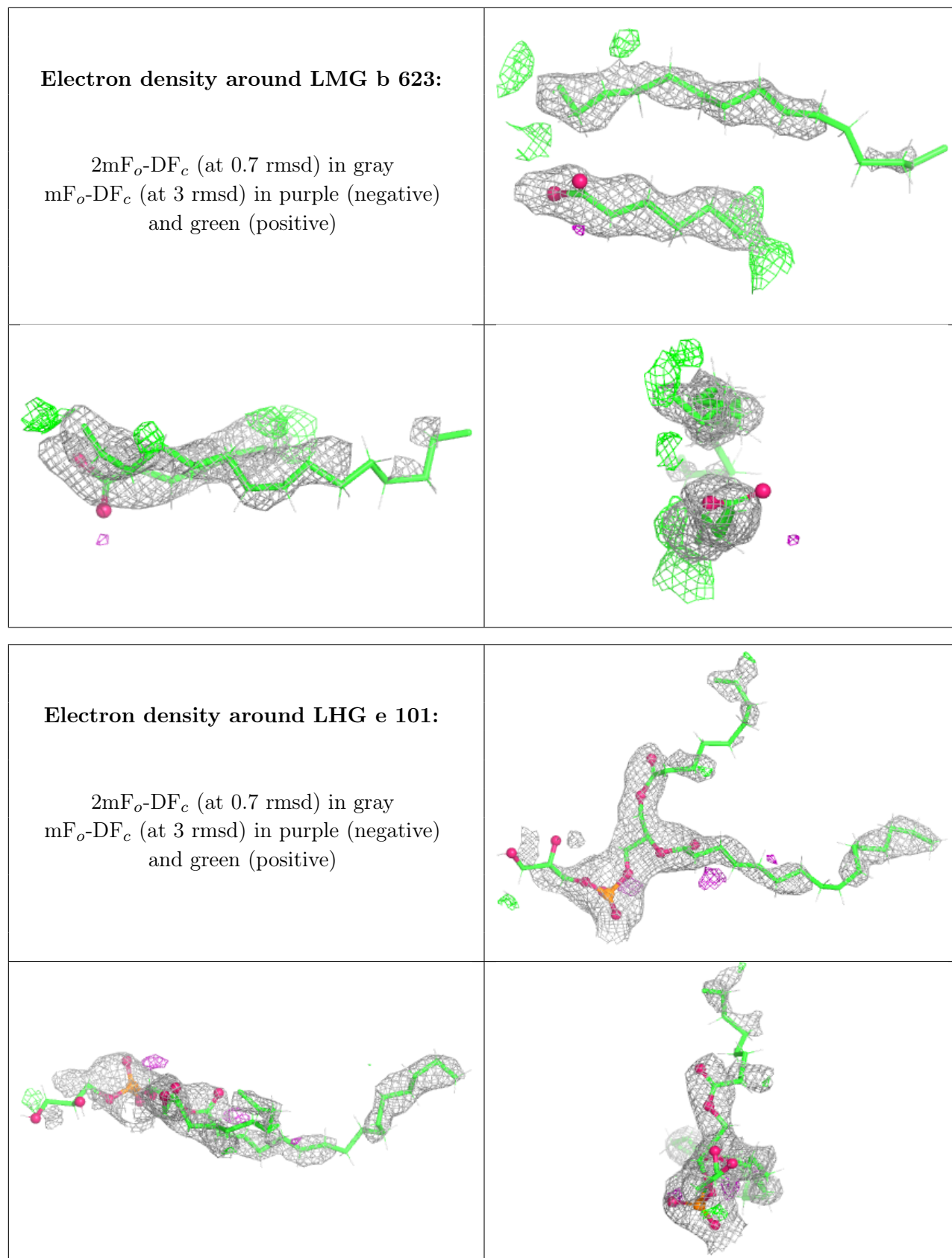
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	b	612	65/65	0.97	0.06	20,33,51,57	0
29	LHG	D	407	49/49	0.97	0.06	21,41,54,68	0
23	CLA	B	613	65/65	0.97	0.05	13,30,63,74	0
23	CLA	b	614	65/65	0.97	0.06	18,32,77,84	0
23	CLA	B	604	65/65	0.97	0.07	18,31,79,87	0
23	CLA	B	605	65/65	0.97	0.06	18,30,44,46	0
23	CLA	A	404	65/65	0.97	0.05	17,27,47,57	0
23	CLA	C	501	65/65	0.97	0.06	18,34,52,58	0
23	CLA	D	401	65/65	0.97	0.05	18,29,53,61	0
23	CLA	D	402	65/65	0.97	0.06	15,32,58,67	0
23	CLA	D	403	65/65	0.97	0.07	23,40,121,137	0
23	CLA	B	607	65/65	0.97	0.06	14,33,65,72	0
23	CLA	B	608	65/65	0.97	0.05	19,35,56,61	0
23	CLA	B	602	65/65	0.97	0.06	22,36,61,63	0
23	CLA	a	411	65/65	0.97	0.06	17,31,44,50	0
23	CLA	b	603	65/65	0.97	0.07	26,42,73,83	0
23	CLA	b	604	65/65	0.97	0.06	18,37,70,77	0
23	CLA	b	605	65/65	0.97	0.07	21,34,88,99	0
33	BCT	a	404	4/4	0.97	0.06	23,23,41,49	0
23	CLA	b	606	65/65	0.97	0.06	21,35,52,57	0
23	CLA	B	610	65/65	0.97	0.06	16,31,44,48	0
23	CLA	d	402	65/65	0.97	0.06	19,33,64,73	0
23	CLA	b	608	65/65	0.97	0.07	18,35,66,74	0
35	HEM	e	102	43/43	0.97	0.09	43,57,78,80	0
33	BCT	A	418	4/4	0.98	0.06	26,33,39,47	0
35	HEM	E	101	43/43	0.98	0.08	35,50,67,72	0
23	CLA	A	408	54/65	0.98	0.06	16,30,74,77	0
32	OEY	a	417[B]	11/11	0.99	0.03	22,28,30,30	11
22	CL	A	403	1/1	0.99	0.04	24,24,24,24	0
22	CL	a	402	1/1	0.99	0.03	28,28,28,28	0
22	CL	a	403	1/1	0.99	0.09	27,27,27,27	0
21	FE2	A	401	1/1	0.99	0.01	30,30,30,30	0
21	FE2	a	401	1/1	0.99	0.02	35,35,35,35	0
22	CL	A	402	1/1	0.99	0.05	29,29,29,29	0
31	OEX	A	416[A]	10/10	0.99	0.03	21,30,34,35	10
32	OEY	A	417[B]	11/11	0.99	0.03	22,26,29,30	11
36	HEC	V	201	43/43	0.99	0.04	24,31,41,41	0
36	HEC	v	201	43/43	0.99	0.05	27,35,51,54	0
31	OEX	a	416[A]	10/10	1.00	0.02	25,31,34,35	10

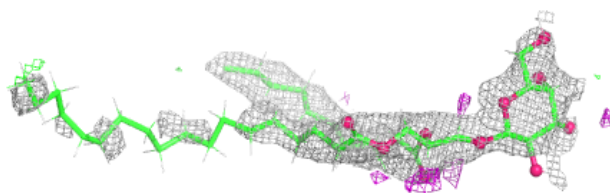
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.



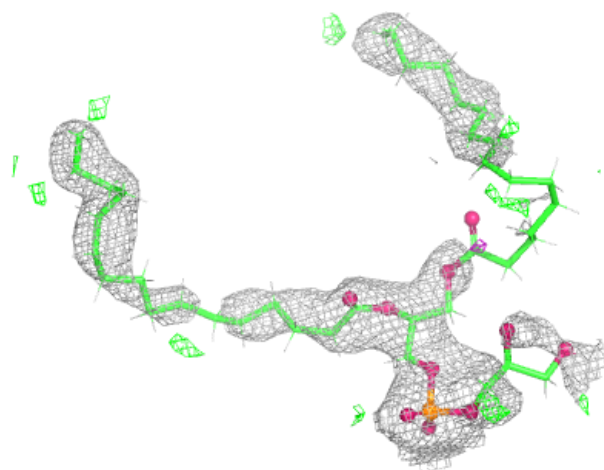
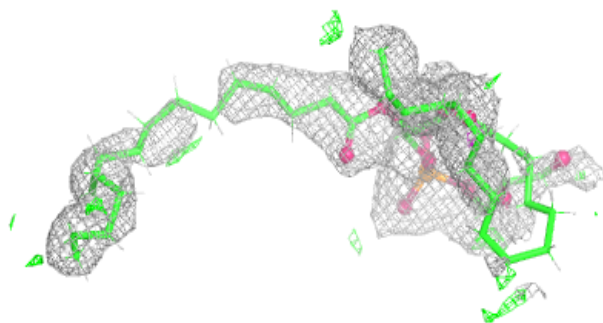
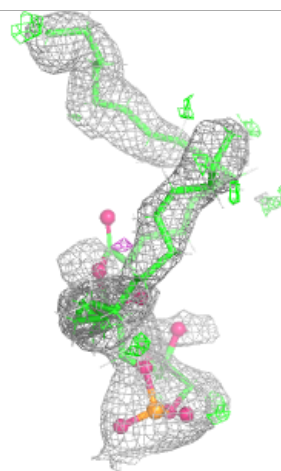
Electron density around LMG c 521:

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



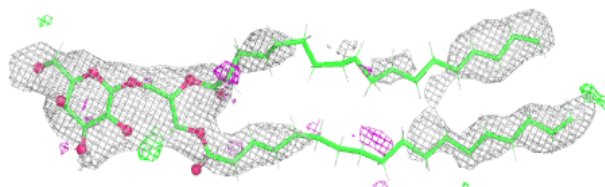
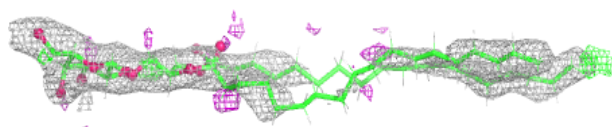
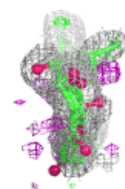
Electron density around LHG A 413:

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

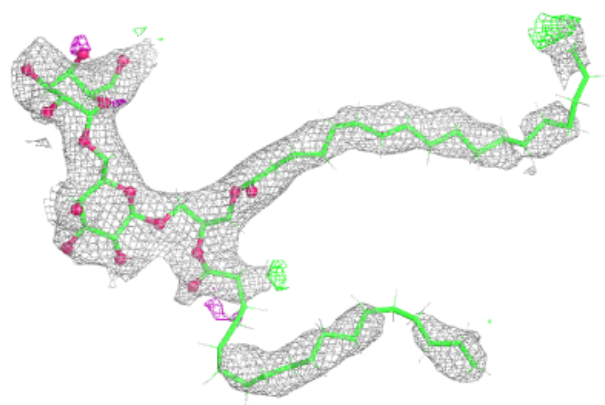
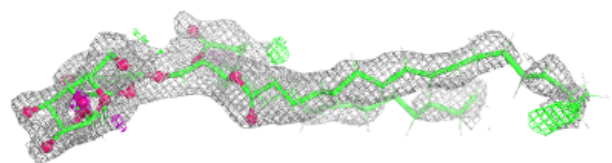


Electron density around LMG b 622:

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

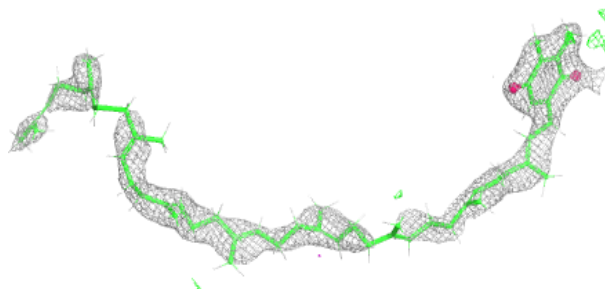
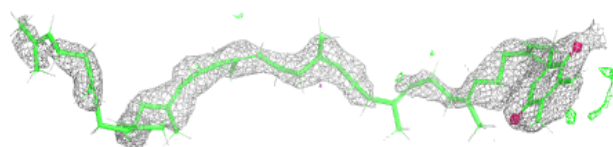
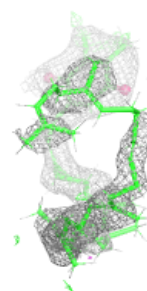
**Electron density around DGD A 415:**

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

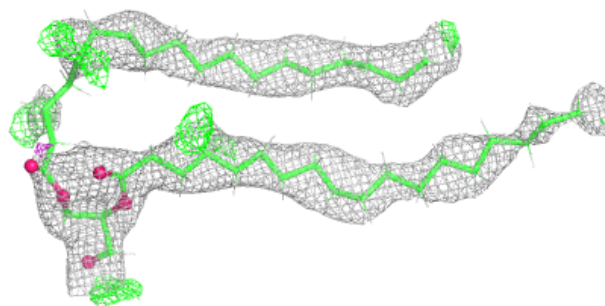
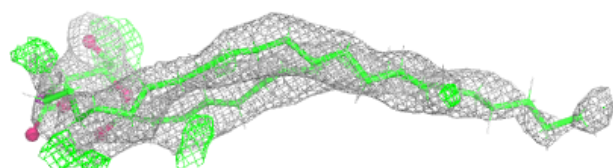
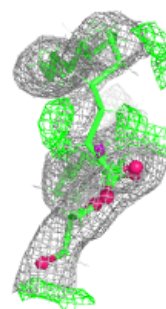


Electron density around PL9 a 410:

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

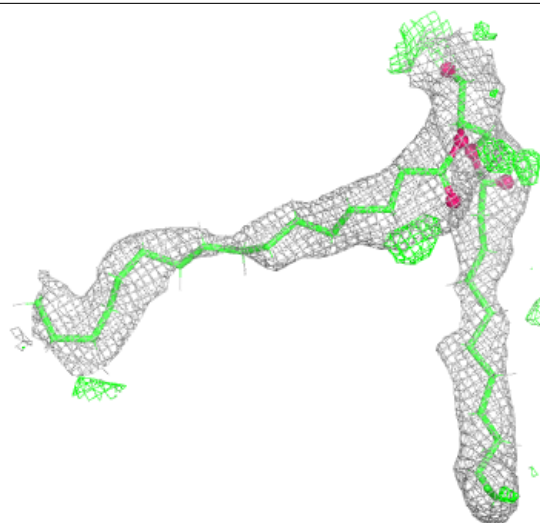
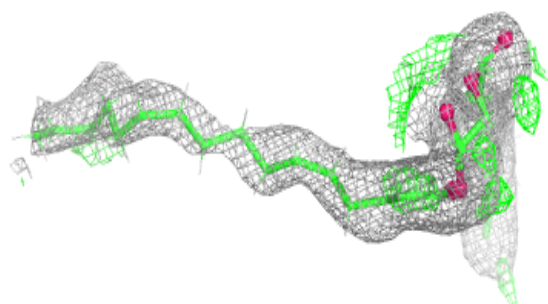
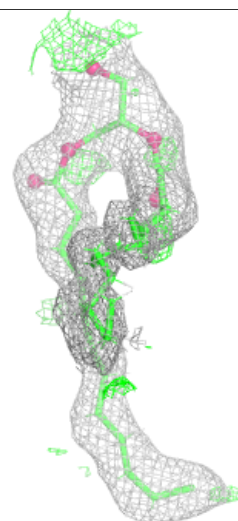
**Electron density around DGD a 414:**

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



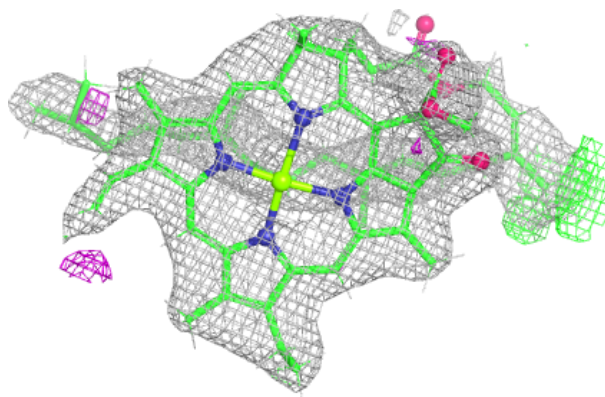
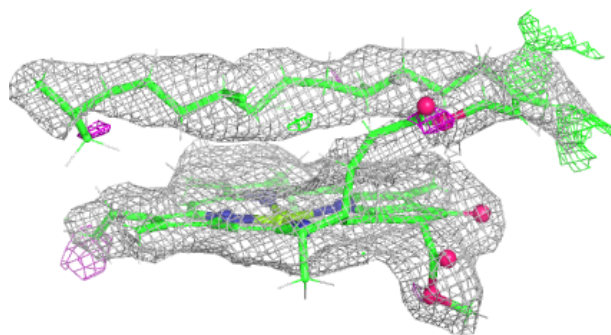
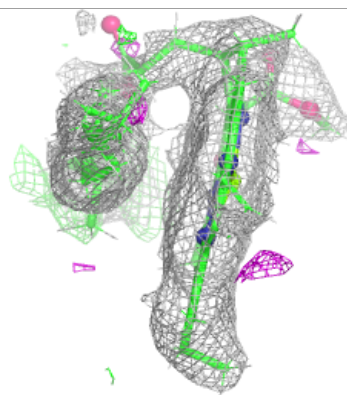
Electron density around SQD a 413:

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

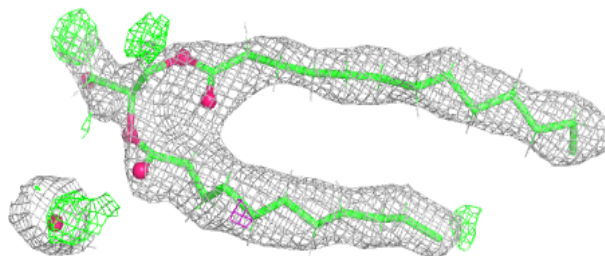
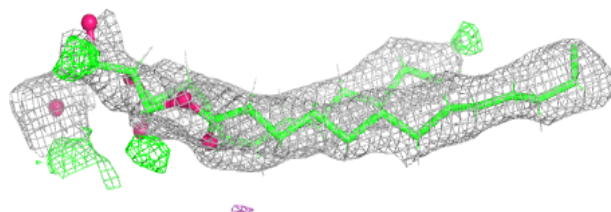
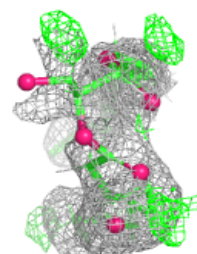


Electron density around CLA h 101:

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

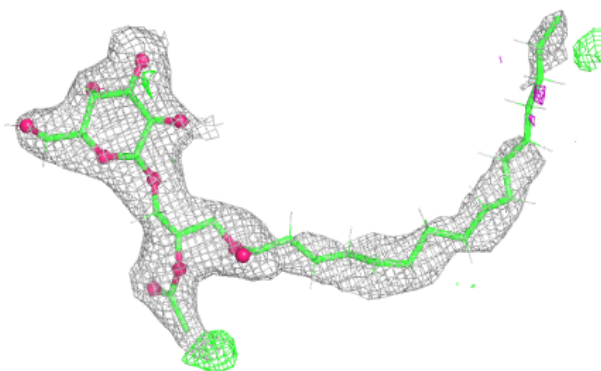
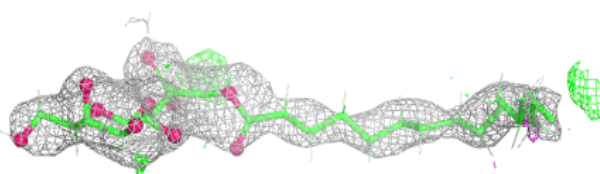
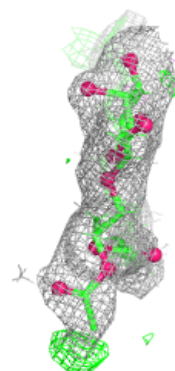
**Electron density around LMG D 409:**

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

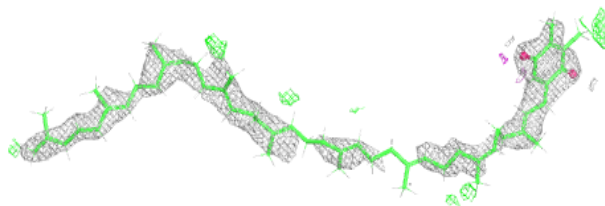
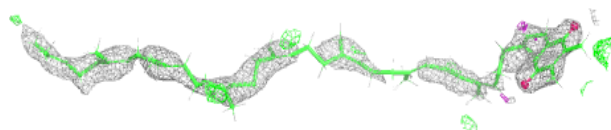
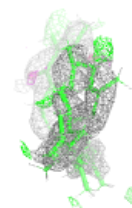


Electron density around LMG c 519:

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

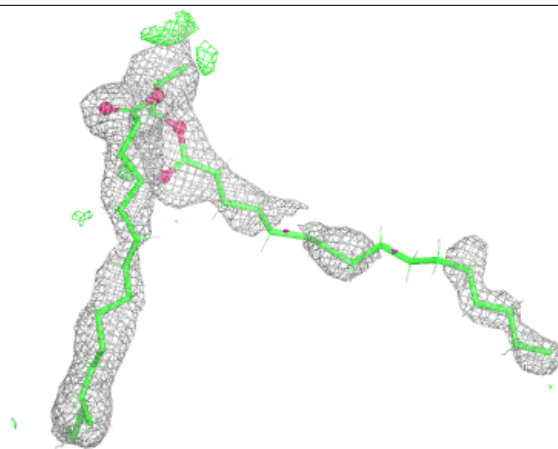
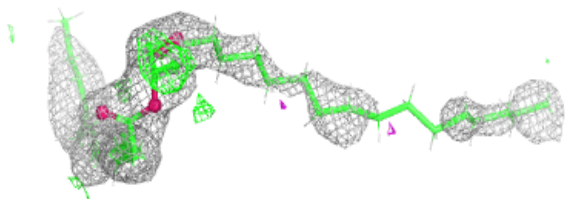
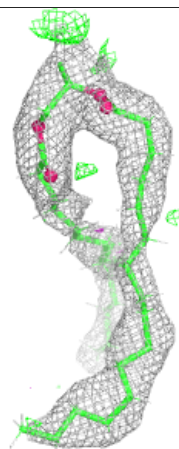
**Electron density around PL9 A 410:**

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



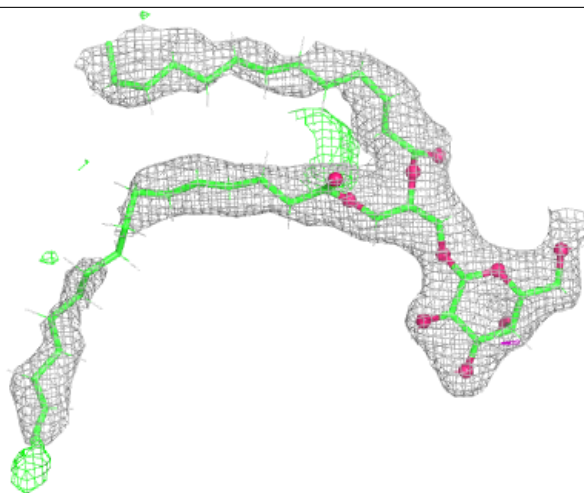
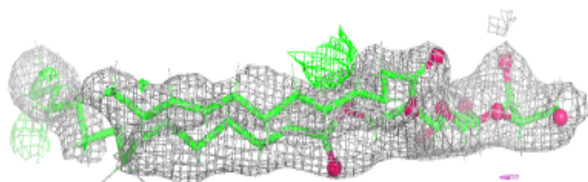
Electron density around SQD A 414:

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



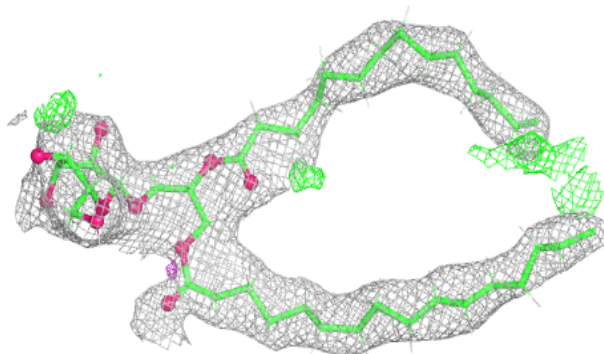
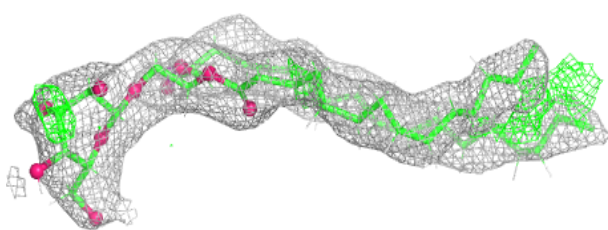
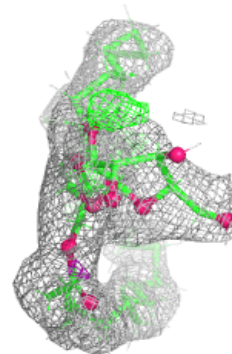
Electron density around LMG C 518:

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

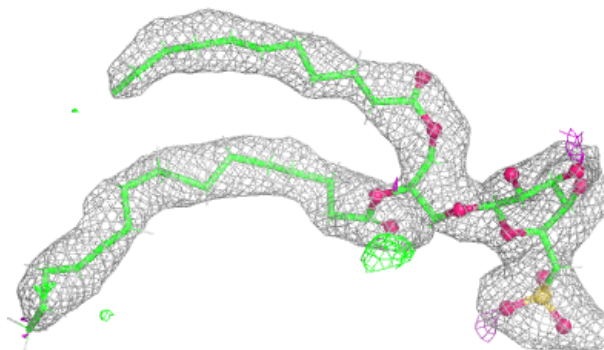
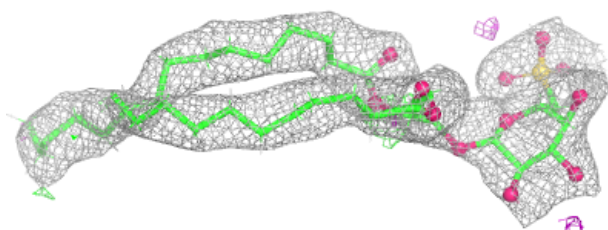
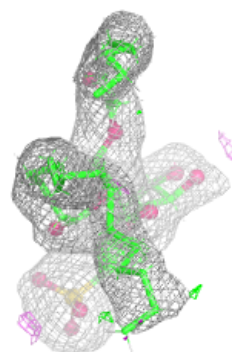


Electron density around LMG c 523:

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and green (positive)

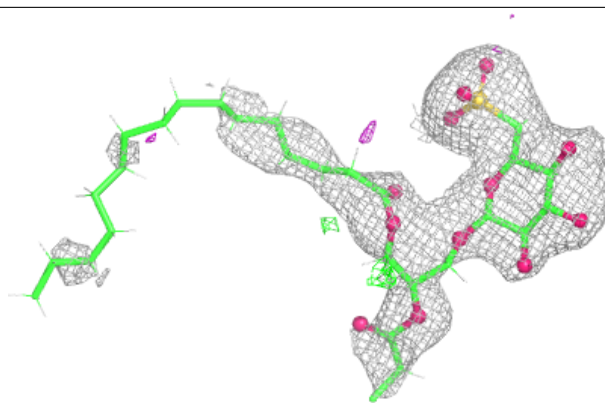
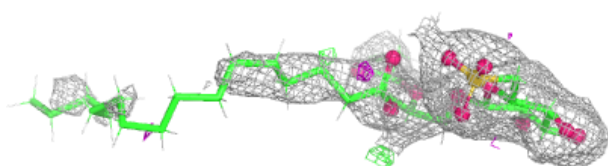
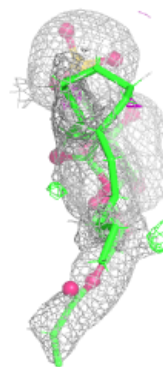
**Electron density around SQD b 601:**

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

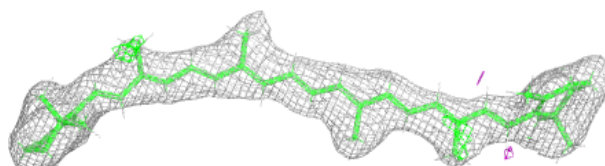
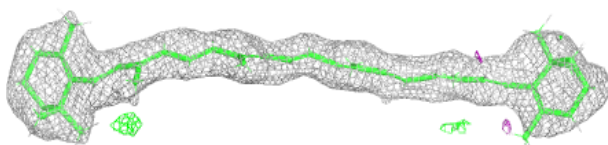
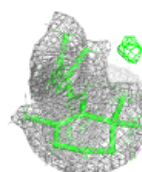


Electron density around SQD f 101:

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

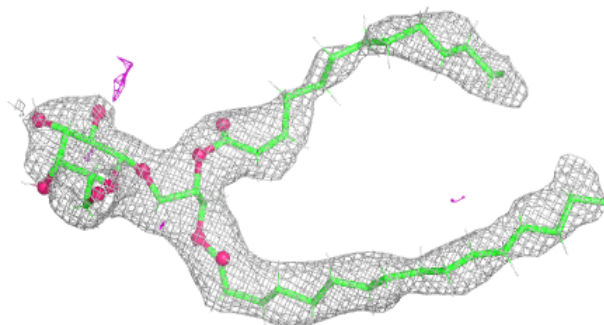
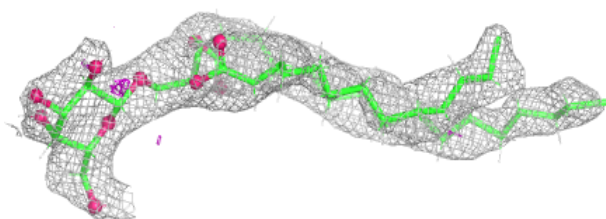
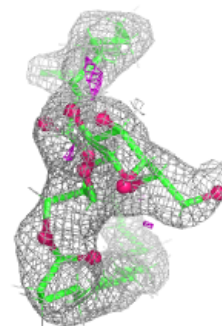
**Electron density around BCR x 101:**

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

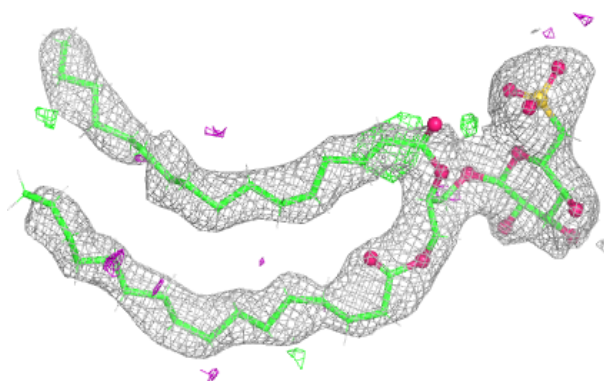
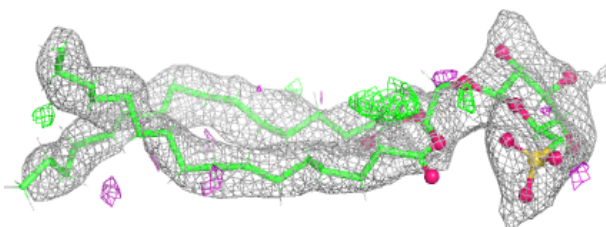
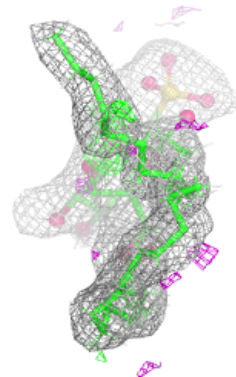


Electron density around LMG A 411:

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

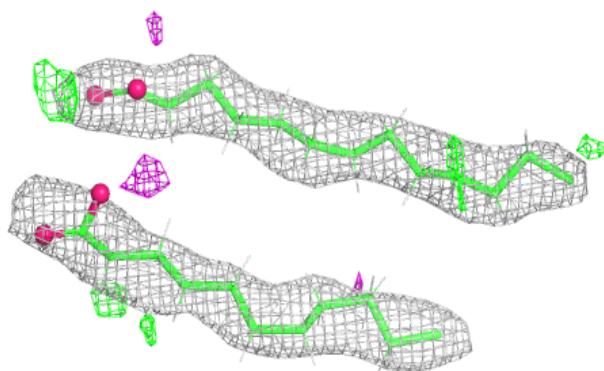
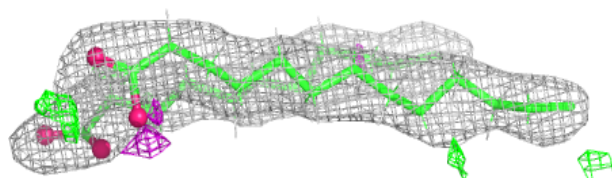
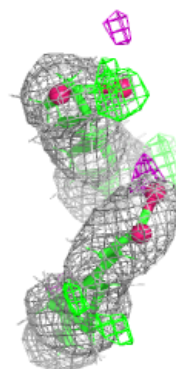
**Electron density around SQD B 624:**

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

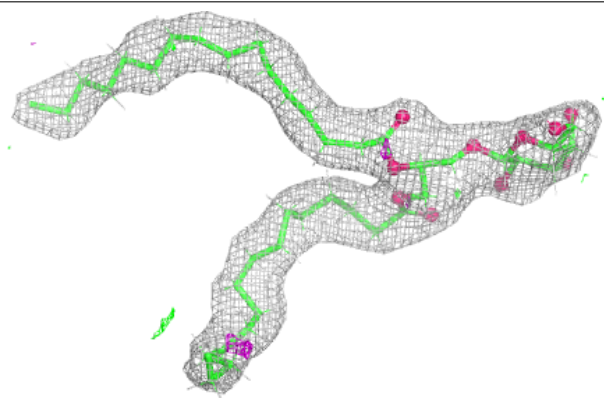
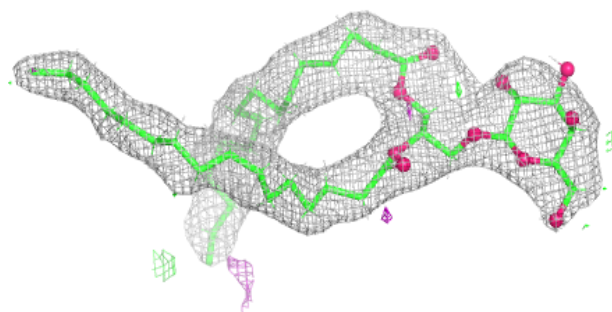
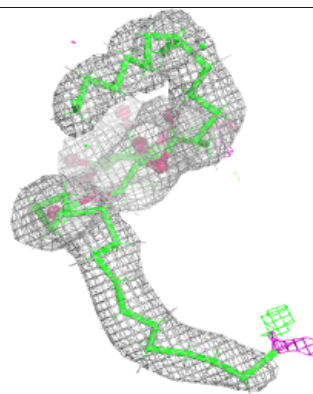


Electron density around LMG B 621:

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

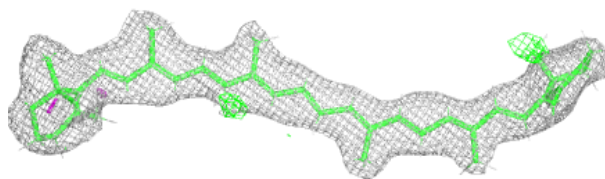
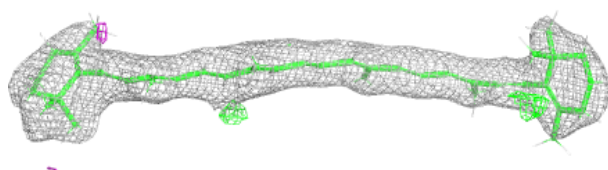
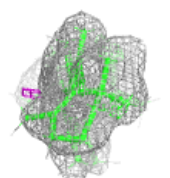
**Electron density around LMG m 101:**

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

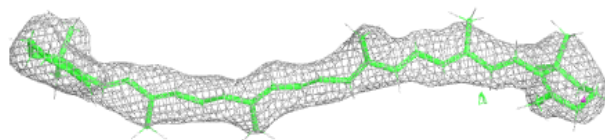
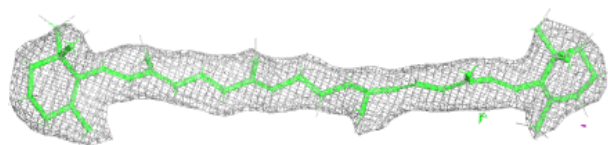
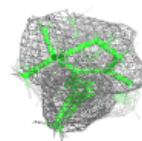


Electron density around BCR K 101:

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

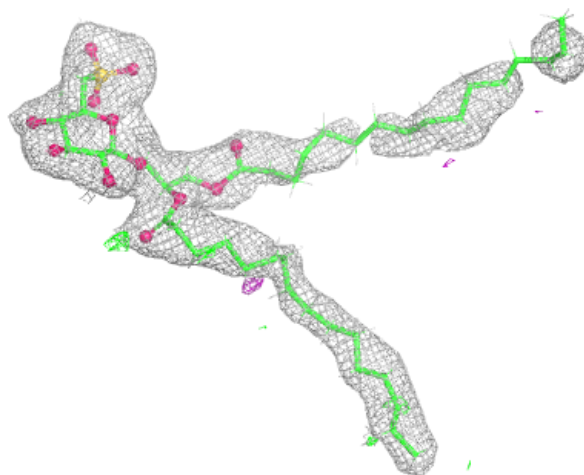
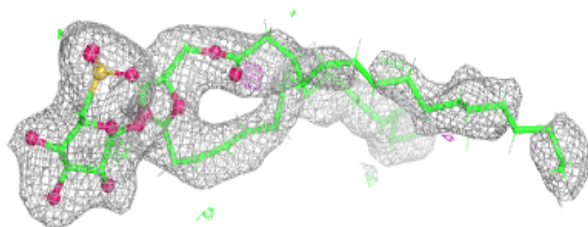
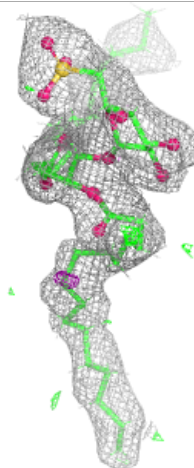
**Electron density around BCR c 514:**

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



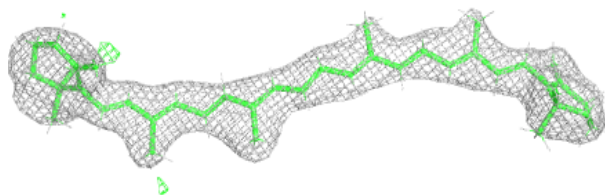
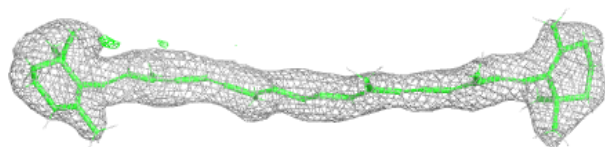
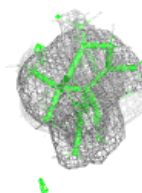
Electron density around SQD a 412:

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

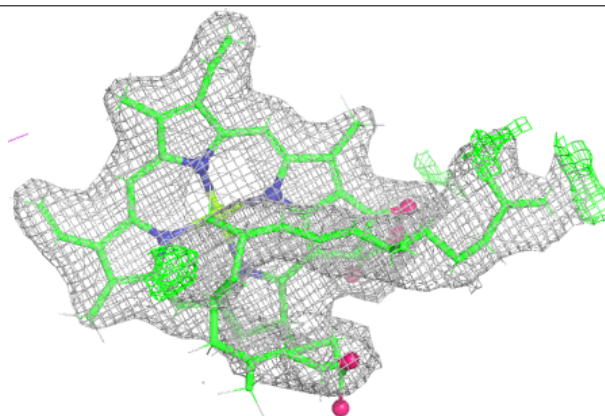
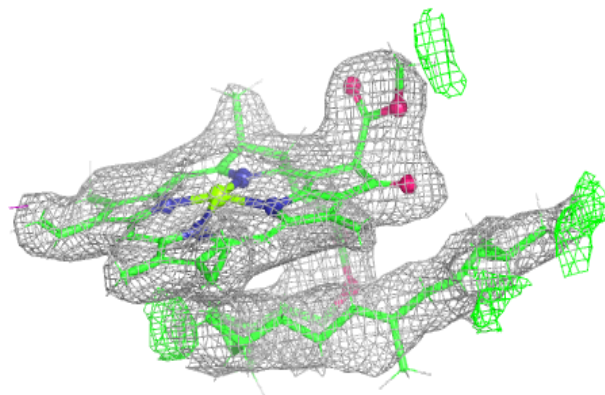
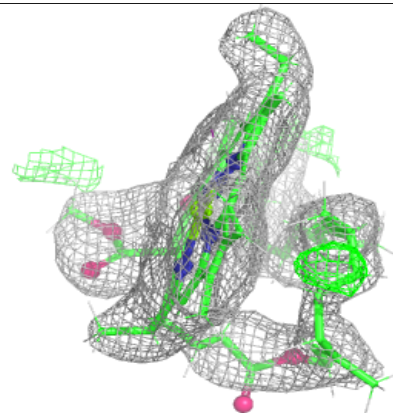


Electron density around BCR k 101:

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

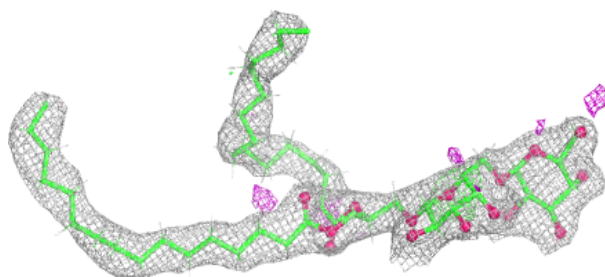
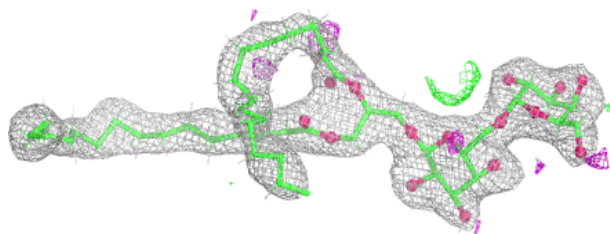
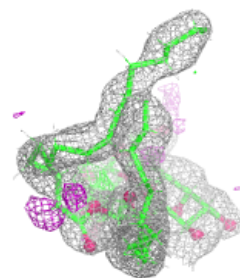
**Electron density around CLA B 601:**

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

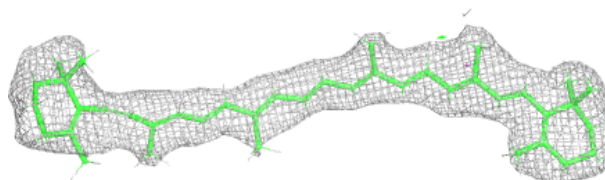
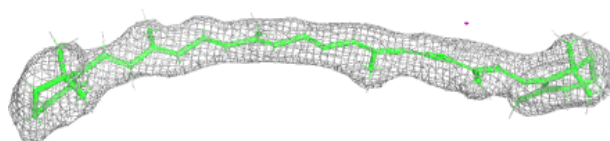
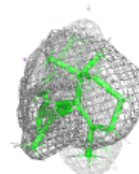


Electron density around DGD h 102:

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

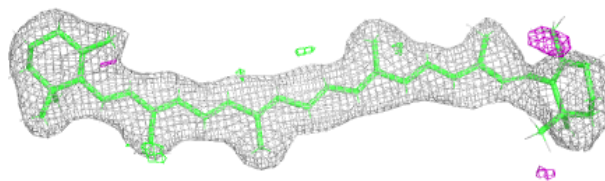
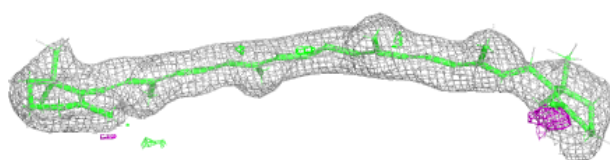
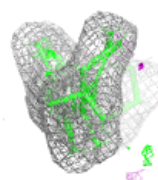
**Electron density around BCR d 404:**

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

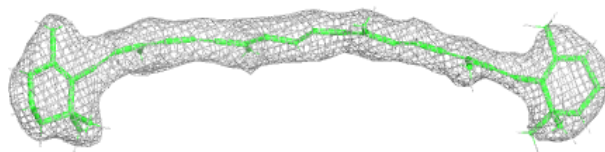
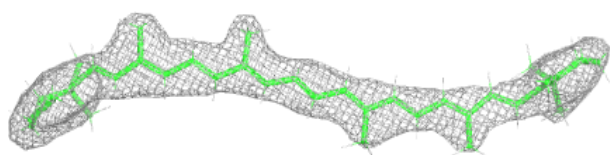
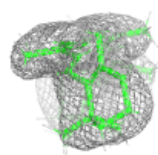


Electron density around BCR D 404:

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

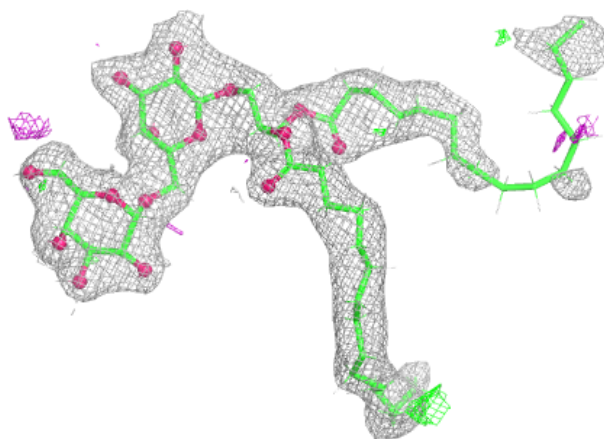
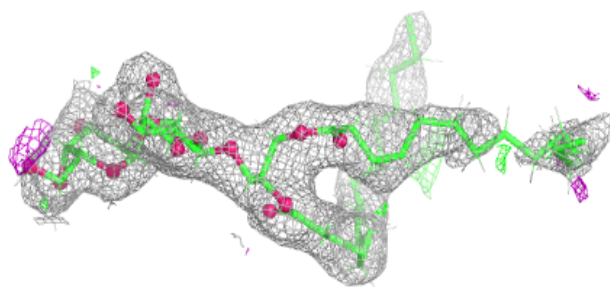
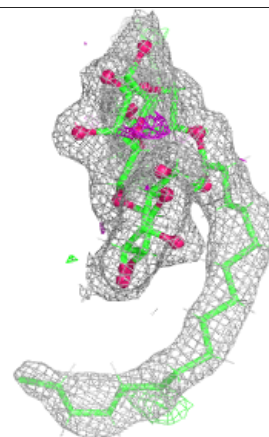
**Electron density around BCR k 102:**

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



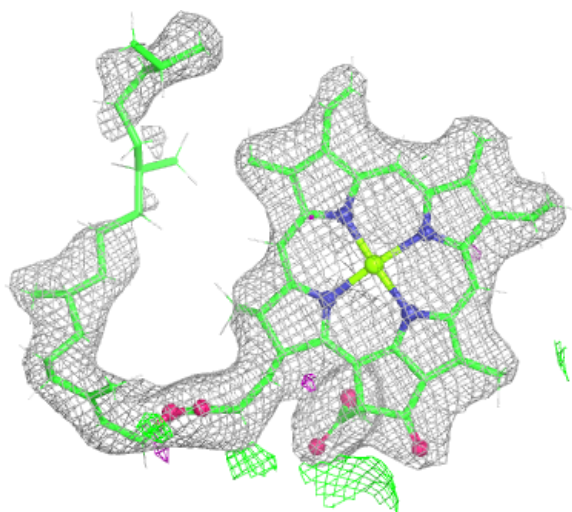
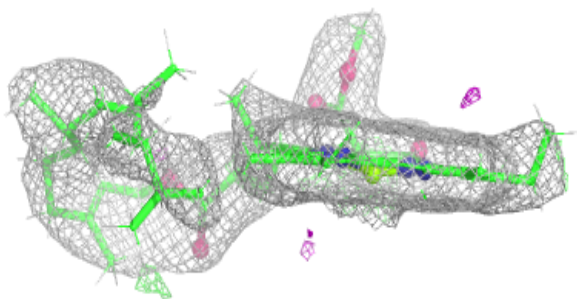
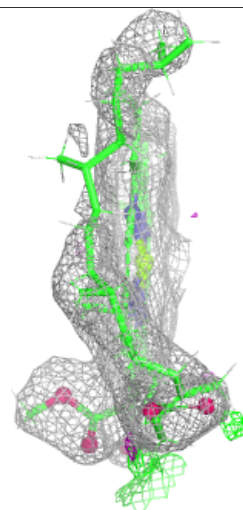
Electron density around DGD C 516:

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



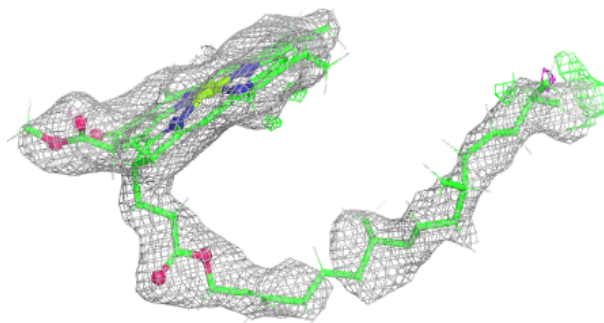
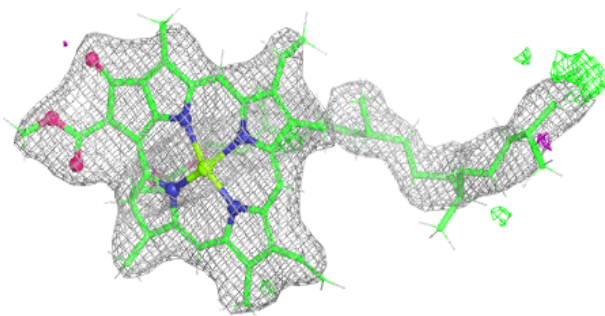
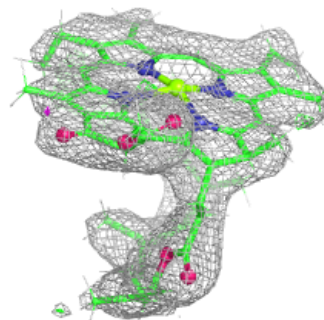
Electron density around CLA c 512:

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

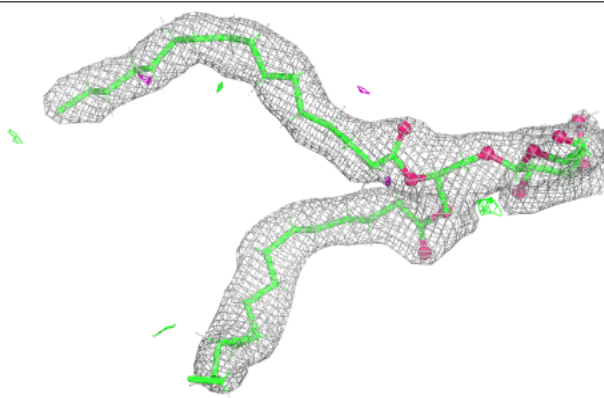
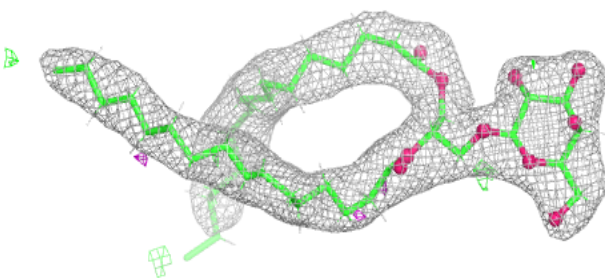
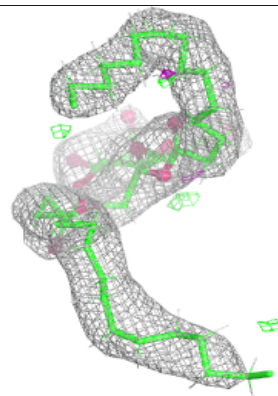


Electron density around CLA C 513:

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

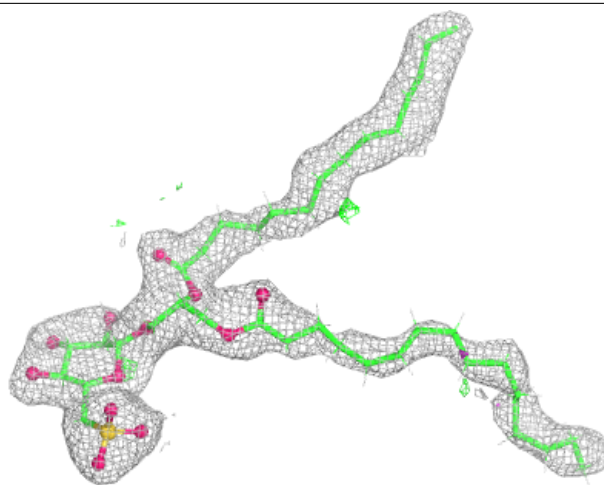
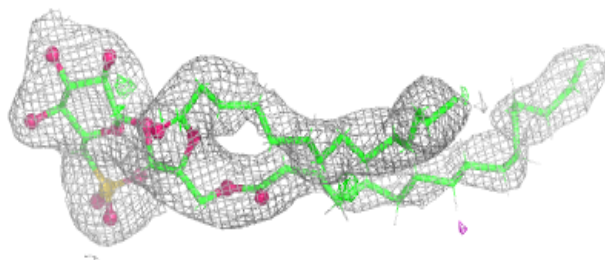
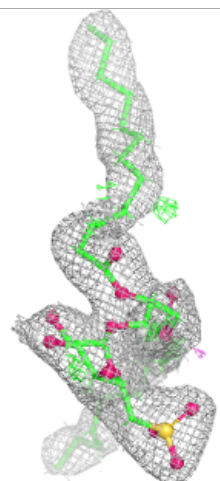
**Electron density around LMG M 101:**

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



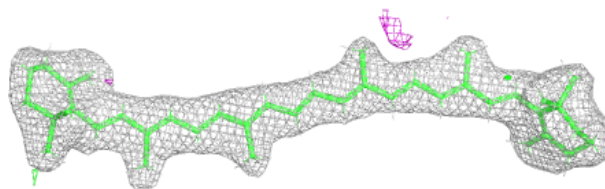
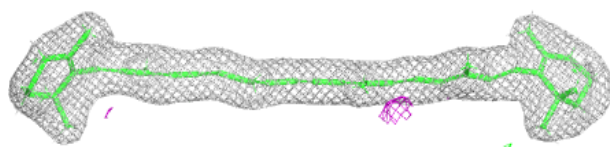
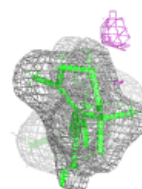
Electron density around SQD A 412:

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

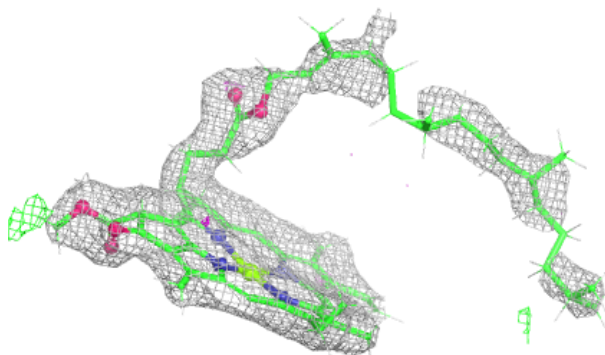
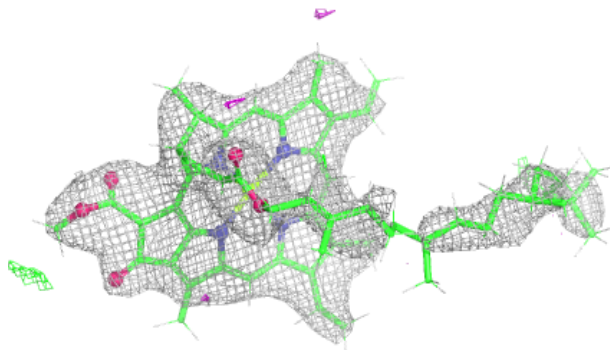
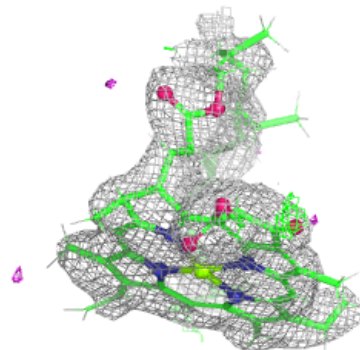


Electron density around BCR b 619:

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

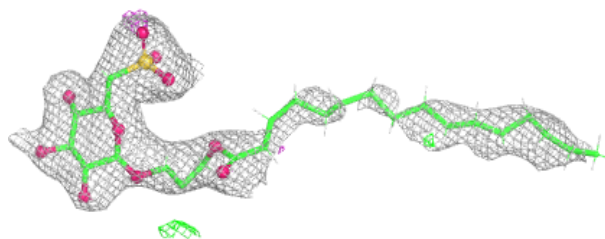
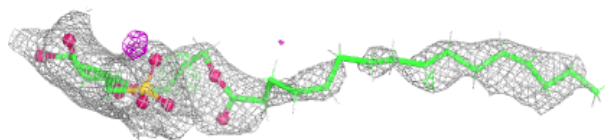
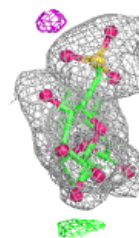
**Electron density around CLA c 513:**

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

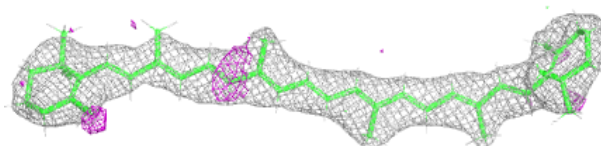
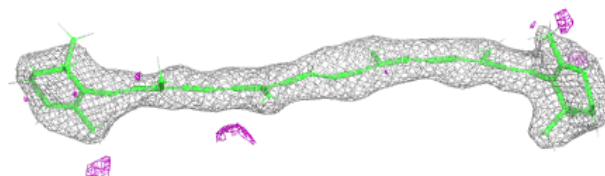
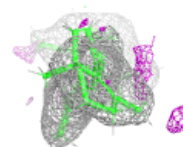


Electron density around SQD F 101:

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

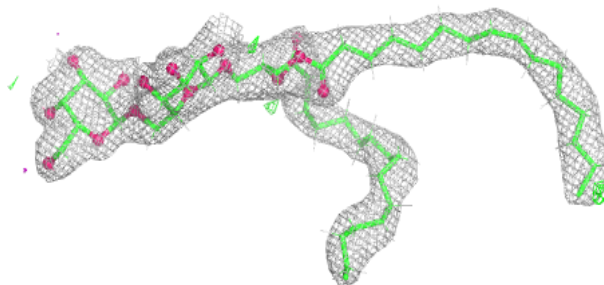
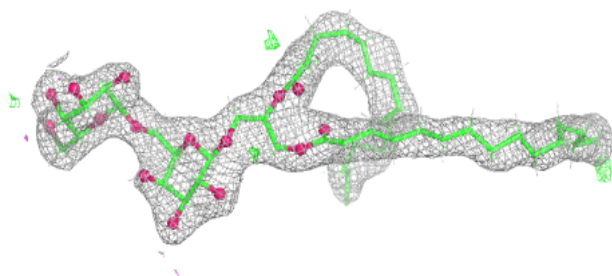
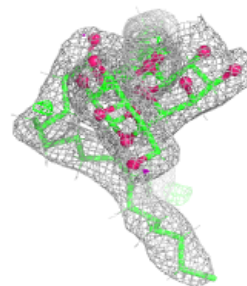
**Electron density around BCR c 515:**

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

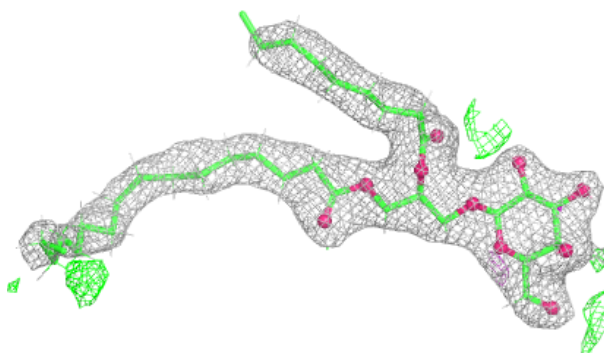
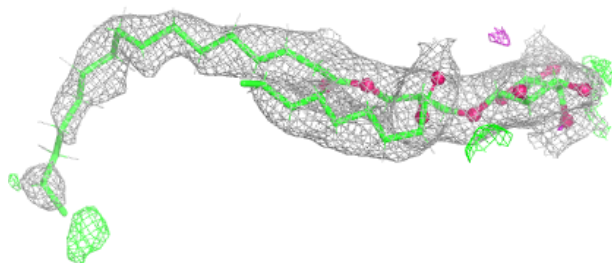
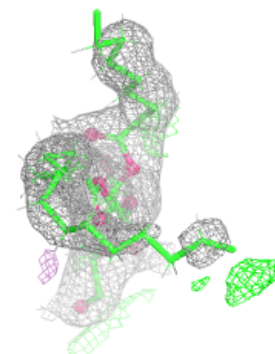


Electron density around DGD H 102:

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

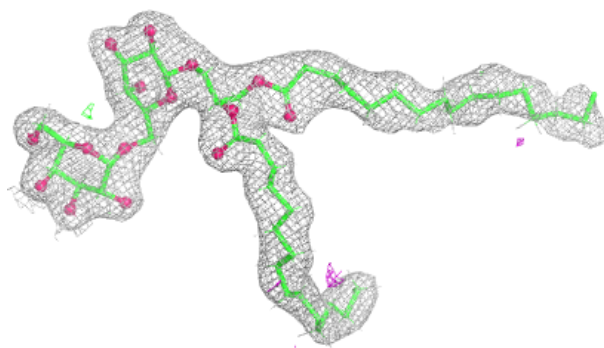
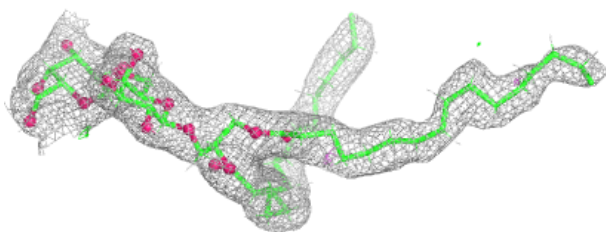
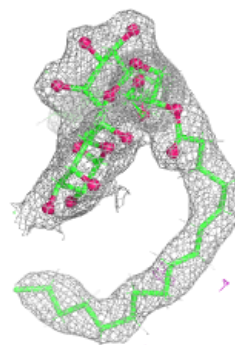
**Electron density around LMG d 409:**

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

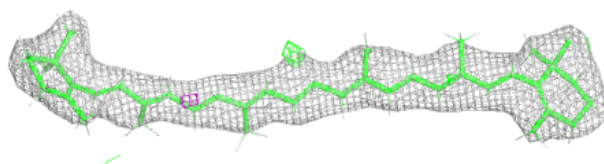
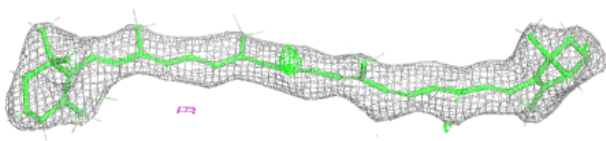
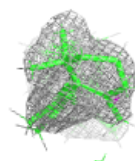


Electron density around DGD c 517:

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

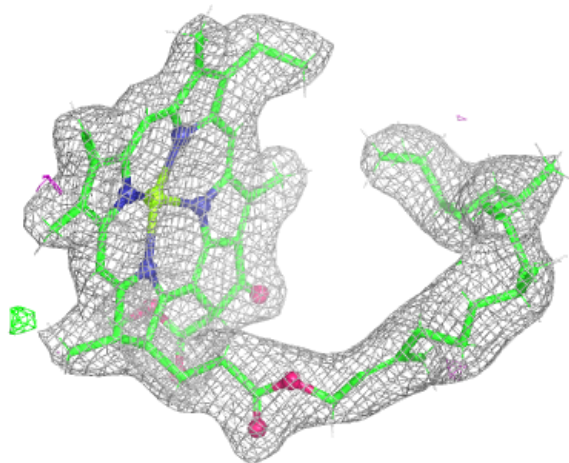
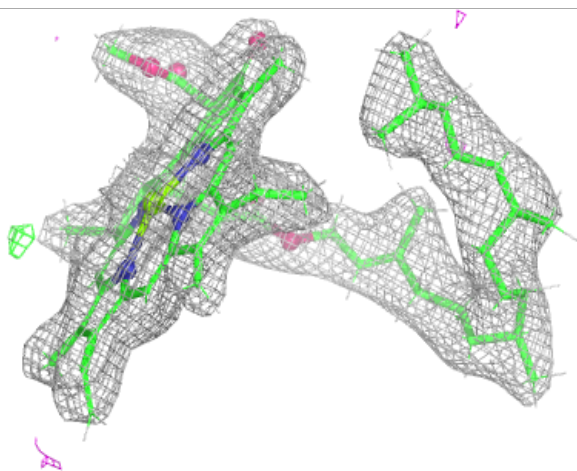
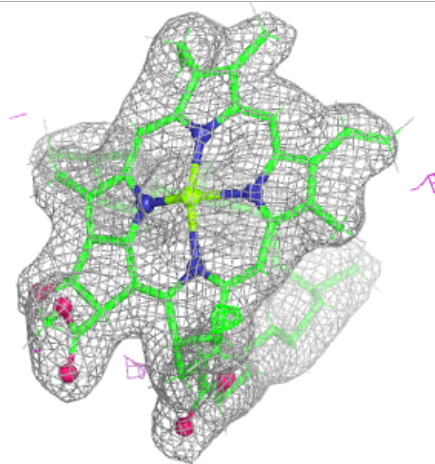
**Electron density around BCR Z 101:**

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



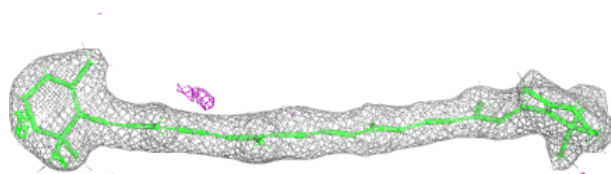
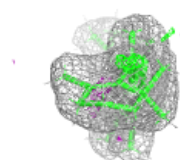
Electron density around CLA C 503:

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



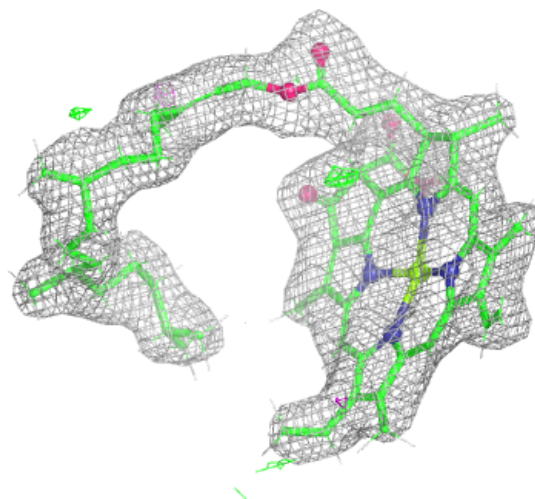
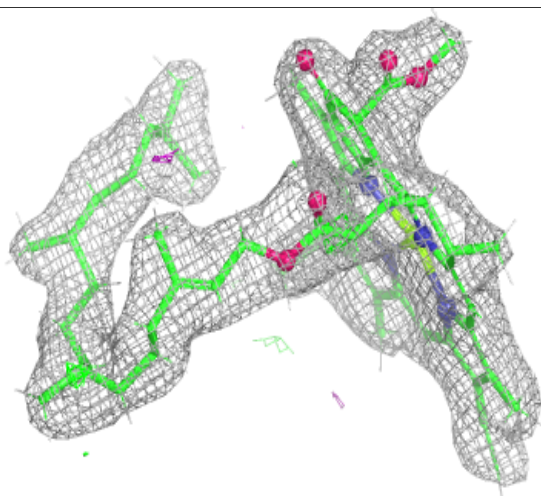
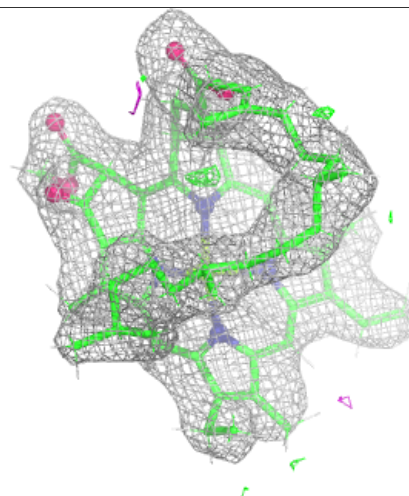
Electron density around BCR b 618:

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



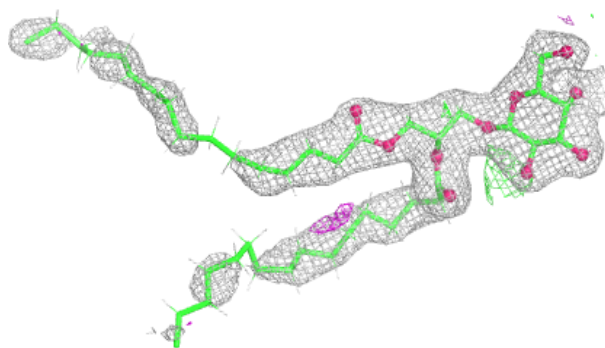
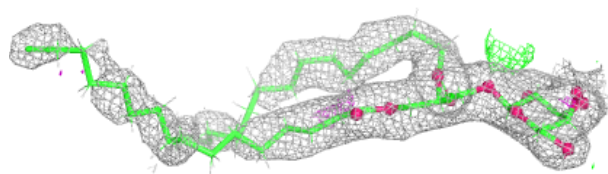
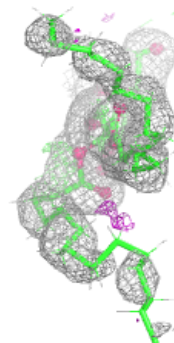
Electron density around CLA c 503:

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

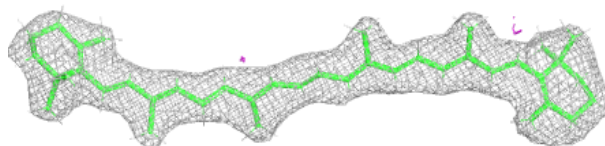
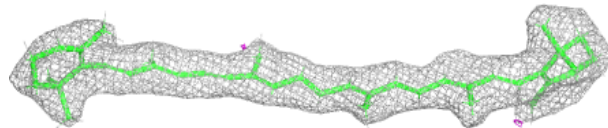
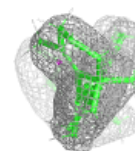


Electron density around LMG D 406:

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

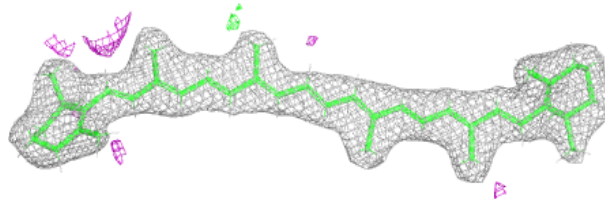
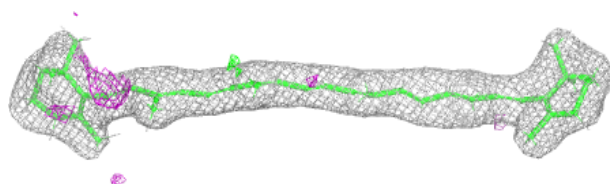
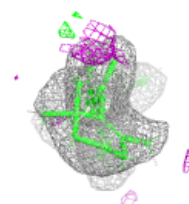
**Electron density around BCR b 620:**

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

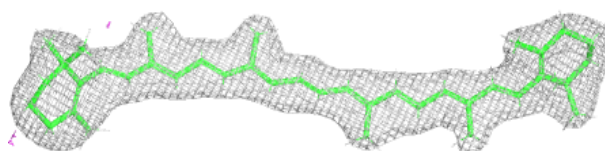
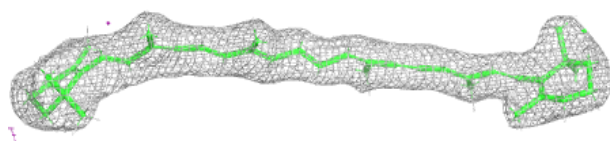
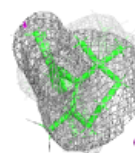


Electron density around BCR B 618:

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

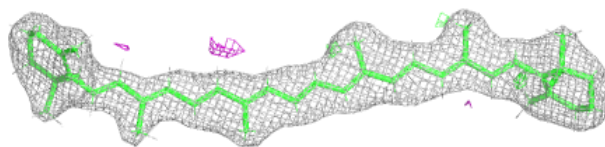
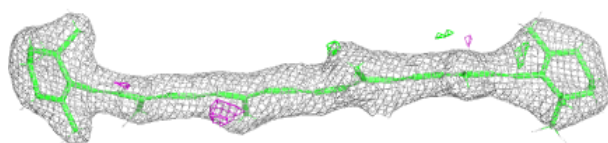
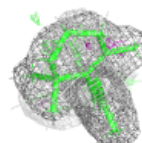
**Electron density around BCR B 619:**

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

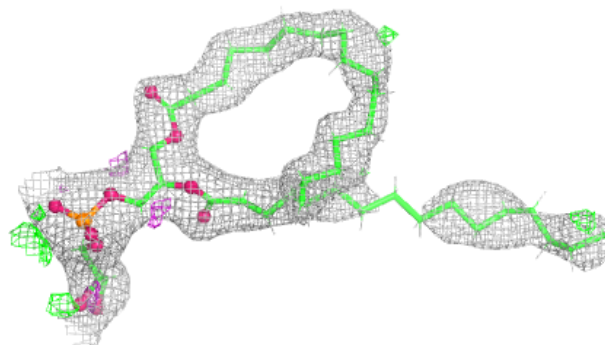
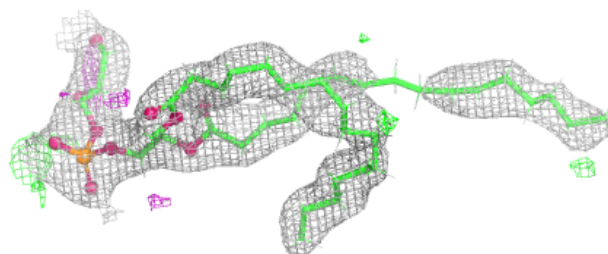
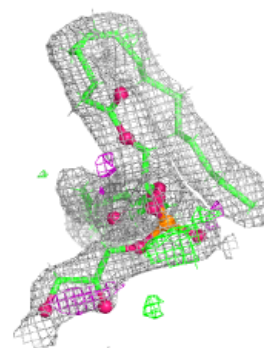


Electron density around BCR C 514:

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

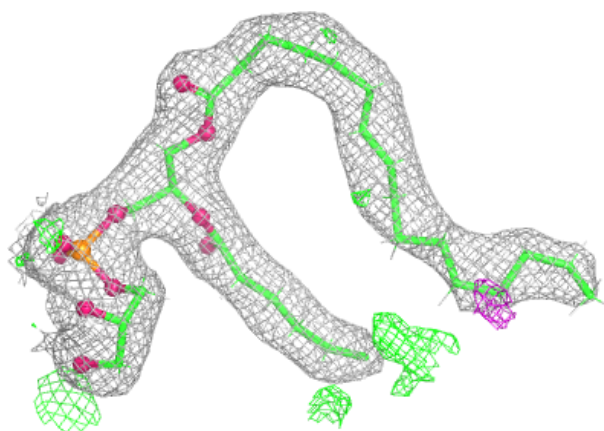
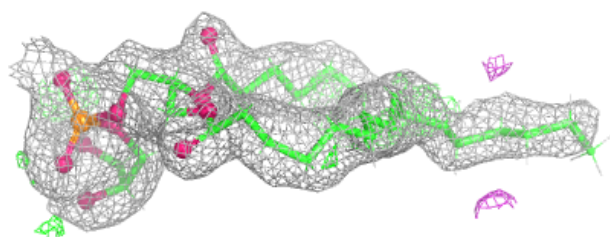
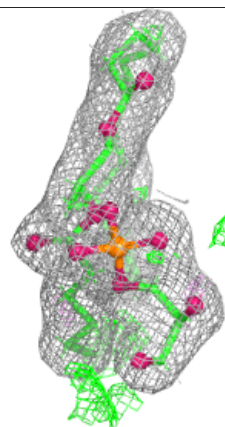
**Electron density around LHG d 406:**

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

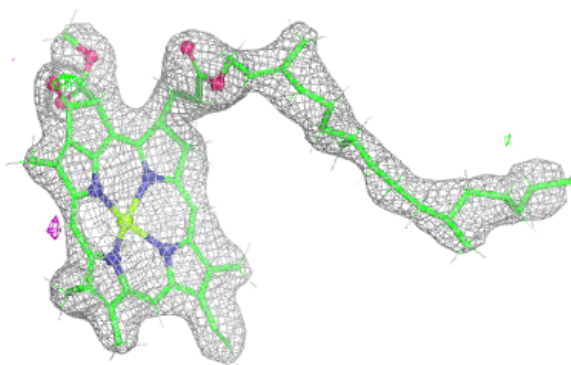
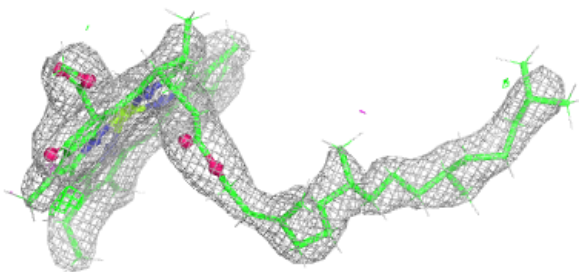
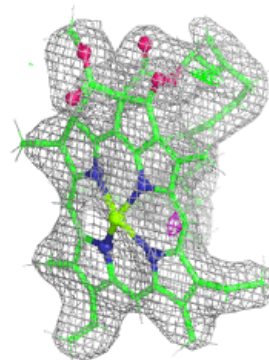


Electron density around LHG d 408:

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

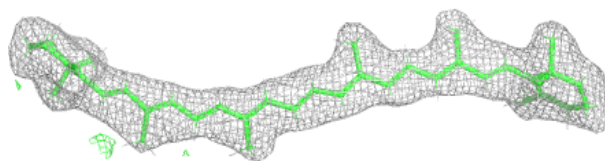
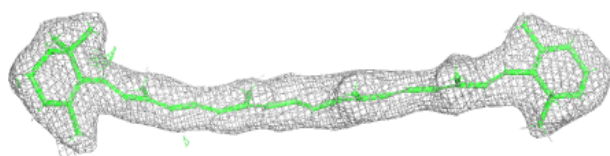
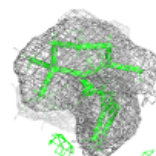
**Electron density around CLA c 511:**

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

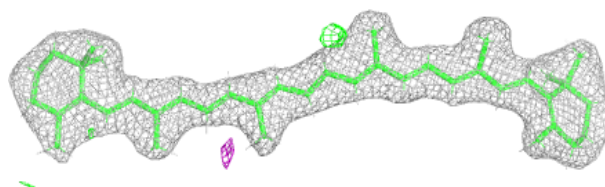
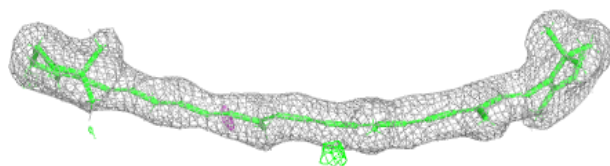
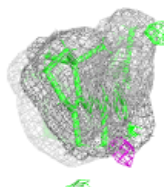


Electron density around BCR H 101:

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

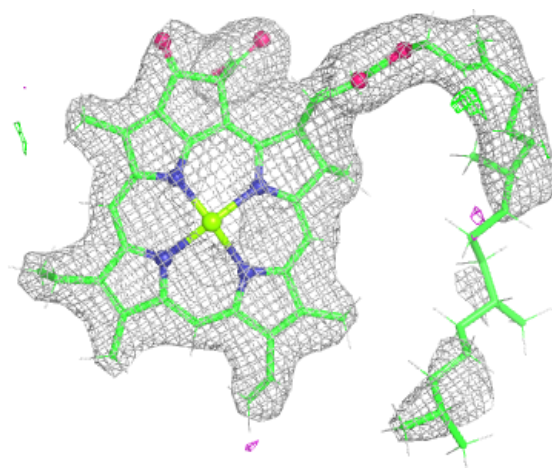
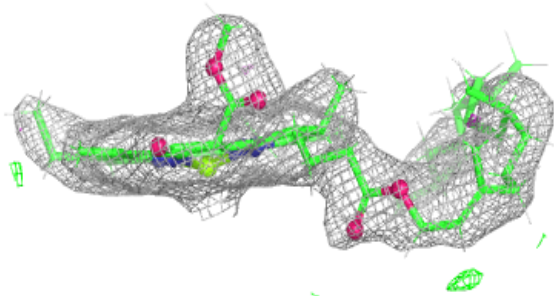
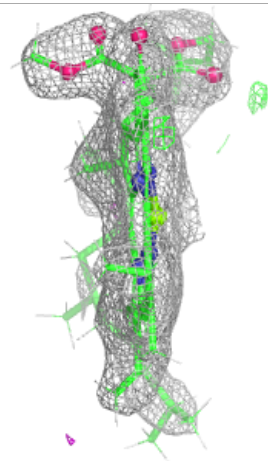
**Electron density around BCR t 101:**

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



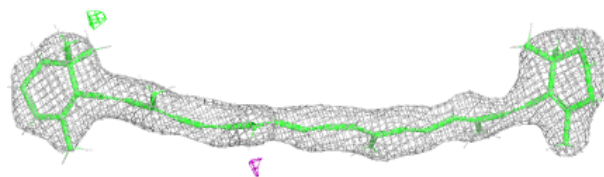
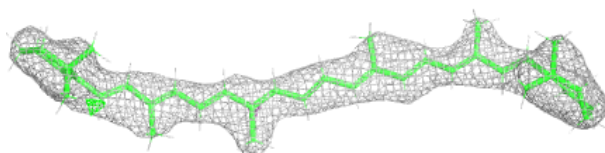
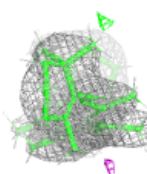
Electron density around CLA C 512:

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

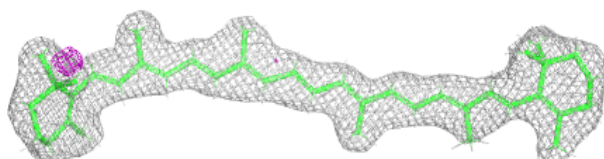
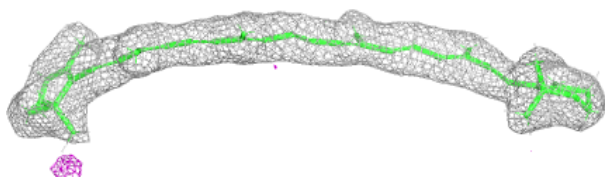
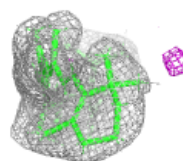


Electron density around BCR K 102:

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

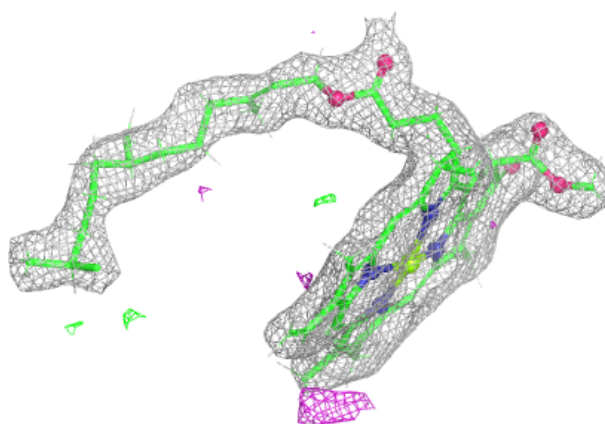
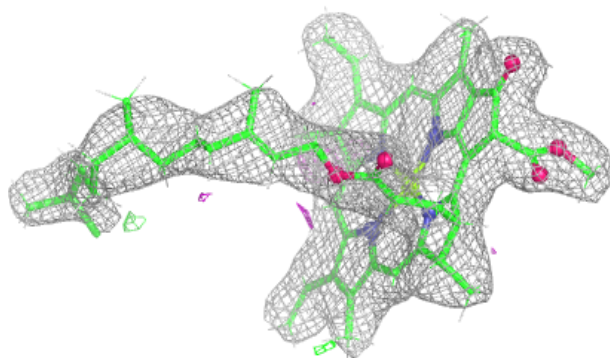
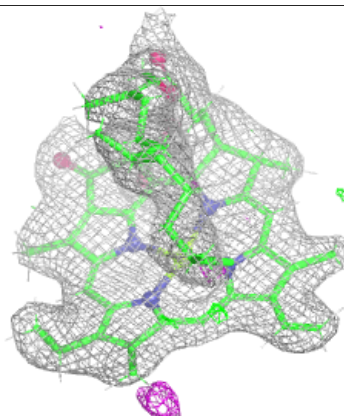
**Electron density around BCR T 101:**

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

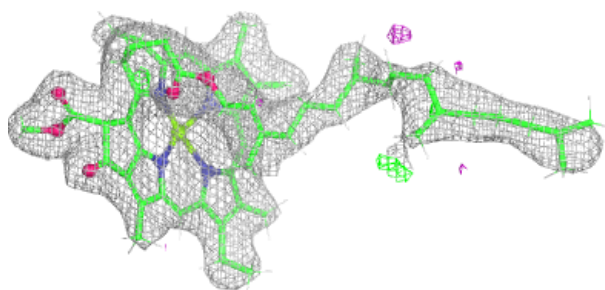
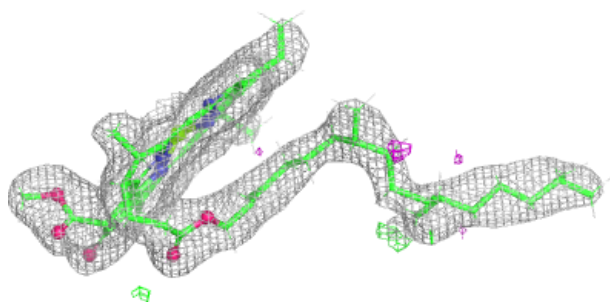
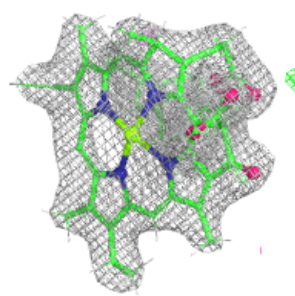


Electron density around CLA c 504:

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

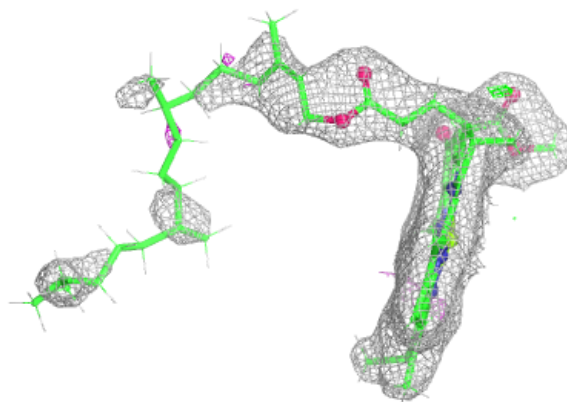
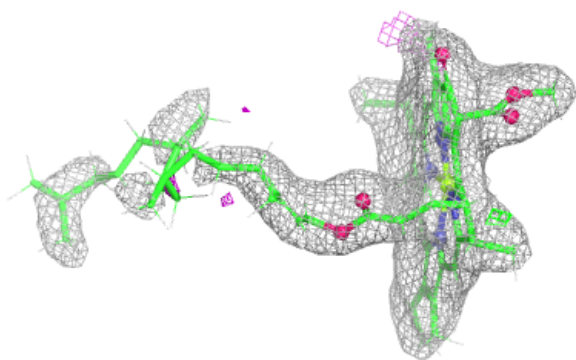
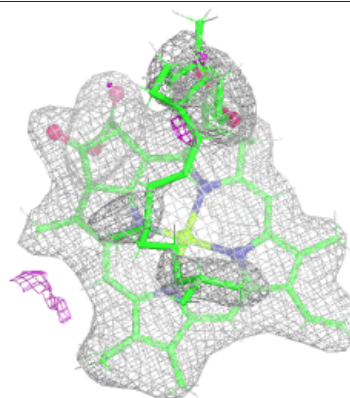
**Electron density around CLA c 505:**

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

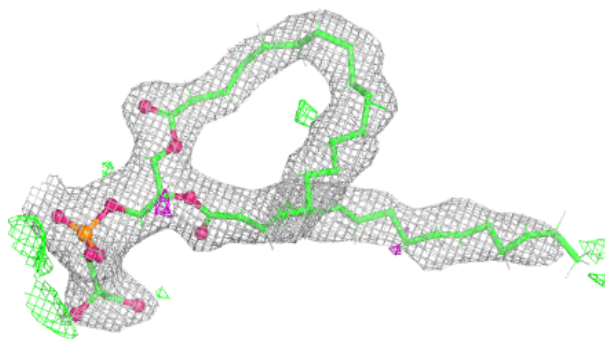
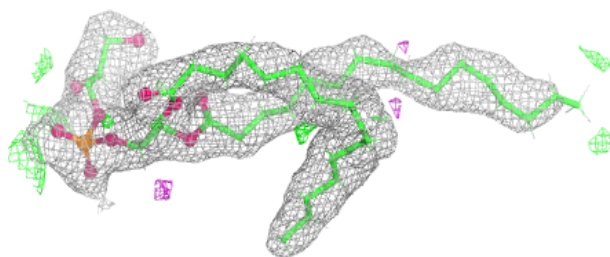
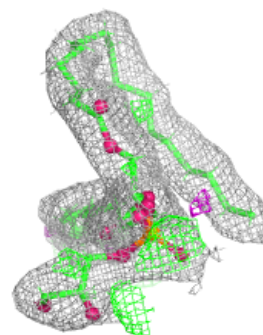


Electron density around CLA c 506:

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

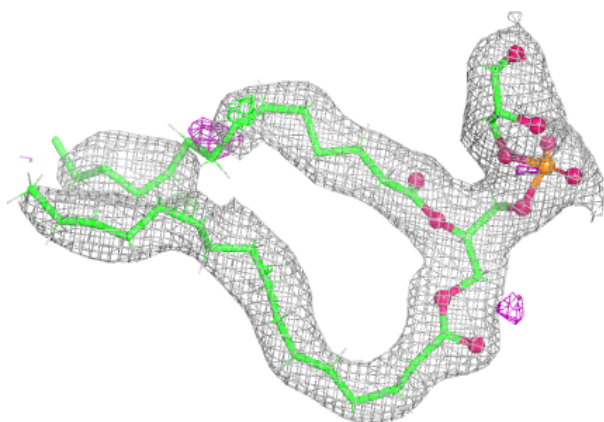
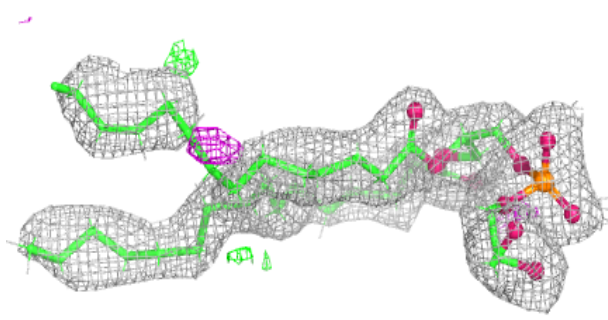
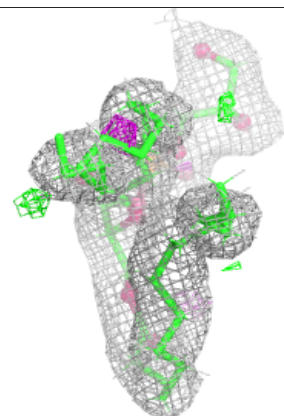
**Electron density around LHG B 623:**

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

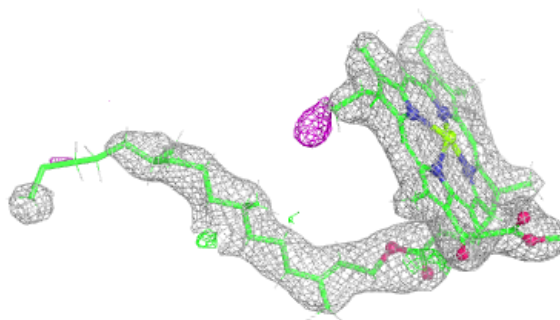
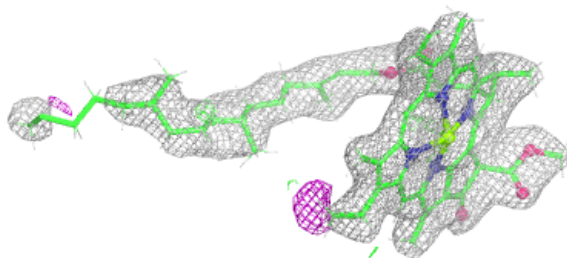
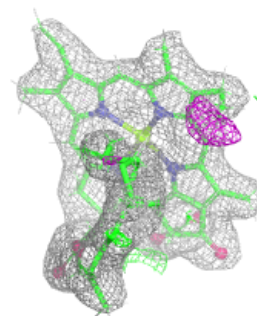


Electron density around LHG D 408:

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

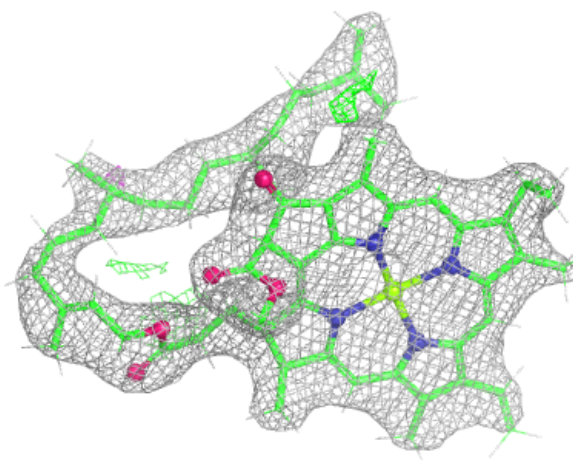
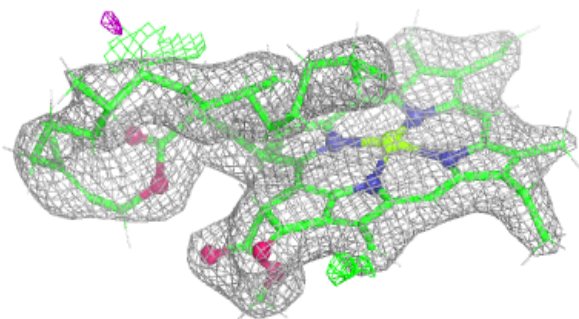
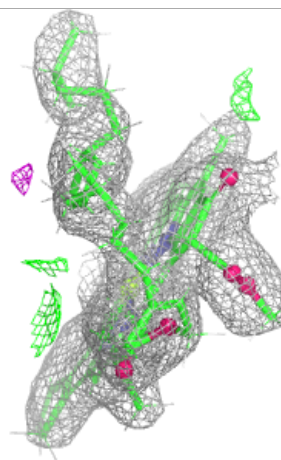
**Electron density around CLA c 508:**

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



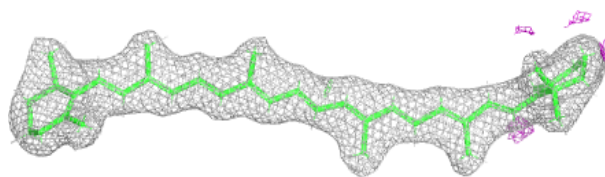
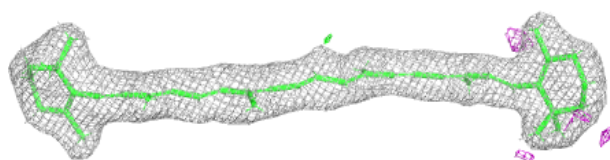
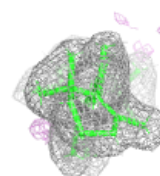
Electron density around CLA c 509:

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



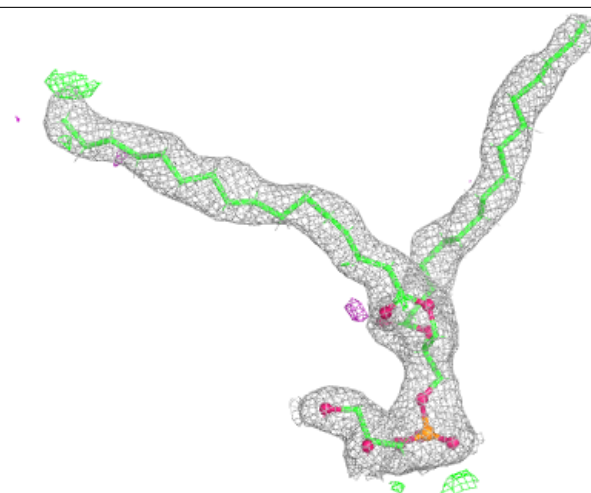
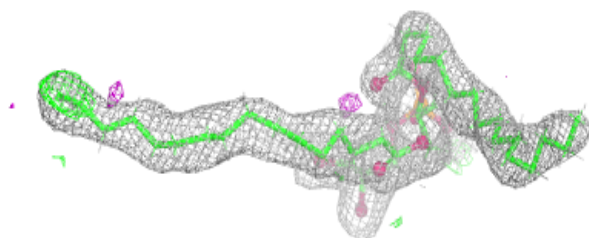
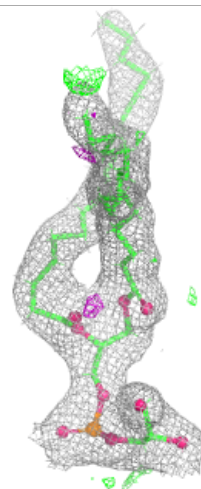
Electron density around BCR a 409:

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



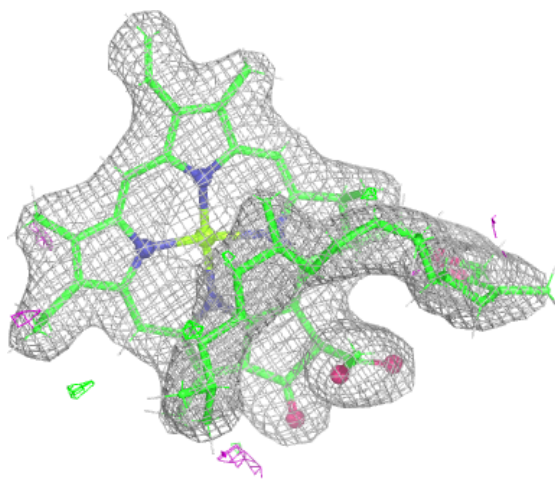
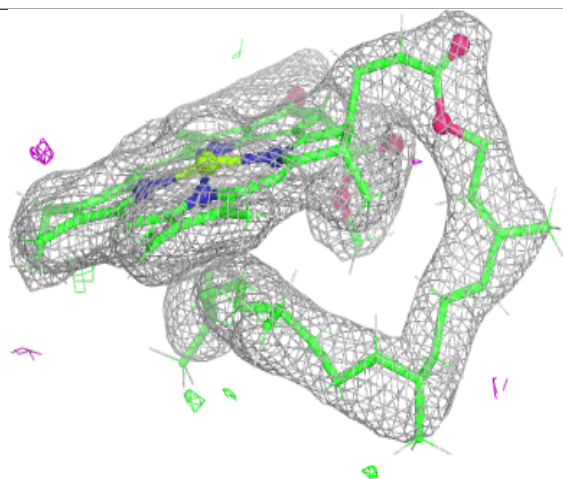
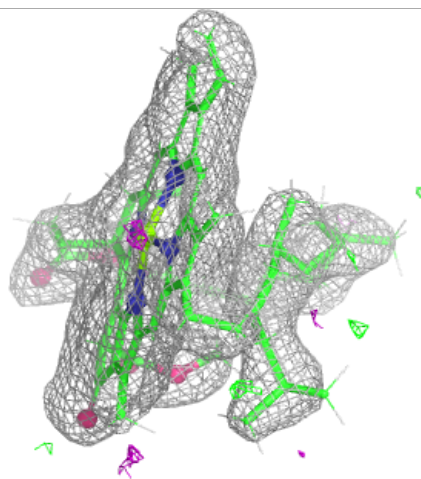
Electron density around LHG 1 101:

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



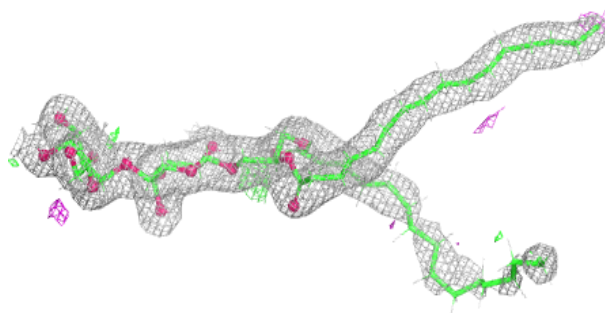
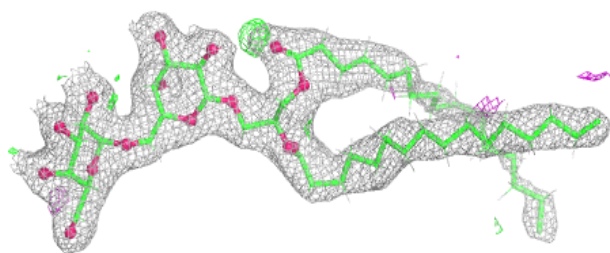
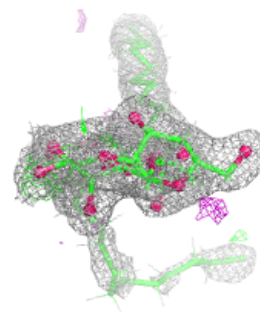
Electron density around CLA c 510:

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

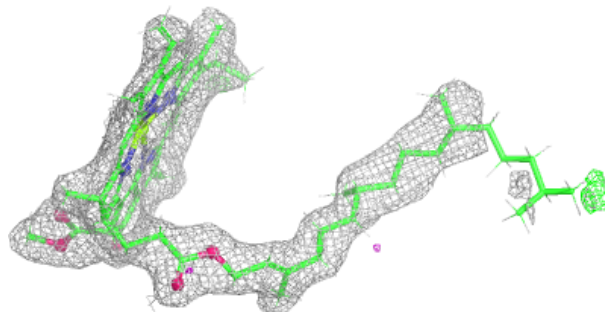
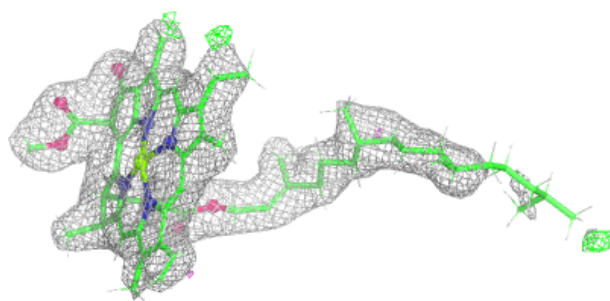
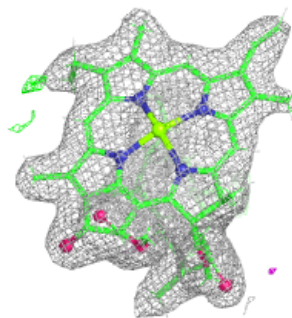


Electron density around DGD C 515:

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

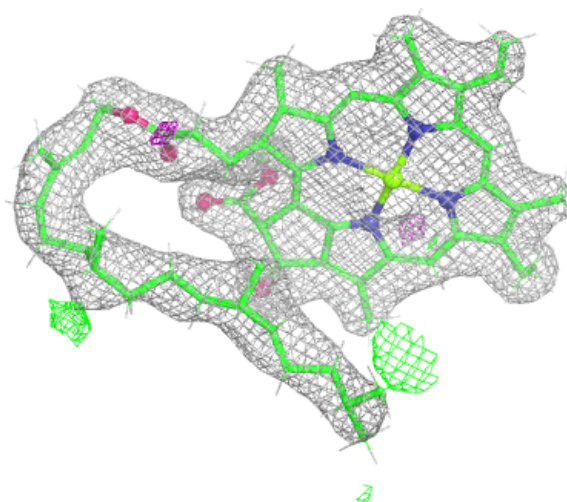
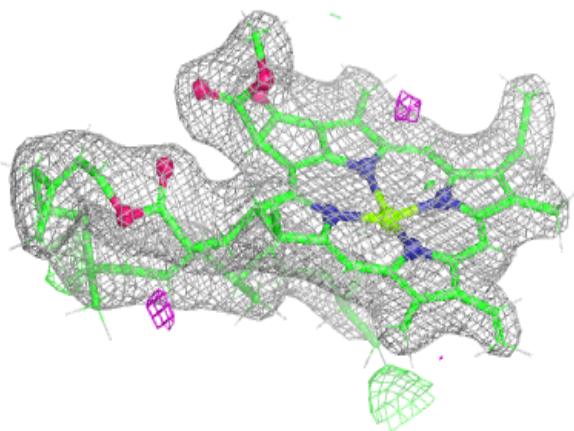
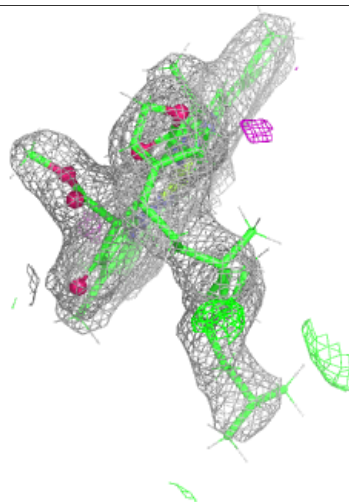
**Electron density around CLA C 508:**

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



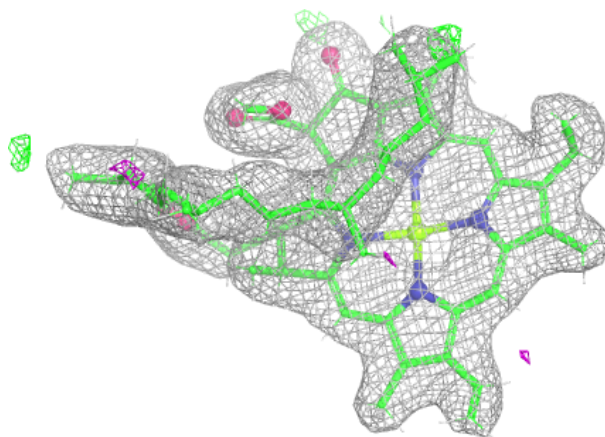
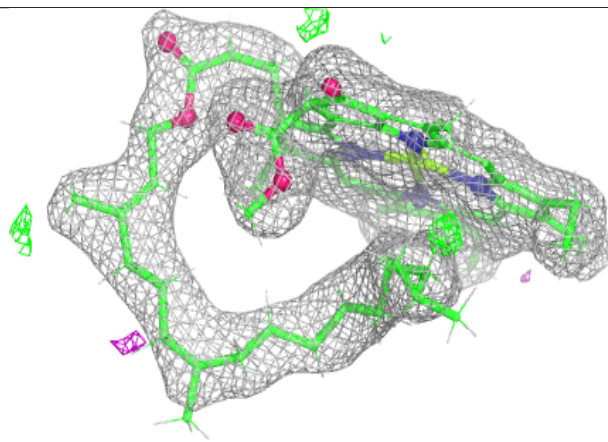
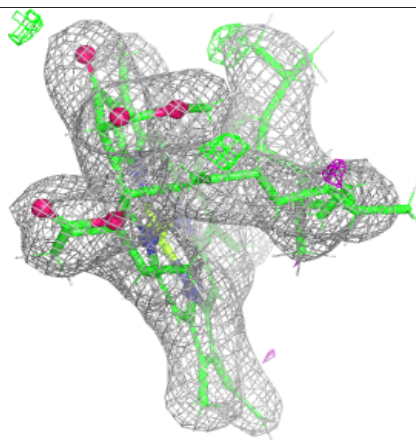
Electron density around CLA C 509:

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



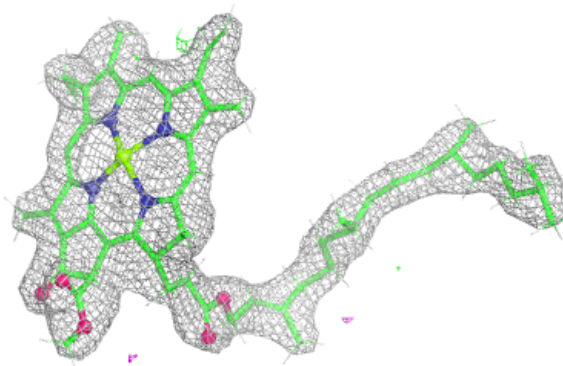
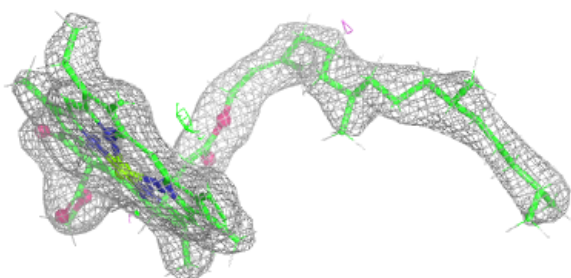
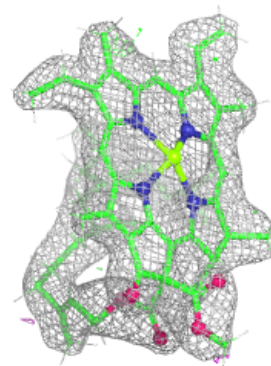
Electron density around CLA C 510:

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

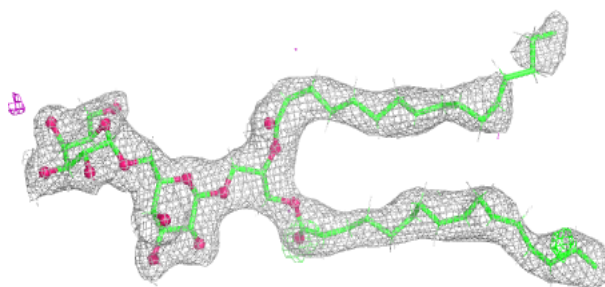
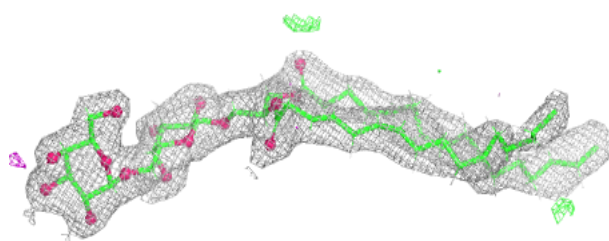
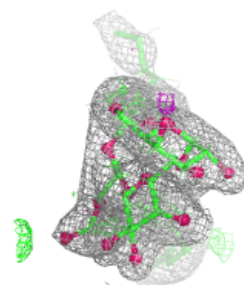


Electron density around CLA C 511:

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

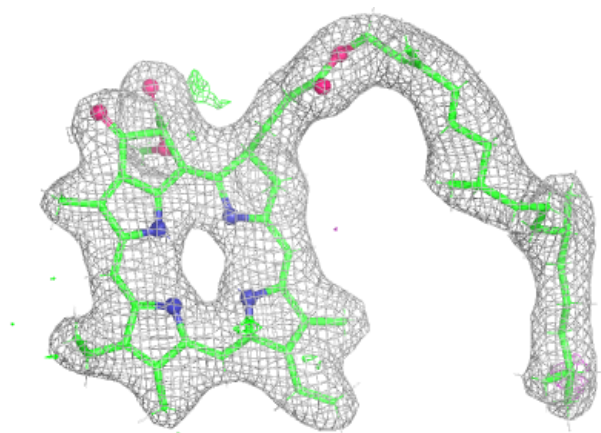
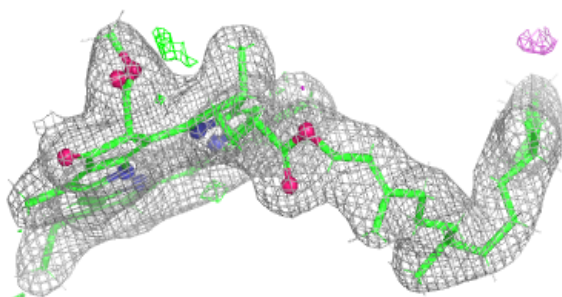
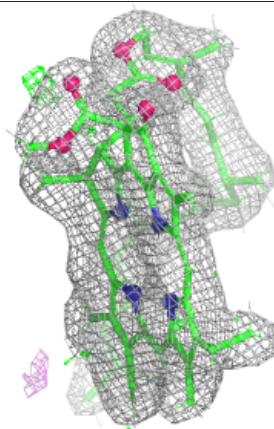
**Electron density around DGD c 518:**

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

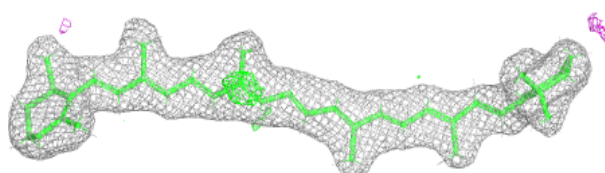
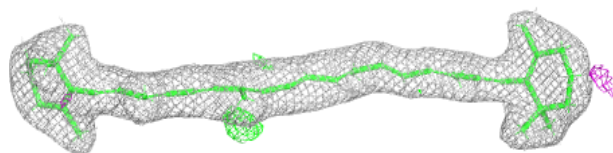
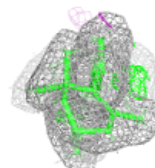


Electron density around PHO d 401:

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

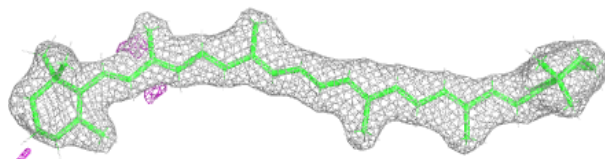
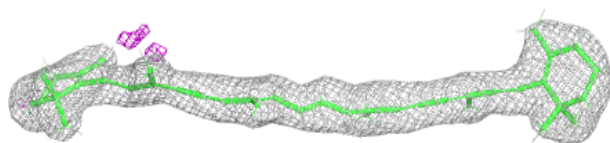
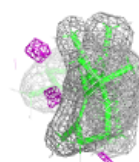
**Electron density around BCR A 409:**

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

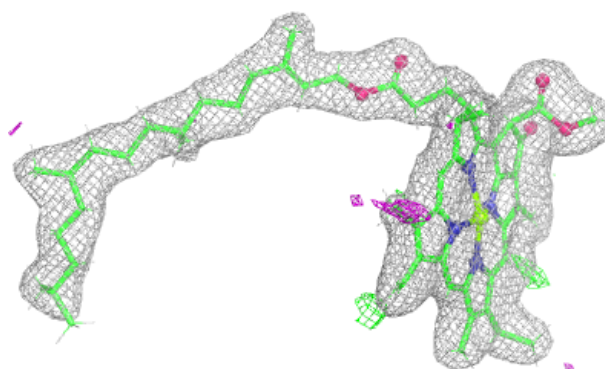
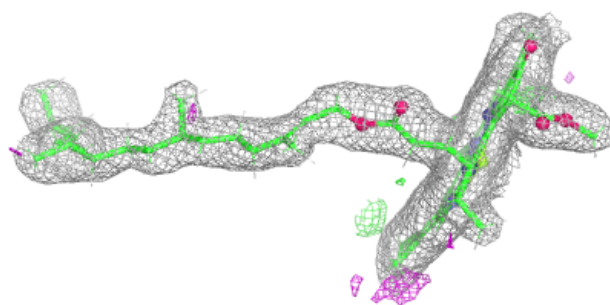
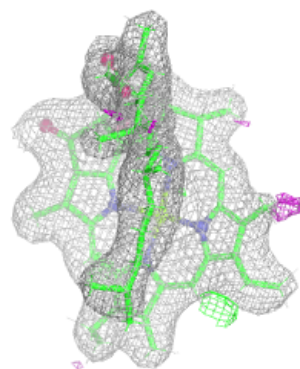


Electron density around BCR B 617:

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

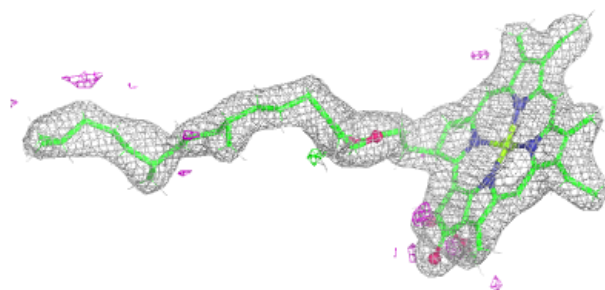
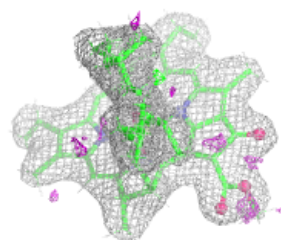
**Electron density around CLA B 609:**

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



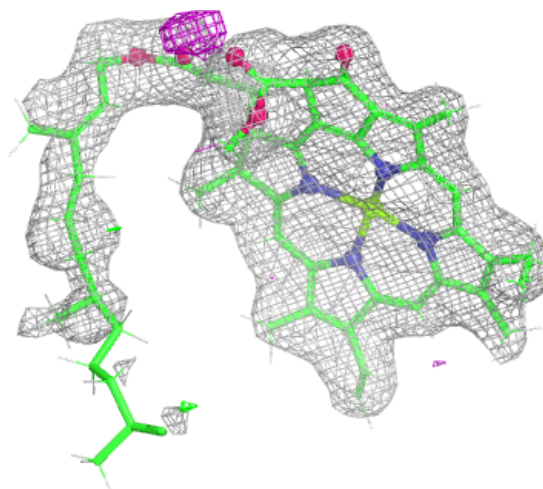
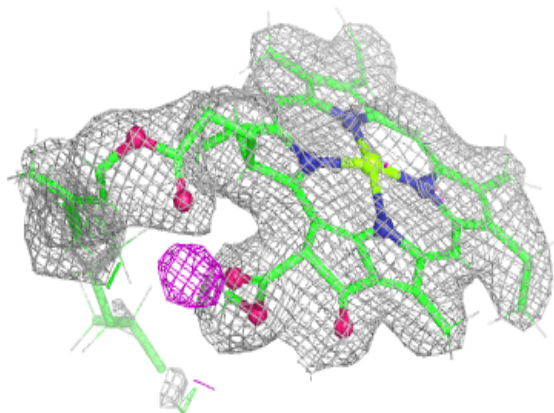
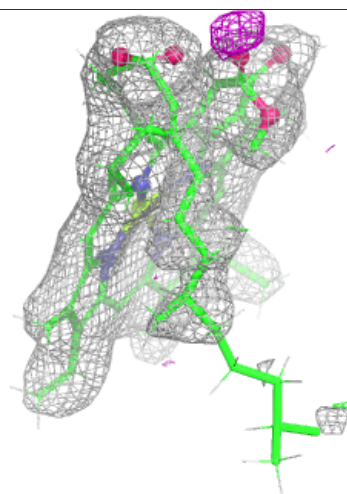
Electron density around CLA C 502:

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



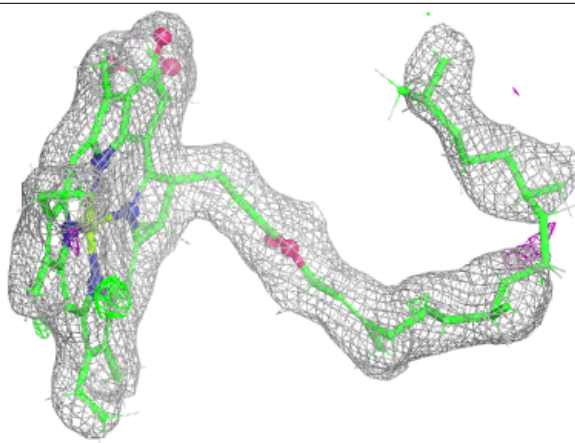
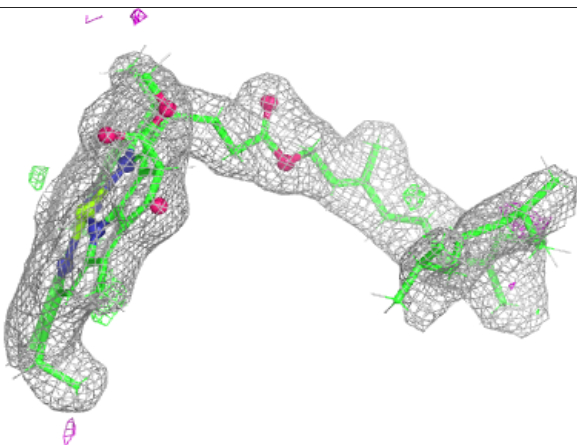
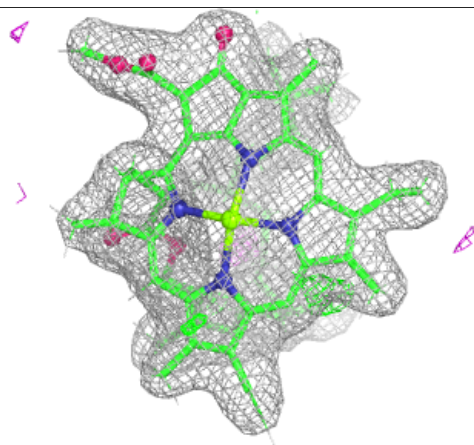
Electron density around CLA b 617:

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

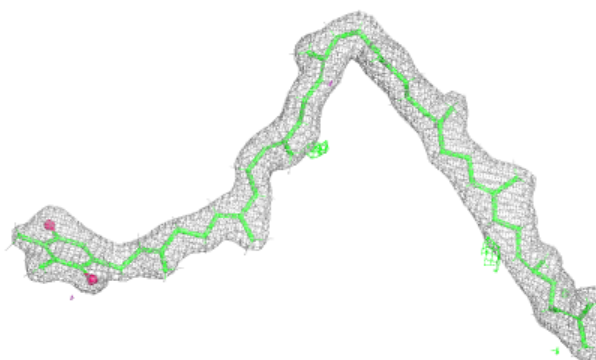
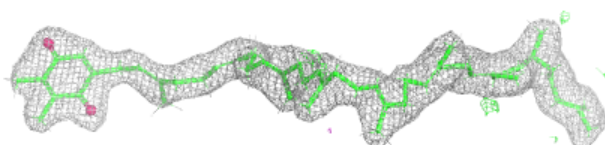
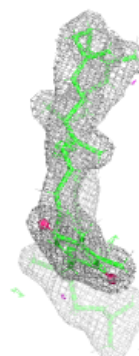


Electron density around CLA B 606:

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

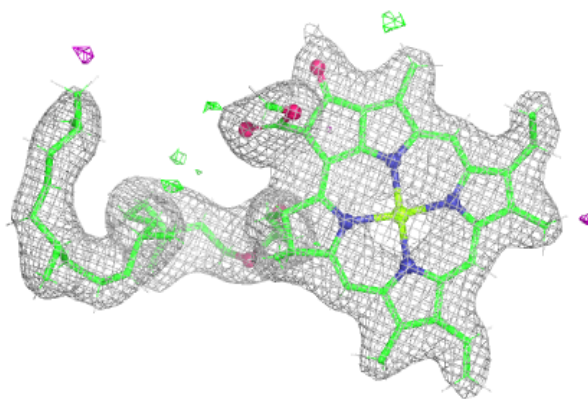
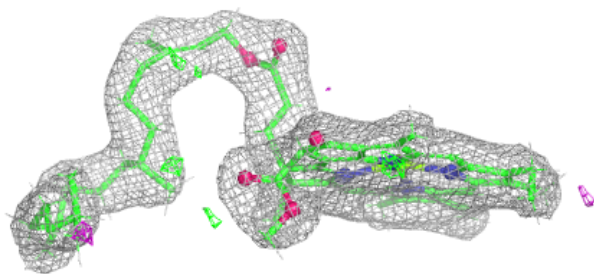
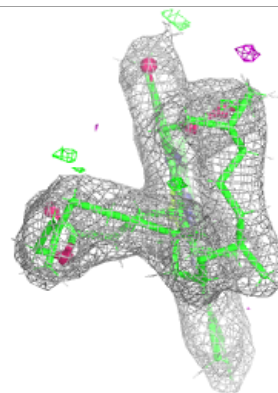
**Electron density around PL9 d 405:**

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

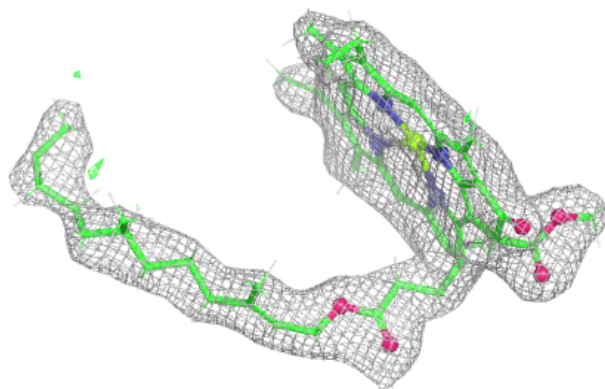
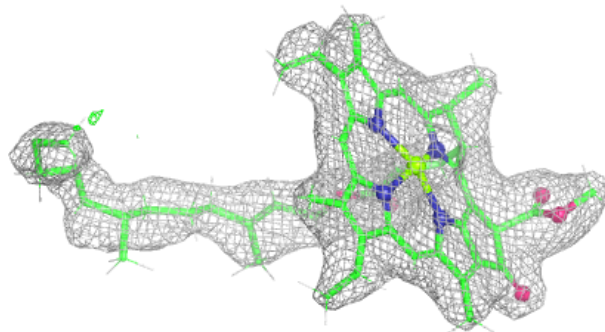
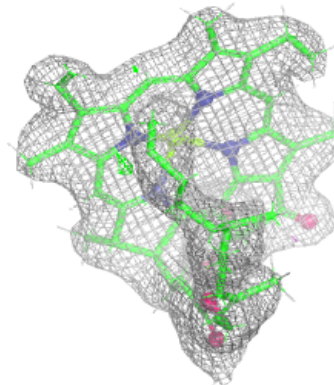


Electron density around CLA B 612:

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

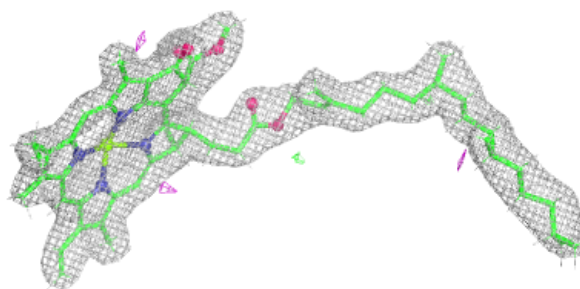
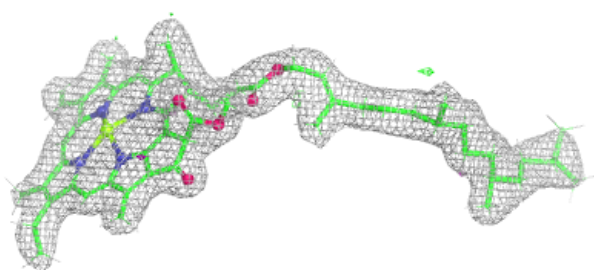
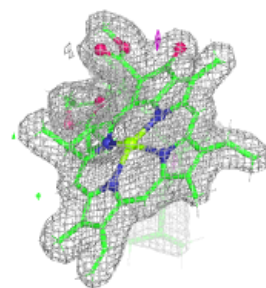
**Electron density around CLA C 504:**

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

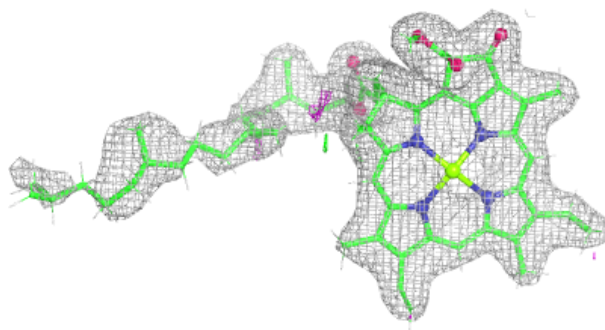
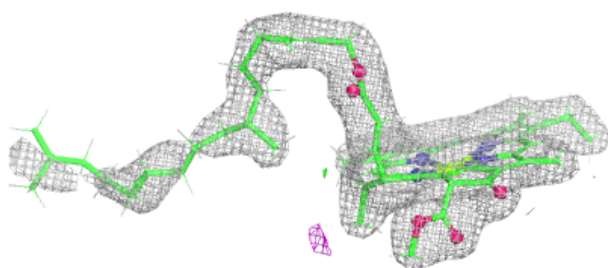


Electron density around CLA a 405:

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

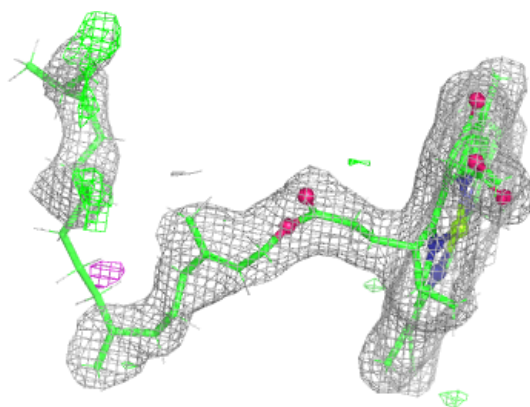
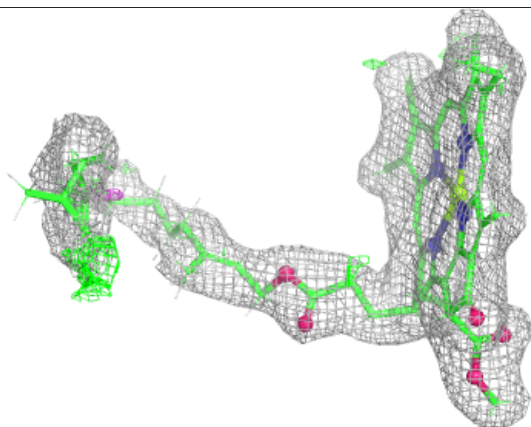
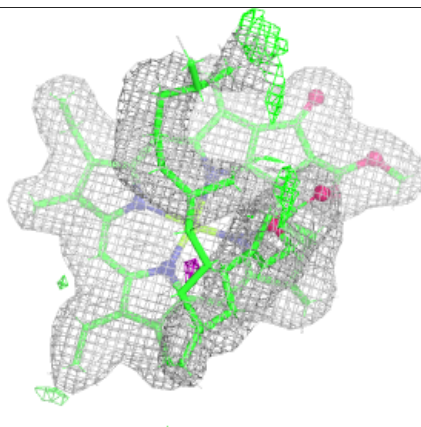
**Electron density around CLA a 406:**

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

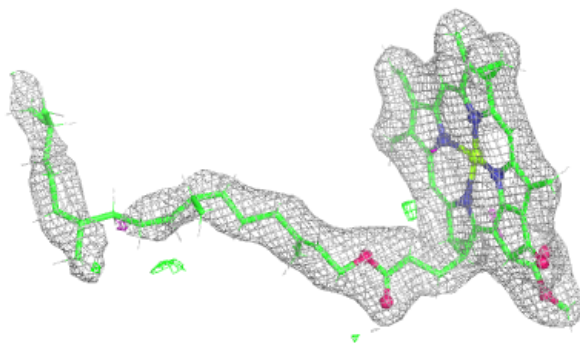
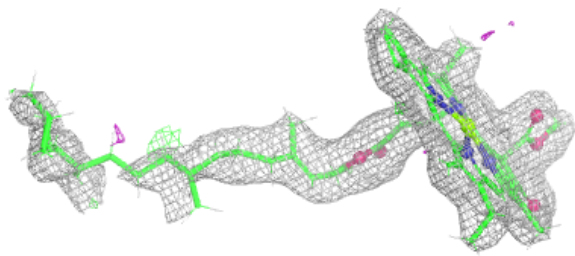
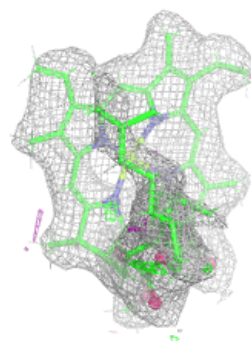


Electron density around CLA a 408:

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

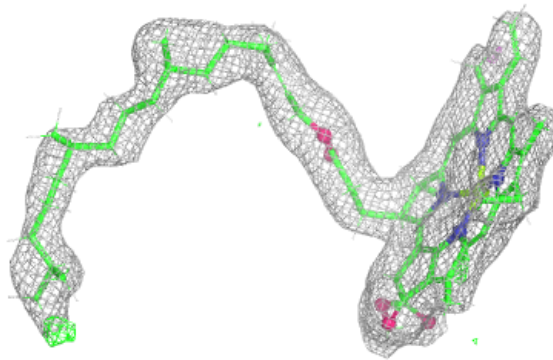
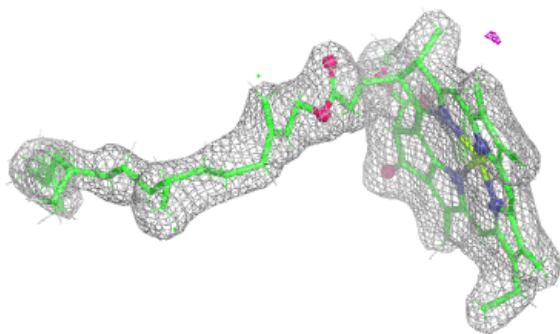
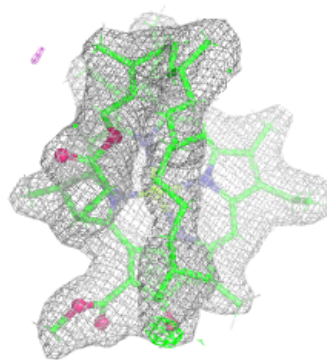
**Electron density around CLA d 403:**

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



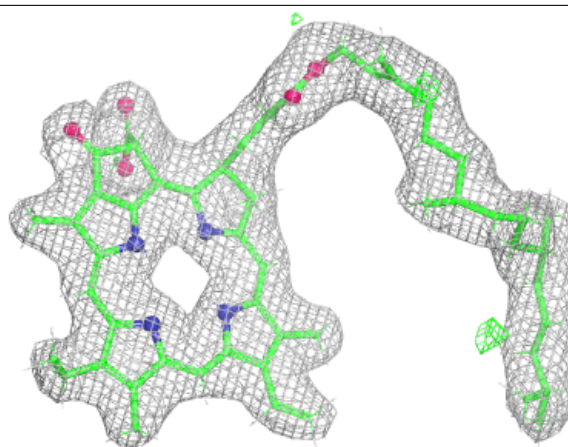
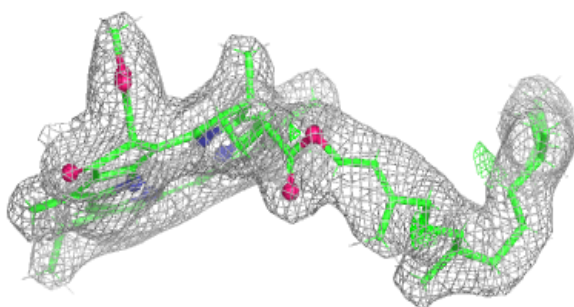
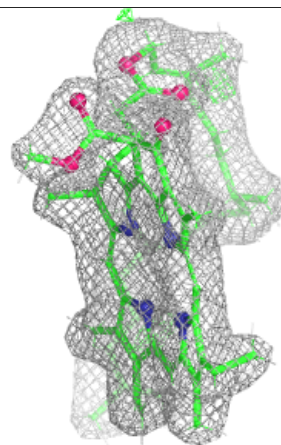
Electron density around CLA b 607:

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



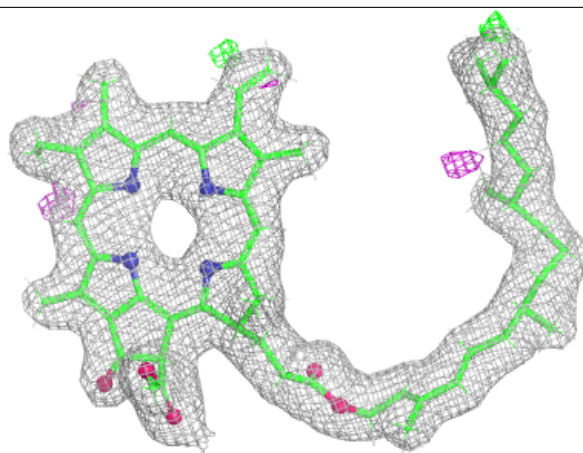
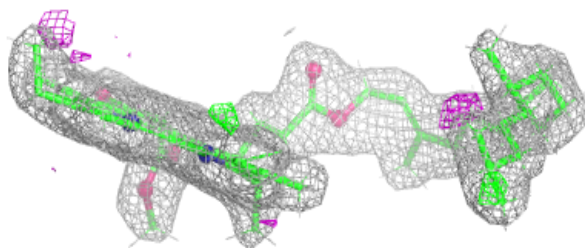
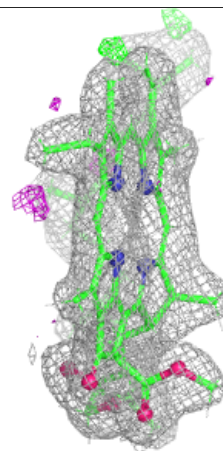
Electron density around PHO A 407:

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



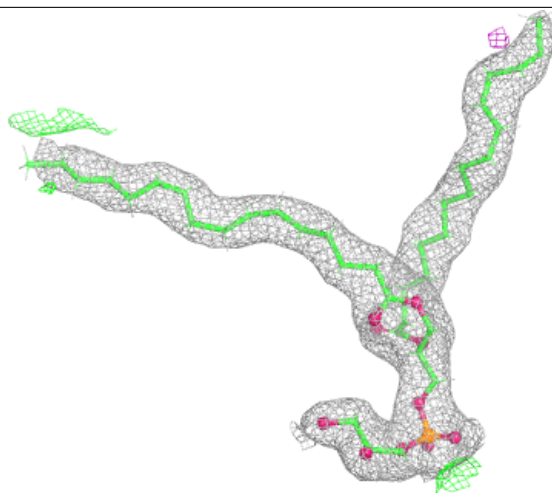
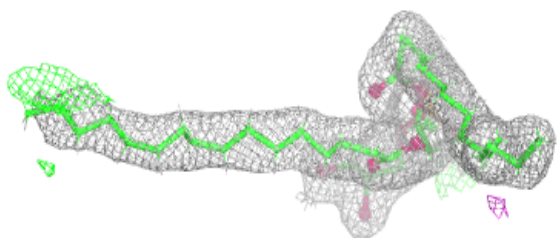
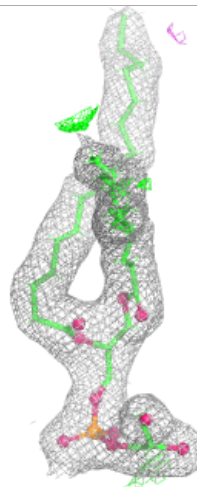
Electron density around PHO a 407:

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



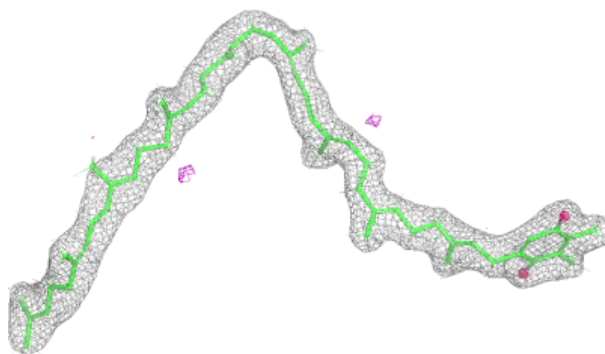
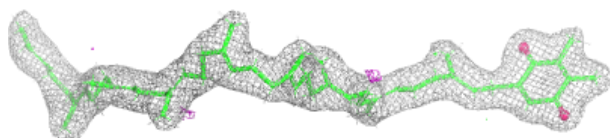
Electron density around LHG B 622:

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

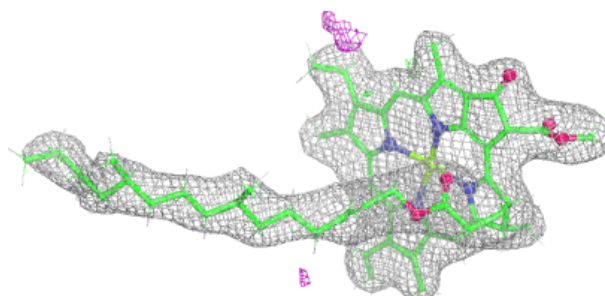
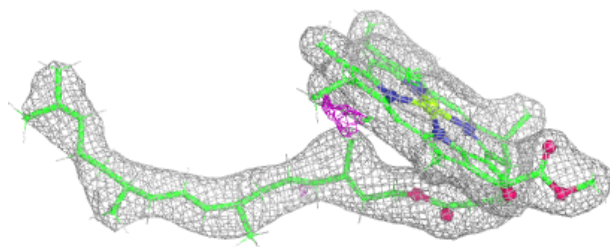
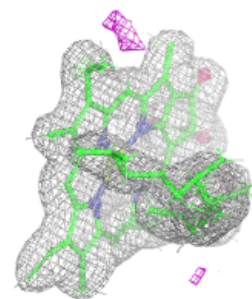


Electron density around PL9 D 405:

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

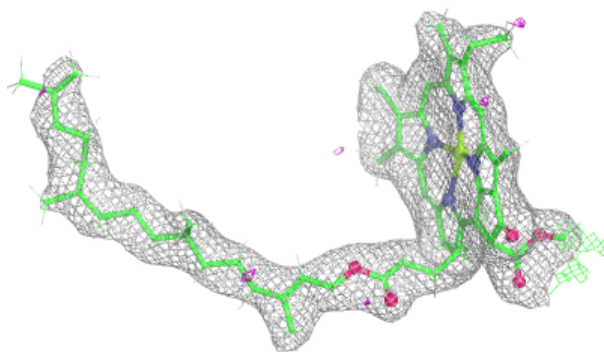
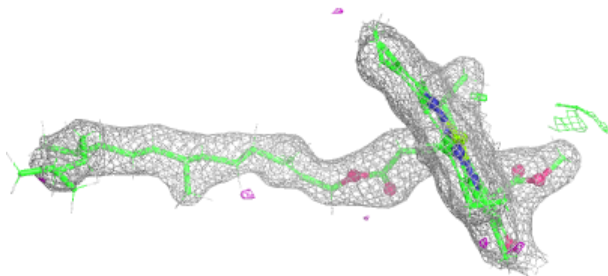
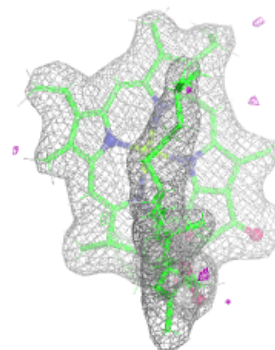
**Electron density around CLA b 609:**

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

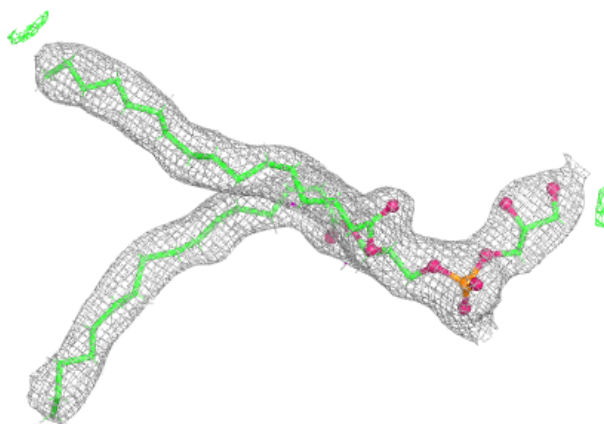
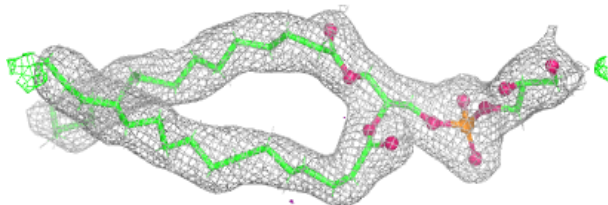
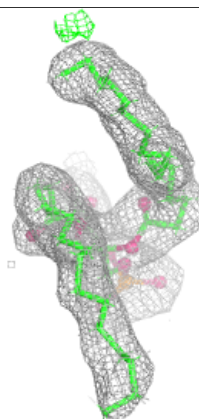


Electron density around CLA b 610:

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

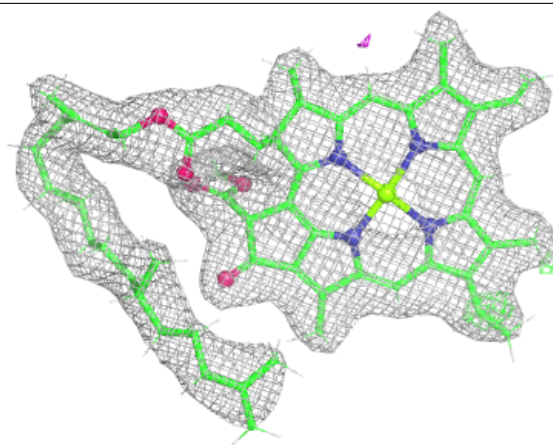
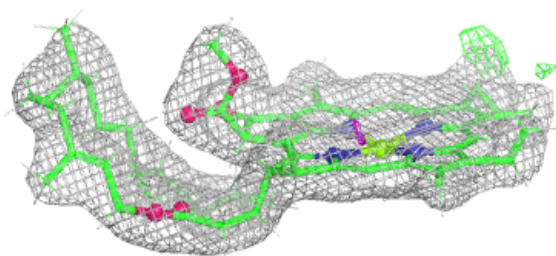
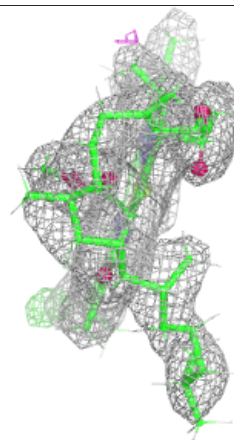
**Electron density around LHG d 407:**

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



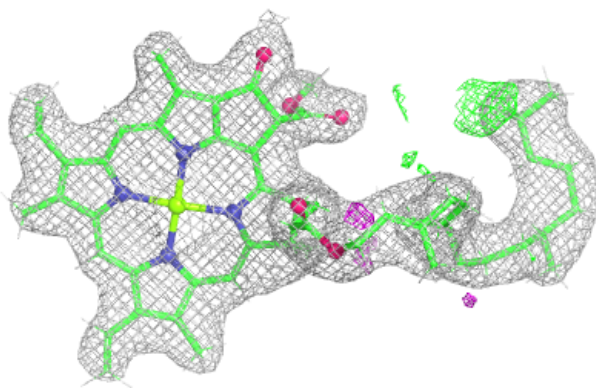
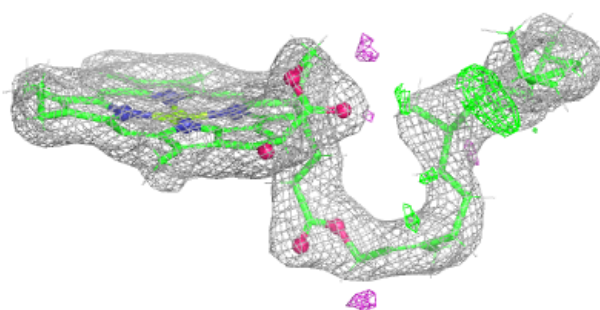
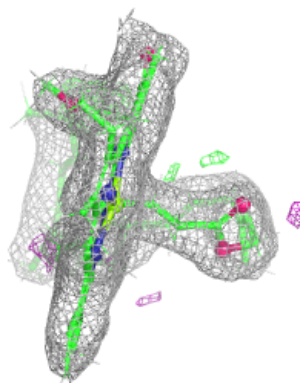
Electron density around CLA b 611:

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

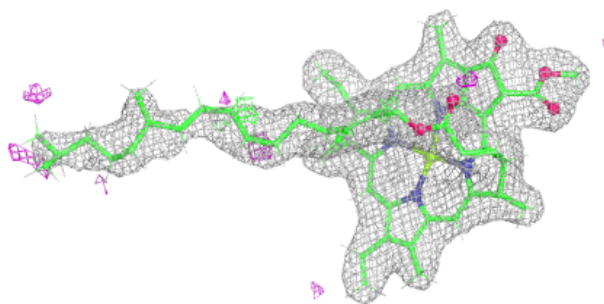
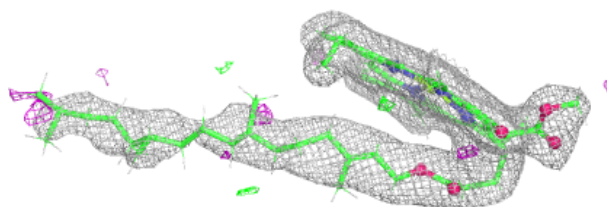
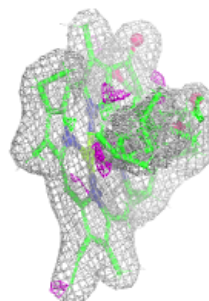


Electron density around CLA b 613:

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

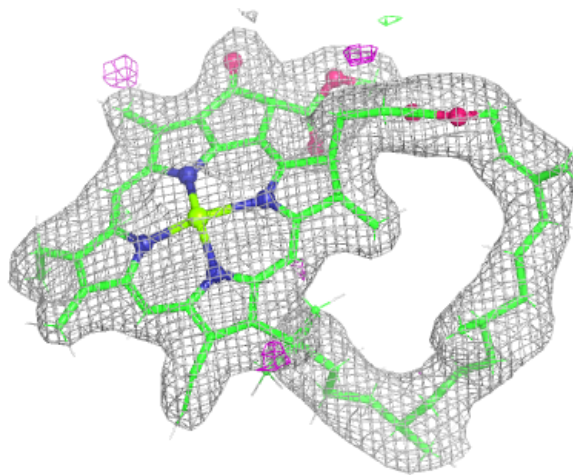
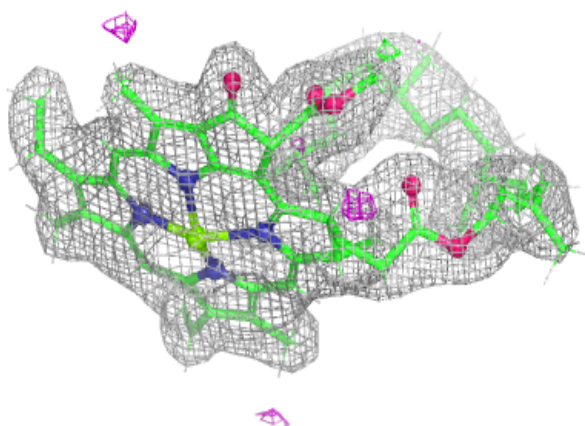
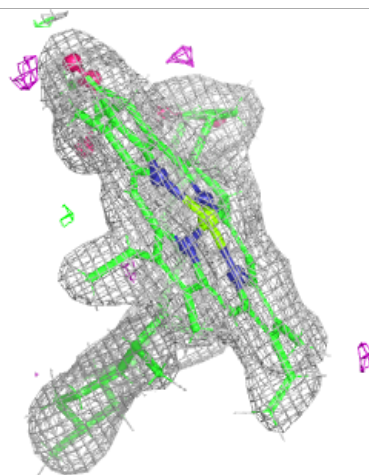
**Electron density around CLA b 615:**

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



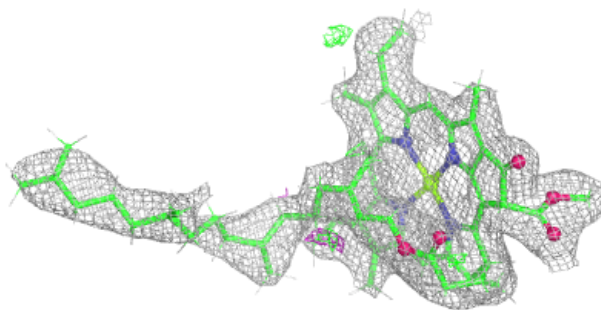
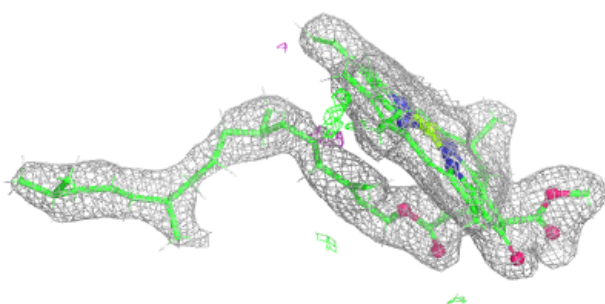
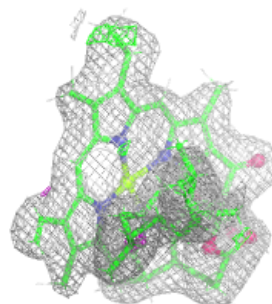
Electron density around CLA b 616:

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

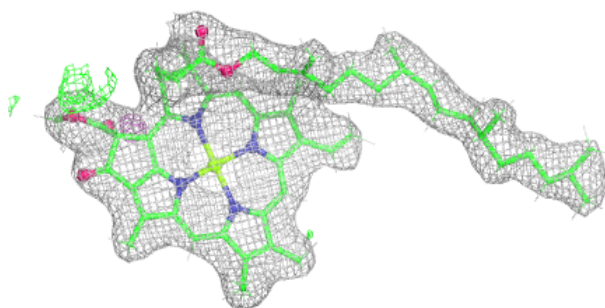
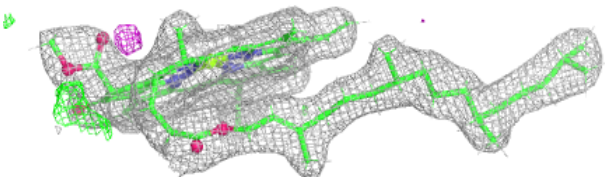
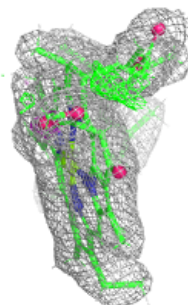


Electron density around CLA C 505:

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

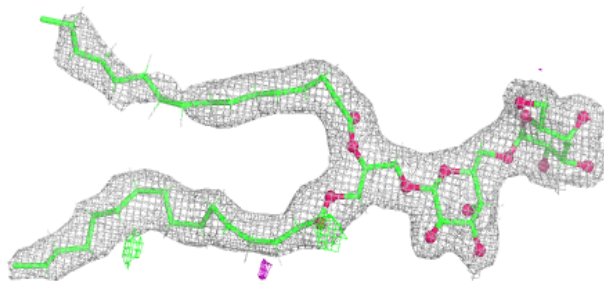
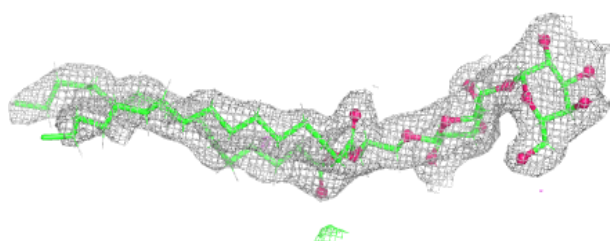
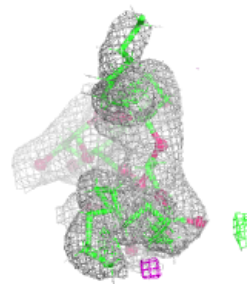
**Electron density around CLA c 501:**

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

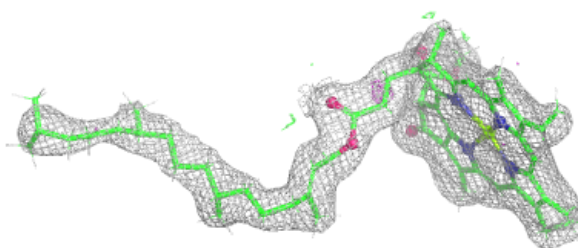
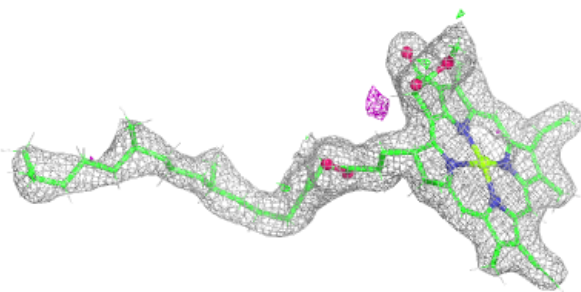
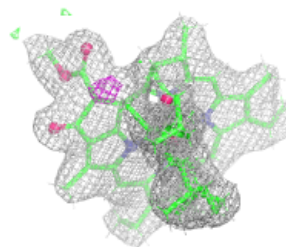


Electron density around DGD C 517:

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

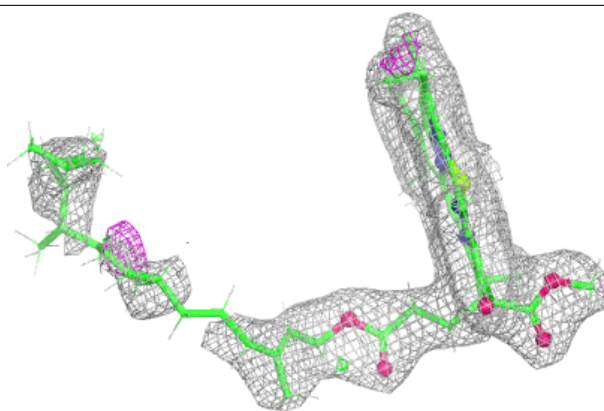
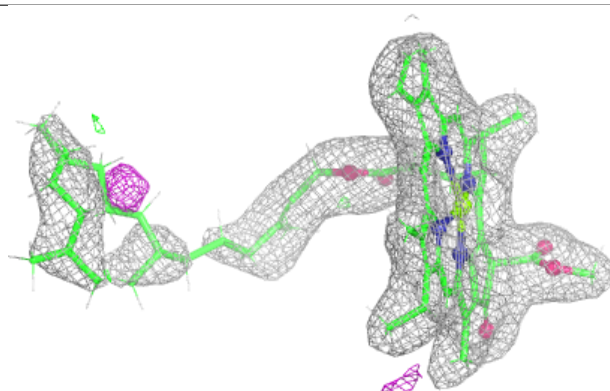
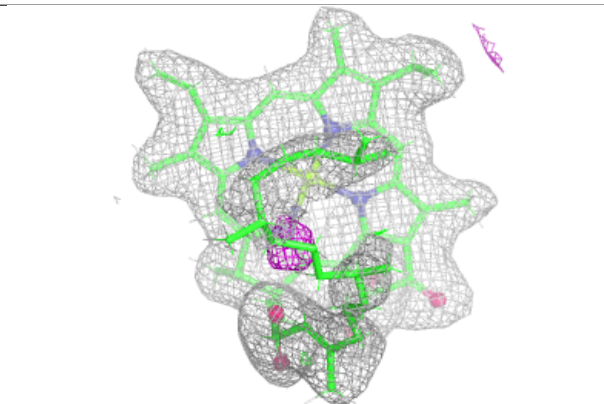
**Electron density around CLA c 502:**

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

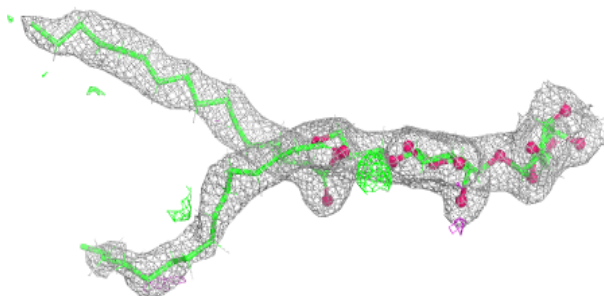
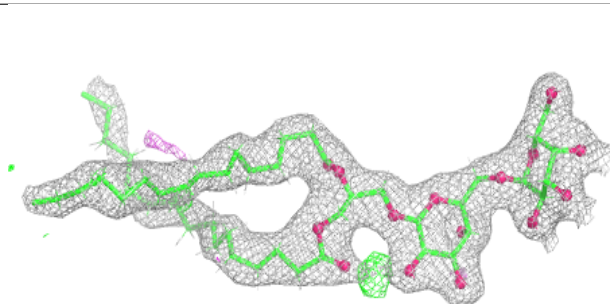
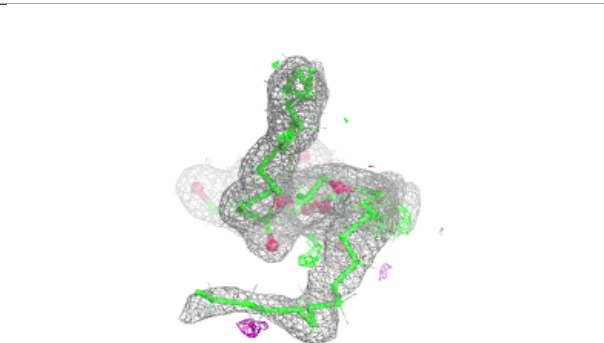


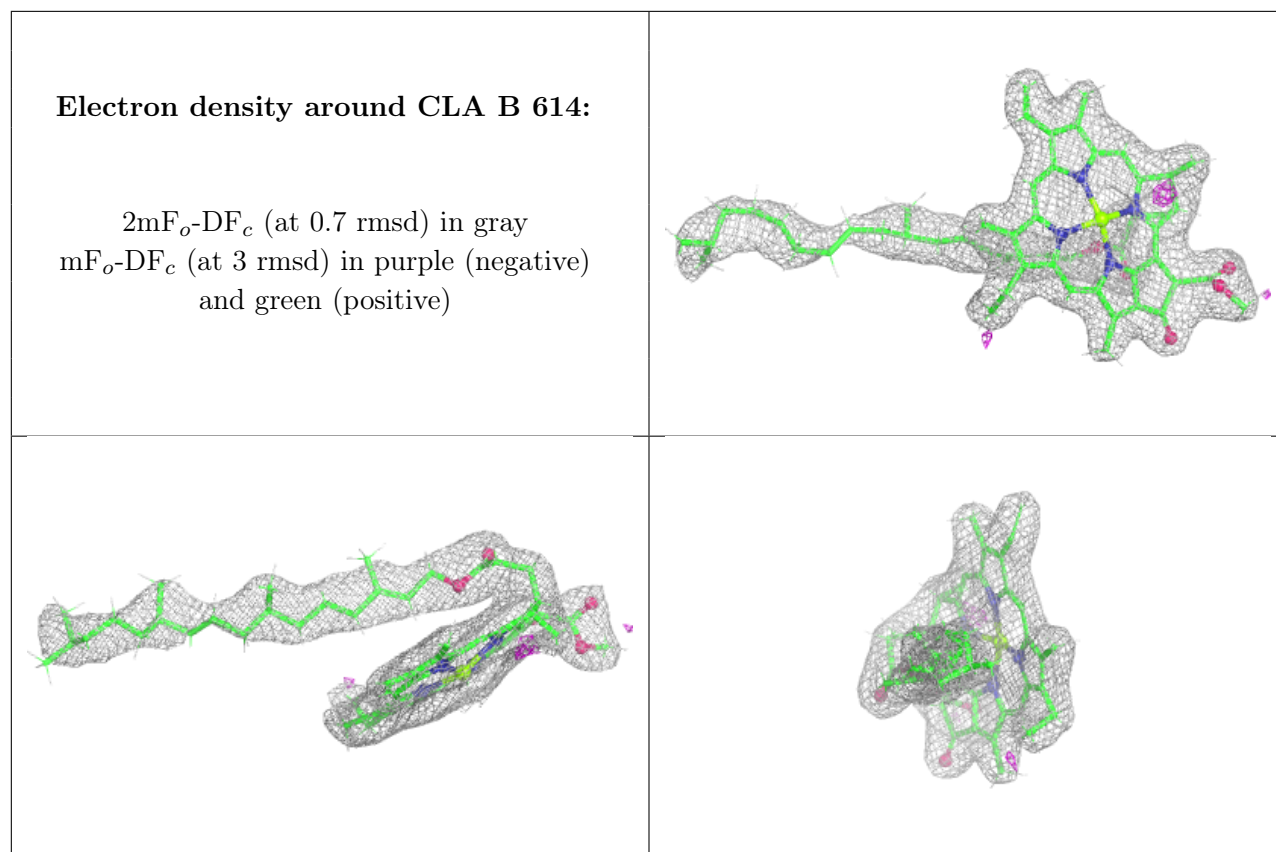
Electron density around CLA C 506:

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

**Electron density around DGD c 516:**

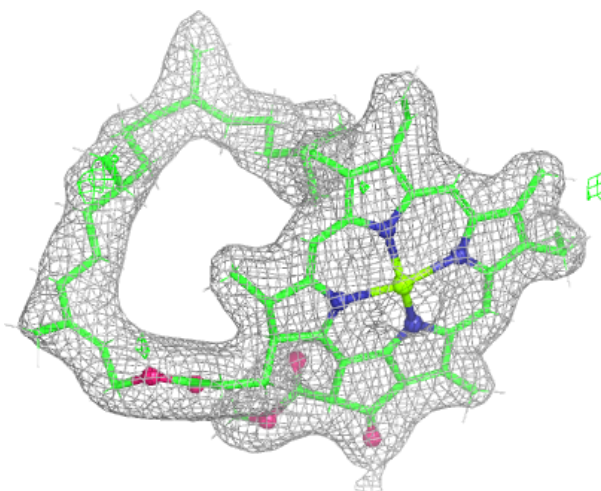
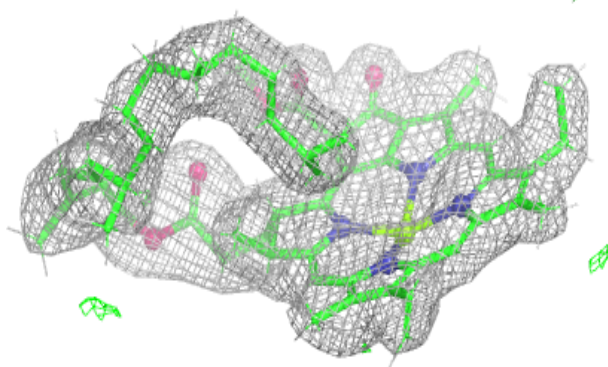
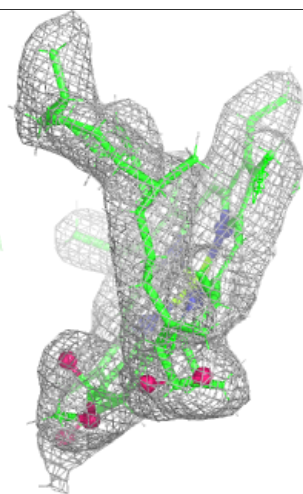
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





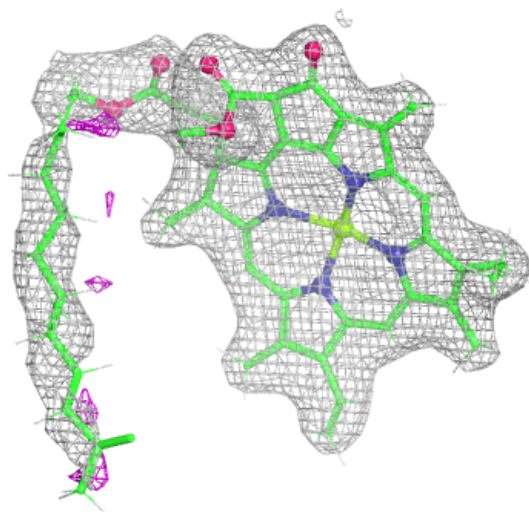
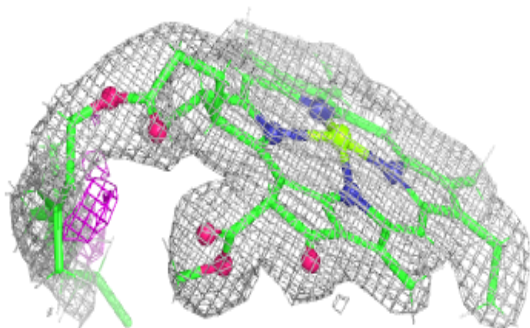
Electron density around CLA B 615:

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



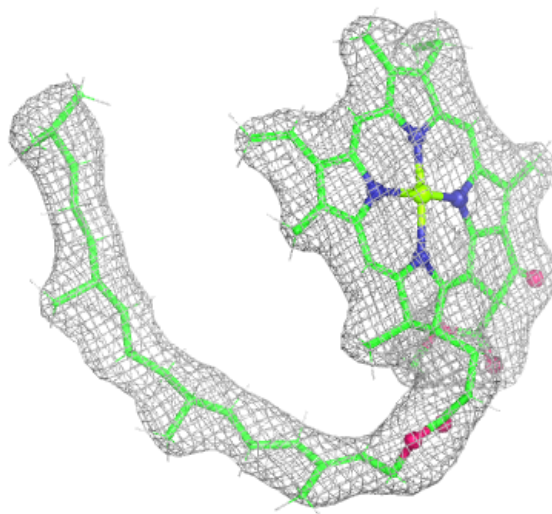
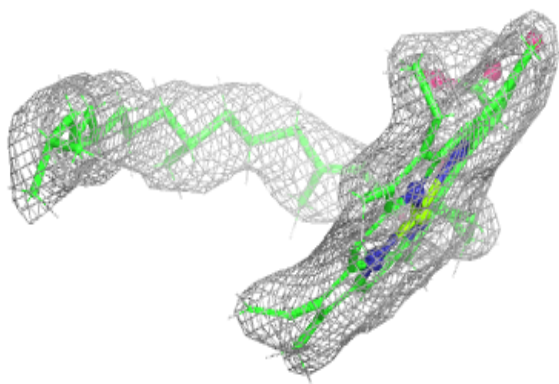
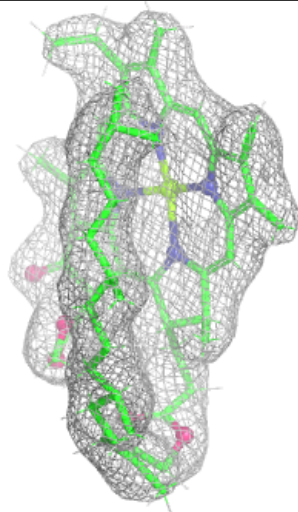
Electron density around CLA B 616:

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



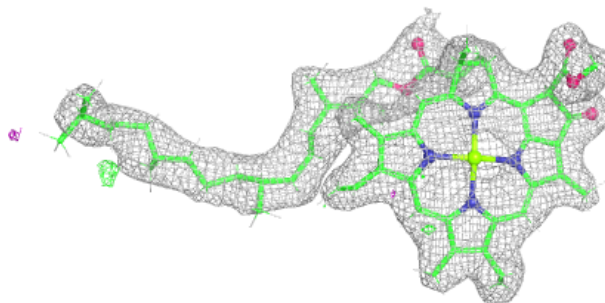
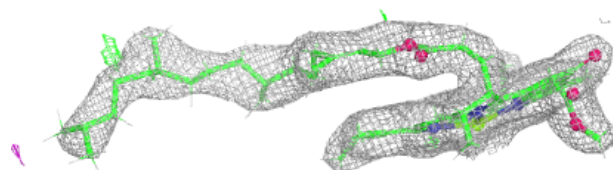
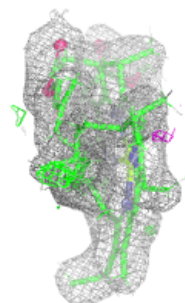
Electron density around CLA c 507:

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



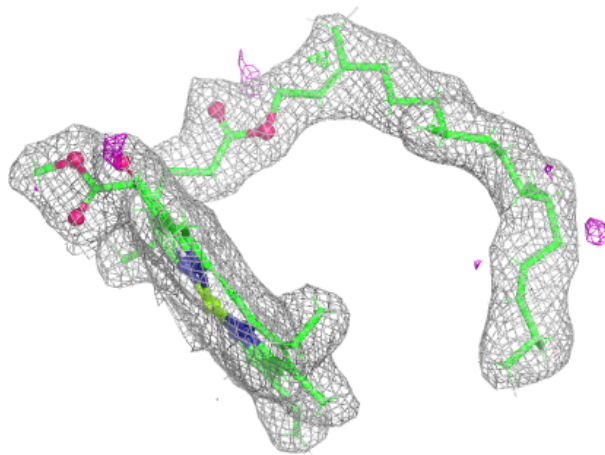
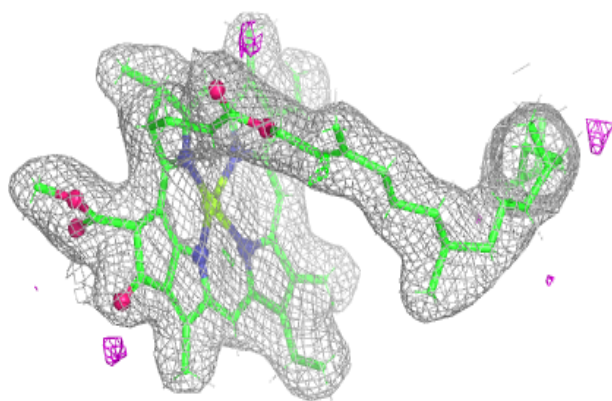
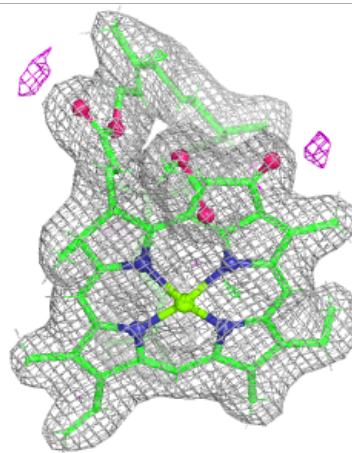
Electron density around CLA B 603:

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



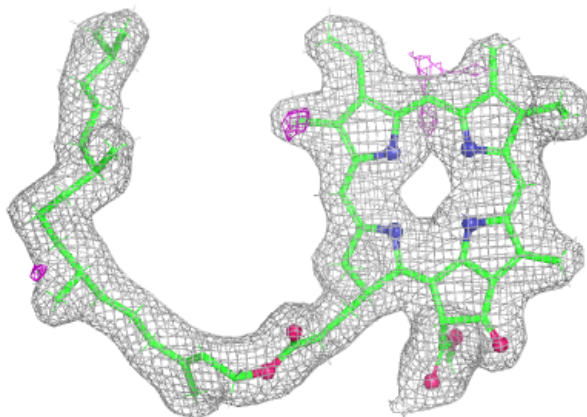
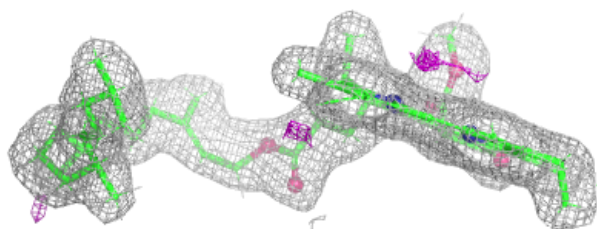
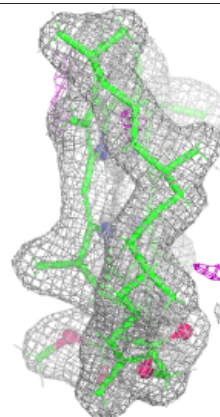
Electron density around CLA B 611:

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



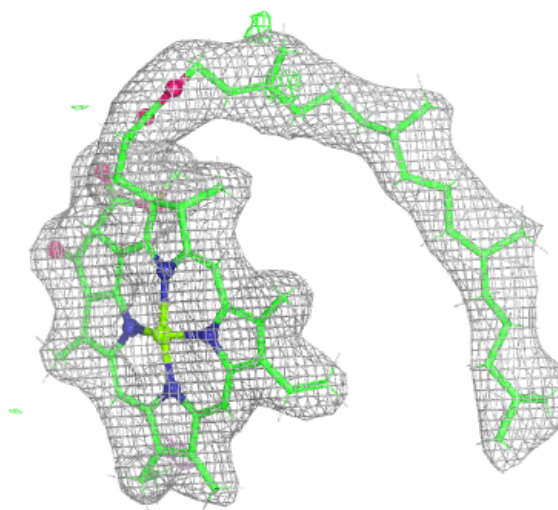
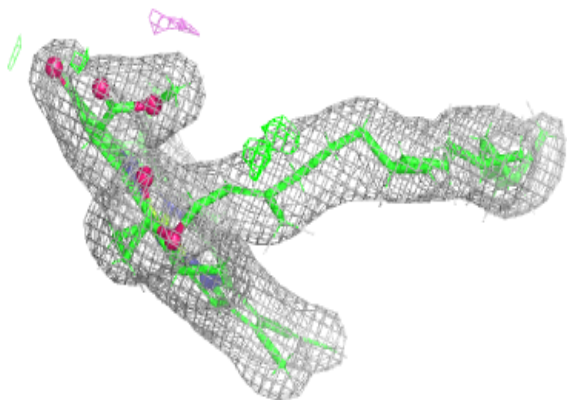
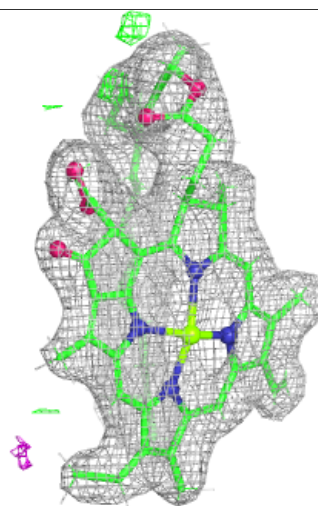
Electron density around PHO A 406:

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



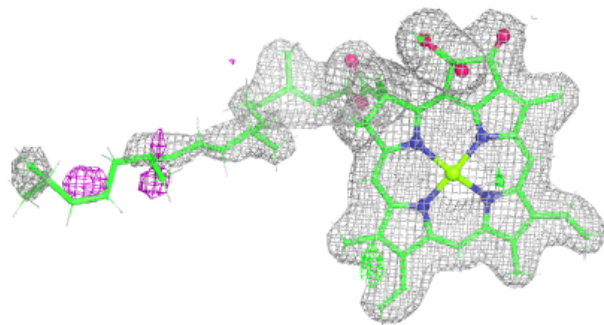
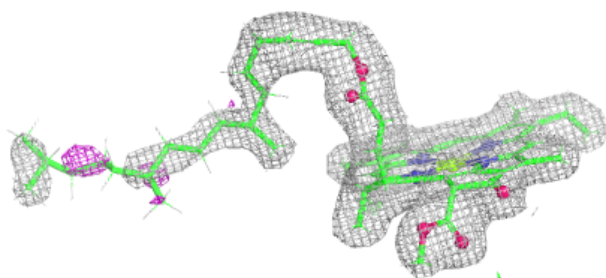
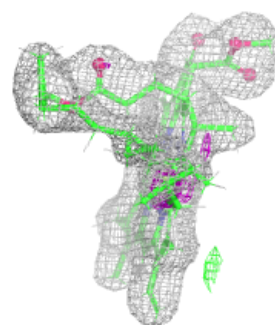
Electron density around CLA C 507:

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



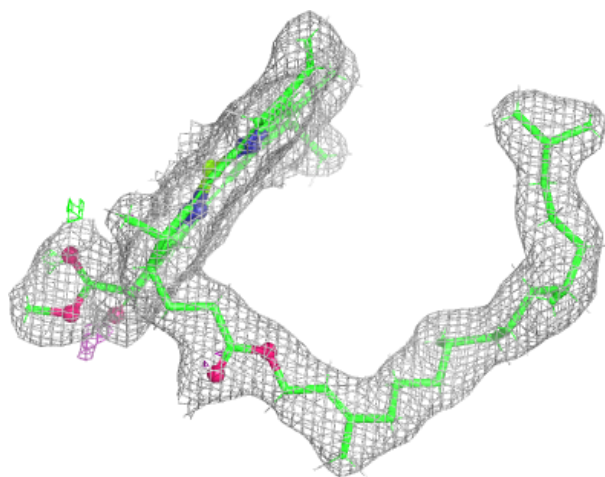
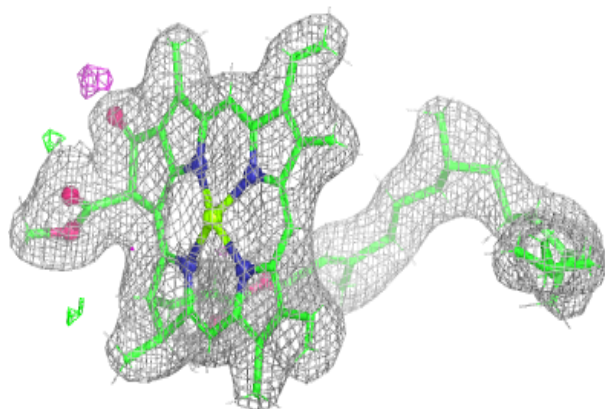
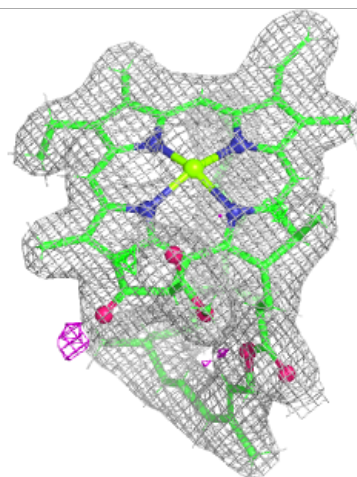
Electron density around CLA A 405:

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



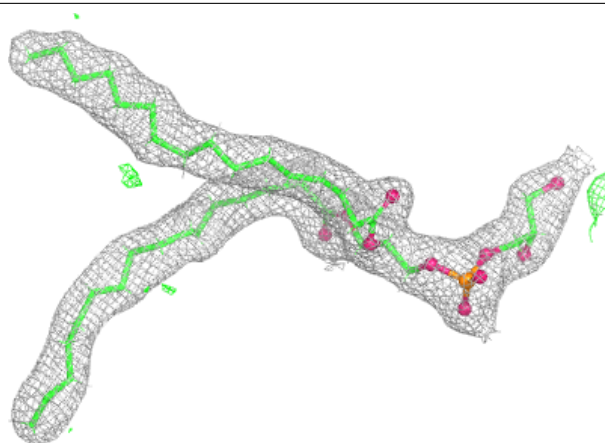
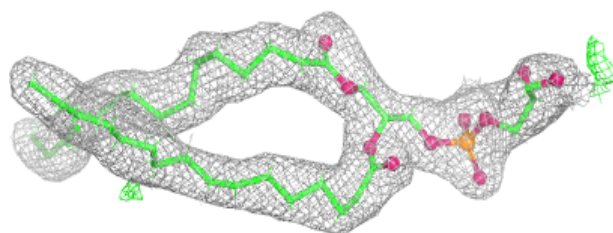
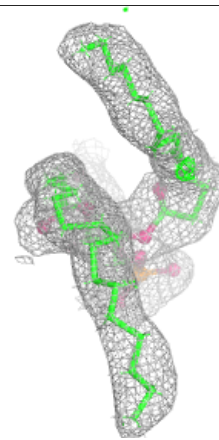
Electron density around CLA b 612:

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



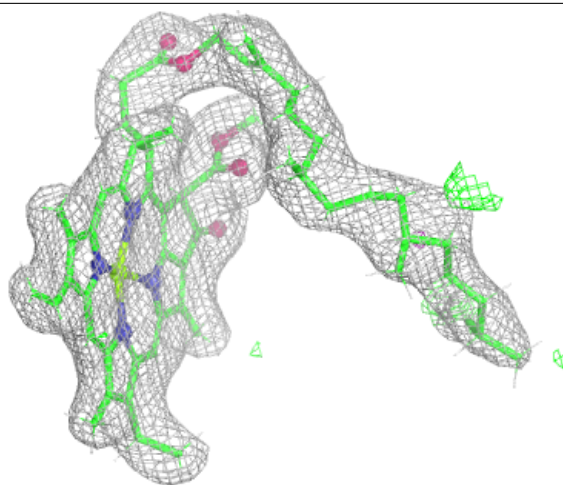
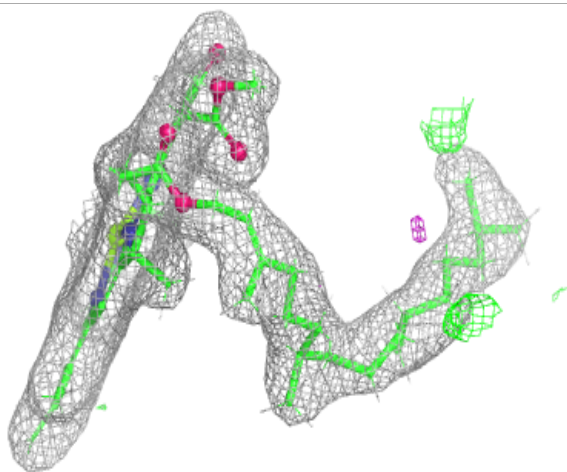
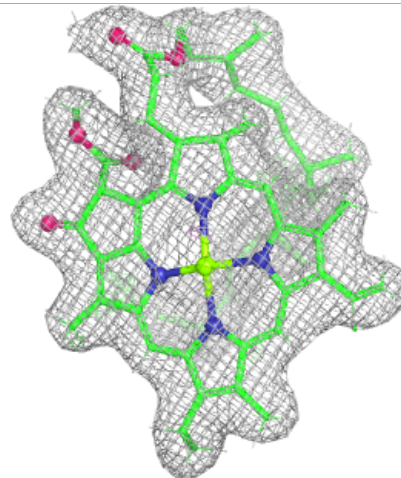
Electron density around LHG D 407:

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



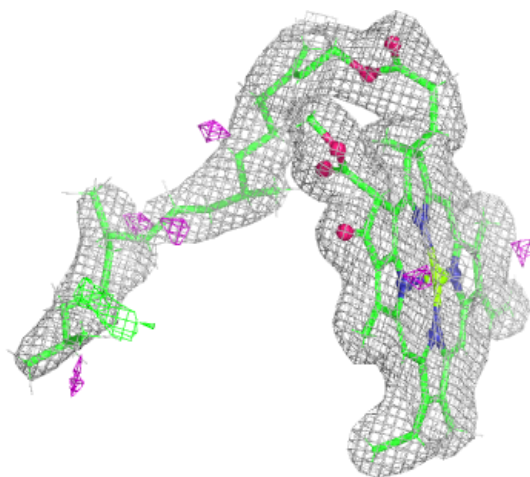
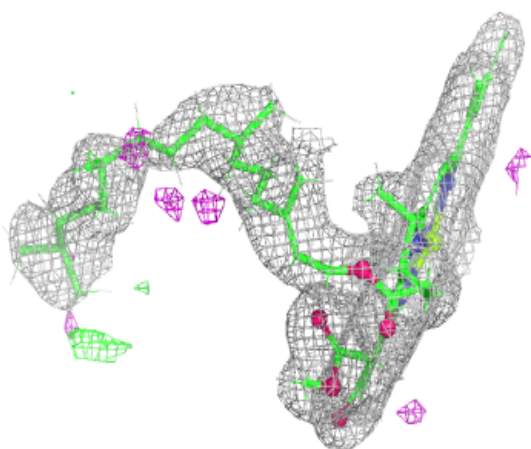
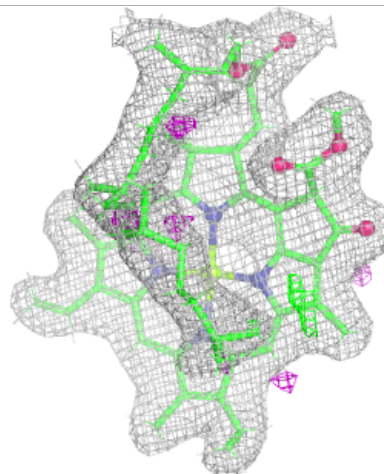
Electron density around CLA B 613:

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



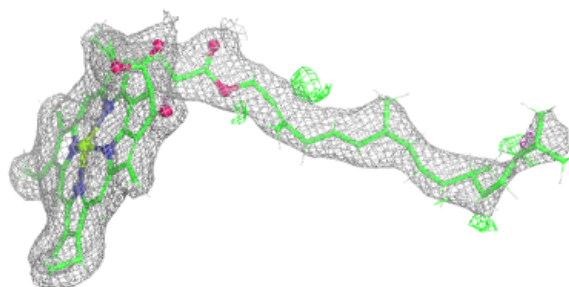
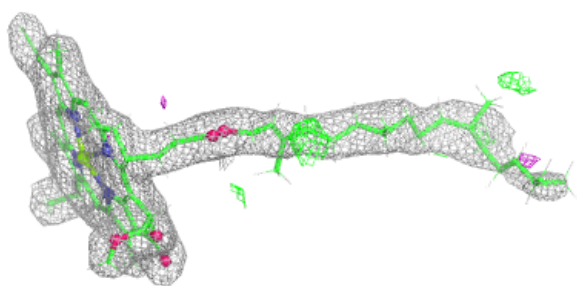
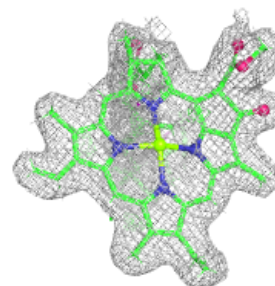
Electron density around CLA b 614:

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

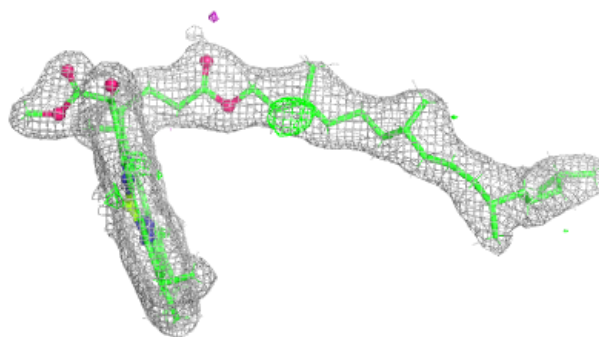
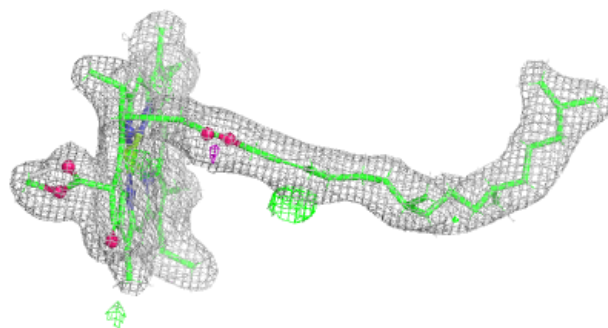
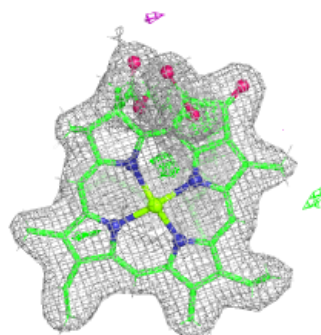


Electron density around CLA B 604:

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

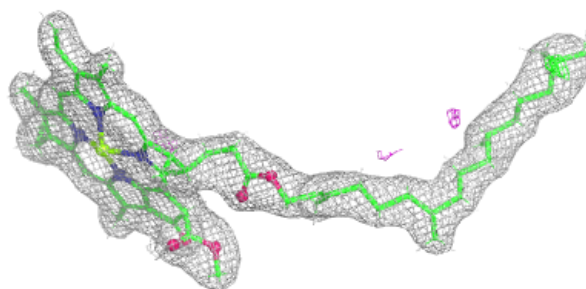
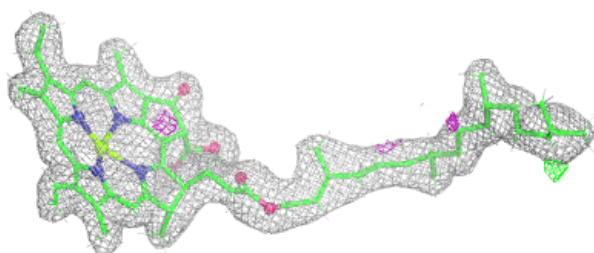
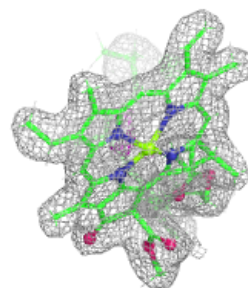
**Electron density around CLA B 605:**

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

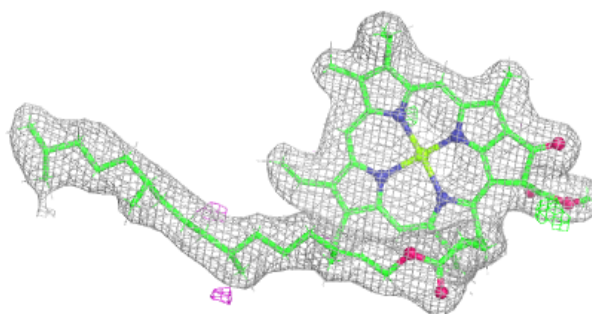
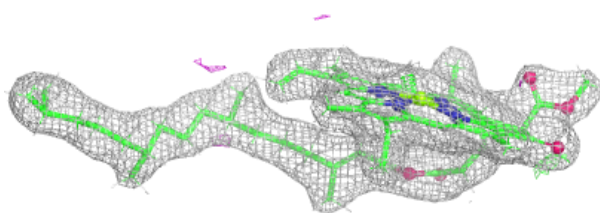
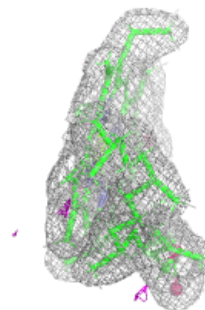


Electron density around CLA A 404:

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

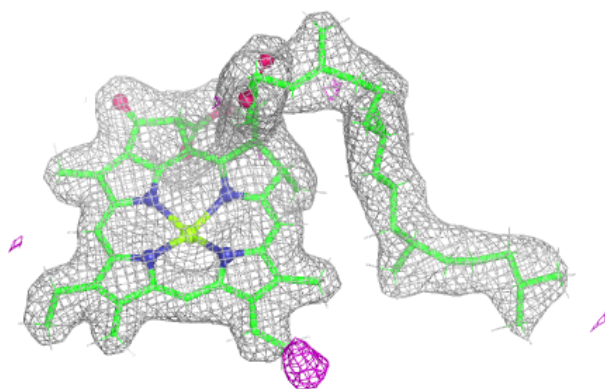
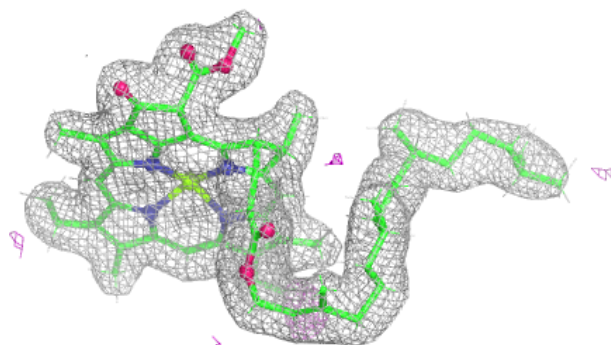
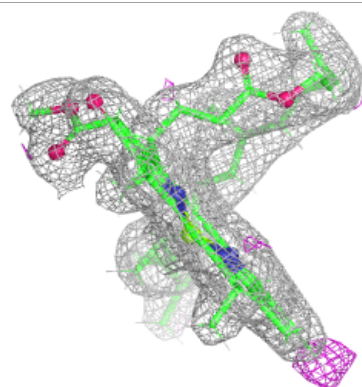
**Electron density around CLA C 501:**

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

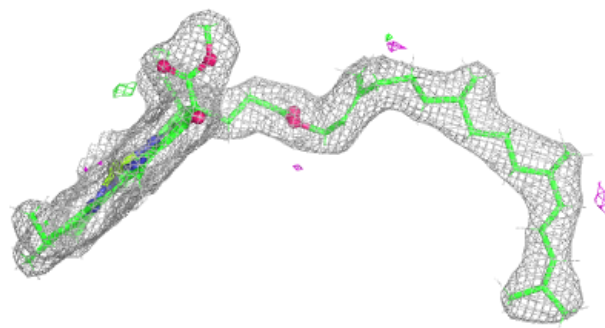
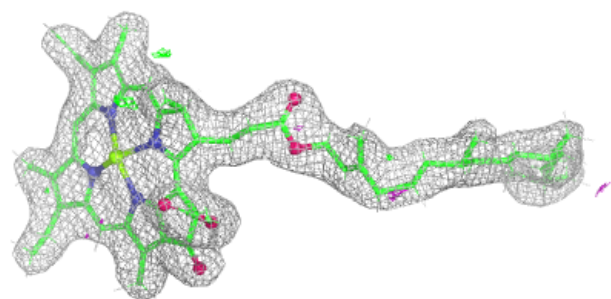
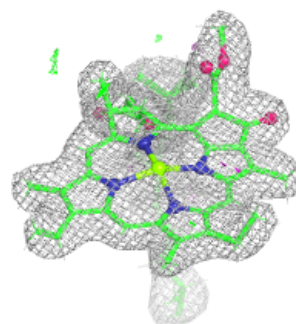


Electron density around CLA D 401:

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

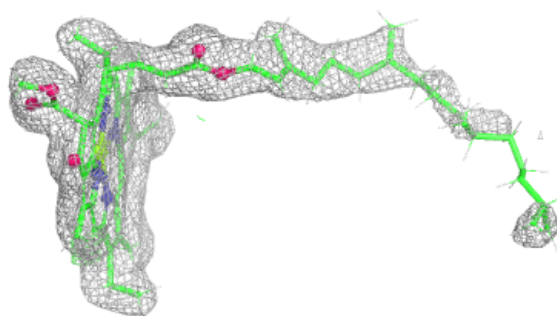
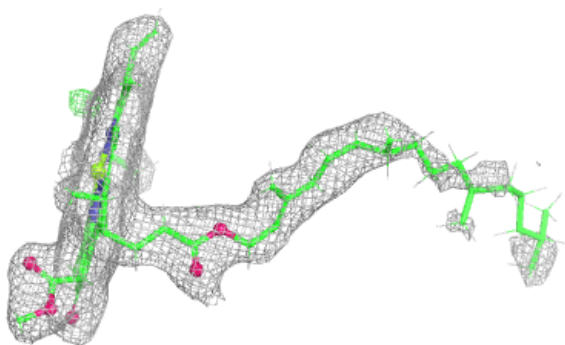
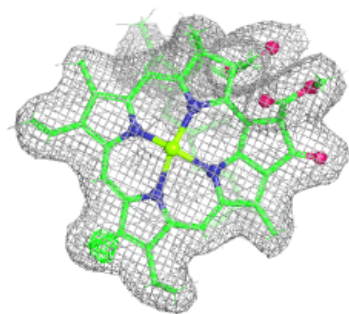
**Electron density around CLA D 402:**

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

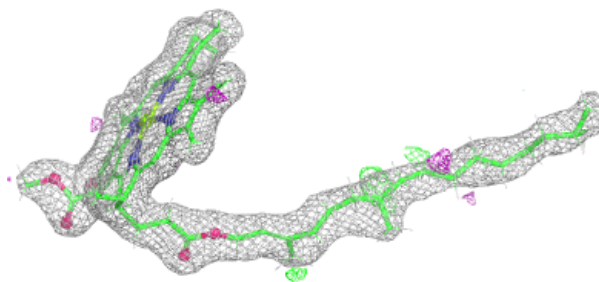
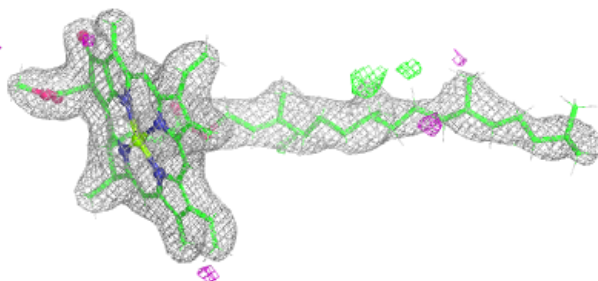
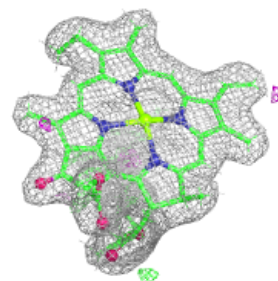


Electron density around CLA D 403:

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

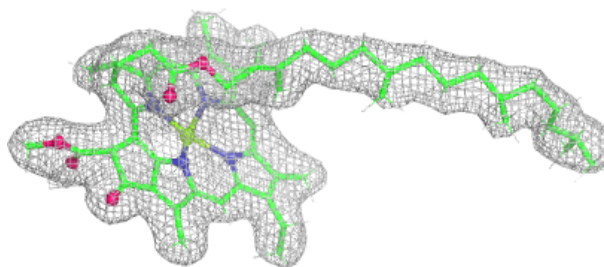
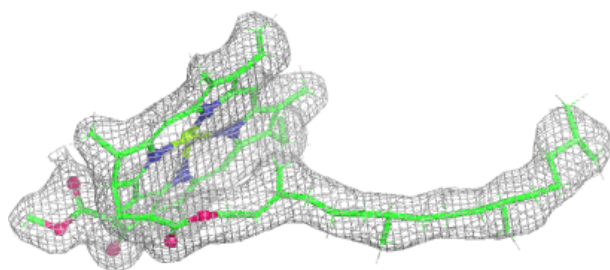
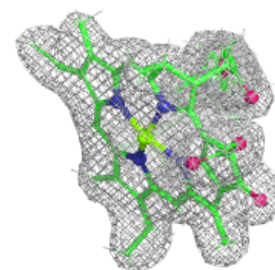
**Electron density around CLA B 607:**

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

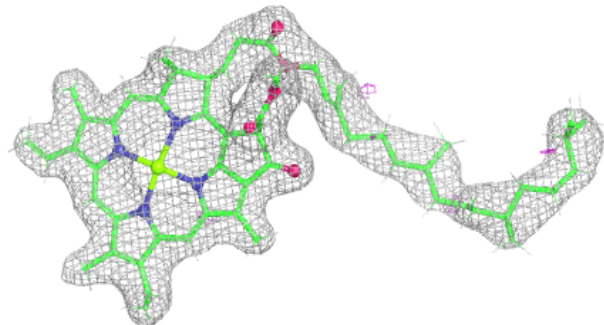
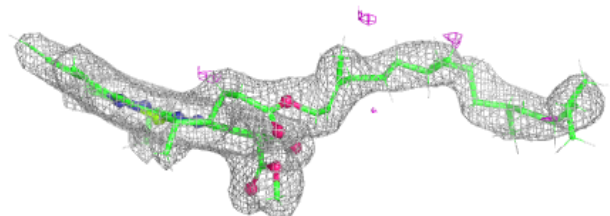
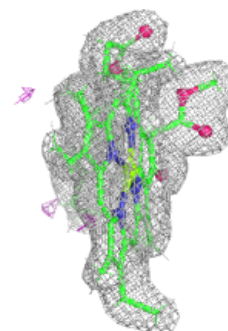


Electron density around CLA B 608:

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

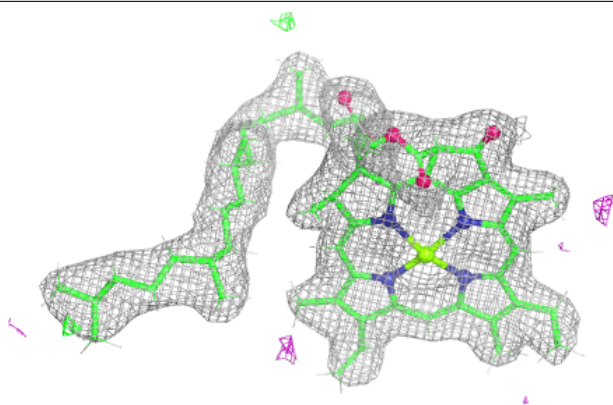
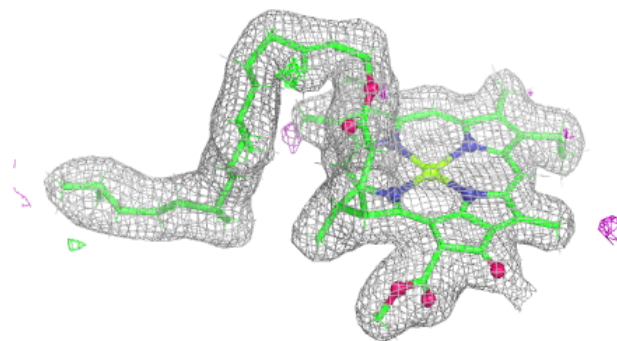
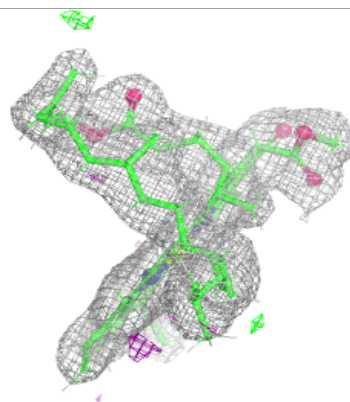
**Electron density around CLA B 602:**

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

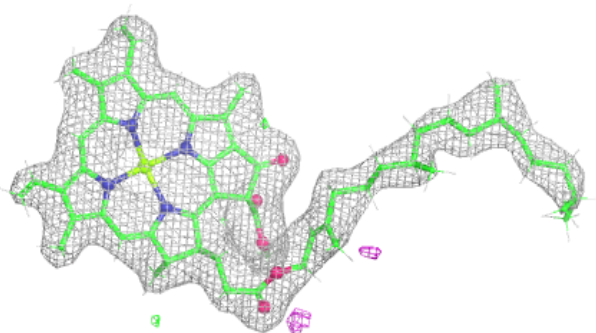
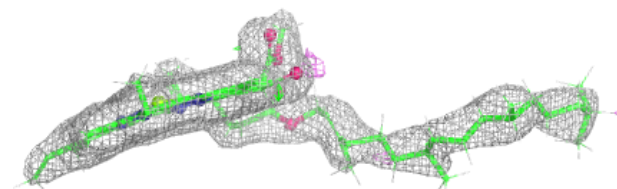
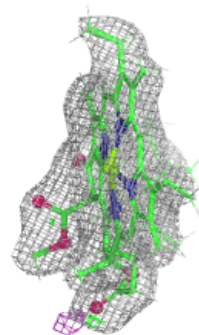


Electron density around CLA a 411:

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

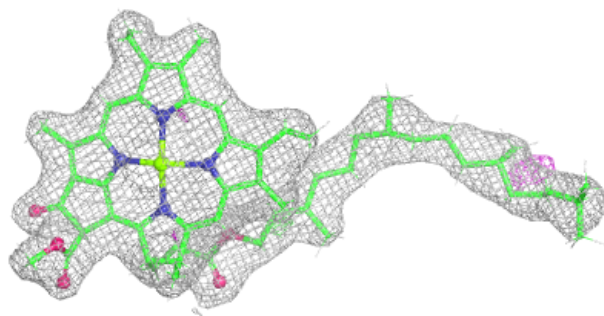
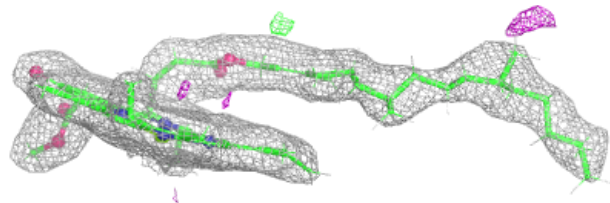
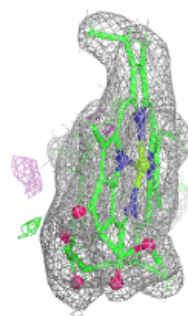
**Electron density around CLA b 603:**

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

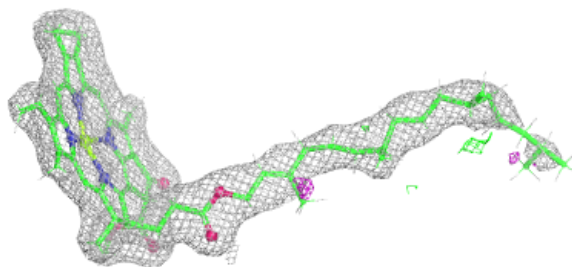
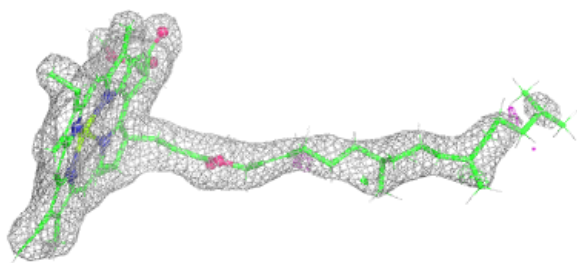
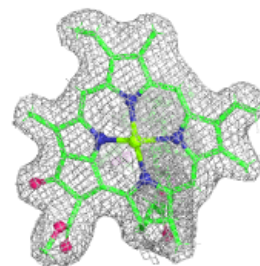


Electron density around CLA b 604:

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

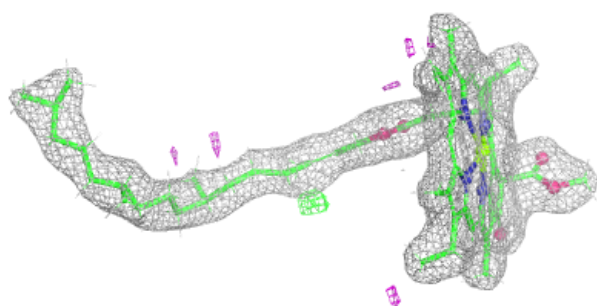
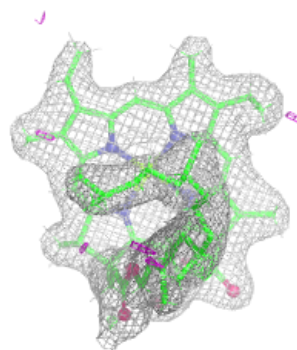
**Electron density around CLA b 605:**

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



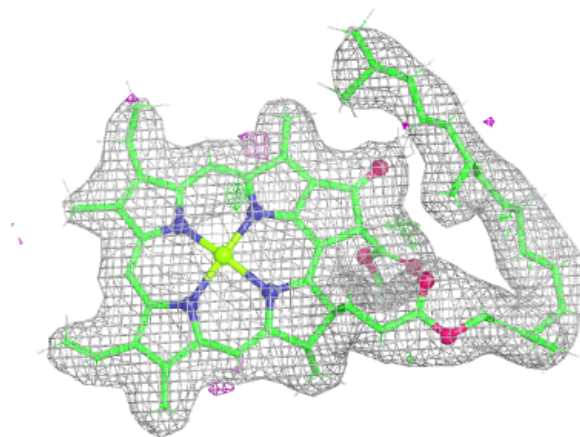
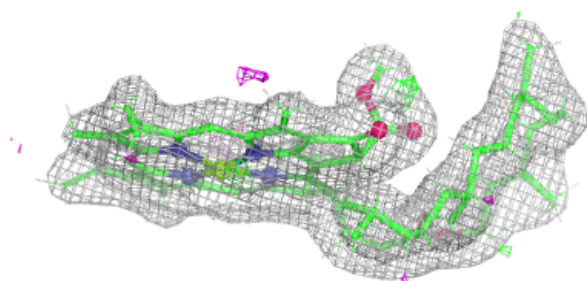
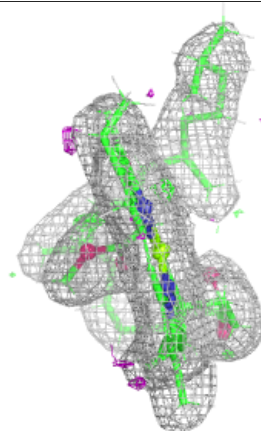
Electron density around CLA b 606:

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



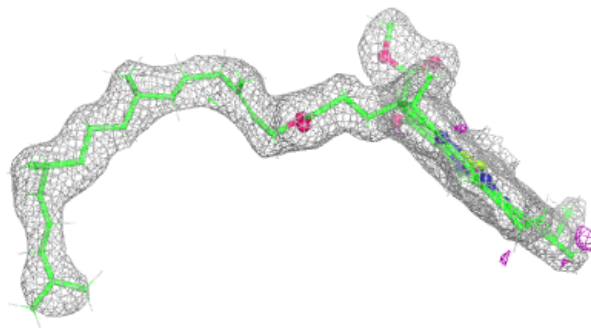
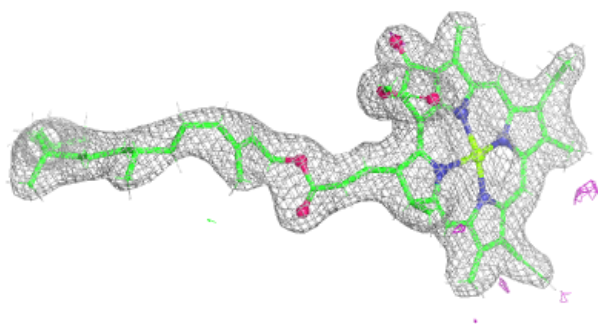
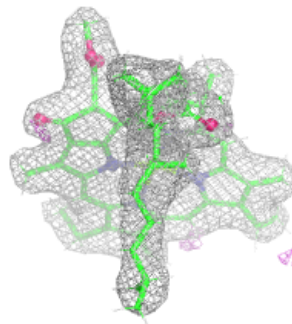
Electron density around CLA B 610:

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

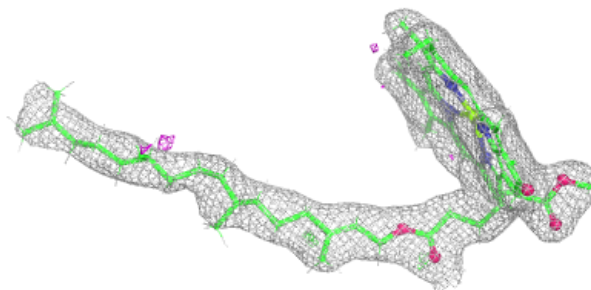
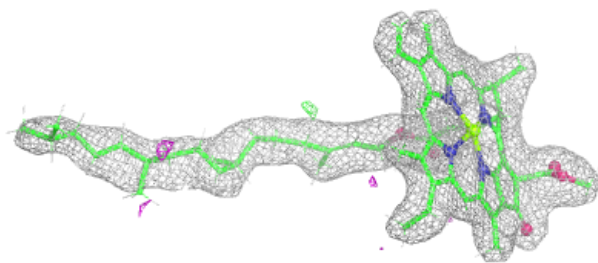
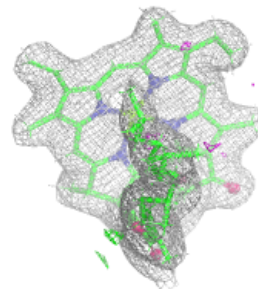


Electron density around CLA d 402:

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

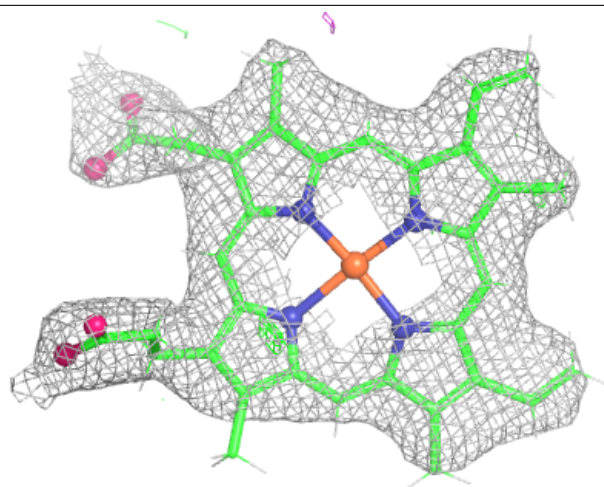
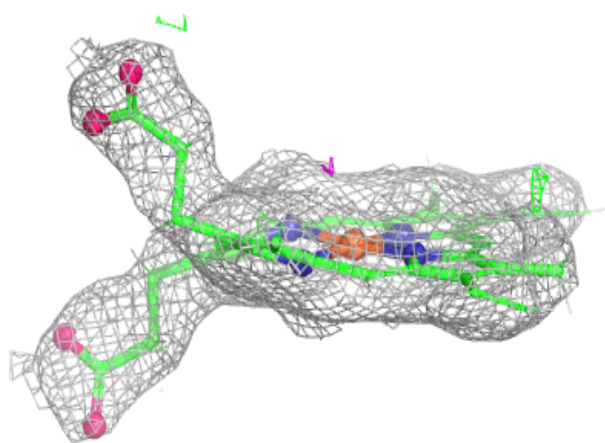
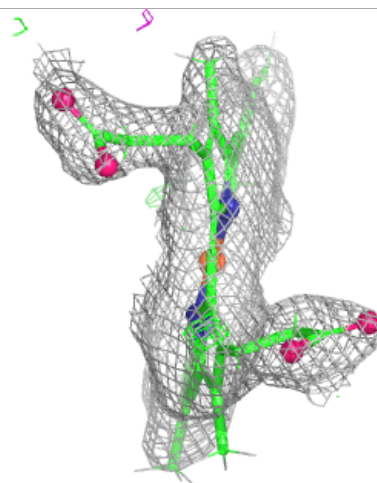
**Electron density around CLA b 608:**

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



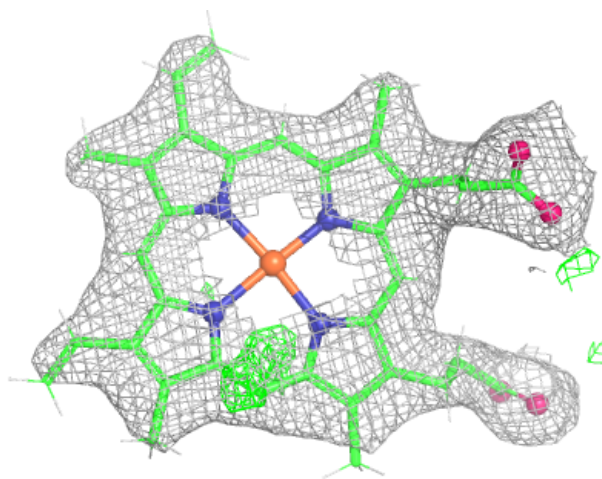
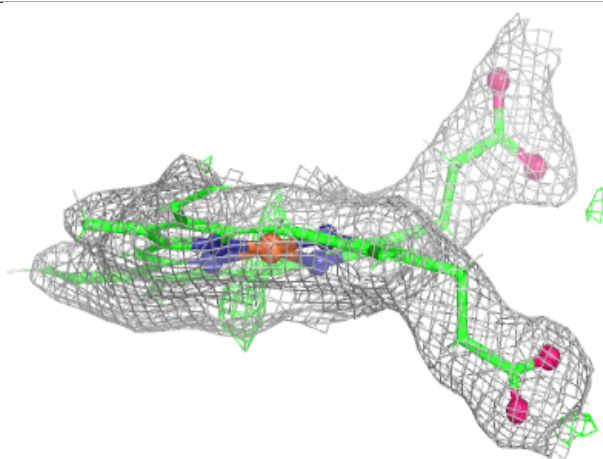
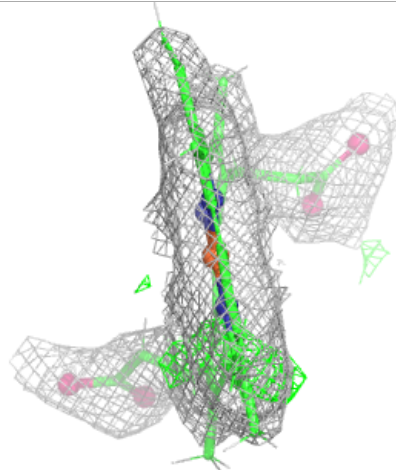
Electron density around HEM e 102:

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



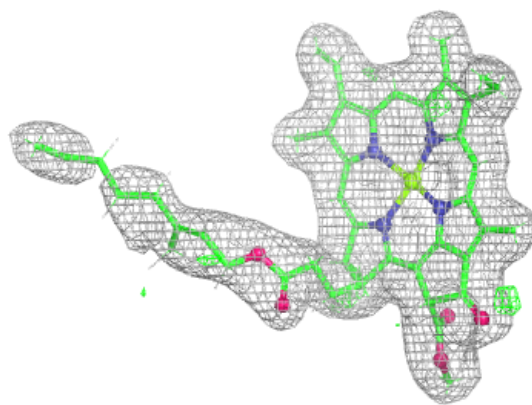
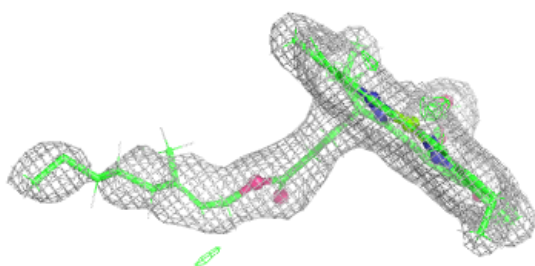
Electron density around HEM E 101:

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



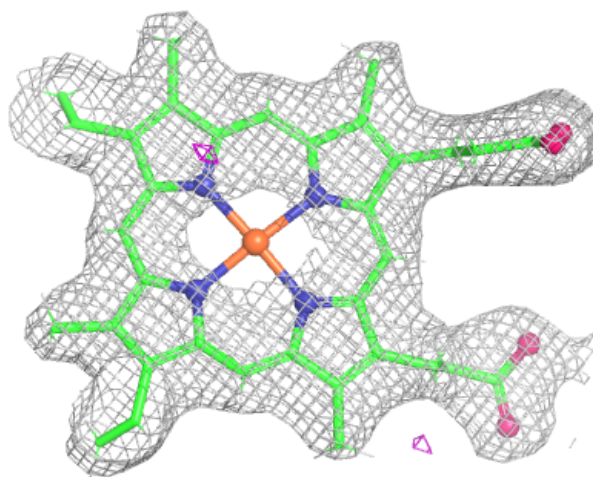
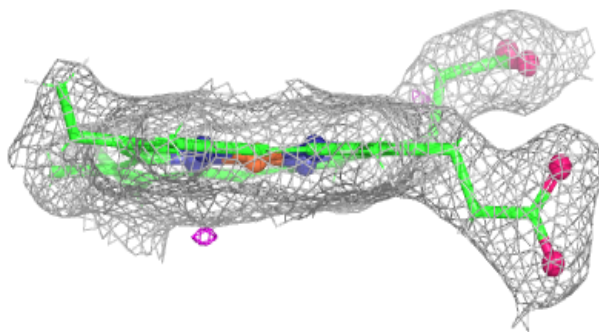
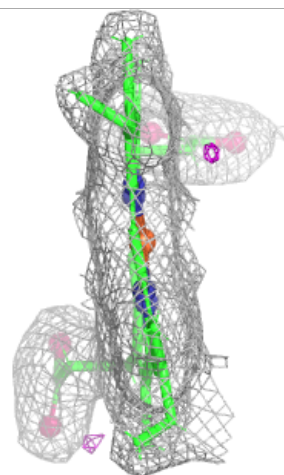
Electron density around CLA A 408:

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



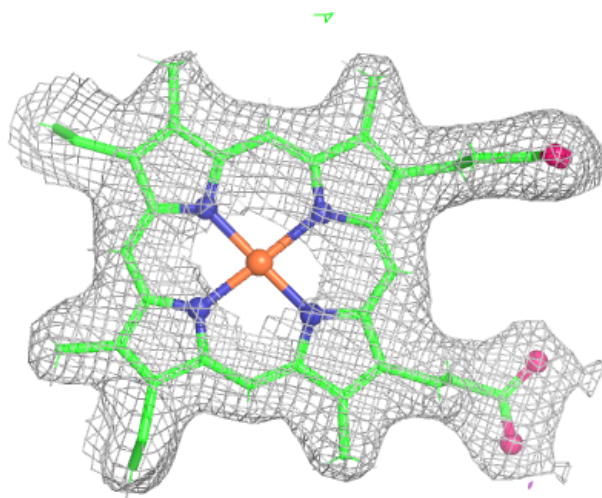
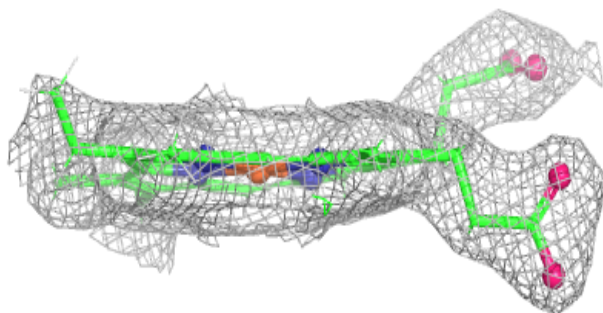
Electron density around HEC V 201:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.