



wwPDB X-ray Structure Validation Summary Report

Mar 7, 2026 – 03:39 AM UTC

PDB ID : 5MX2 / pdb_00005mx2
Title : Photosystem II depleted of the Mn4CaO5 cluster at 2.55 Å resolution
Authors : Zhang, M.; Bommer, M.; Chatterjee, R.; Hussain, R.; Kern, J.; Yano, J.; Dau, H.; Dobbek, H.; Zouni, A.
Deposited on : 2017-01-20
Resolution : 2.20 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

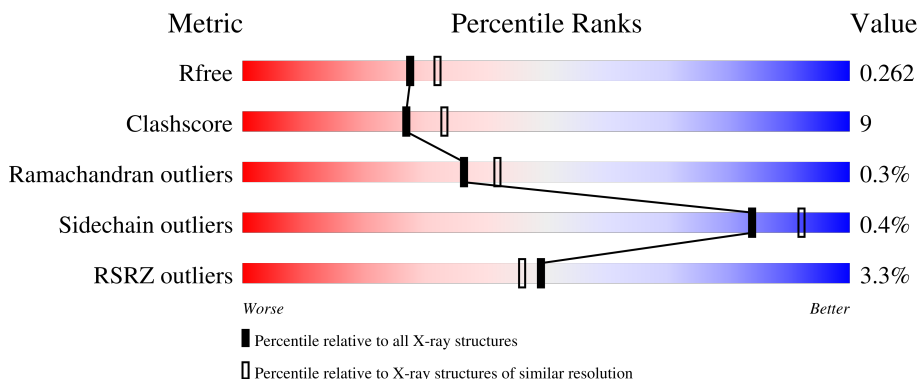
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

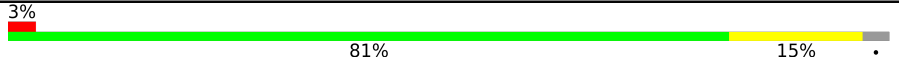
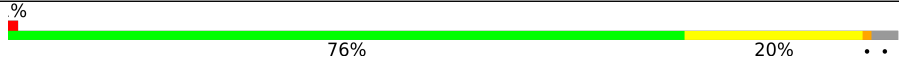



The reported resolution of this entry is 2.20 Å.

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.








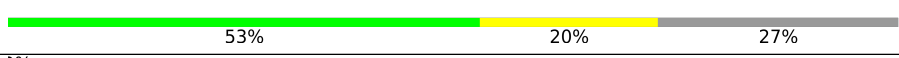

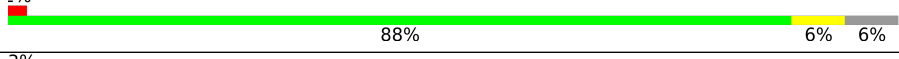
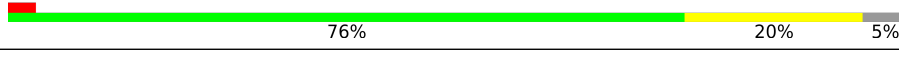
















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	 3% 81% 15% .
1	a	344	 % 76% 20% ..
2	B	510	 2% 82% 17% .
2	b	510	 2% 81% 18% .
3	C	461	 % 84% 13% .




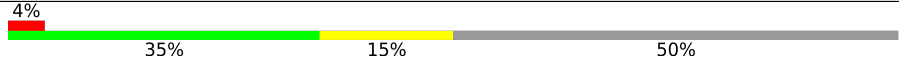
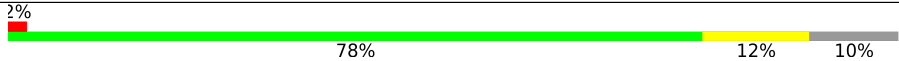
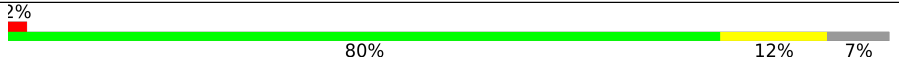
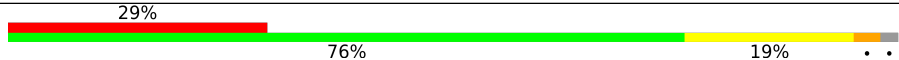
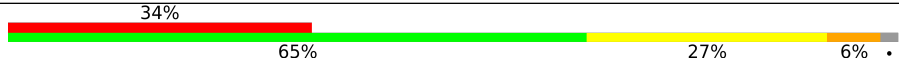
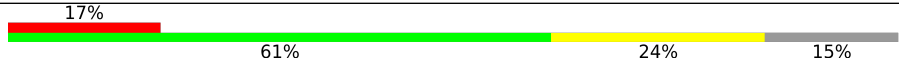
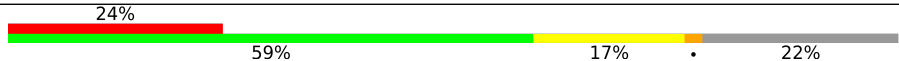
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Mol	Chain	Length	Quality of chain
3	c	461	 80% 17%
4	D	352	 81% 15%
4	d	352	 72% 25%
5	E	84	 71% 25%
5	e	84	 70% 24% 6%
6	F	45	 53% 20% 27%
6	f	45	 56% 16% 27%
7	H	66	 88% 6% 6%
7	h	66	 76% 20% 5%
8	I	38	 74% 13% 13%
8	i	38	 87% 13%
9	J	40	 80% 18%
9	j	40	 68% 15% 18%
10	K	46	 61% 15% 24%
10	k	46	 57% 22% 22%
11	L	37	 81% 16%
11	l	37	 89% 8%
12	M	36	 75% 14% 11%
12	m	36	 75% 14% 11%
13	O	272	 69% 19% 11%
13	o	272	 69% 19% 11%
14	T	32	 66% 22% 12%
14	t	32	 62% 28% 9%
15	U	134	 57% 15% 28%
15	u	134	 63% 9% 28%

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Mol	Chain	Length	Quality of chain
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	412	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	407	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 50407 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	2617	1714	430	458	15	0	0	0
1	a	333	2617	1714	430	458	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	3980	2611	665	691	13	0	0	0
2	b	503	3958	2599	657	689	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	447	3455	2264	576	602	13	0	0	0
3	c	448	3466	2270	580	603	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	340	2706	1794	440	460	12	0	0	0
4	d	340	2706	1794	440	460	12	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			656	428	106	122			
5	e	79	Total	C	N	O	0	0	0
			645	422	104	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	62	Total	C	N	O	S	0	0	0
			493	330	79	82	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			
8	i	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			
9	j	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	35	Total	C	N	O	0	0	0
			272	192	37	43			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	36	284	198	41	45	0	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	L	36	296	197	47	52	0	0	0
11	l	36	296	197	47	52	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	32	249	167	36	45	1	0	0	0
12	m	32	249	167	36	45	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	242	1859	1162	314	379	4	0	0	0
13	o	241	1852	1158	313	377	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	28	241	170	34	35	2	0	0	0
14	t	29	249	176	35	36	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	U	96	765	486	128	151	0	0	0
15	u	96	765	486	128	151	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	21	Total	C	N	O	S	0	0	0
			155	102	28	23	2			
17	y	23	Total	C	N	O	S	0	0	0
			171	113	30	25	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	S	0	0	0
			270	182	41	47				
18	x	38	Total	C	N	O	S	0	0	0
			281	188	45	48				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			

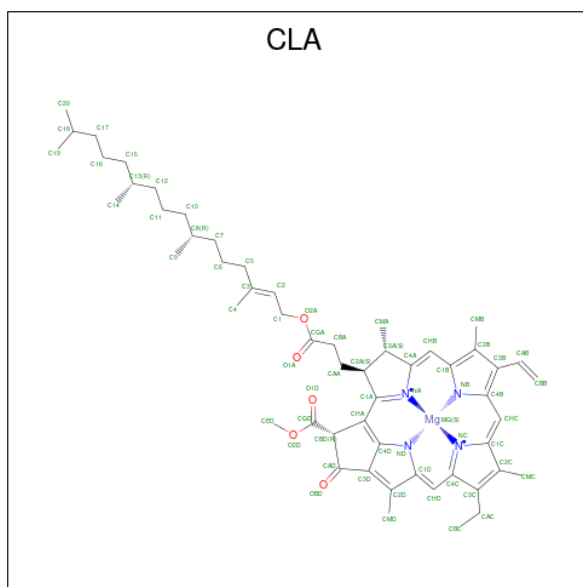
- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	35	Total	C	N	O	S	0	0	0
			282	191	49	42				
20	r	32	Total	C	N	O	S	0	0	0
			257	176	45	36				

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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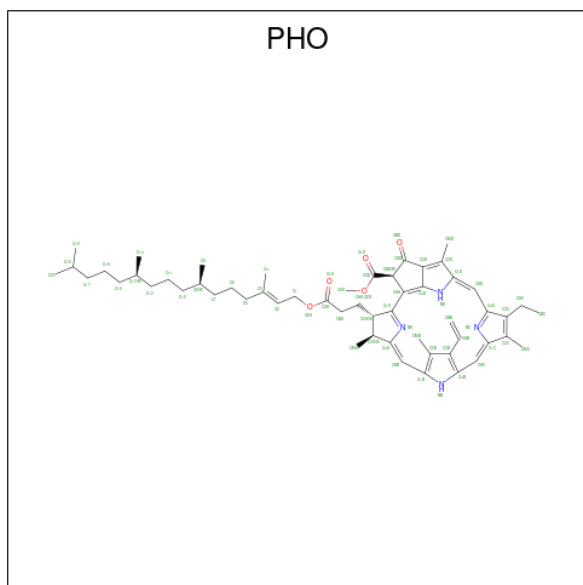
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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

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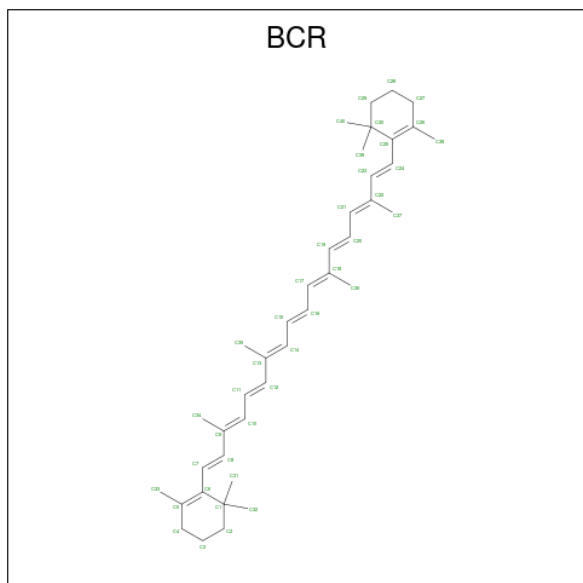
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



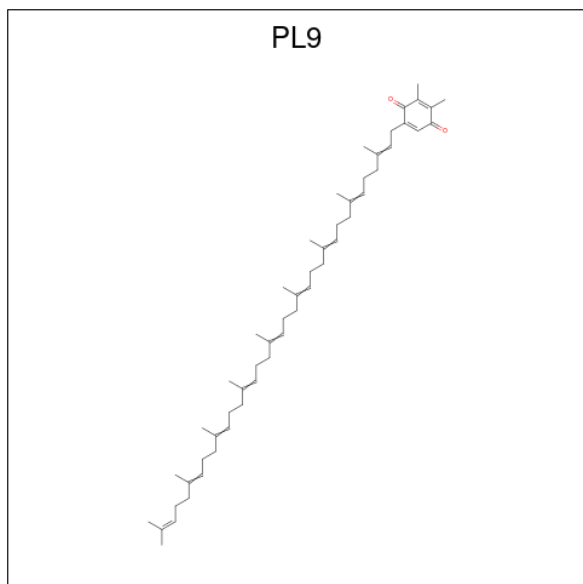
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
23	A	1	64	55	4	5	0	0
23	D	1	64	55	4	5	0	0
23	a	1	64	55	4	5	0	0
23	a	1	64	55	4	5	0	0

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



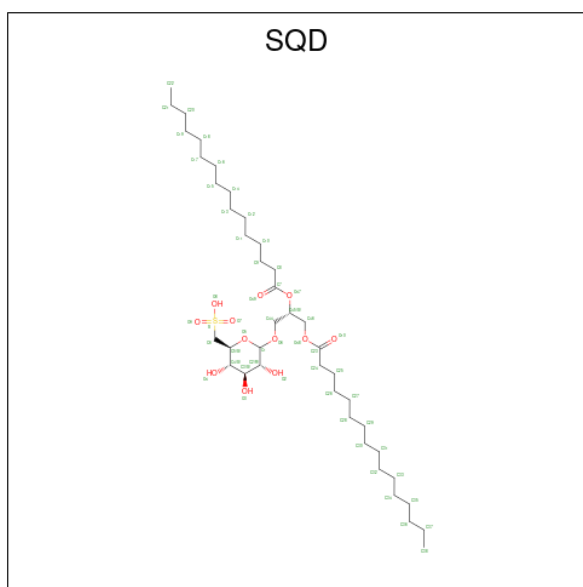
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total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

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



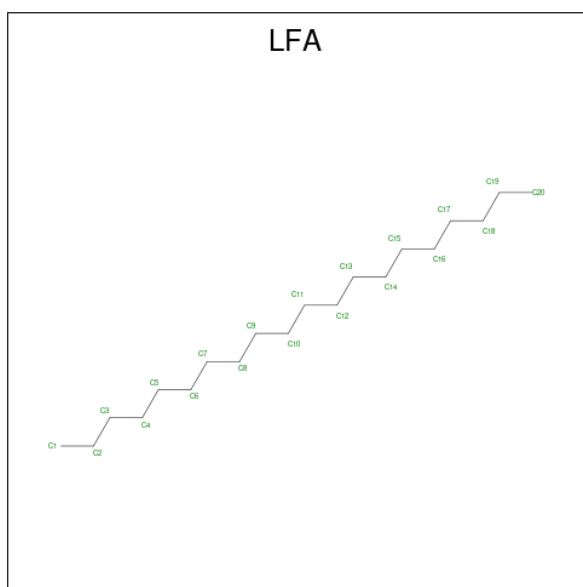
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			55	53	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	a	1	Total	C	O	0	0
			55	53	2		
25	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 26 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
			Total	C	O	S		
26	A	1	54	41	12	1	0	0
26	A	1	54	41	12	1	0	0
26	D	1	43	30	12	1	0	0
26	L	1	48	35	12	1	0	0
26	a	1	54	41	12	1	0	0
26	a	1	50	41	9		0	0
26	b	1	54	41	12	1	0	0
26	f	1	43	30	12	1	0	0

- Molecule 27 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 14 14	0	0
27	A	1	Total C 11 11	0	0
27	B	1	Total C 10 10	0	0
27	B	1	Total C 16 16	0	0
27	B	1	Total C 13 13	0	0
27	B	1	Total C 15 15	0	0
27	B	1	Total C 9 9	0	0
27	B	1	Total C 10 10	0	0
27	B	1	Total C 14 14	0	0
27	B	1	Total C 12 12	0	0
27	C	1	Total C 15 15	0	0
27	D	1	Total C 15 15	0	0
27	D	1	Total C 8 8	0	0
27	D	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	1	Total C 14 14	0	0
27	J	1	Total C 11 11	0	0
27	M	1	Total C 10 10	0	0
27	M	1	Total C 16 16	0	0
27	T	1	Total C 12 12	0	0
27	a	1	Total C 7 7	0	0
27	b	1	Total C 15 15	0	0
27	b	1	Total C 10 10	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 16 16	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 11 11	0	0
27	b	1	Total C 9 9	0	0
27	b	1	Total C 15 15	0	0
27	c	1	Total C 9 9	0	0
27	c	1	Total C 15 15	0	0
27	d	1	Total C 15 15	0	0
27	d	1	Total C 9 9	0	0
27	d	1	Total C 16 16	0	0
27	i	1	Total C 16 16	0	0
27	i	1	Total C 7 7	0	0

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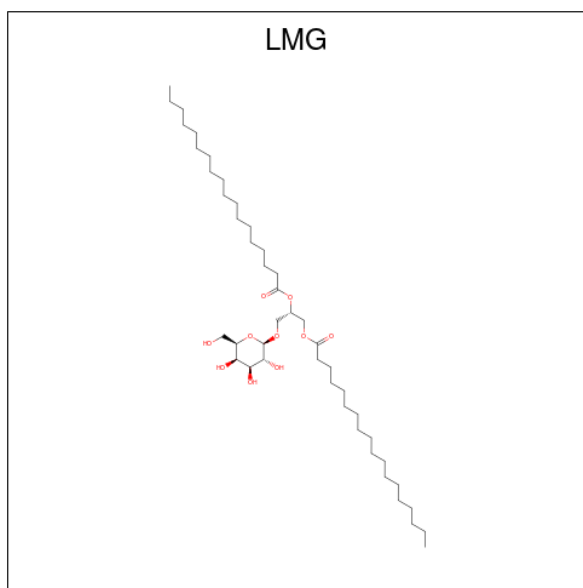
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	j	1	Total C 15 15	0	0
27	m	1	Total C 10 10	0	0
27	m	1	Total C 15 15	0	0
27	t	1	Total C 15 15	0	0

- Molecule 28 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



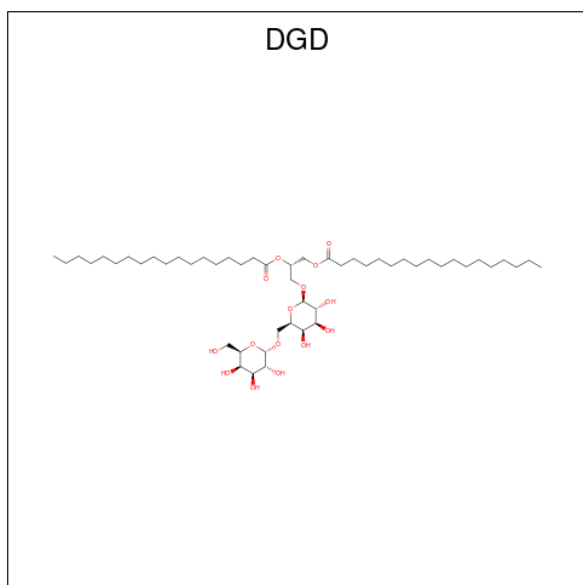
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total C O 51 41 10	0	0
29	B	1	Total C O 36 26 10	0	0
29	C	1	Total C O 51 41 10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	C	1	Total	C	O	0	0
			48	38	10		
29	C	1	Total	C	O	0	0
			44	34	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			39	29	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			41	31	10		
29	f	1	Total	C	O	0	0
			51	41	10		
29	m	1	Total	C	O	0	0
			51	41	10		

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



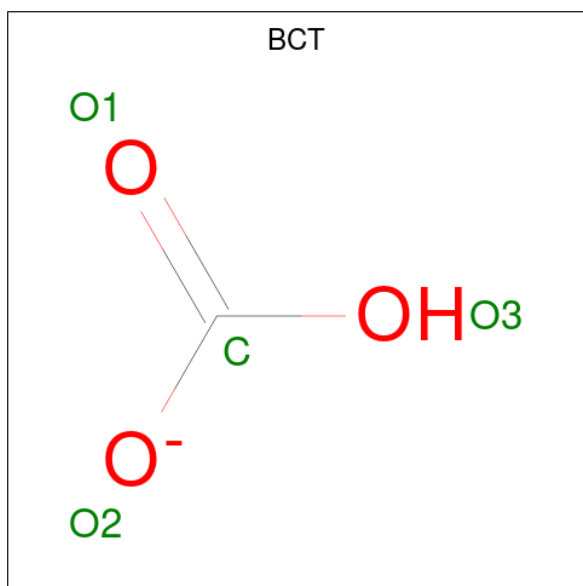
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			62	47	15		
30	C	1	Total	C	O	0	0
			56	41	15		

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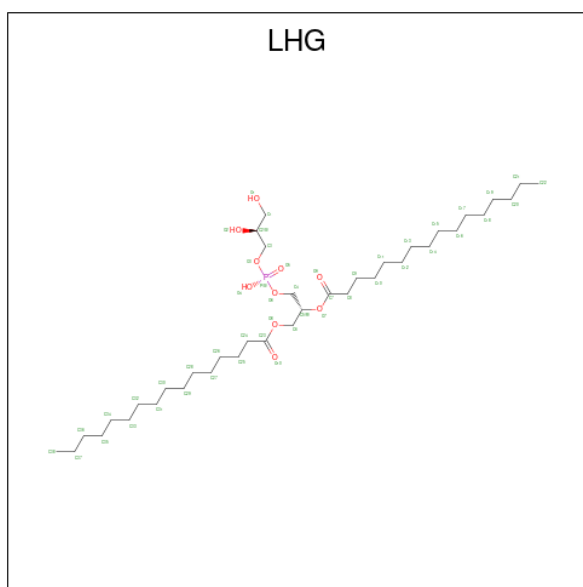
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			62	47	15		
30	H	1	Total	C	O	0	0
			60	45	15		
30	c	1	Total	C	O	0	0
			62	47	15		
30	c	1	Total	C	O	0	0
			55	40	15		
30	c	1	Total	C	O	0	0
			62	47	15		
30	h	1	Total	C	O	0	0
			62	47	15		

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



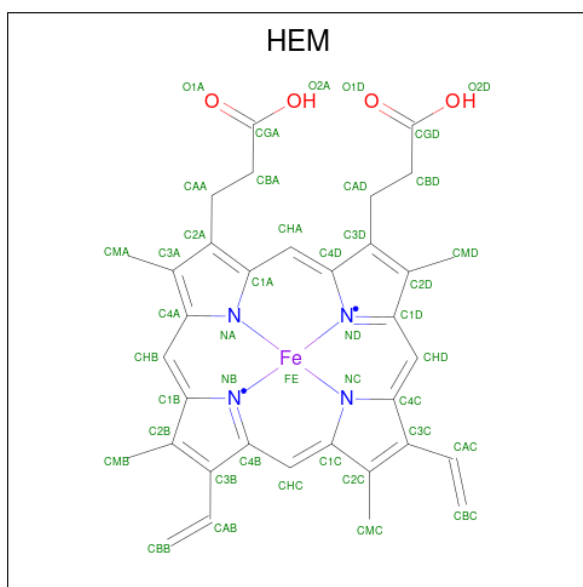
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	D	1	Total	C	O	0	0
			4	1	3		
31	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



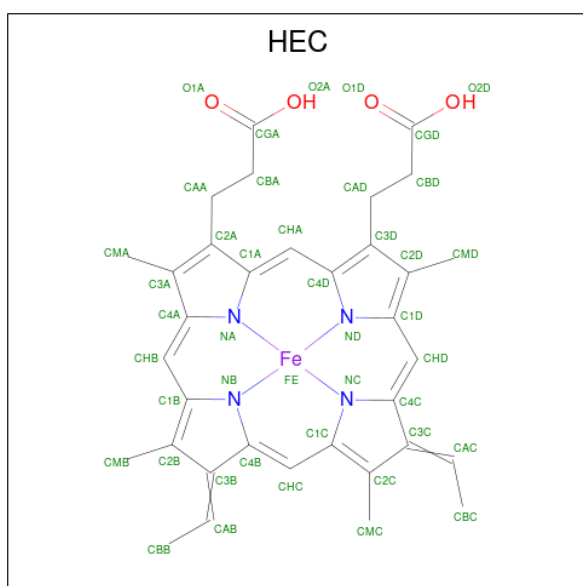
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
32	D	1	49	38	10	1	0	0
32	D	1	49	38	10	1	0	0
32	D	1	49	38	10	1	0	0
32	E	1	42	31	10	1	0	0
32	L	1	49	38	10	1	0	0
32	b	1	49	38	10	1	0	0
32	d	1	49	38	10	1	0	0
32	d	1	49	38	10	1	0	0
32	e	1	42	31	10	1	0	0
32	l	1	49	38	10	1	0	0

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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



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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	70	Total O 70 70	0	0
35	B	84	Total O 84 84	0	0
35	C	62	Total O 62 62	0	0
35	D	72	Total O 72 72	0	0
35	E	5	Total O 5 5	0	0
35	F	1	Total O 1 1	0	0
35	H	17	Total O 17 17	0	0
35	J	1	Total O 1 1	0	0
35	K	1	Total O 1 1	0	0
35	L	5	Total O 5 5	0	0
35	M	3	Total O 3 3	0	0
35	O	30	Total O 30 30	0	0
35	T	2	Total O 2 2	0	0
35	U	2	Total O 2 2	0	0
35	V	12	Total O 12 12	0	0
35	X	3	Total O 3 3	0	0
35	a	77	Total O 77 77	0	0
35	b	72	Total O 72 72	0	0
35	c	65	Total O 65 65	0	0
35	d	51	Total O 51 51	0	0
35	e	5	Total O 5 5	0	0

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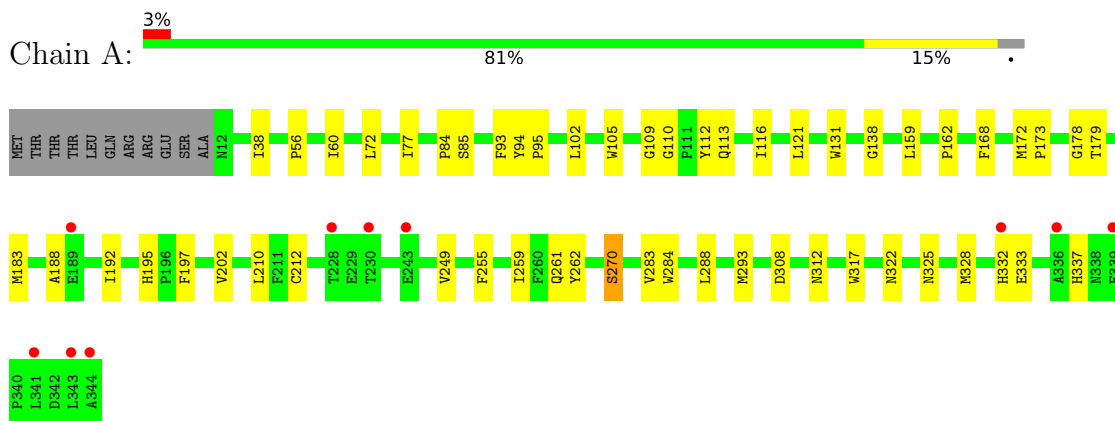
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	f	2	Total O 2 2	0	0
35	h	3	Total O 3 3	0	0
35	l	5	Total O 5 5	0	0
35	m	2	Total O 2 2	0	0
35	o	25	Total O 25 25	0	0
35	t	3	Total O 3 3	0	0
35	u	12	Total O 12 12	0	0
35	v	11	Total O 11 11	0	0

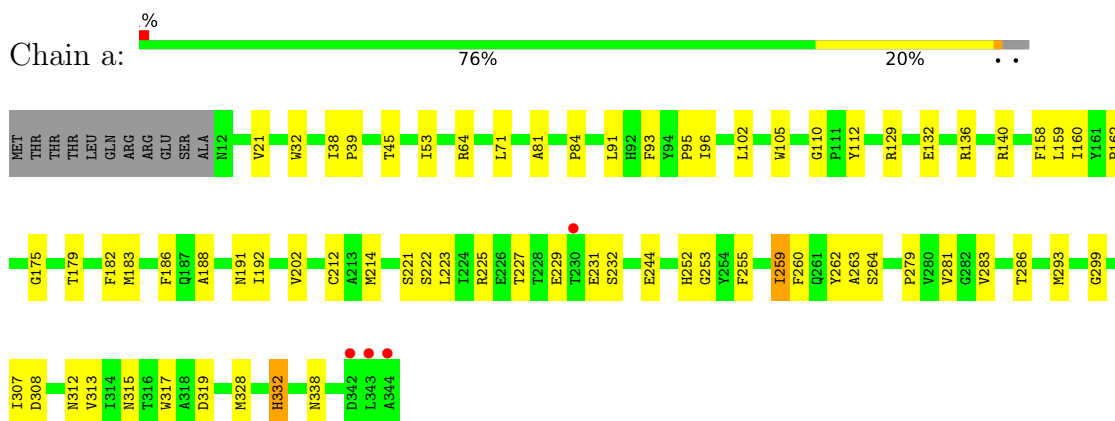
3 Residue-property plots [i](#)

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

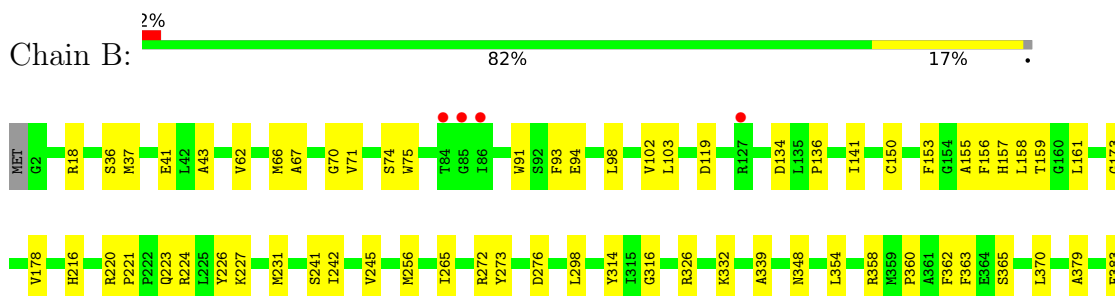
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

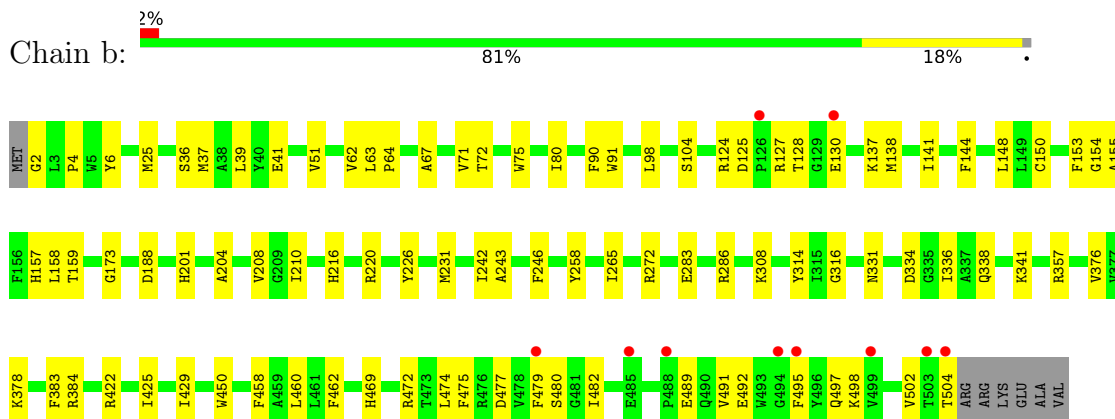


- Molecule 2: Photosystem II CP47 reaction center protein

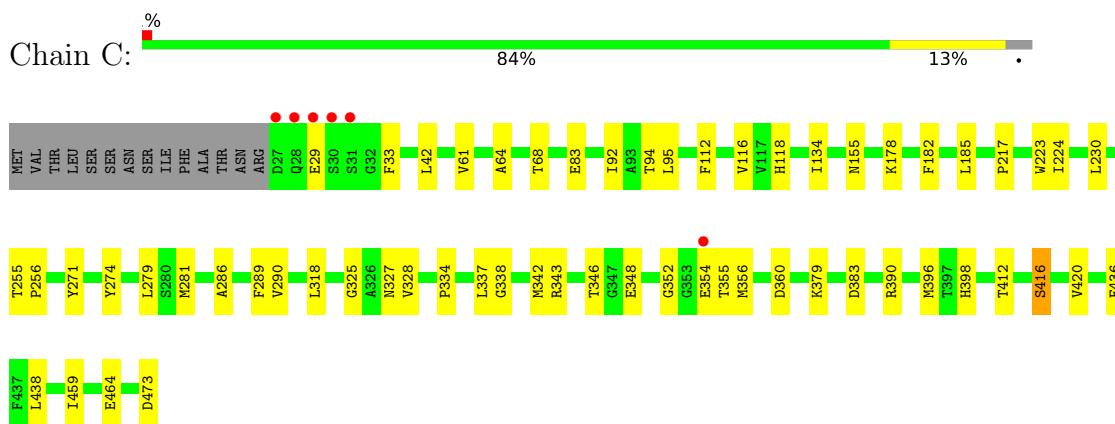




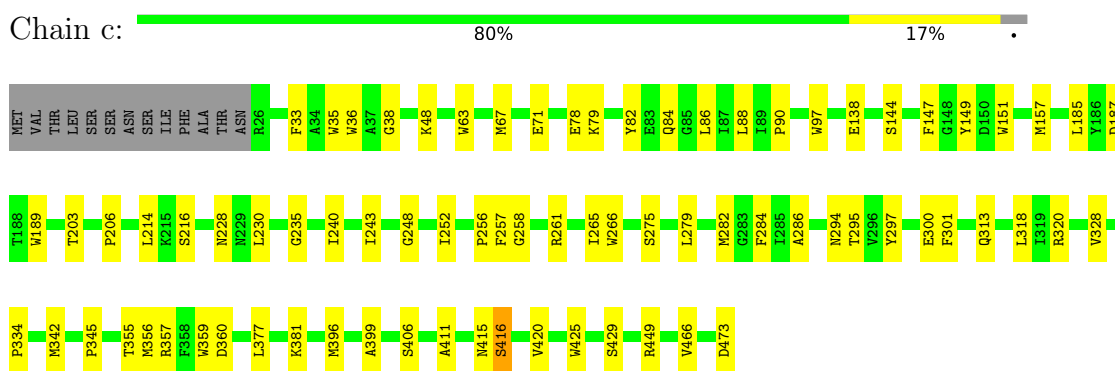
• Molecule 2: Photosystem II CP47 reaction center protein



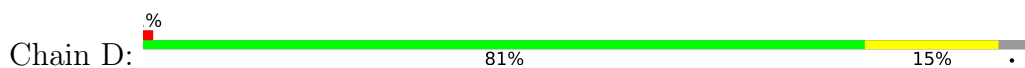
• Molecule 3: Photosystem II CP43 reaction center protein

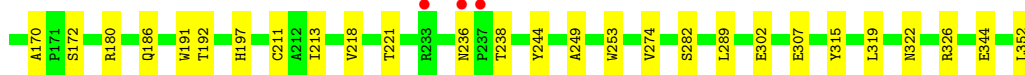


• Molecule 3: Photosystem II CP43 reaction center protein

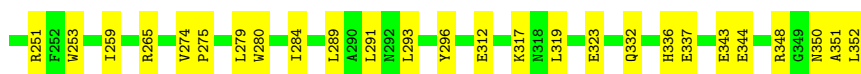


• Molecule 4: Photosystem II D2 protein





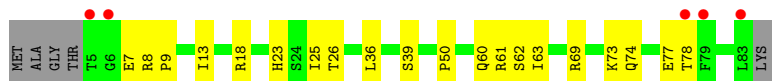
● Molecule 4: Photosystem II D2 protein



● Molecule 5: Cytochrome b559 subunit alpha



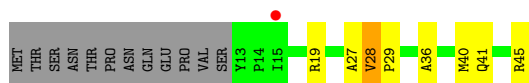
● Molecule 5: Cytochrome b559 subunit alpha



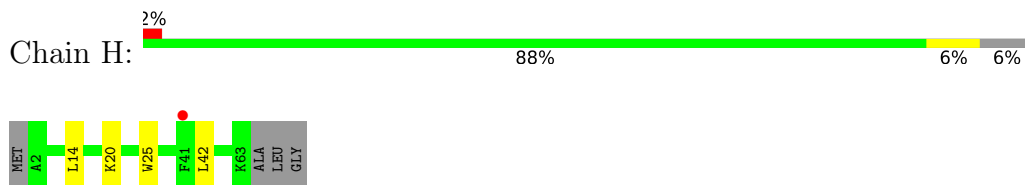
● Molecule 6: Cytochrome b559 subunit beta



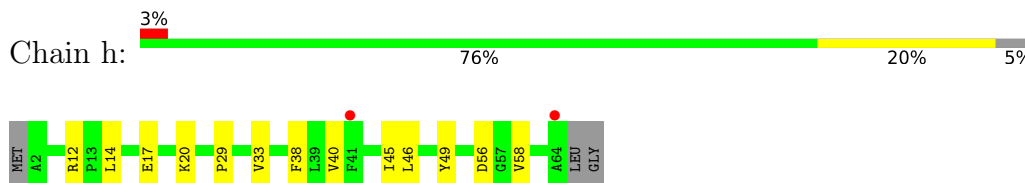
● Molecule 6: Cytochrome b559 subunit beta



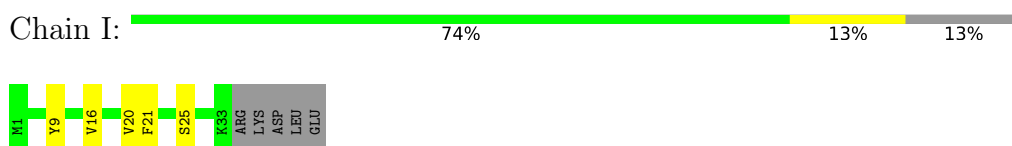
- Molecule 7: Photosystem II reaction center protein H



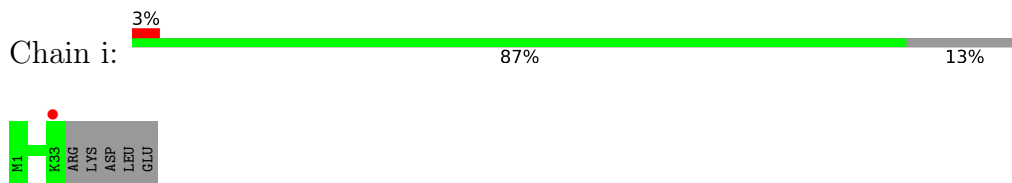
- Molecule 7: Photosystem II reaction center protein H



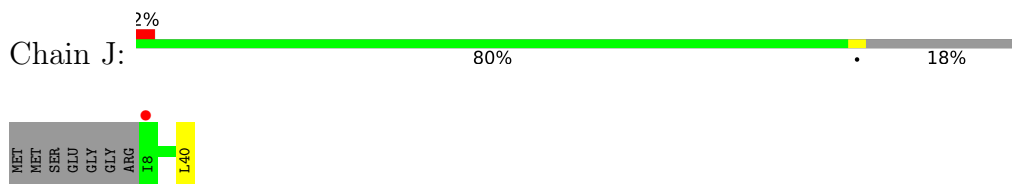
- Molecule 8: Photosystem II reaction center protein I



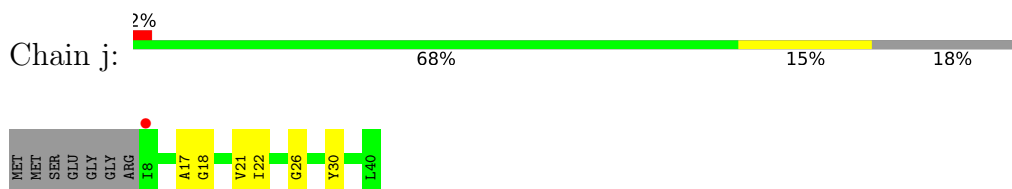
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

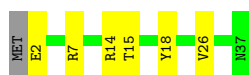
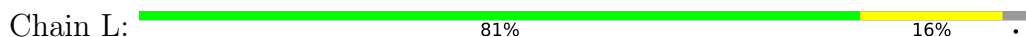




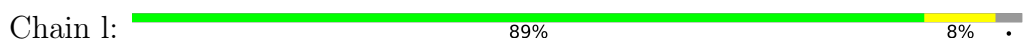
• Molecule 10: Photosystem II reaction center protein K



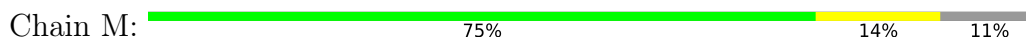
• Molecule 11: Photosystem II reaction center protein L



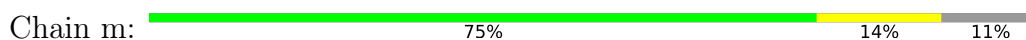
• Molecule 11: Photosystem II reaction center protein L



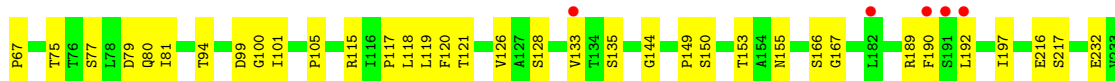
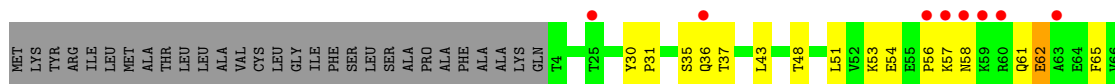
• Molecule 12: Photosystem II reaction center protein M

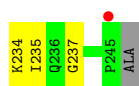


• Molecule 12: Photosystem II reaction center protein M

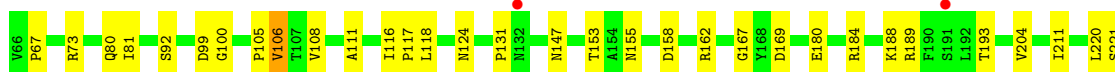


• Molecule 13: Photosystem II manganese-stabilizing polypeptide





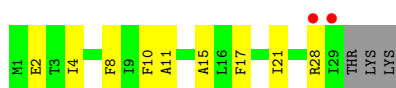
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



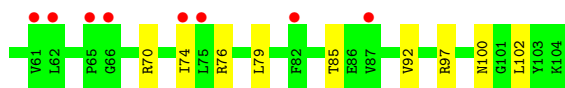
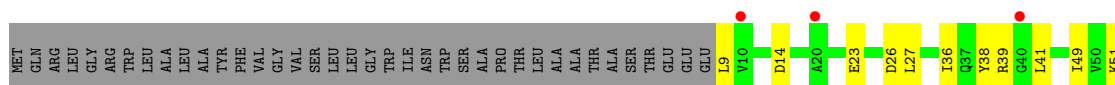
- Molecule 14: Photosystem II reaction center protein T



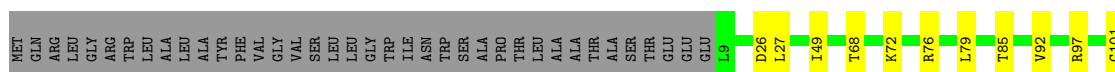
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein

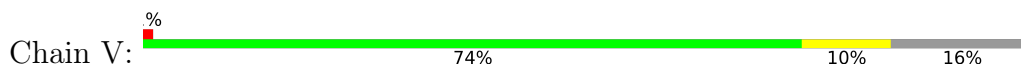


- Molecule 15: Photosystem II 12 kDa extrinsic protein





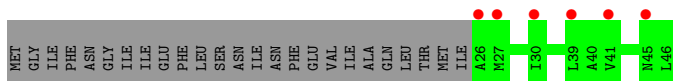
• Molecule 16: Cytochrome c-550



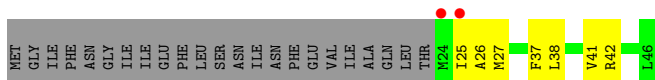
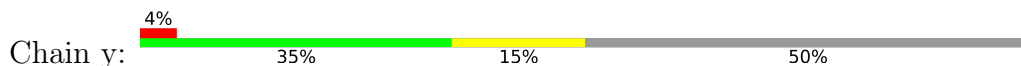
• Molecule 16: Cytochrome c-550



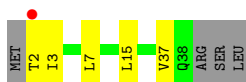
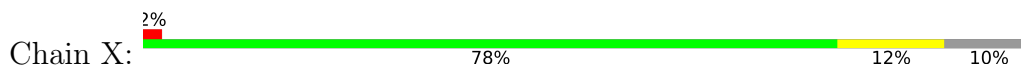
• Molecule 17: Photosystem II reaction center protein Ycf12



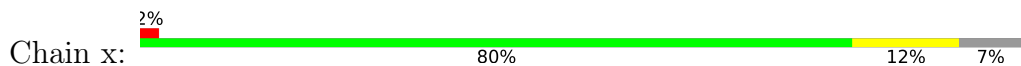
• Molecule 17: Photosystem II reaction center protein Ycf12

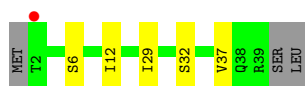


• Molecule 18: Photosystem II reaction center X protein

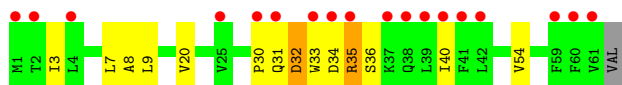
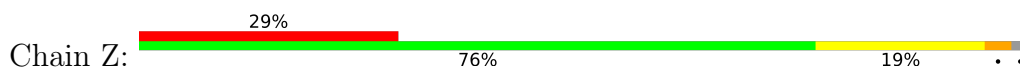


• Molecule 18: Photosystem II reaction center X protein

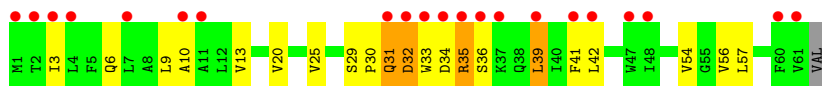




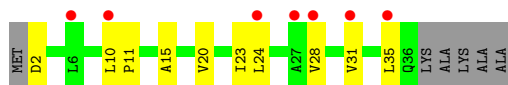
● Molecule 19: Photosystem II reaction center protein Z



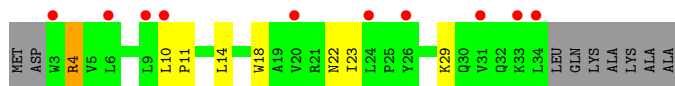
● Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.33Å 219.62Å 304.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 2.20 49.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.65-2.20) 92.6 (49.65-2.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.211 , 0.260 0.213 , 0.262	Depositor DCC
R_{free} test set	18229 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtrriage
Anisotropy	0.673	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50407	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	0/2702	0.51	0/3685
1	a	0.47	0/2702	0.52	0/3685
2	B	0.48	0/4120	0.51	0/5614
2	b	0.46	1/4098 (0.0%)	0.50	0/5586
3	C	0.43	0/3568	0.45	0/4858
3	c	0.44	2/3579 (0.1%)	0.46	0/4872
4	D	0.52	0/2801	0.52	0/3818
4	d	0.47	0/2801	0.51	0/3818
5	E	0.36	0/675	0.43	0/922
5	e	0.49	1/664 (0.2%)	0.47	0/907
6	F	0.36	0/278	0.41	0/379
6	f	0.33	0/278	0.43	0/379
7	H	0.42	0/506	0.48	0/690
7	h	0.37	0/511	0.41	0/697
8	I	0.41	0/273	0.43	0/370
8	i	0.40	0/273	0.41	0/370
9	J	0.37	0/244	0.39	0/332
9	j	0.29	0/244	0.32	0/332
10	K	0.32	0/282	0.42	0/391
10	k	0.34	0/294	0.50	0/405
11	L	0.49	0/303	0.48	0/412
11	l	0.47	0/303	0.48	0/412
12	M	0.47	0/252	0.49	0/344
12	m	0.41	0/252	0.41	0/344
13	O	0.38	0/1890	0.45	0/2564
13	o	0.41	0/1883	0.47	0/2554
14	T	0.50	0/250	0.43	0/338
14	t	0.44	0/258	0.42	0/349
15	U	0.24	0/776	0.37	0/1052
15	u	0.37	0/776	0.45	0/1052
16	V	0.38	0/1085	0.40	0/1473
16	v	0.37	0/1085	0.44	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.22	0/156	0.38	0/207
17	y	0.27	0/172	0.37	0/228
18	X	0.37	0/273	0.33	0/370
18	x	0.25	0/284	0.33	0/384
19	Z	0.27	0/482	0.46	0/659
19	z	0.34	0/482	0.60	1/659 (0.2%)
20	R	0.25	0/288	0.37	0/395
20	r	0.28	0/263	0.57	0/361
All	All	0.44	4/42406 (0.0%)	0.48	1/57740 (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
1	a	0	1
19	z	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ILE	C-N	-8.62	1.13	1.33
2	b	2	GLY	C-N	-6.22	1.20	1.33
3	c	399	ALA	C-N	-6.04	1.19	1.33
3	c	78	GLU	C-N	-5.73	1.21	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	39	LEU	CA-CB-CG	5.72	136.31	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	81	ALA	Peptide
19	z	35	ARG	Peptide

5.2 Too-close contacts [i](#)

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	2617	0	2514	43	0
1	a	2617	0	2514	57	0
2	B	3980	0	3841	65	0
2	b	3958	0	3815	80	0
3	C	3455	0	3376	46	0
3	c	3466	0	3389	71	0
4	D	2706	0	2608	45	0
4	d	2706	0	2608	75	0
5	E	656	0	638	21	0
5	e	645	0	628	22	0
6	F	269	0	277	10	0
6	f	269	0	277	8	0
7	H	493	0	513	4	0
7	h	498	0	518	13	0
8	I	266	0	282	4	0
8	i	266	0	282	0	0
9	J	238	0	249	1	0
9	j	238	0	249	6	0
10	K	272	0	279	5	0
10	k	284	0	292	8	0
11	L	296	0	304	6	0
11	l	296	0	304	2	0
12	M	249	0	268	5	0
12	m	249	0	268	5	0
13	O	1859	0	1833	37	0
13	o	1852	0	1826	39	0
14	T	241	0	244	4	0
14	t	249	0	255	11	0
15	U	765	0	767	13	0
15	u	765	0	767	7	0
16	V	1064	0	1073	13	0
16	v	1064	0	1073	18	0
17	Y	155	0	175	0	0
17	y	171	0	195	4	0
18	X	270	0	299	4	0
18	x	281	0	312	3	0
19	Z	471	0	507	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	471	0	507	17	0
20	R	282	0	313	7	0
20	r	257	0	290	9	0
21	A	2	0	0	1	0
21	a	2	0	0	1	0
22	A	260	0	288	9	0
22	B	975	0	1080	35	0
22	C	845	0	936	41	0
22	D	130	0	144	6	0
22	H	65	0	72	1	0
22	a	195	0	216	12	0
22	b	1040	0	1152	39	0
22	c	845	0	936	52	0
22	d	195	0	216	7	0
23	A	64	0	74	1	0
23	D	64	0	74	2	0
23	a	128	0	148	5	0
24	A	40	0	56	1	0
24	B	120	0	168	9	0
24	C	80	0	112	5	0
24	D	40	0	56	4	0
24	H	40	0	56	4	0
24	K	80	0	112	5	0
24	T	40	0	56	1	0
24	a	40	0	56	1	0
24	b	120	0	168	6	0
24	c	120	0	168	12	0
24	d	40	0	56	3	0
24	h	40	0	56	6	0
24	k	40	0	56	4	0
24	t	40	0	56	8	0
25	A	55	0	80	6	0
25	D	55	0	80	6	0
25	a	55	0	80	4	0
25	d	55	0	80	3	0
26	A	108	0	156	4	0
26	D	43	0	53	1	0
26	L	48	0	63	4	0
26	a	104	0	153	5	0
26	b	54	0	78	8	0
26	f	43	0	53	2	0
27	A	25	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	B	99	0	187	9	0
27	C	15	0	29	0	0
27	D	33	0	57	2	0
27	I	14	0	24	0	0
27	J	11	0	18	0	0
27	M	26	0	47	4	0
27	T	12	0	23	0	0
27	a	7	0	10	0	0
27	b	100	0	183	6	0
27	c	24	0	43	3	0
27	d	40	0	77	2	0
27	i	23	0	41	0	0
27	j	15	0	29	4	0
27	m	25	0	45	1	0
27	t	15	0	29	3	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	B	87	0	114	2	0
29	C	143	0	196	9	0
29	D	51	0	72	1	0
29	b	39	0	48	2	0
29	c	143	0	196	14	0
29	f	51	0	72	2	0
29	m	51	0	72	3	0
30	C	180	0	234	7	0
30	H	60	0	78	3	0
30	c	179	0	232	16	0
30	h	62	0	82	7	0
31	D	4	0	0	0	0
31	a	4	0	0	0	0
32	D	147	0	222	19	0
32	E	42	0	57	4	0
32	L	49	0	74	6	0
32	b	49	0	74	2	0
32	d	98	0	148	20	0
32	e	42	0	57	2	0
32	l	49	0	74	1	0
33	E	43	0	30	9	0
33	e	43	0	30	7	0
34	V	43	0	30	2	0
34	v	43	0	30	1	0
35	A	70	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	84	0	0	3	0
35	C	62	0	0	2	0
35	D	72	0	0	2	0
35	E	5	0	0	0	0
35	F	1	0	0	0	0
35	H	17	0	0	1	0
35	J	1	0	0	0	0
35	K	1	0	0	0	0
35	L	5	0	0	1	0
35	M	3	0	0	0	0
35	O	30	0	0	2	0
35	T	2	0	0	0	0
35	U	2	0	0	0	0
35	V	12	0	0	0	0
35	X	3	0	0	0	0
35	a	77	0	0	5	0
35	b	72	0	0	0	0
35	c	65	0	0	6	0
35	d	51	0	0	2	0
35	e	5	0	0	1	0
35	f	2	0	0	0	0
35	h	3	0	0	0	0
35	l	5	0	0	0	0
35	m	2	0	0	0	0
35	o	25	0	0	4	0
35	t	3	0	0	0	0
35	u	12	0	0	1	0
35	v	11	0	0	3	0
All	All	50407	0	51279	931	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 9.

The worst 5 of 931 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)
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.43	0.99
3:c:189:TRP:HE1	3:c:295:THR:HG22	1.36	0.89
2:b:357:ARG:NH2	4:d:337:GLU:O	2.07	0.88
32:D:409:LHG:H352	32:D:409:LHG:H151	1.53	0.88
11:L:7:ARG:NH2	26:L:101:SQD:O8	2.09	0.85

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	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	36	42
1	a	331/344 (96%)	319 (96%)	11 (3%)	1 (0%)	36	42
2	B	503/510 (99%)	478 (95%)	25 (5%)	0	100	100
2	b	501/510 (98%)	479 (96%)	22 (4%)	0	100	100
3	C	445/461 (96%)	433 (97%)	11 (2%)	1 (0%)	43	51
3	c	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	43	51
4	D	338/352 (96%)	327 (97%)	11 (3%)	0	100	100
4	d	338/352 (96%)	321 (95%)	17 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	30 (97%)	1 (3%)	0	100	100
7	H	60/66 (91%)	56 (93%)	4 (7%)	0	100	100
7	h	61/66 (92%)	55 (90%)	6 (10%)	0	100	100
8	I	31/38 (82%)	30 (97%)	1 (3%)	0	100	100
8	i	31/38 (82%)	31 (100%)	0	0	100	100
9	J	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
9	j	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
10	K	33/46 (72%)	32 (97%)	1 (3%)	0	100	100
10	k	34/46 (74%)	33 (97%)	1 (3%)	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	30/36 (83%)	30 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	222 (92%)	15 (6%)	3 (1%)	9	8
13	o	239/272 (88%)	223 (93%)	14 (6%)	2 (1%)	16	16
14	T	26/32 (81%)	26 (100%)	0	0	100	100
14	t	27/32 (84%)	25 (93%)	2 (7%)	0	100	100
15	U	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
15	u	94/134 (70%)	89 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	19
16	v	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
17	Y	19/46 (41%)	18 (95%)	1 (5%)	0	100	100
17	y	21/46 (46%)	21 (100%)	0	0	100	100
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100	100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
19	Z	59/62 (95%)	54 (92%)	2 (3%)	3 (5%)	1	0
19	z	59/62 (95%)	53 (90%)	3 (5%)	3 (5%)	1	0
20	R	33/41 (80%)	32 (97%)	0	1 (3%)	3	1
20	r	30/41 (73%)	30 (100%)	0	0	100	100
All	All	5173/5700 (91%)	4951 (96%)	205 (4%)	17 (0%)	36	42

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	32	ASP
19	Z	35	ARG
3	c	416	SER
19	z	30	PRO

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	269 (100%)	1 (0%)	84	92
1	a	270/280 (96%)	268 (99%)	2 (1%)	76	87
2	B	403/407 (99%)	402 (100%)	1 (0%)	87	94
2	b	401/407 (98%)	401 (100%)	0	100	100
3	C	349/362 (96%)	346 (99%)	3 (1%)	70	84
3	c	350/362 (97%)	348 (99%)	2 (1%)	78	89
4	D	275/283 (97%)	275 (100%)	0	100	100
4	d	275/283 (97%)	275 (100%)	0	100	100
5	E	71/73 (97%)	70 (99%)	1 (1%)	59	75
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	26 (96%)	1 (4%)	30	41
7	H	53/55 (96%)	53 (100%)	0	100	100
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	66
8	I	30/35 (86%)	30 (100%)	0	100	100
8	i	30/35 (86%)	30 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	23/28 (82%)	23 (100%)	0	100	100
10	K	28/37 (76%)	28 (100%)	0	100	100
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	33 (97%)	1 (3%)	37	51
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	29 (100%)	0	100	100
13	O	206/228 (90%)	205 (100%)	1 (0%)	81	90
13	o	205/228 (90%)	204 (100%)	1 (0%)	81	90
14	T	25/29 (86%)	24 (96%)	1 (4%)	28	38
14	t	26/29 (90%)	26 (100%)	0	100	100
15	U	83/112 (74%)	82 (99%)	1 (1%)	63	78
15	u	83/112 (74%)	83 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	117/138 (85%)	117 (100%)	0	100	100
17	Y	15/37 (40%)	15 (100%)	0	100	100
17	y	17/37 (46%)	17 (100%)	0	100	100
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	47
19	Z	51/52 (98%)	51 (100%)	0	100	100
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	30/33 (91%)	30 (100%)	0	100	100
20	r	27/33 (82%)	26 (96%)	1 (4%)	30	41
All	All	4297/4660 (92%)	4278 (100%)	19 (0%)	84	92

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	h	56	ASP
18	x	6	SER
20	r	4	ARG
13	o	106	VAL
15	U	23	GLU

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

Mol	Chain	Res	Type
4	d	186	GLN
11	l	37	ASN
4	d	224	GLN
5	e	82	GLN
12	m	32	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 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
22	CLA	B	614	-	69,73,73	1.36	9 (13%)	82,113,113	1.33	10 (12%)
22	CLA	b	610	-	69,73,73	1.52	8 (11%)	82,113,113	1.33	7 (8%)
22	CLA	C	514	-	69,73,73	1.66	9 (13%)	82,113,113	1.17	9 (10%)
30	DGD	C	519	-	63,63,67	0.83	3 (4%)	77,77,81	1.10	7 (9%)
22	CLA	D	404	-	69,73,73	1.86	12 (17%)	82,113,113	1.19	9 (10%)
22	CLA	C	507	-	69,73,73	1.82	12 (17%)	82,113,113	1.36	10 (12%)
22	CLA	C	512	3	69,73,73	1.56	9 (13%)	82,113,113	1.22	8 (9%)
27	LFA	D	413	-	7,7,19	0.13	0	6,6,18	0.33	0
22	CLA	A	403	-	69,73,73	1.55	9 (13%)	82,113,113	1.43	8 (9%)
27	LFA	M	101	-	9,9,19	0.18	0	8,8,18	0.64	0
22	CLA	C	505	35	69,73,73	1.74	10 (14%)	82,113,113	1.18	9 (10%)
22	CLA	B	610	-	69,73,73	1.55	9 (13%)	82,113,113	1.38	11 (13%)
27	LFA	D	411	-	14,14,19	0.10	0	13,13,18	0.25	0
27	LFA	B	623	-	12,12,19	0.07	0	11,11,18	0.23	0
22	CLA	b	613	-	69,73,73	1.50	9 (13%)	82,113,113	1.31	9 (10%)
29	LMG	C	520	-	48,48,55	0.94	2 (4%)	56,56,63	1.16	5 (8%)
26	SQD	a	410	-	52,54,54	1.05	3 (5%)	62,65,65	1.34	11 (17%)
29	LMG	b	624	-	39,39,55	1.12	3 (7%)	47,47,63	1.12	6 (12%)
22	CLA	c	504	-	69,73,73	1.60	9 (13%)	82,113,113	1.17	8 (9%)
24	BCR	H	102	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
22	CLA	B	615	-	69,73,73	1.70	9 (13%)	82,113,113	1.43	10 (12%)
27	LFA	b	630	-	14,14,19	0.09	0	13,13,18	0.37	0
31	BCT	D	401	28	3,3,3	0.86	0	2,3,3	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEC	V	201	16	46,50,50	1.78	6 (13%)	58,82,82	1.05	4 (6%)
27	LFA	i	102	-	6,6,19	0.11	0	5,5,18	0.16	0
22	CLA	a	405	35	69,73,73	1.48	8 (11%)	82,113,113	1.24	9 (10%)
24	BCR	b	621	-	41,41,41	0.84	1 (2%)	56,56,56	1.87	14 (25%)
27	LFA	J	101	-	10,10,19	0.12	0	9,9,18	0.36	0
27	LFA	b	625	-	15,15,19	0.09	0	14,14,18	0.38	0
29	LMG	c	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.17	6 (10%)
22	CLA	B	605	-	69,73,73	1.50	8 (11%)	82,113,113	1.31	7 (8%)
22	CLA	C	504	-	69,73,73	1.47	7 (10%)	82,113,113	1.10	9 (10%)
22	CLA	B	603	-	69,73,73	1.55	7 (10%)	82,113,113	1.28	9 (10%)
22	CLA	A	412	35	69,73,73	1.54	10 (14%)	82,113,113	1.21	9 (10%)
22	CLA	a	404	-	69,73,73	1.53	7 (10%)	82,113,113	1.28	7 (8%)
22	CLA	c	507	-	69,73,73	1.67	8 (11%)	82,113,113	1.38	10 (12%)
22	CLA	b	604	-	69,73,73	1.60	10 (14%)	82,113,113	1.31	10 (12%)
22	CLA	b	617	-	69,73,73	1.51	9 (13%)	82,113,113	1.24	9 (10%)
24	BCR	c	523	-	41,41,41	0.86	1 (2%)	56,56,56	1.86	13 (23%)
26	SQD	b	601	-	52,54,54	1.06	3 (5%)	62,65,65	1.52	13 (20%)
27	LFA	d	408	-	14,14,19	0.12	0	13,13,18	0.42	0
22	CLA	b	603	35	69,73,73	1.59	7 (10%)	82,113,113	1.14	10 (12%)
22	CLA	c	506	-	69,73,73	1.57	9 (13%)	82,113,113	1.11	8 (9%)
22	CLA	B	607	-	69,73,73	1.55	9 (13%)	82,113,113	1.19	7 (8%)
22	CLA	c	505	35	69,73,73	1.66	9 (13%)	82,113,113	1.15	8 (9%)
22	CLA	c	512	3	69,73,73	1.57	9 (13%)	82,113,113	1.23	9 (10%)
22	CLA	B	602	-	69,73,73	1.59	9 (13%)	82,113,113	1.29	10 (12%)
27	LFA	a	411	-	6,6,19	0.10	0	5,5,18	0.22	0
27	LFA	j	101	-	14,14,19	0.11	0	13,13,18	0.43	0
23	PHO	a	414	-	58,69,69	1.36	7 (12%)	55,99,99	1.72	4 (7%)
32	LHG	D	408	-	48,48,48	0.88	3 (6%)	51,54,54	1.19	4 (7%)
27	LFA	i	101	-	15,15,19	0.12	0	14,14,18	0.38	0
23	PHO	a	406	-	58,69,69	1.15	6 (10%)	55,99,99	1.66	4 (7%)
27	LFA	m	102	-	14,14,19	0.13	0	13,13,18	0.40	0
22	CLA	A	406	-	69,73,73	2.01	14 (20%)	82,113,113	1.17	9 (10%)
31	BCT	a	413	28	3,3,3	0.87	0	2,3,3	0.23	0
23	PHO	D	402	-	58,69,69	1.23	7 (12%)	55,99,99	1.76	6 (10%)
26	SQD	L	101	-	46,48,54	1.15	3 (6%)	56,59,65	3.33	10 (17%)
29	LMG	m	103	-	51,51,55	0.84	3 (5%)	59,59,63	1.38	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	a	408	-	41,41,41	0.88	1 (2%)	56,56,56	1.44	11 (19%)
24	BCR	c	524	-	41,41,41	0.78	1 (2%)	56,56,56	1.74	14 (25%)
33	HEM	E	102	6,5	50,50,50	1.42	9 (18%)	67,82,82	1.15	5 (7%)
26	SQD	a	412	-	50,50,54	0.89	2 (4%)	58,58,65	1.18	6 (10%)
23	PHO	A	405	-	58,69,69	1.25	8 (13%)	55,99,99	1.68	4 (7%)
22	CLA	c	510	-	69,73,73	1.70	10 (14%)	82,113,113	1.21	12 (14%)
22	CLA	d	402	-	69,73,73	1.51	9 (13%)	82,113,113	1.09	4 (4%)
27	LFA	M	102	-	15,15,19	0.21	0	14,14,18	0.65	0
22	CLA	B	611	-	69,73,73	1.72	8 (11%)	82,113,113	1.18	7 (8%)
29	LMG	B	619	-	51,51,55	0.93	2 (3%)	59,59,63	1.05	2 (3%)
29	LMG	D	410	-	51,51,55	0.96	2 (3%)	59,59,63	0.94	2 (3%)
24	BCR	d	404	-	41,41,41	0.93	2 (4%)	56,56,56	2.21	16 (28%)
27	LFA	B	627	-	13,13,19	0.12	0	12,12,18	0.51	0
24	BCR	c	515	-	41,41,41	0.87	2 (4%)	56,56,56	1.40	7 (12%)
26	SQD	D	412	-	41,43,54	1.18	3 (7%)	51,54,65	1.74	10 (19%)
24	BCR	B	617	-	41,41,41	0.85	2 (4%)	56,56,56	1.62	13 (23%)
24	BCR	k	101	-	41,41,41	0.86	1 (2%)	56,56,56	1.84	12 (21%)
22	CLA	b	611	-	69,73,73	1.72	12 (17%)	82,113,113	1.25	8 (9%)
29	LMG	c	501	-	51,51,55	0.87	3 (5%)	59,59,63	1.25	5 (8%)
22	CLA	b	615	-	69,73,73	1.90	11 (15%)	82,113,113	1.25	8 (9%)
27	LFA	B	626	-	9,9,19	0.11	0	8,8,18	0.45	0
27	LFA	B	625	-	8,8,19	0.11	0	7,7,18	0.31	0
27	LFA	b	623	-	11,11,19	0.09	0	10,10,18	0.39	0
24	BCR	K	101	-	41,41,41	0.81	2 (4%)	56,56,56	1.66	11 (19%)
27	LFA	A	410	-	13,13,19	0.09	0	12,12,18	0.33	0
27	LFA	b	626	-	11,11,19	0.09	0	10,10,18	0.30	0
30	DGD	h	102	-	63,63,67	0.82	2 (3%)	77,77,81	1.01	3 (3%)
27	LFA	d	409	-	8,8,19	0.11	0	7,7,18	0.26	0
22	CLA	C	503	-	69,73,73	1.59	8 (11%)	82,113,113	1.13	9 (10%)
22	CLA	b	614	-	69,73,73	1.83	11 (15%)	82,113,113	1.29	10 (12%)
32	LHG	b	628	-	48,48,48	0.90	3 (6%)	51,54,54	1.13	5 (9%)
22	CLA	C	510	-	69,73,73	1.80	10 (14%)	82,113,113	1.18	9 (10%)
27	LFA	C	521	-	14,14,19	0.08	0	13,13,18	0.33	0
22	CLA	C	513	-	69,73,73	1.66	9 (13%)	82,113,113	1.18	10 (12%)
22	CLA	B	612	-	69,73,73	1.60	9 (13%)	82,113,113	1.22	7 (8%)
29	LMG	B	621	-	36,36,55	1.06	2 (5%)	44,44,63	1.23	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DGD	c	516	-	63,63,67	0.84	3 (4%)	77,77,81	1.14	6 (7%)
22	CLA	H	101	35	69,73,73	1.64	10 (14%)	82,113,113	1.13	7 (8%)
22	CLA	C	511	-	69,73,73	1.56	7 (10%)	82,113,113	1.25	11 (13%)
22	CLA	c	503	-	69,73,73	1.70	9 (13%)	82,113,113	1.23	10 (12%)
29	LMG	C	522	-	44,44,55	1.06	3 (6%)	52,52,63	1.60	9 (17%)
22	CLA	C	509	-	69,73,73	1.58	8 (11%)	82,113,113	1.16	9 (10%)
27	LFA	I	101	-	13,13,19	0.09	0	12,12,18	0.36	0
29	LMG	C	501	-	51,51,55	0.89	2 (3%)	59,59,63	1.10	3 (5%)
32	LHG	e	101	-	41,41,48	0.98	2 (4%)	44,47,54	1.07	3 (6%)
22	CLA	B	606	35	69,73,73	1.83	10 (14%)	82,113,113	1.22	10 (12%)
32	LHG	D	409	-	48,48,48	0.87	3 (6%)	51,54,54	1.03	2 (3%)
22	CLA	b	618	-	69,73,73	1.71	11 (15%)	82,113,113	1.26	8 (9%)
27	LFA	B	628	-	11,11,19	0.10	0	10,10,18	0.37	0
33	HEM	e	102	6,5	50,50,50	1.39	7 (14%)	67,82,82	1.01	3 (4%)
22	CLA	c	514	-	69,73,73	1.78	10 (14%)	82,113,113	1.21	10 (12%)
24	BCR	K	102	-	41,41,41	0.84	1 (2%)	56,56,56	1.92	12 (21%)
22	CLA	c	509	-	69,73,73	1.61	9 (13%)	82,113,113	1.26	8 (9%)
32	LHG	D	407	-	48,48,48	0.90	3 (6%)	51,54,54	1.20	4 (7%)
25	PL9	A	408	-	55,55,55	0.64	2 (3%)	68,69,69	2.00	22 (32%)
22	CLA	b	606	-	69,73,73	1.62	10 (14%)	82,113,113	1.38	11 (13%)
24	BCR	B	616	-	41,41,41	0.84	1 (2%)	56,56,56	1.70	11 (19%)
27	LFA	b	627	-	10,10,19	0.09	0	9,9,18	0.35	0
22	CLA	B	613	-	69,73,73	1.55	10 (14%)	82,113,113	1.30	5 (6%)
26	SQD	f	102	-	41,43,54	1.19	4 (9%)	51,54,65	1.63	10 (19%)
24	BCR	B	618	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	15 (26%)
30	DGD	H	103	-	61,61,67	0.84	2 (3%)	75,75,81	1.20	5 (6%)
22	CLA	c	508	35	69,73,73	1.73	10 (14%)	82,113,113	1.29	8 (9%)
22	CLA	C	502	-	69,73,73	1.72	11 (15%)	82,113,113	1.37	12 (14%)
32	LHG	L	102	-	48,48,48	0.95	2 (4%)	51,54,54	1.12	3 (5%)
27	LFA	d	410	-	15,15,19	0.08	0	14,14,18	0.36	0
22	CLA	C	508	35	69,73,73	1.78	9 (13%)	82,113,113	1.21	10 (12%)
22	CLA	a	407	-	69,73,73	1.86	10 (14%)	82,113,113	1.19	10 (12%)
22	CLA	b	609	35	69,73,73	1.84	11 (15%)	82,113,113	1.31	10 (12%)
29	LMG	c	522	-	41,41,55	1.04	2 (4%)	49,49,63	1.61	11 (22%)
22	CLA	c	502	-	69,73,73	1.73	9 (13%)	82,113,113	1.27	9 (10%)
27	LFA	B	620	-	9,9,19	0.18	0	8,8,18	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LFA	T	102	-	11,11,19	0.13	0	10,10,18	0.42	0
24	BCR	b	620	-	41,41,41	0.78	0	56,56,56	1.52	9 (16%)
30	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.23	7 (9%)
27	LFA	B	624	-	14,14,19	0.09	0	13,13,18	0.31	0
32	LHG	d	406	-	48,48,48	0.93	4 (8%)	51,54,54	1.17	5 (9%)
27	LFA	b	629	-	8,8,19	0.11	0	7,7,18	0.32	0
27	LFA	t	101	-	14,14,19	0.14	0	13,13,18	0.52	0
32	LHG	E	101	-	41,41,48	1.01	2 (4%)	44,47,54	1.09	3 (6%)
22	CLA	B	609	35	69,73,73	1.85	11 (15%)	82,113,113	1.31	10 (12%)
22	CLA	B	608	-	69,73,73	1.60	8 (11%)	82,113,113	1.22	10 (12%)
22	CLA	c	511	-	69,73,73	1.65	9 (13%)	82,113,113	1.27	7 (8%)
24	BCR	C	515	-	41,41,41	0.79	1 (2%)	56,56,56	1.80	17 (30%)
27	LFA	c	520	-	8,8,19	0.11	0	7,7,18	0.37	0
30	DGD	c	517	-	56,56,67	0.89	2 (3%)	70,70,81	1.10	4 (5%)
22	CLA	b	607	-	69,73,73	1.48	10 (14%)	82,113,113	1.24	8 (9%)
27	LFA	B	622	-	15,15,19	0.11	0	14,14,18	0.32	0
22	CLA	D	403	-	69,73,73	1.62	8 (11%)	82,113,113	1.37	7 (8%)
27	LFA	b	602	-	14,14,19	0.12	0	13,13,18	0.43	0
22	CLA	b	608	-	69,73,73	1.65	11 (15%)	82,113,113	1.29	8 (9%)
22	CLA	c	513	-	69,73,73	1.61	9 (13%)	82,113,113	1.19	8 (9%)
24	BCR	A	407	-	41,41,41	0.82	0	56,56,56	1.57	11 (19%)
30	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	1.04	2 (2%)
24	BCR	D	405	-	41,41,41	0.93	2 (4%)	56,56,56	1.90	13 (23%)
22	CLA	B	601	-	69,73,73	1.58	8 (11%)	82,113,113	1.33	7 (8%)
24	BCR	T	101	-	41,41,41	0.90	2 (4%)	56,56,56	2.03	14 (25%)
32	LHG	d	407	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	3 (5%)
27	LFA	D	414	-	9,9,19	0.19	0	8,8,18	0.51	0
24	BCR	t	102	-	41,41,41	0.86	1 (2%)	56,56,56	1.94	14 (25%)
26	SQD	A	409	-	52,54,54	1.05	3 (5%)	62,65,65	1.63	11 (17%)
25	PL9	a	409	-	55,55,55	0.61	2 (3%)	68,69,69	1.79	18 (26%)
34	HEC	v	201	16	46,50,50	1.80	6 (13%)	58,82,82	1.09	4 (6%)
22	CLA	A	404	35	69,73,73	1.52	8 (11%)	82,113,113	1.21	9 (10%)
22	CLA	B	604	-	69,73,73	1.45	8 (11%)	82,113,113	1.28	8 (9%)
22	CLA	C	506	-	69,73,73	1.64	9 (13%)	82,113,113	1.19	8 (9%)
22	CLA	b	616	-	69,73,73	1.51	8 (11%)	82,113,113	1.14	6 (7%)
24	BCR	b	619	-	41,41,41	0.85	1 (2%)	56,56,56	1.80	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PL9	d	405	-	55,55,55	0.66	3 (5%)	68,69,69	1.74	15 (22%)
27	LFA	A	413	-	10,10,19	0.08	0	9,9,18	0.43	0
22	CLA	d	403	-	69,73,73	1.88	11 (15%)	82,113,113	1.18	9 (10%)
24	BCR	h	101	-	41,41,41	0.79	0	56,56,56	1.82	14 (25%)
26	SQD	A	411	-	52,54,54	1.07	3 (5%)	62,65,65	1.31	8 (12%)
27	LFA	c	521	-	14,14,19	0.09	0	13,13,18	0.34	0
22	CLA	b	612	35	69,73,73	1.84	11 (15%)	82,113,113	1.44	7 (8%)
25	PL9	D	406	-	55,55,55	0.72	3 (5%)	68,69,69	1.62	15 (22%)
24	BCR	C	516	-	41,41,41	0.94	2 (4%)	56,56,56	1.76	10 (17%)
22	CLA	d	401	35	69,73,73	1.62	9 (13%)	82,113,113	1.19	11 (13%)
30	DGD	C	518	-	57,57,67	0.86	2 (3%)	71,71,81	1.27	9 (12%)
22	CLA	b	605	-	69,73,73	1.71	10 (14%)	82,113,113	1.25	6 (7%)
27	LFA	m	101	-	9,9,19	0.13	0	8,8,18	0.44	0
32	LHG	l	101	-	48,48,48	0.88	3 (6%)	51,54,54	1.23	5 (9%)
29	LMG	f	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.09	5 (8%)
27	LFA	b	622	-	9,9,19	0.13	0	8,8,18	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	614	-	1/1/15/20	10/39/115/115	-
22	CLA	b	610	-	1/1/15/20	3/39/115/115	-
22	CLA	C	514	-	1/1/15/20	1/39/115/115	-
30	DGD	C	519	-	-	6/51/91/95	0/2/2/2
22	CLA	D	404	-	1/1/15/20	5/39/115/115	-
22	CLA	C	507	-	1/1/15/20	4/39/115/115	-
22	CLA	C	512	3	1/1/15/20	1/39/115/115	-
27	LFA	D	413	-	-	2/5/5/17	-
22	CLA	A	403	-	1/1/15/20	1/39/115/115	-
27	LFA	M	101	-	-	2/7/7/17	-
22	CLA	C	505	35	1/1/15/20	5/39/115/115	-
22	CLA	B	610	-	1/1/15/20	3/39/115/115	-
27	LFA	D	411	-	-	5/12/12/17	-
27	LFA	B	623	-	-	6/10/10/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	613	-	1/1/15/20	7/39/115/115	-
29	LMG	C	520	-	-	10/43/63/70	0/1/1/1
26	SQD	a	410	-	-	14/49/69/69	0/1/1/1
29	LMG	b	624	-	-	13/34/54/70	0/1/1/1
22	CLA	c	504	-	1/1/15/20	4/39/115/115	-
24	BCR	H	102	-	-	3/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/15/20	7/39/115/115	-
27	LFA	b	630	-	-	6/12/12/17	-
34	HEC	V	201	16	-	5/14/54/54	-
27	LFA	i	102	-	-	2/4/4/17	-
22	CLA	a	405	35	1/1/15/20	5/39/115/115	-
24	BCR	b	621	-	-	8/29/63/63	0/2/2/2
27	LFA	J	101	-	-	1/8/8/17	-
27	LFA	b	625	-	-	6/13/13/17	-
29	LMG	c	519	-	-	10/46/66/70	0/1/1/1
22	CLA	B	605	-	1/1/15/20	5/39/115/115	-
22	CLA	C	504	-	1/1/15/20	5/39/115/115	-
22	CLA	B	603	-	1/1/15/20	1/39/115/115	-
22	CLA	A	412	35	1/1/15/20	0/39/115/115	-
22	CLA	a	404	-	1/1/15/20	2/39/115/115	-
22	CLA	c	507	-	1/1/15/20	5/39/115/115	-
22	CLA	b	604	-	1/1/15/20	5/39/115/115	-
22	CLA	b	617	-	1/1/15/20	3/39/115/115	-
24	BCR	c	523	-	-	2/29/63/63	0/2/2/2
26	SQD	b	601	-	-	11/49/69/69	0/1/1/1
27	LFA	d	408	-	-	5/12/12/17	-
22	CLA	b	603	35	1/1/15/20	8/39/115/115	-
22	CLA	c	506	-	1/1/15/20	7/39/115/115	-
22	CLA	B	607	-	1/1/15/20	2/39/115/115	-
22	CLA	c	505	35	1/1/15/20	4/39/115/115	-
22	CLA	c	512	3	1/1/15/20	0/39/115/115	-
22	CLA	B	602	-	1/1/15/20	4/39/115/115	-
27	LFA	a	411	-	-	1/4/4/17	-
27	LFA	j	101	-	-	3/12/12/17	-
23	PHO	a	414	-	-	0/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	D	408	-	-	10/53/53/53	-
27	LFA	i	101	-	-	6/13/13/17	-
23	PHO	a	406	-	-	3/37/103/103	0/5/6/6
27	LFA	m	102	-	-	4/12/12/17	-
22	CLA	A	406	-	1/1/15/20	2/39/115/115	-
23	PHO	D	402	-	-	4/37/103/103	0/5/6/6
26	SQD	L	101	-	-	18/43/63/69	0/1/1/1
29	LMG	m	103	-	-	17/46/66/70	0/1/1/1
24	BCR	a	408	-	-	2/29/63/63	0/2/2/2
24	BCR	c	524	-	-	2/29/63/63	0/2/2/2
33	HEM	E	102	6,5	-	6/14/54/54	-
26	SQD	a	412	-	-	15/44/64/69	0/1/1/1
23	PHO	A	405	-	-	0/37/103/103	0/5/6/6
22	CLA	c	510	-	1/1/15/20	3/39/115/115	-
22	CLA	d	402	-	1/1/15/20	3/39/115/115	-
27	LFA	M	102	-	-	5/13/13/17	-
22	CLA	B	611	-	1/1/15/20	3/39/115/115	-
29	LMG	B	619	-	-	15/46/66/70	0/1/1/1
29	LMG	D	410	-	-	5/46/66/70	0/1/1/1
24	BCR	d	404	-	-	4/29/63/63	0/2/2/2
27	LFA	B	627	-	-	8/11/11/17	-
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
26	SQD	D	412	-	-	6/38/58/69	0/1/1/1
24	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	BCR	k	101	-	-	5/29/63/63	0/2/2/2
22	CLA	b	611	-	1/1/15/20	6/39/115/115	-
29	LMG	c	501	-	-	17/46/66/70	0/1/1/1
22	CLA	b	615	-	1/1/15/20	4/39/115/115	-
27	LFA	B	626	-	-	4/7/7/17	-
27	LFA	B	625	-	-	0/6/6/17	-
27	LFA	b	623	-	-	0/9/9/17	-
24	BCR	K	101	-	-	4/29/63/63	0/2/2/2
27	LFA	A	410	-	-	6/11/11/17	-
27	LFA	b	626	-	-	6/9/9/17	-
30	DGD	h	102	-	-	18/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LFA	d	409	-	-	2/6/6/17	-
22	CLA	C	503	-	1/1/15/20	4/39/115/115	-
22	CLA	b	614	-	1/1/15/20	3/39/115/115	-
32	LHG	b	628	-	-	12/53/53/53	-
22	CLA	C	510	-	1/1/15/20	6/39/115/115	-
27	LFA	C	521	-	-	5/12/12/17	-
22	CLA	C	513	-	1/1/15/20	2/39/115/115	-
22	CLA	B	612	-	1/1/15/20	2/39/115/115	-
29	LMG	B	621	-	-	8/31/51/70	0/1/1/1
30	DGD	c	516	-	-	13/51/91/95	0/2/2/2
22	CLA	H	101	35	1/1/15/20	9/39/115/115	-
22	CLA	C	511	-	1/1/15/20	1/39/115/115	-
22	CLA	c	503	-	1/1/15/20	2/39/115/115	-
29	LMG	C	522	-	-	16/39/59/70	0/1/1/1
22	CLA	C	509	-	1/1/15/20	2/39/115/115	-
27	LFA	I	101	-	-	6/11/11/17	-
29	LMG	C	501	-	-	15/46/66/70	0/1/1/1
32	LHG	e	101	-	-	13/46/46/53	-
22	CLA	B	606	35	1/1/15/20	6/39/115/115	-
32	LHG	D	409	-	-	17/53/53/53	-
22	CLA	b	618	-	1/1/15/20	4/39/115/115	-
27	LFA	B	628	-	-	2/9/9/17	-
33	HEM	e	102	6,5	-	7/14/54/54	-
22	CLA	c	514	-	1/1/15/20	1/39/115/115	-
24	BCR	K	102	-	-	2/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/15/20	3/39/115/115	-
32	LHG	D	407	-	-	15/53/53/53	-
25	PL9	A	408	-	-	8/53/73/73	0/1/1/1
22	CLA	b	606	-	1/1/15/20	6/39/115/115	-
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
27	LFA	b	627	-	-	3/8/8/17	-
22	CLA	B	613	-	1/1/15/20	10/39/115/115	-
26	SQD	f	102	-	-	17/38/58/69	0/1/1/1
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	H	103	-	-	12/49/89/95	0/2/2/2
22	CLA	c	508	35	1/1/15/20	4/39/115/115	-
22	CLA	C	502	-	1/1/15/20	1/39/115/115	-
32	LHG	L	102	-	-	15/53/53/53	-
27	LFA	d	410	-	-	5/13/13/17	-
22	CLA	C	508	35	1/1/15/20	2/39/115/115	-
22	CLA	a	407	-	1/1/15/20	4/39/115/115	-
22	CLA	b	609	35	1/1/15/20	5/39/115/115	-
29	LMG	c	522	-	-	10/36/56/70	0/1/1/1
22	CLA	c	502	-	1/1/15/20	4/39/115/115	-
27	LFA	B	620	-	-	5/7/7/17	-
27	LFA	T	102	-	-	2/9/9/17	-
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
30	DGD	C	517	-	-	14/51/91/95	0/2/2/2
27	LFA	B	624	-	-	8/12/12/17	-
32	LHG	d	406	-	-	16/53/53/53	-
27	LFA	b	629	-	-	0/6/6/17	-
27	LFA	t	101	-	-	3/12/12/17	-
32	LHG	E	101	-	-	20/46/46/53	-
22	CLA	B	609	35	1/1/15/20	3/39/115/115	-
22	CLA	B	608	-	1/1/15/20	6/39/115/115	-
22	CLA	c	511	-	1/1/15/20	3/39/115/115	-
24	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	LFA	c	520	-	-	0/6/6/17	-
30	DGD	c	517	-	-	14/44/84/95	0/2/2/2
22	CLA	b	607	-	1/1/15/20	8/39/115/115	-
27	LFA	B	622	-	-	2/13/13/17	-
22	CLA	D	403	-	1/1/15/20	3/39/115/115	-
27	LFA	b	602	-	-	5/12/12/17	-
22	CLA	b	608	-	1/1/15/20	4/39/115/115	-
22	CLA	c	513	-	1/1/15/20	2/39/115/115	-
24	BCR	A	407	-	-	3/29/63/63	0/2/2/2
30	DGD	c	518	-	-	18/51/91/95	0/2/2/2
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
22	CLA	B	601	-	1/1/15/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	T	101	-	-	8/29/63/63	0/2/2/2
32	LHG	d	407	-	-	25/53/53/53	-
27	LFA	D	414	-	-	0/7/7/17	-
24	BCR	t	102	-	-	6/29/63/63	0/2/2/2
26	SQD	A	409	-	-	11/49/69/69	0/1/1/1
25	PL9	a	409	-	-	15/53/73/73	0/1/1/1
34	HEC	v	201	16	-	5/14/54/54	-
22	CLA	A	404	35	1/1/15/20	2/39/115/115	-
22	CLA	B	604	-	1/1/15/20	11/39/115/115	-
22	CLA	C	506	-	1/1/15/20	6/39/115/115	-
22	CLA	b	616	-	1/1/15/20	11/39/115/115	-
24	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	PL9	d	405	-	-	11/53/73/73	0/1/1/1
27	LFA	A	413	-	-	5/8/8/17	-
22	CLA	d	403	-	1/1/15/20	8/39/115/115	-
24	BCR	h	101	-	-	3/29/63/63	0/2/2/2
26	SQD	A	411	-	-	22/49/69/69	0/1/1/1
27	LFA	c	521	-	-	4/12/12/17	-
22	CLA	b	612	35	1/1/15/20	7/39/115/115	-
25	PL9	D	406	-	-	13/53/73/73	0/1/1/1
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
22	CLA	d	401	35	1/1/15/20	3/39/115/115	-
30	DGD	C	518	-	-	14/45/85/95	0/2/2/2
22	CLA	b	605	-	1/1/15/20	5/39/115/115	-
27	LFA	m	101	-	-	1/7/7/17	-
32	LHG	l	101	-	-	20/53/53/53	-
29	LMG	f	101	-	-	8/46/66/70	0/1/1/1
27	LFA	b	622	-	-	3/7/7/17	-

The worst 5 of 843 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	609	CLA	MG-ND	-8.30	1.89	2.05
22	A	406	CLA	MG-NB	-8.25	1.89	2.05
22	D	404	CLA	MG-NB	-8.11	1.89	2.05
22	d	403	CLA	MG-NB	-8.10	1.89	2.05
22	c	508	CLA	MG-NB	-8.07	1.89	2.05

The worst 5 of 1216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	101	SQD	O9-S-C6	-14.76	84.72	106.76
26	L	101	SQD	O8-S-O9	-10.70	84.64	111.40
23	D	402	PHO	C4D-CHA-CBD	-10.32	103.51	108.45
26	L	101	SQD	O9-S-O7	-10.30	80.32	113.82
23	a	414	PHO	C4D-CHA-CBD	-10.08	103.62	108.45

5 of 70 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	403	CLA	ND
22	A	404	CLA	ND
22	A	406	CLA	ND
22	A	412	CLA	ND
22	B	601	CLA	ND

5 of 1105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C2B-C3B-CAB-CBB
22	B	604	CLA	C4B-C3B-CAB-CBB
22	B	613	CLA	C4B-C3B-CAB-CBB
22	B	613	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

161 monomers are involved in 421 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	514	CLA	2	0
30	C	519	DGD	1	0
22	D	404	CLA	3	0
22	C	507	CLA	2	0
22	C	512	CLA	4	0
27	D	413	LFA	1	0
22	A	403	CLA	2	0
27	M	101	LFA	2	0
22	C	505	CLA	2	0
22	B	610	CLA	1	0
27	B	623	LFA	2	0
22	b	613	CLA	1	0
29	C	520	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	a	410	SQD	3	0
29	b	624	LMG	2	0
22	c	504	CLA	6	0
24	H	102	BCR	4	0
22	B	615	CLA	3	0
34	V	201	HEC	2	0
22	a	405	CLA	5	0
27	b	625	LFA	1	0
29	c	519	LMG	6	0
22	B	605	CLA	3	0
22	C	504	CLA	6	0
22	B	603	CLA	3	0
22	A	412	CLA	2	0
22	a	404	CLA	4	0
22	c	507	CLA	4	0
22	b	604	CLA	5	0
22	b	617	CLA	3	0
24	c	523	BCR	2	0
26	b	601	SQD	8	0
22	b	603	CLA	4	0
22	c	506	CLA	5	0
22	B	607	CLA	5	0
22	c	505	CLA	8	0
22	c	512	CLA	4	0
22	B	602	CLA	4	0
27	j	101	LFA	4	0
23	a	414	PHO	3	0
32	D	408	LHG	4	0
23	a	406	PHO	2	0
22	A	406	CLA	4	0
23	D	402	PHO	2	0
26	L	101	SQD	4	0
29	m	103	LMG	3	0
24	a	408	BCR	1	0
24	c	524	BCR	6	0
33	E	102	HEM	9	0
26	a	412	SQD	2	0
23	A	405	PHO	1	0
22	c	510	CLA	5	0
22	d	402	CLA	3	0
27	M	102	LFA	2	0
22	B	611	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	619	LMG	2	0
29	D	410	LMG	1	0
24	d	404	BCR	3	0
27	B	627	LFA	1	0
24	c	515	BCR	4	0
26	D	412	SQD	1	0
24	B	617	BCR	5	0
24	k	101	BCR	4	0
22	b	611	CLA	5	0
29	c	501	LMG	6	0
22	b	615	CLA	1	0
27	B	626	LFA	2	0
27	b	623	LFA	3	0
24	K	101	BCR	2	0
27	b	626	LFA	1	0
30	h	102	DGD	7	0
27	d	409	LFA	1	0
22	C	503	CLA	4	0
22	b	614	CLA	3	0
32	b	628	LHG	2	0
22	C	510	CLA	2	0
22	C	513	CLA	1	0
22	B	612	CLA	2	0
30	c	516	DGD	6	0
22	H	101	CLA	1	0
22	C	511	CLA	4	0
22	c	503	CLA	3	0
29	C	522	LMG	2	0
22	C	509	CLA	4	0
29	C	501	LMG	5	0
32	e	101	LHG	2	0
22	B	606	CLA	2	0
32	D	409	LHG	10	0
22	b	618	CLA	1	0
27	B	628	LFA	1	0
33	e	102	HEM	7	0
22	c	514	CLA	4	0
24	K	102	BCR	3	0
22	c	509	CLA	5	0
32	D	407	LHG	5	0
25	A	408	PL9	6	0
22	b	606	CLA	3	0

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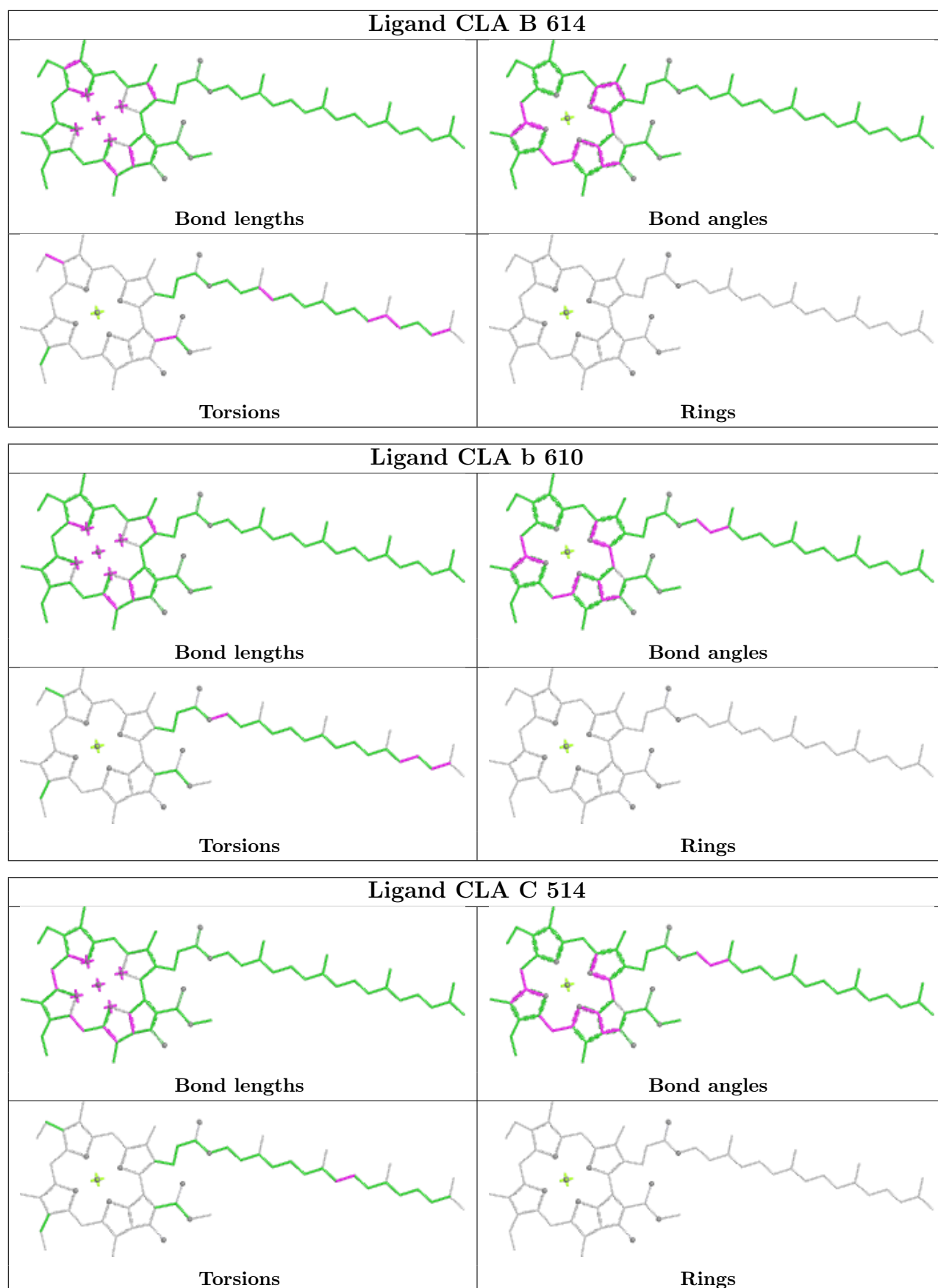
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	616	BCR	3	0
22	B	613	CLA	2	0
26	f	102	SQD	2	0
24	B	618	BCR	1	0
30	H	103	DGD	3	0
22	c	508	CLA	4	0
22	C	502	CLA	8	0
32	L	102	LHG	6	0
27	d	410	LFA	1	0
22	C	508	CLA	3	0
22	a	407	CLA	3	0
22	b	609	CLA	1	0
29	c	522	LMG	2	0
22	c	502	CLA	5	0
27	B	620	LFA	1	0
24	b	620	BCR	3	0
30	C	517	DGD	4	0
27	B	624	LFA	1	0
32	d	406	LHG	6	0
27	t	101	LFA	3	0
32	E	101	LHG	4	0
22	B	609	CLA	1	0
22	B	608	CLA	5	0
22	c	511	CLA	7	0
24	C	515	BCR	2	0
27	c	520	LFA	1	0
30	c	517	DGD	7	0
22	b	607	CLA	5	0
27	B	622	LFA	1	0
22	D	403	CLA	3	0
22	b	608	CLA	4	0
22	c	513	CLA	1	0
24	A	407	BCR	1	0
30	c	518	DGD	3	0
24	D	405	BCR	4	0
22	B	601	CLA	1	0
24	T	101	BCR	1	0
32	d	407	LHG	14	0
27	D	414	LFA	1	0
24	t	102	BCR	8	0
26	A	409	SQD	2	0
25	a	409	PL9	4	0

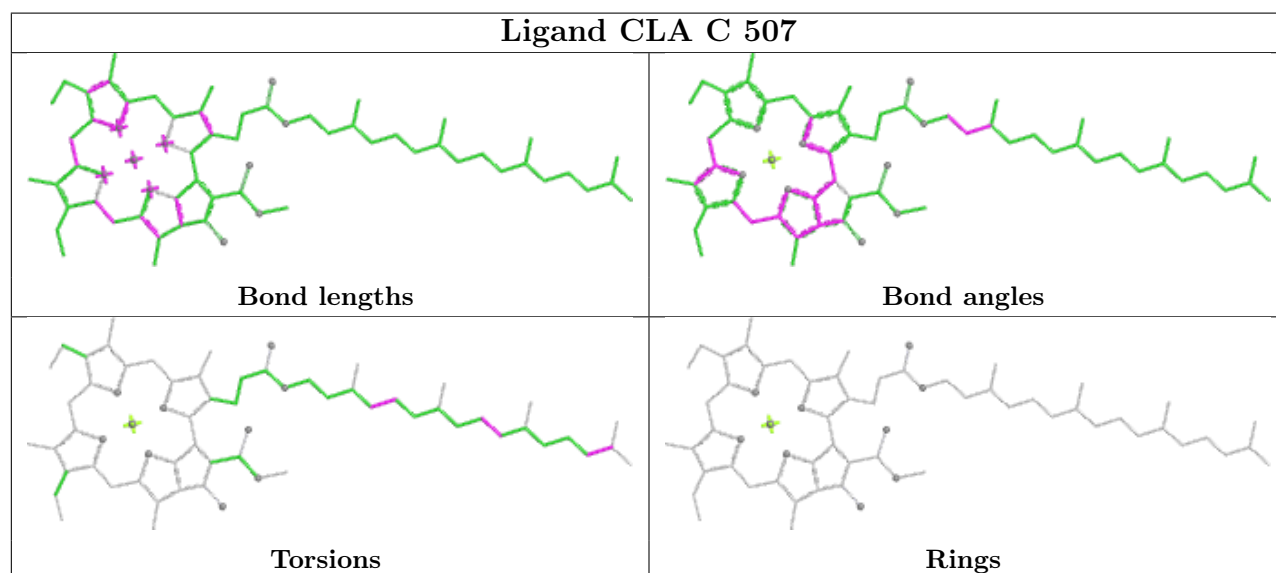
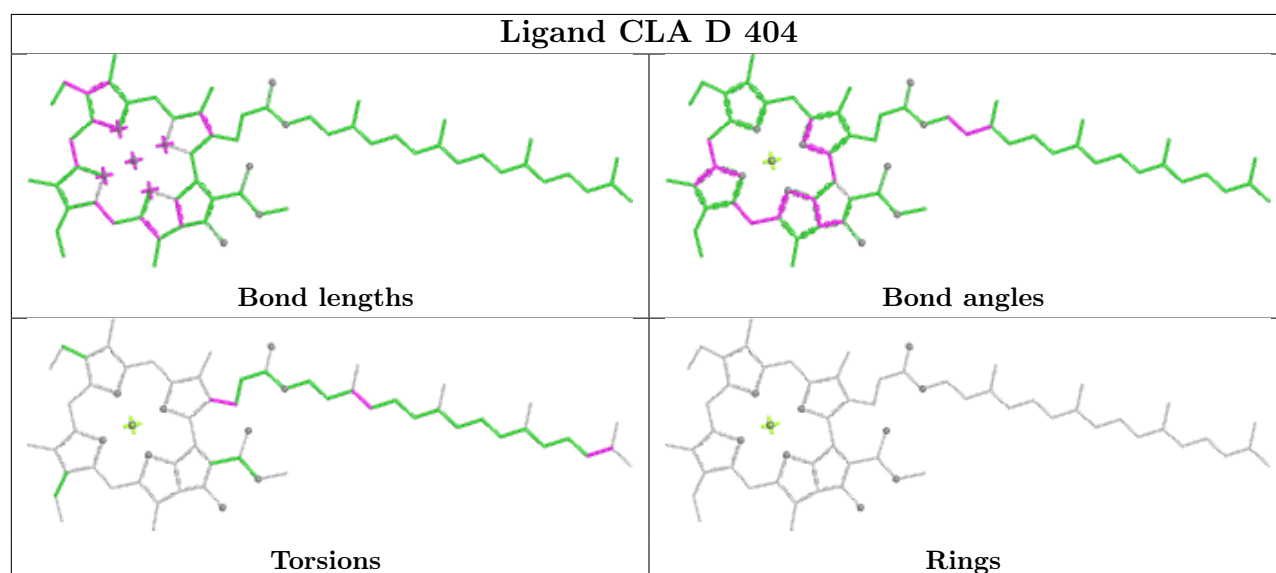
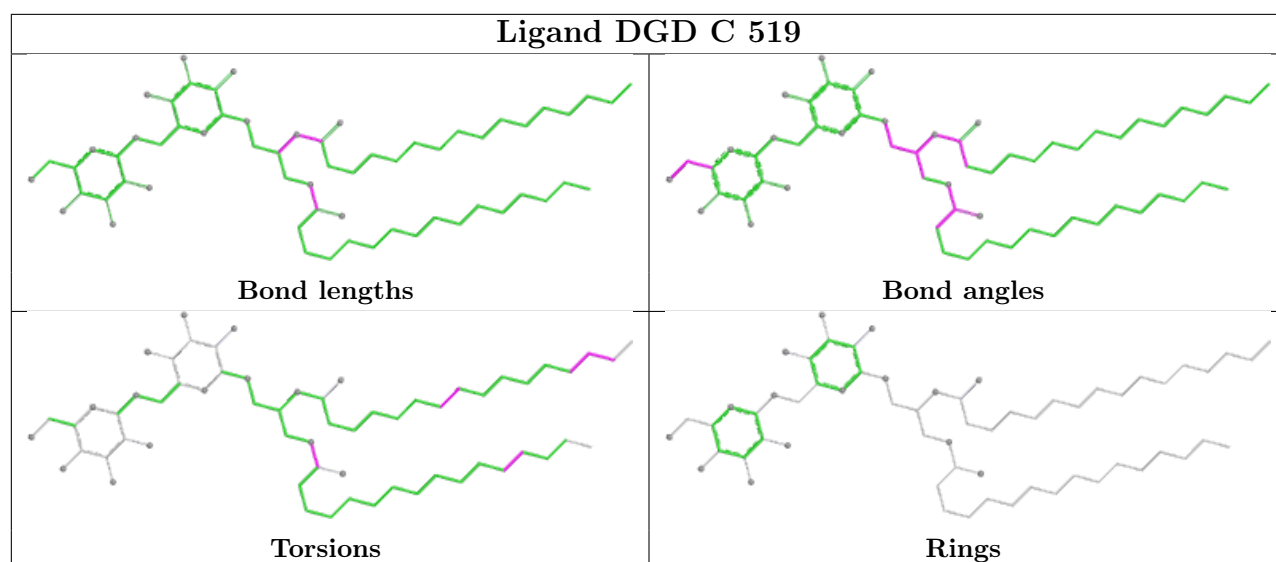
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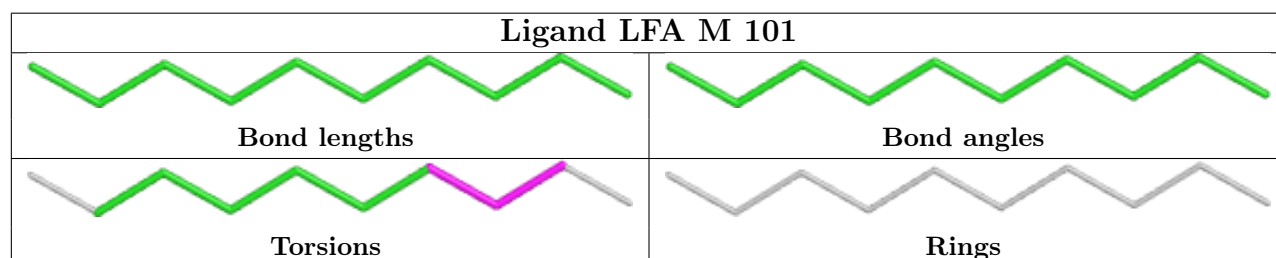
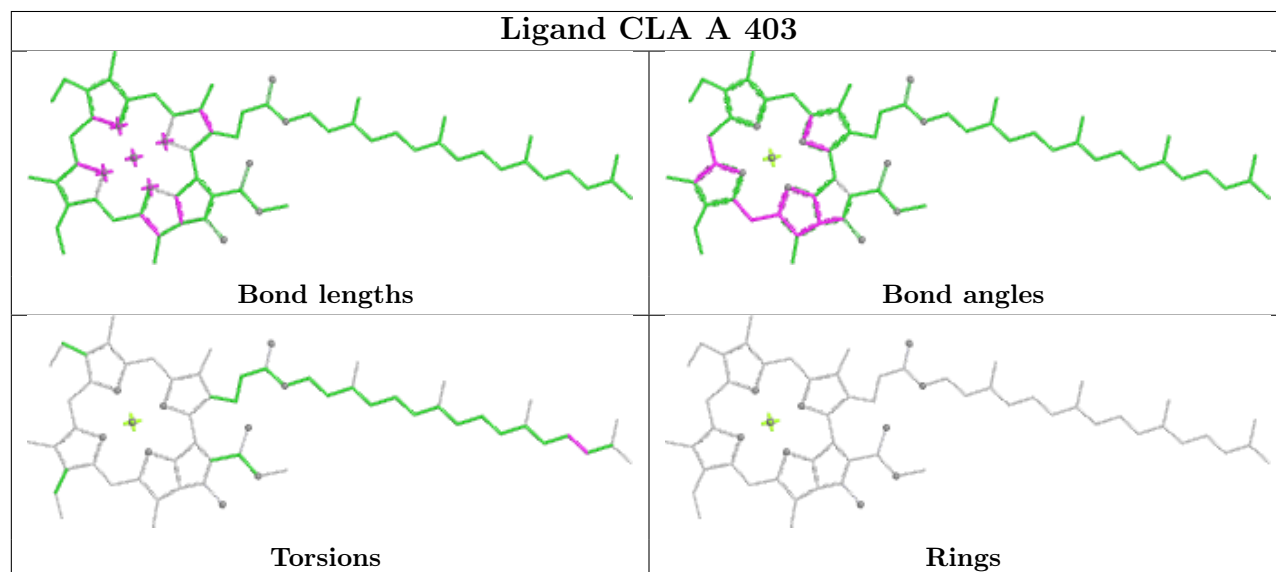
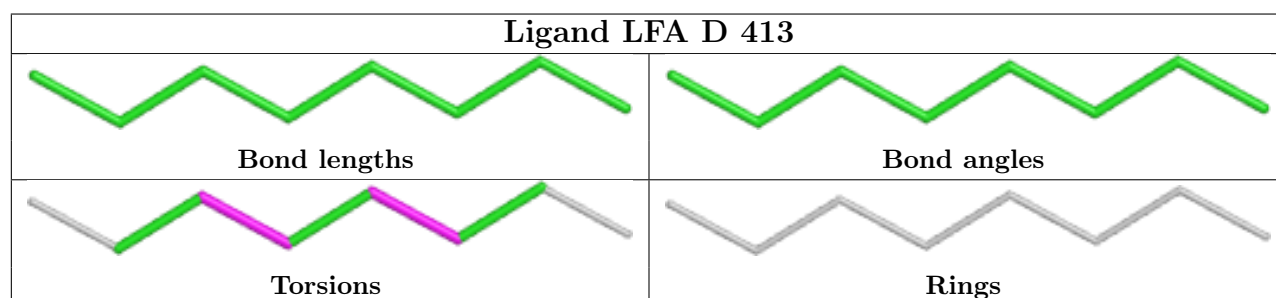
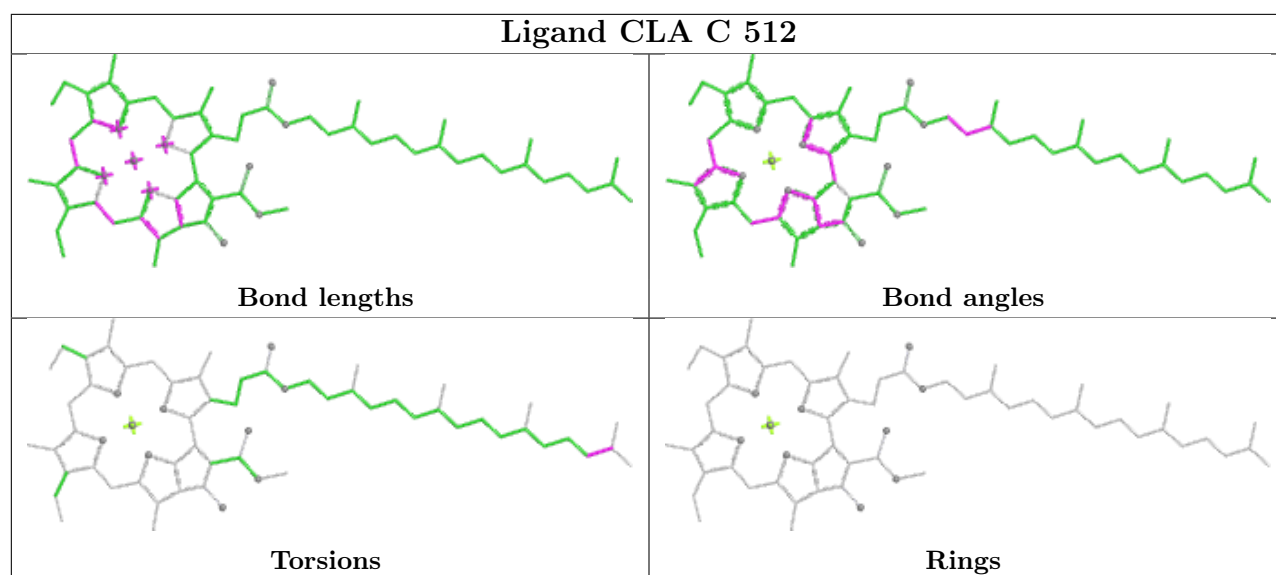
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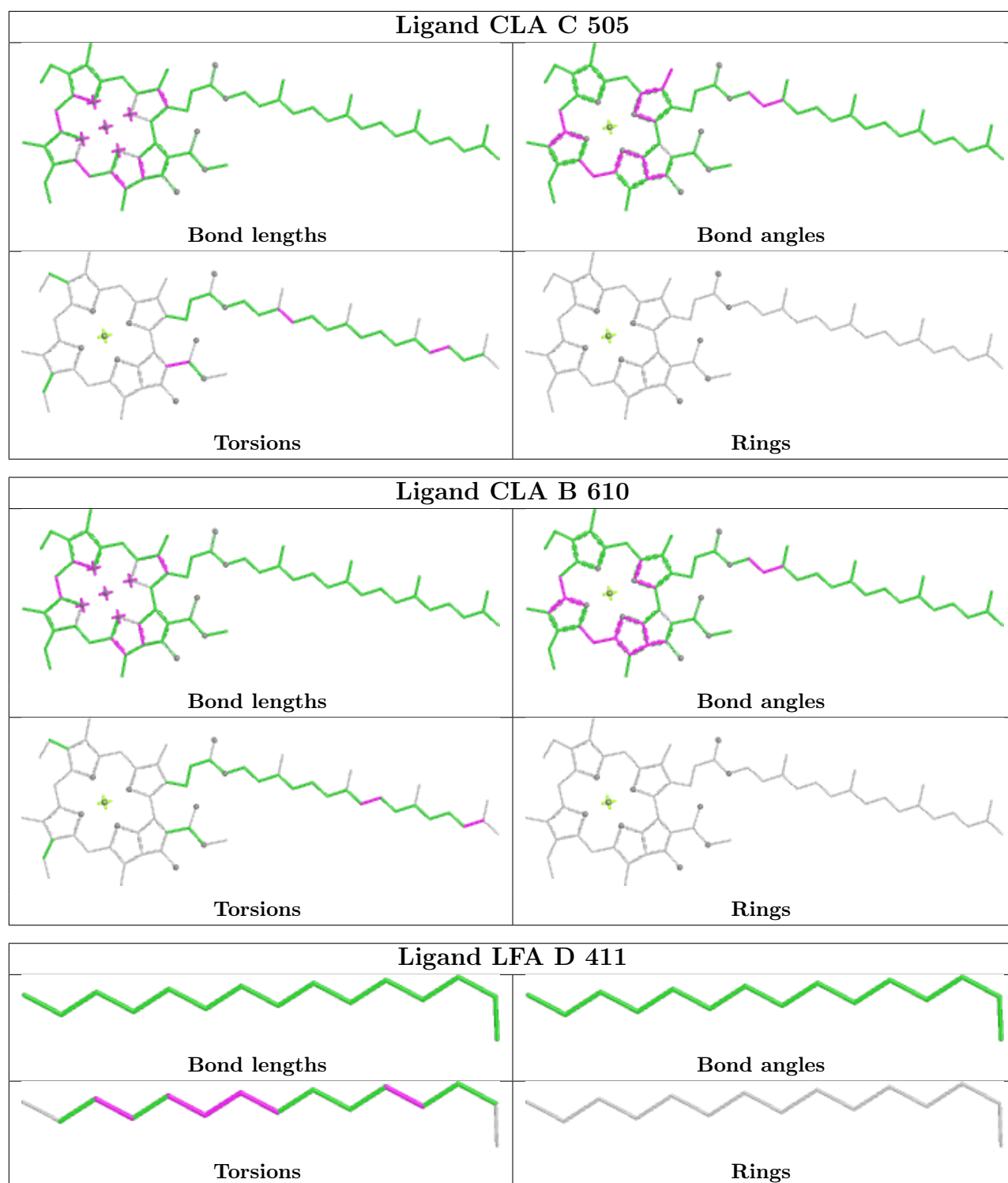
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	v	201	HEC	1	0
22	A	404	CLA	1	0
22	B	604	CLA	9	0
22	C	506	CLA	6	0
22	b	616	CLA	5	0
24	b	619	BCR	3	0
25	d	405	PL9	3	0
27	A	413	LFA	1	0
22	d	403	CLA	2	0
24	h	101	BCR	6	0
26	A	411	SQD	2	0
27	c	521	LFA	2	0
22	b	612	CLA	1	0
25	D	406	PL9	6	0
24	C	516	BCR	3	0
22	d	401	CLA	2	0
30	C	518	DGD	2	0
22	b	605	CLA	4	0
27	m	101	LFA	1	0
32	l	101	LHG	1	0
29	f	101	LMG	2	0
27	b	622	LFA	1	0

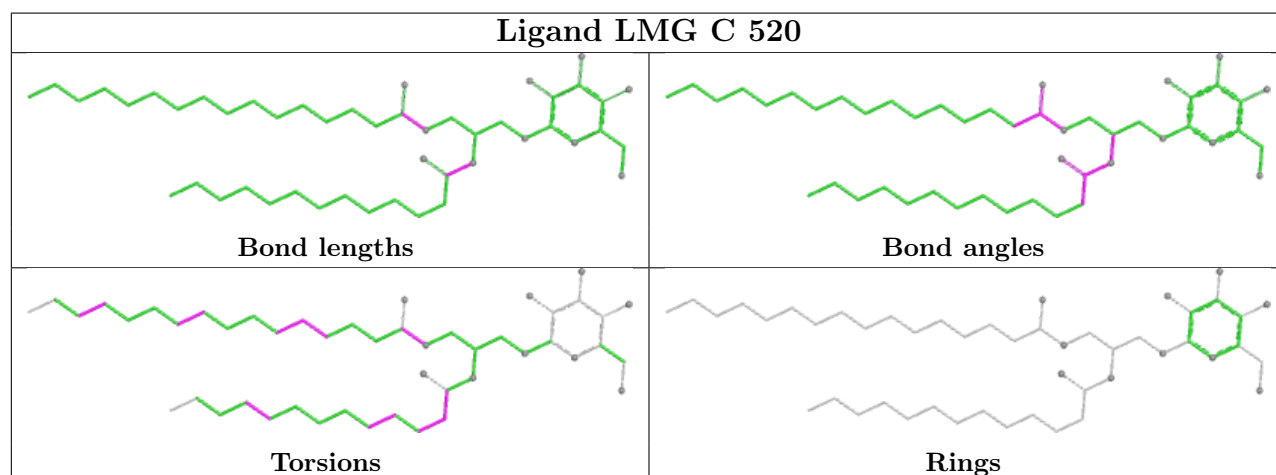
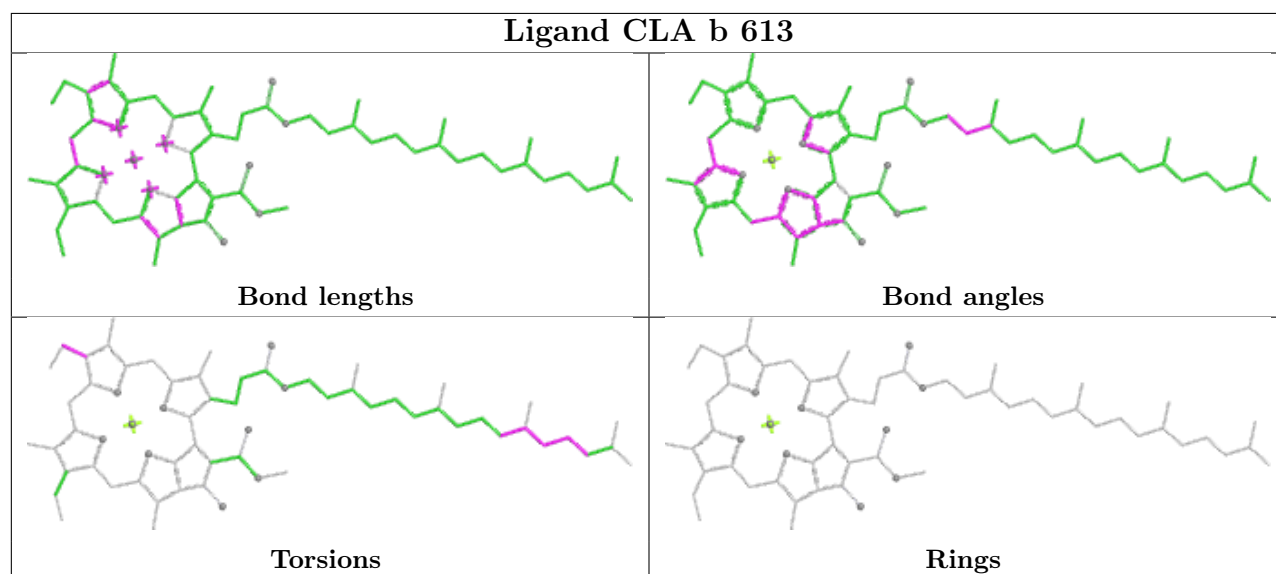
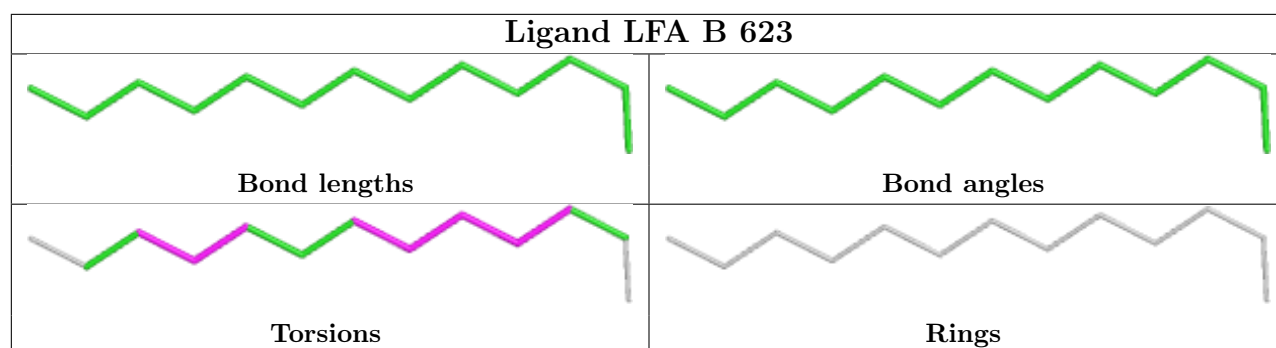
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

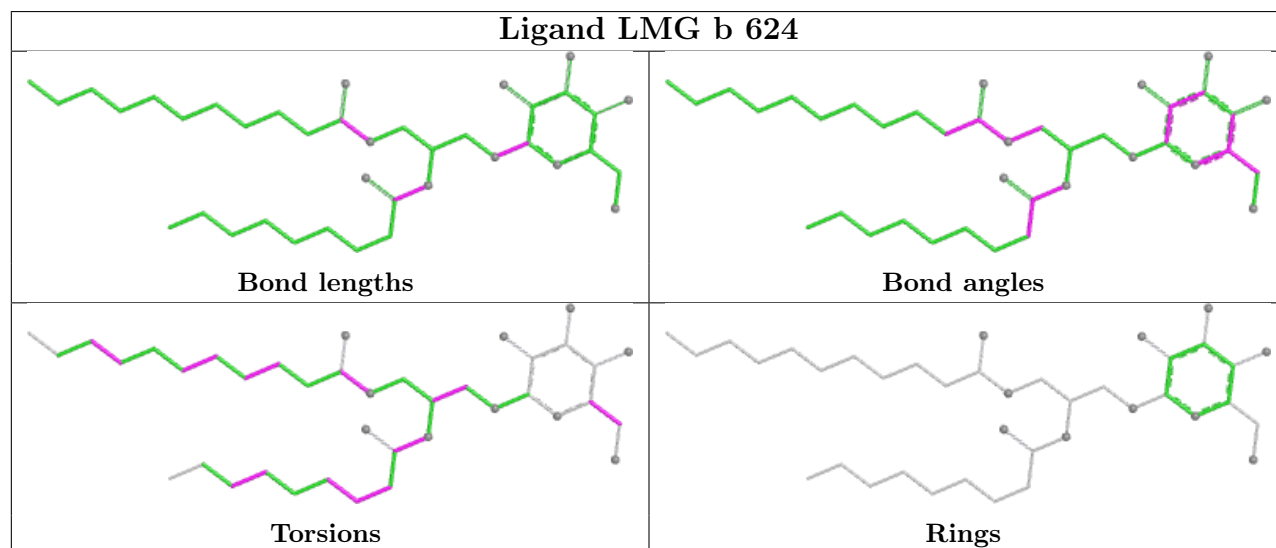
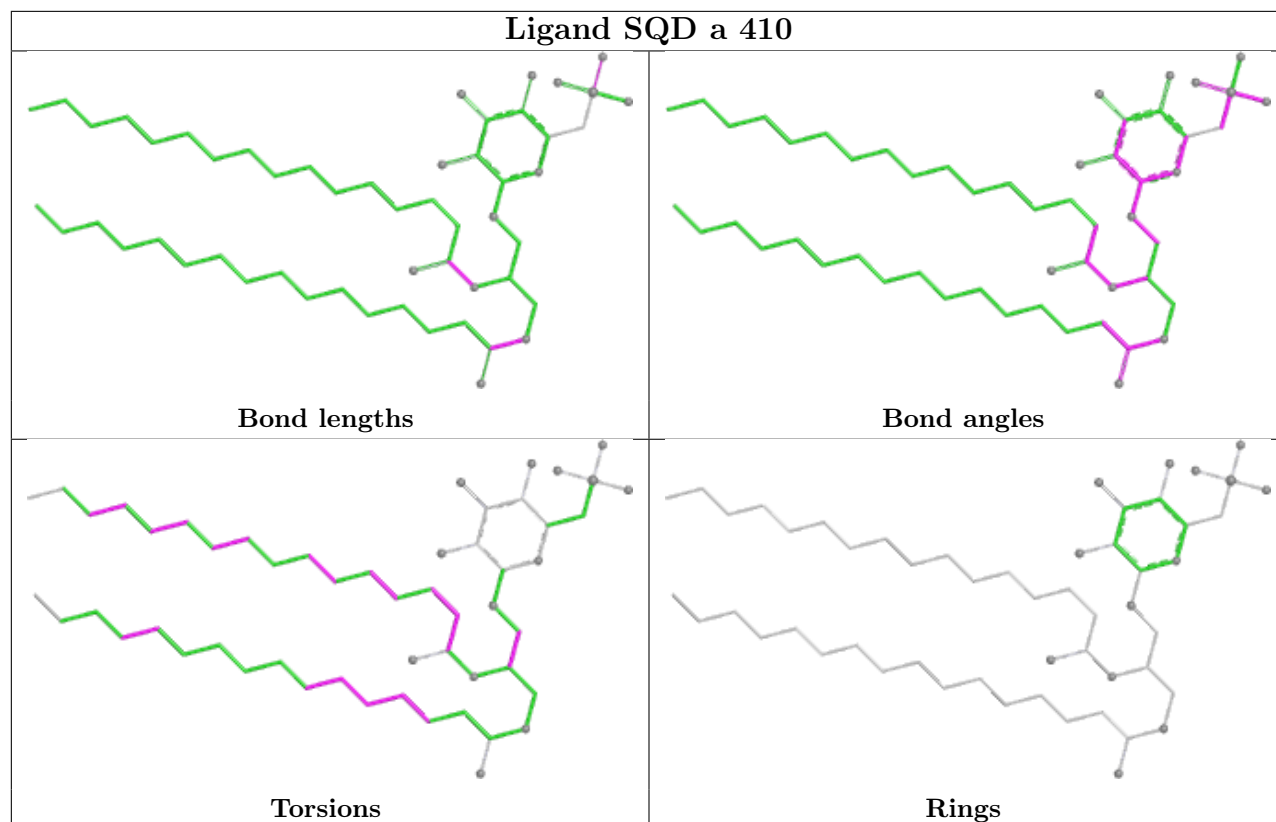


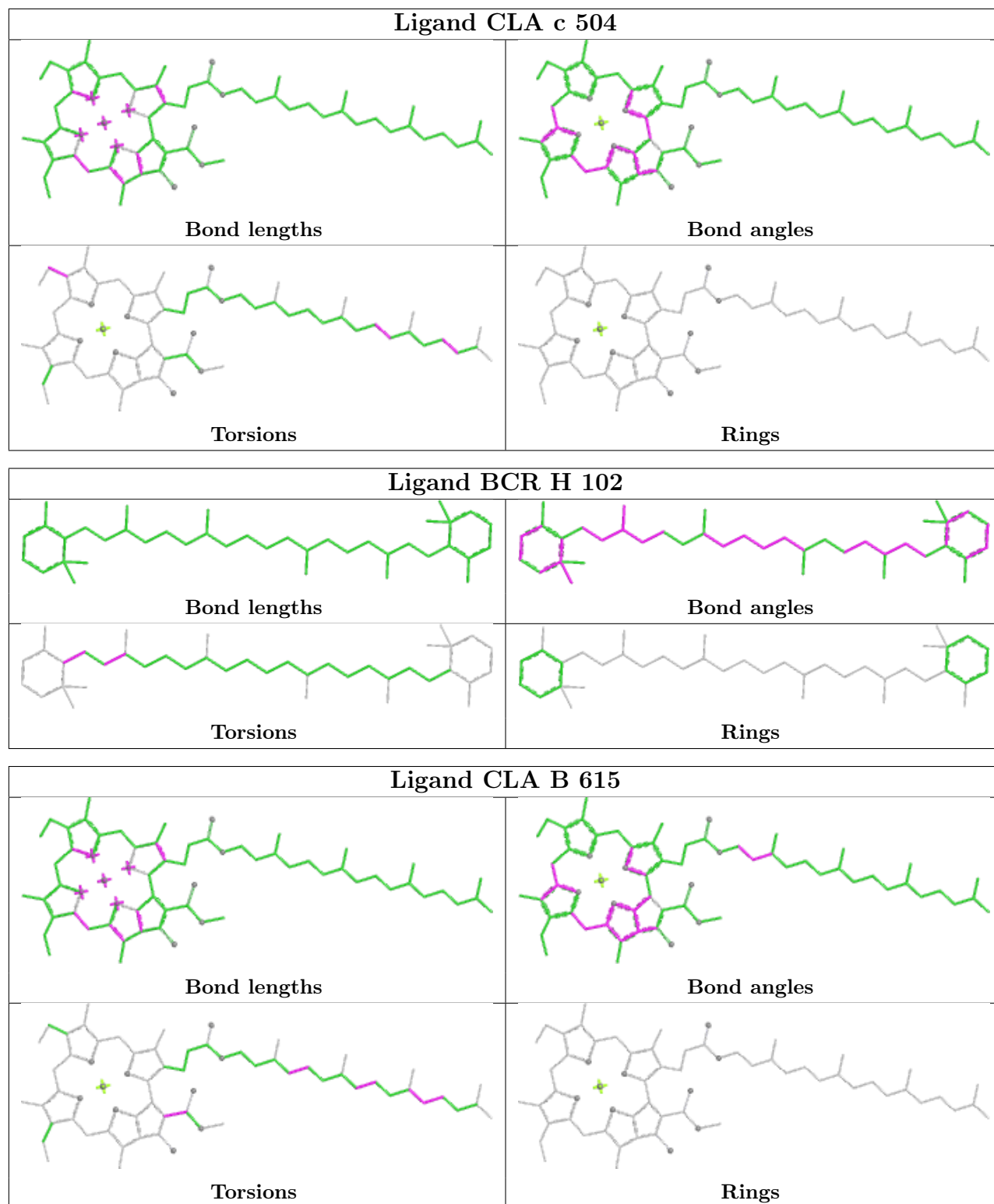


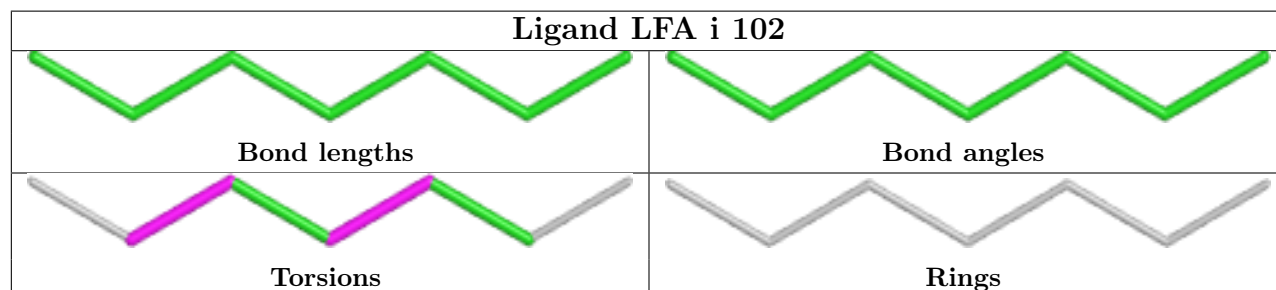
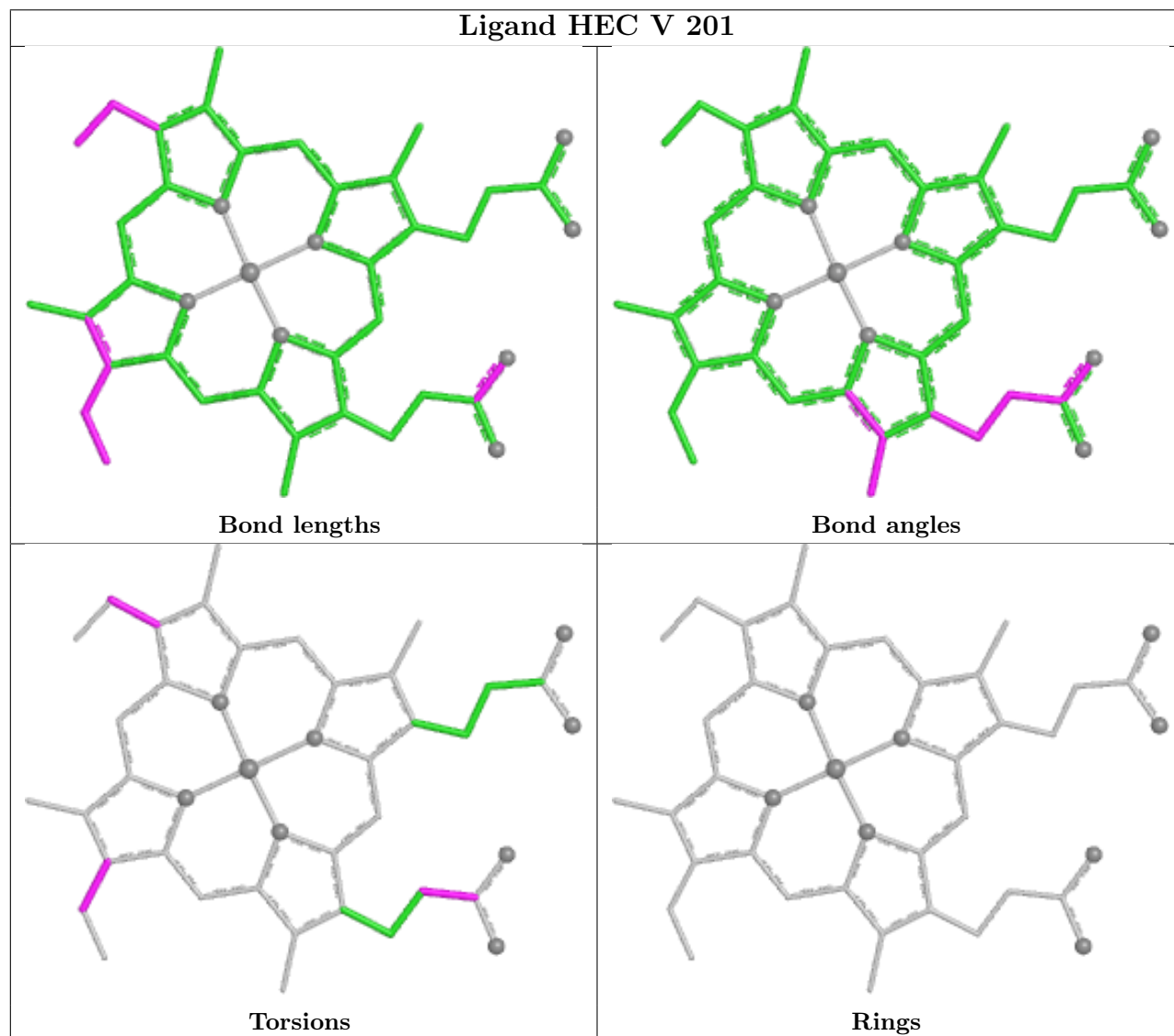
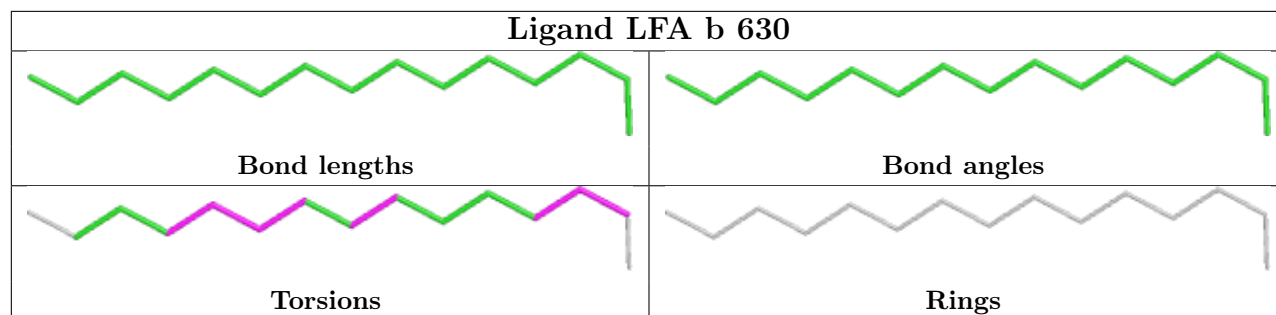


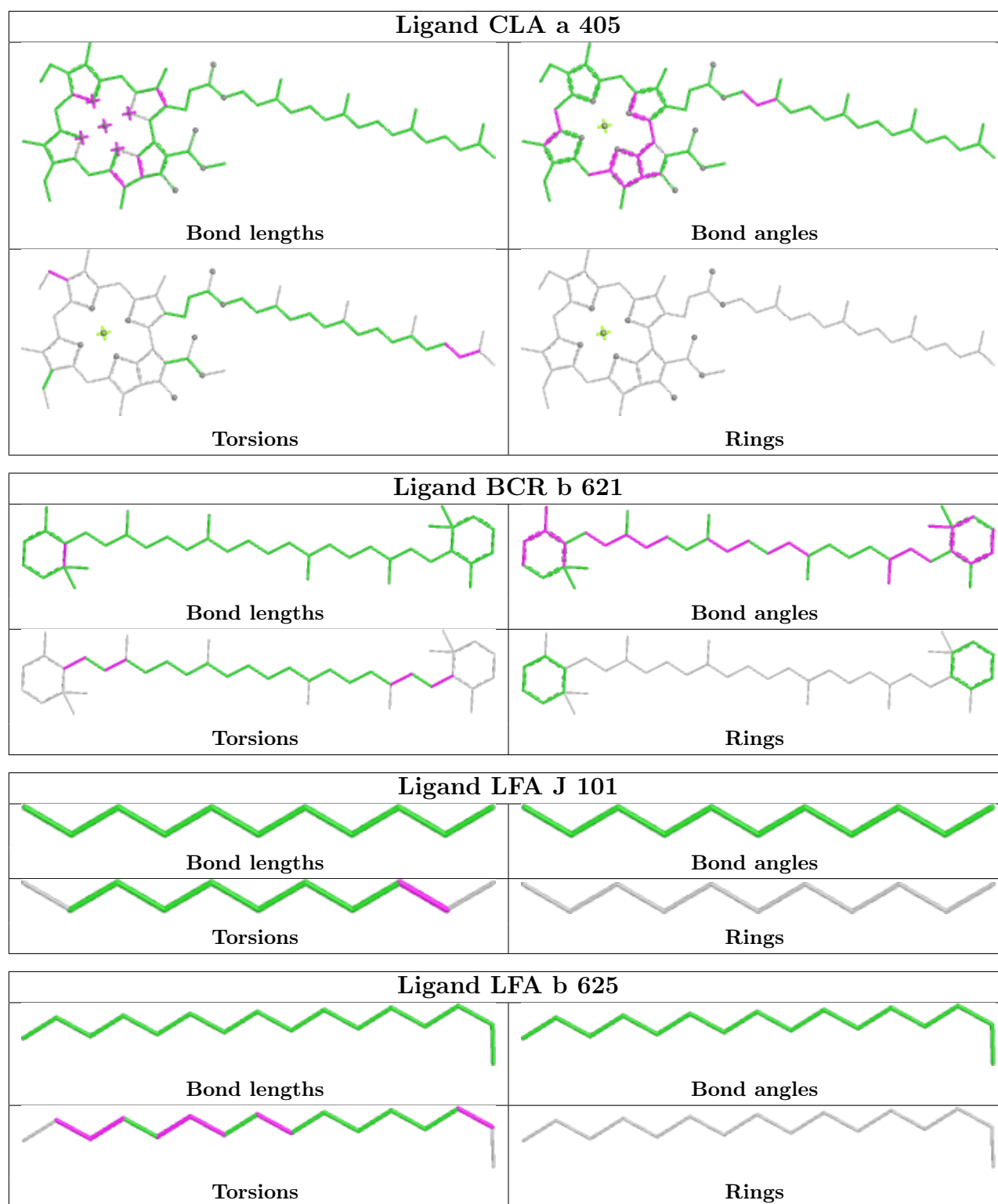


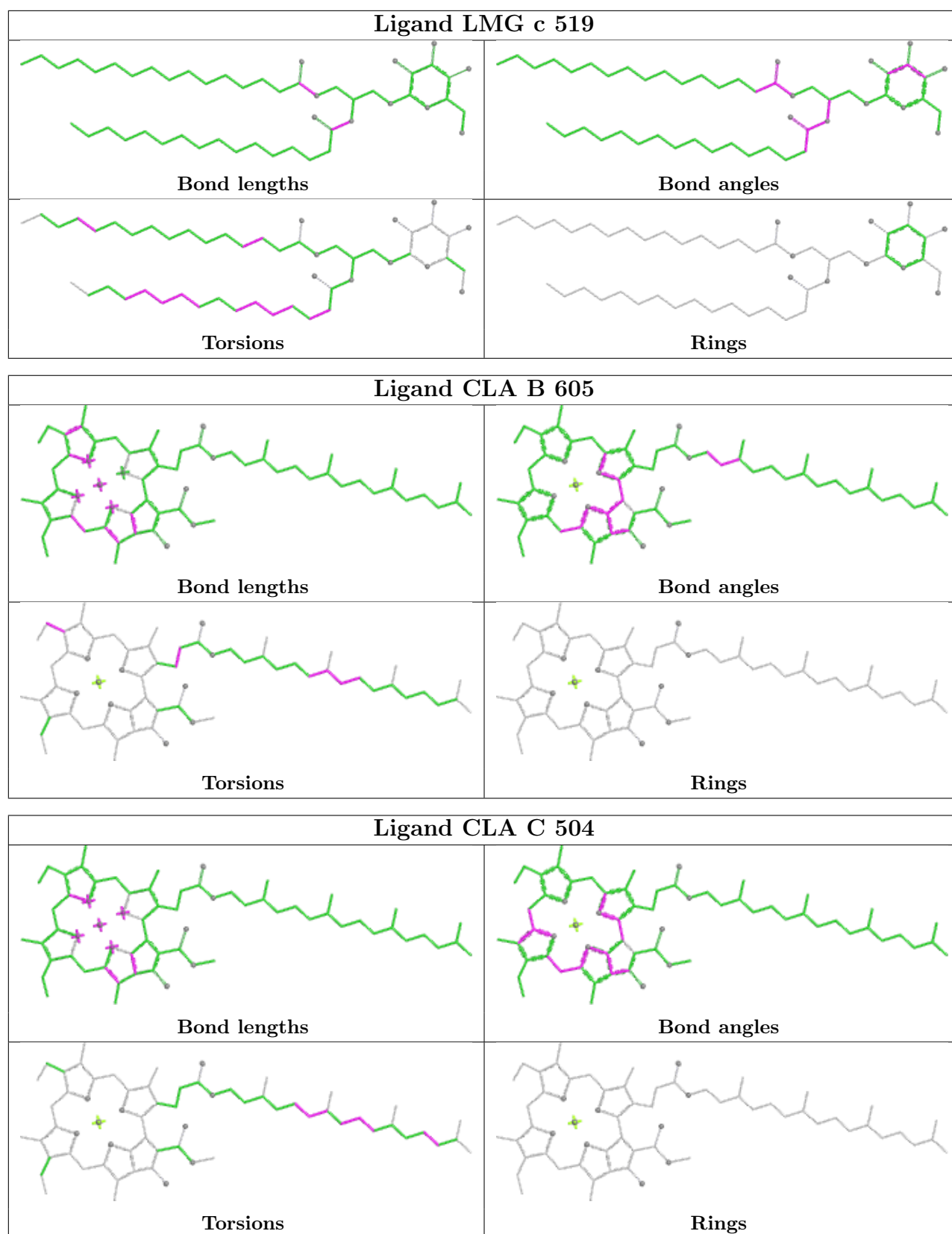


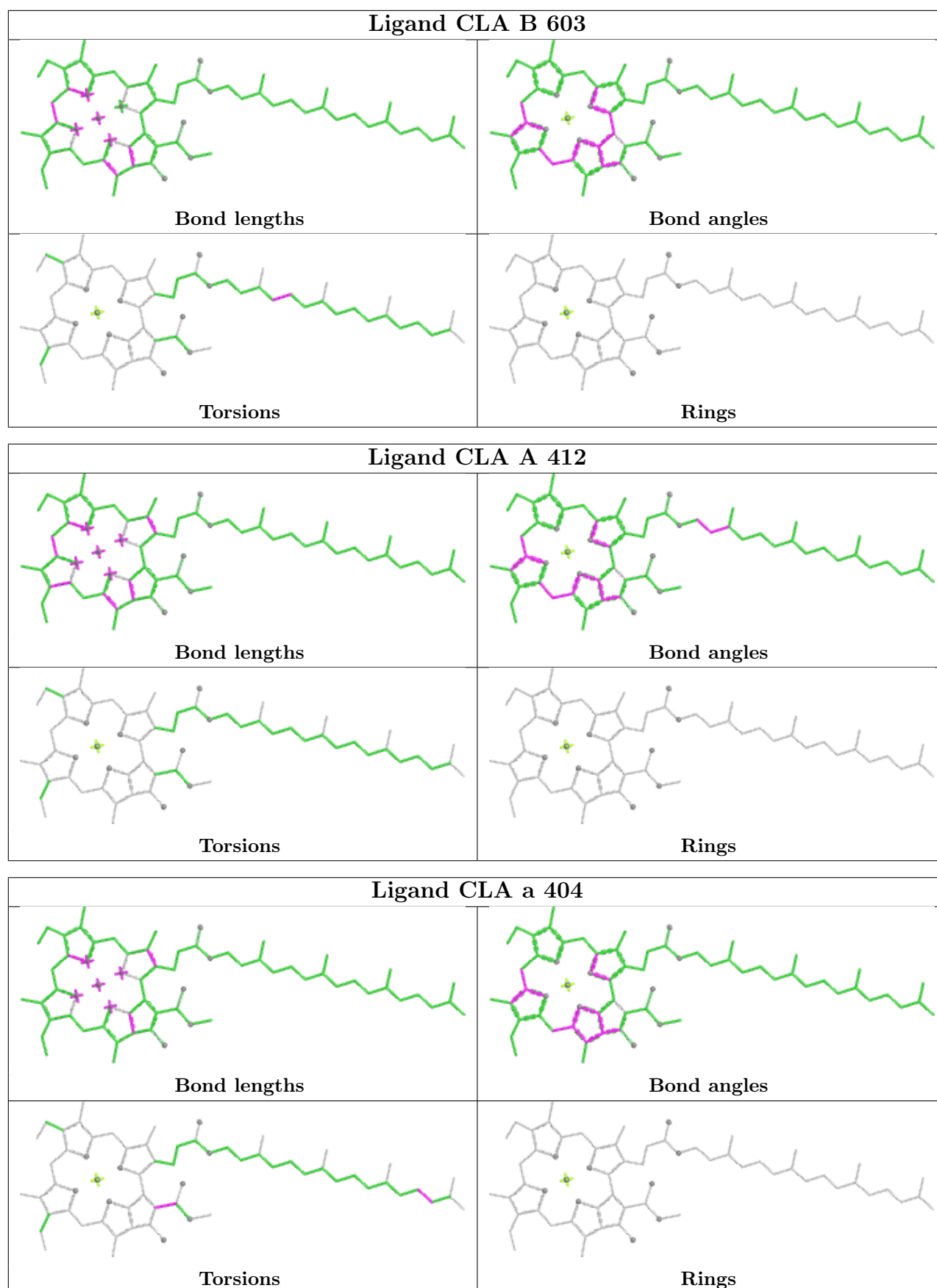


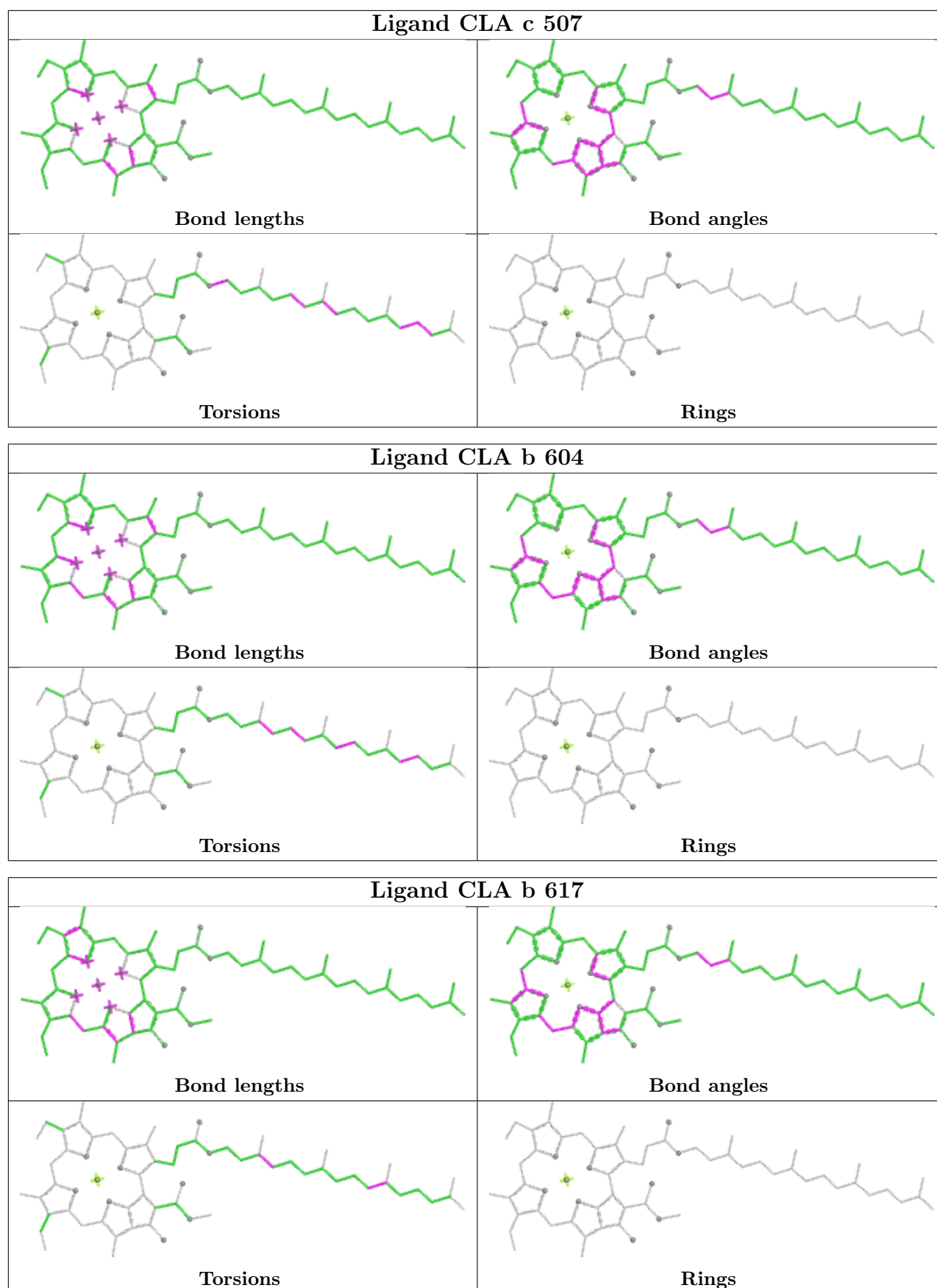


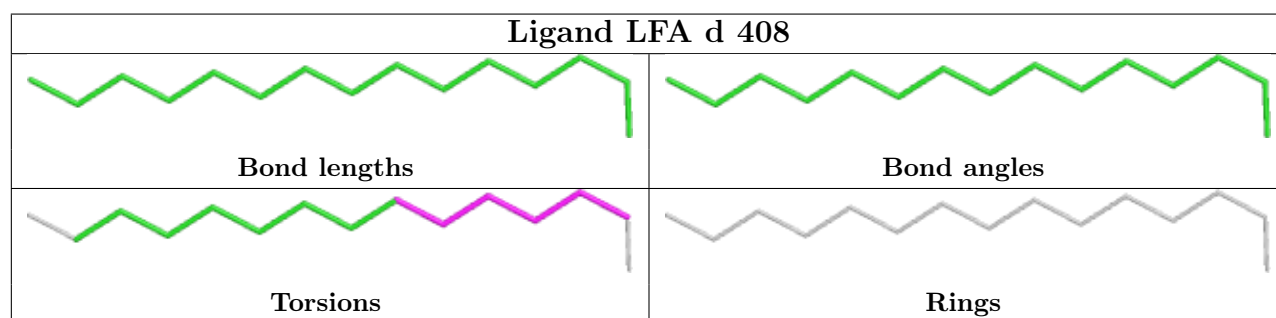
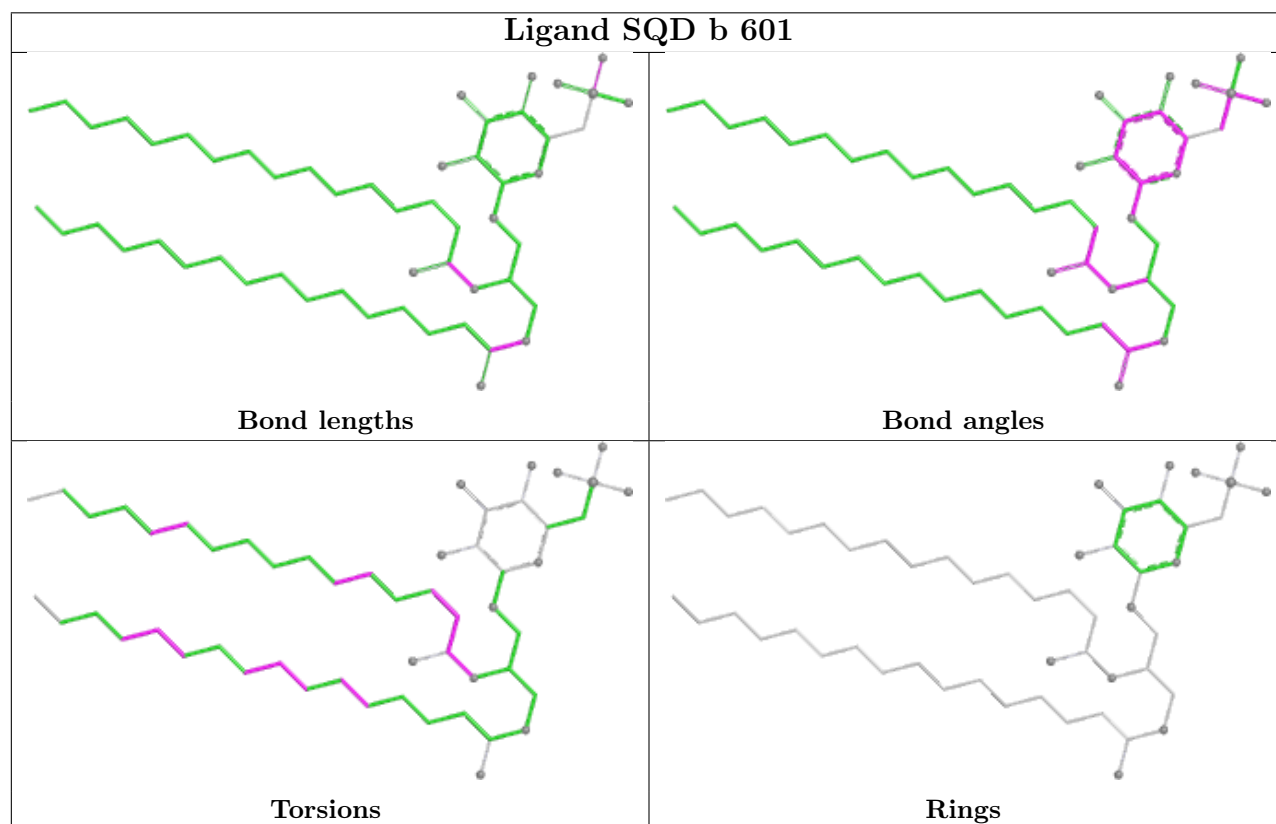
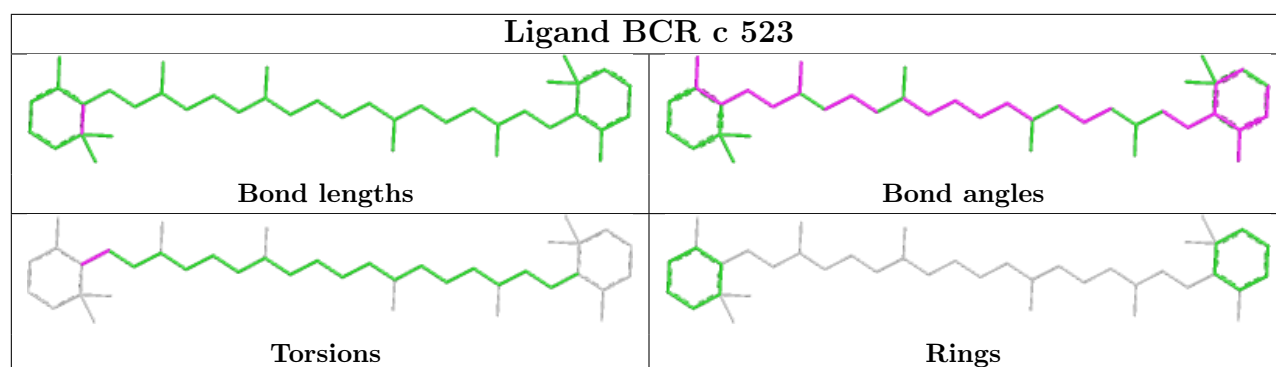


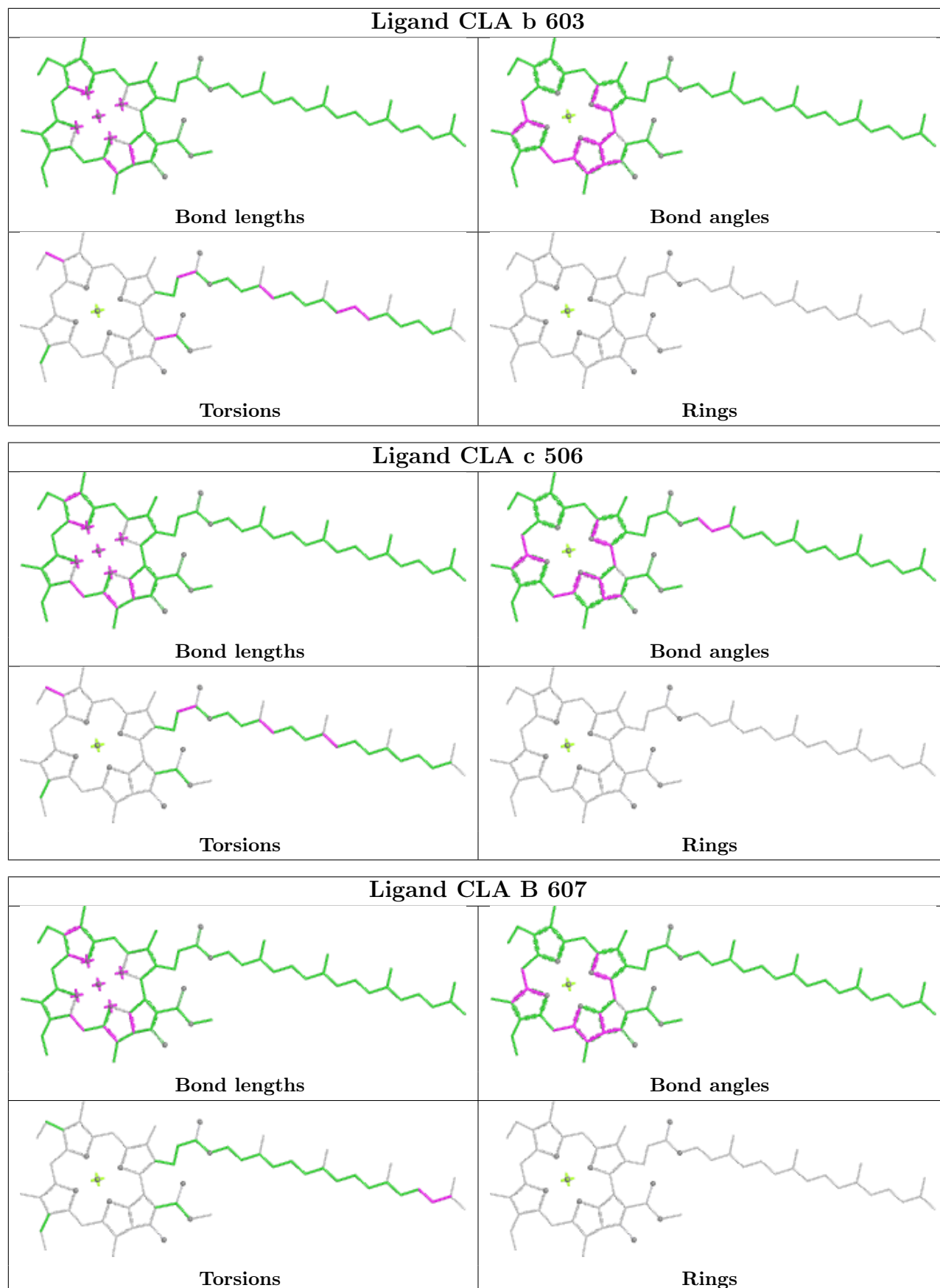


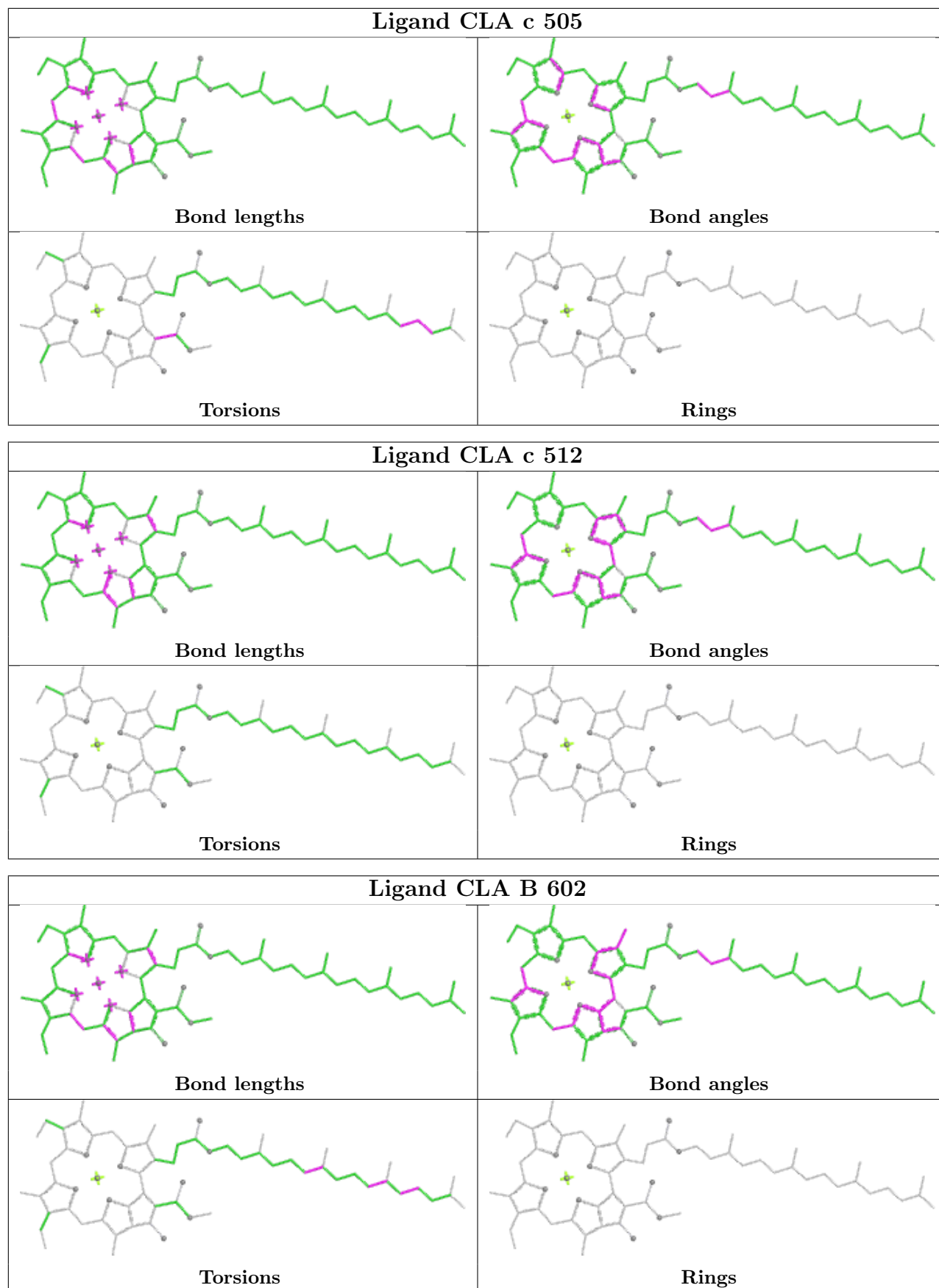


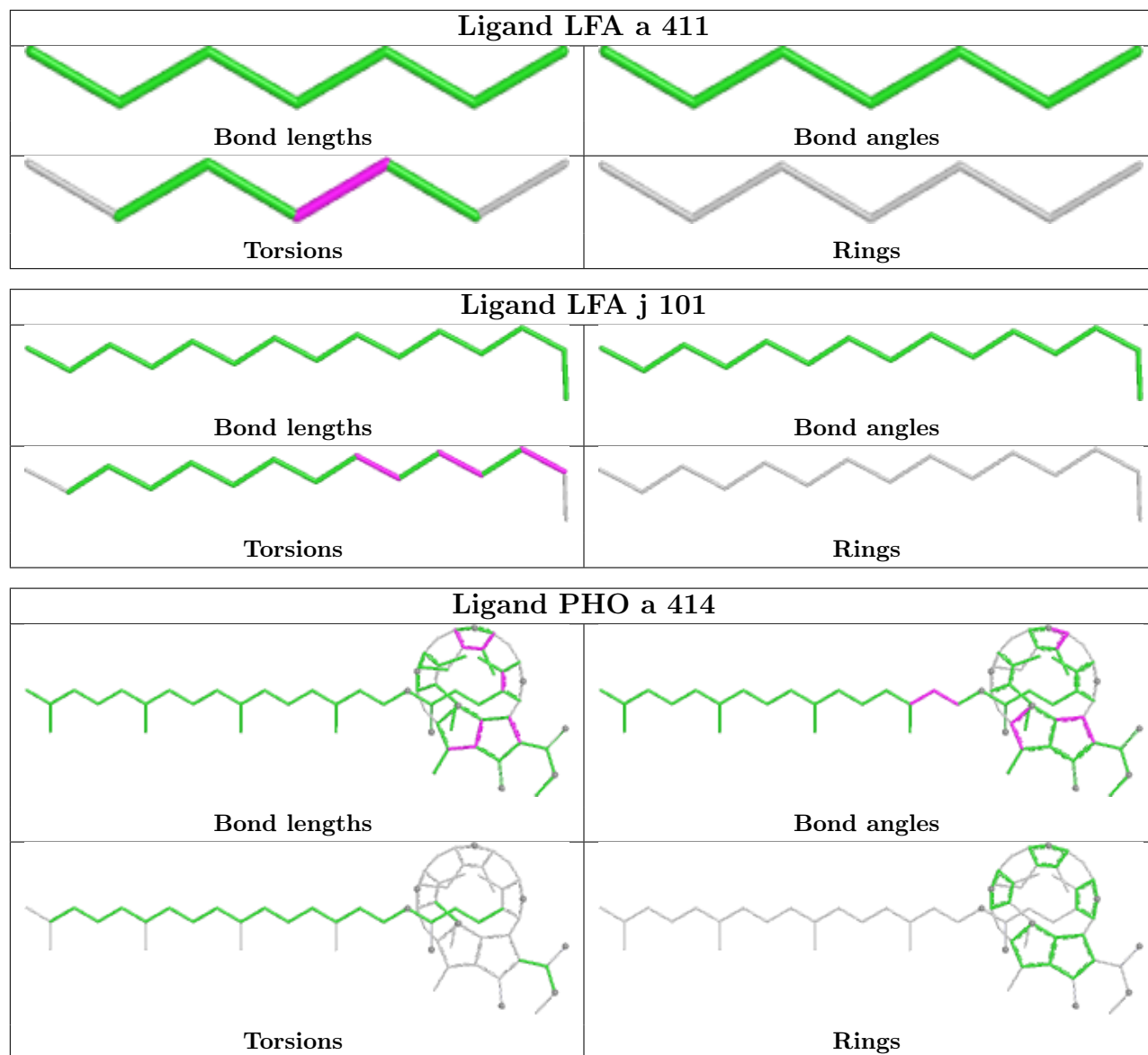


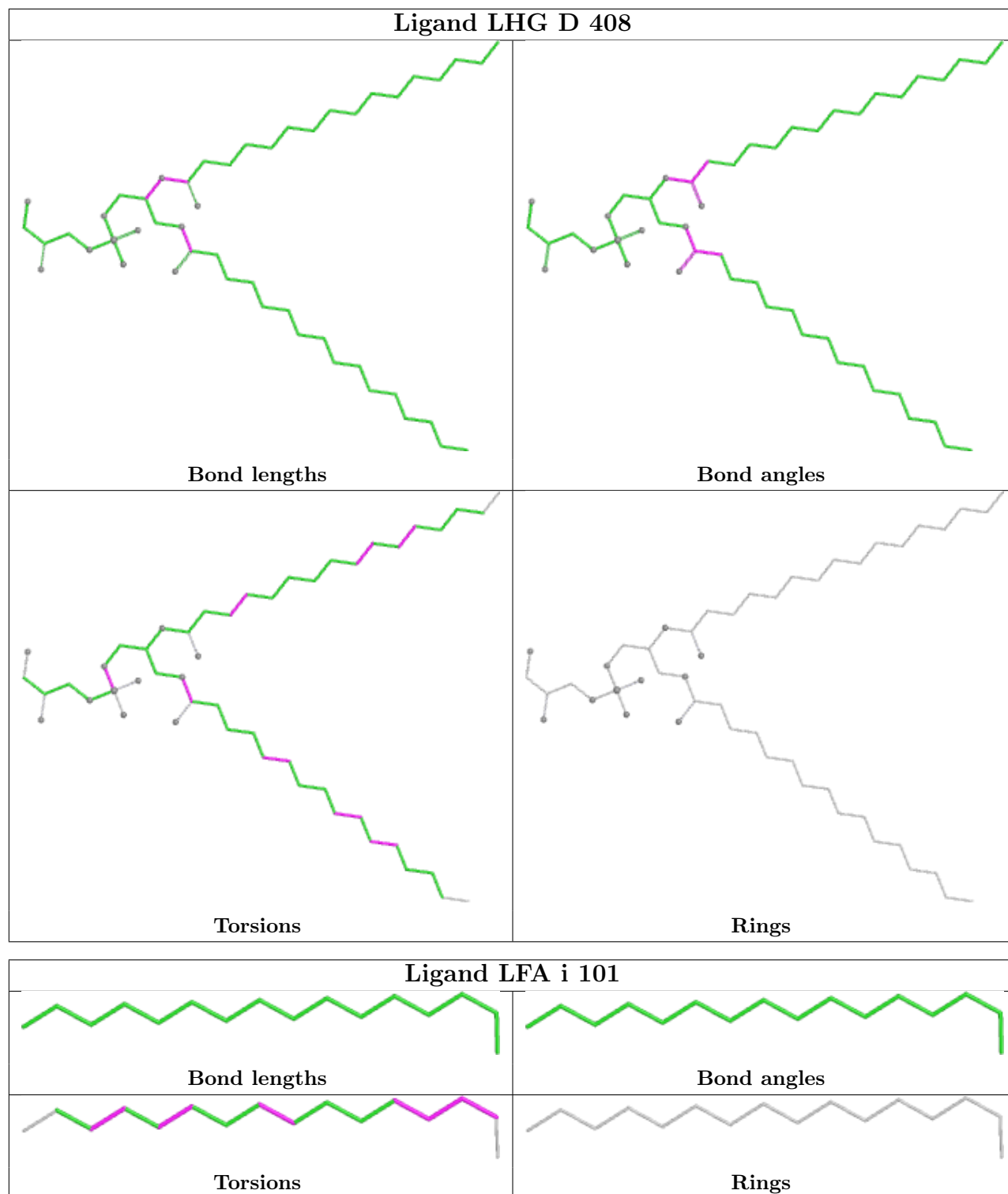


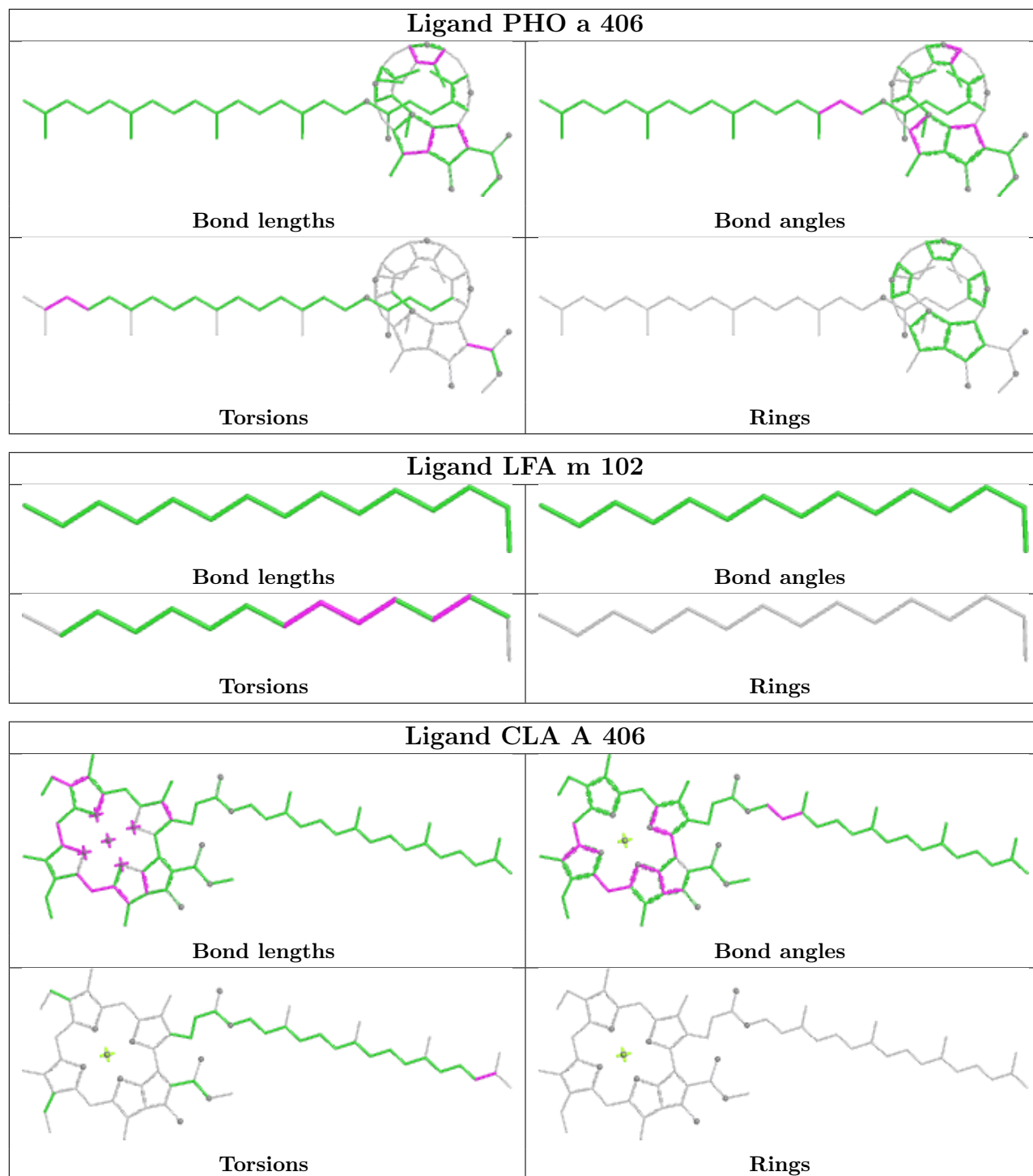


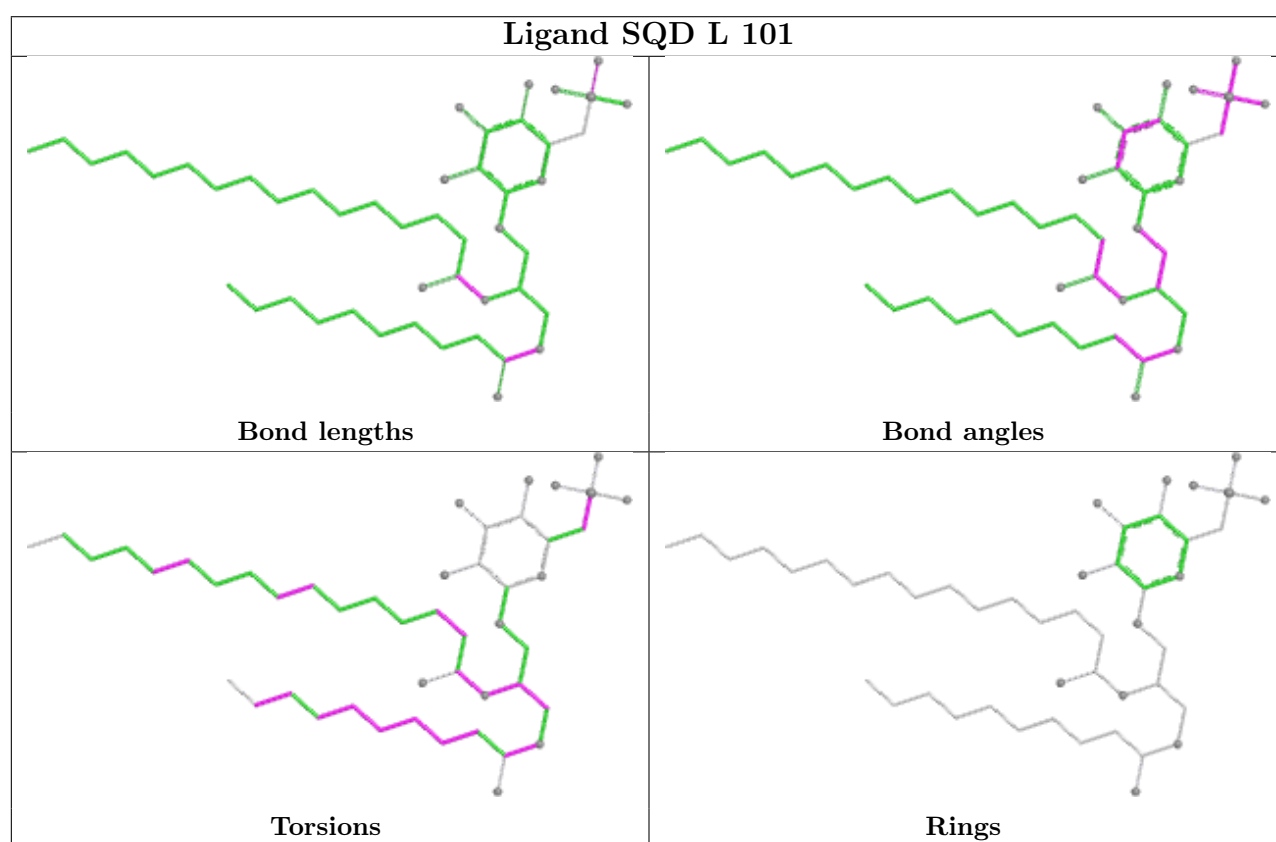
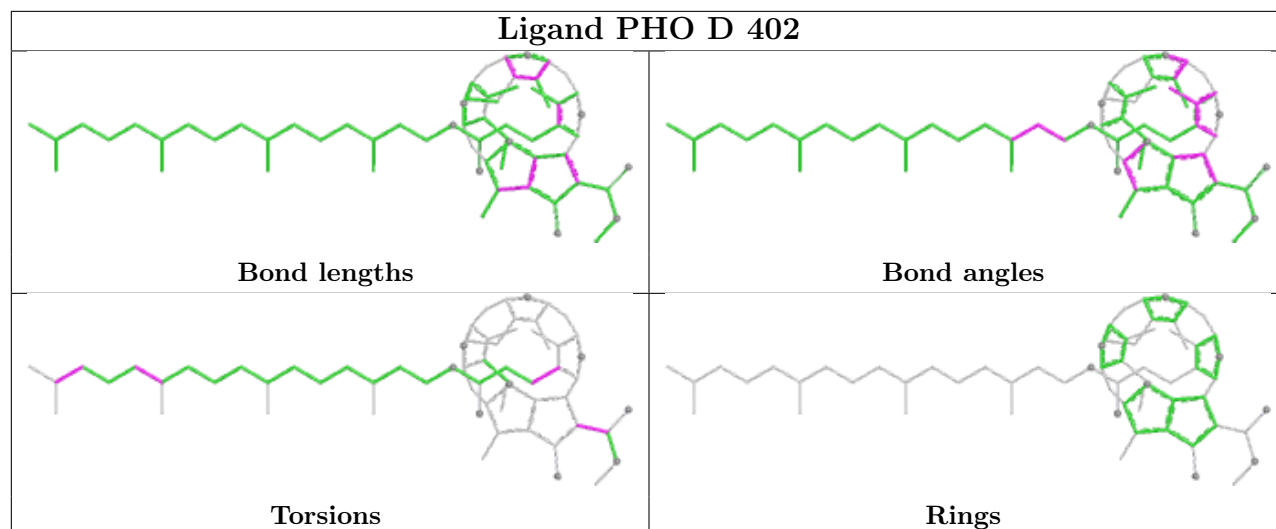


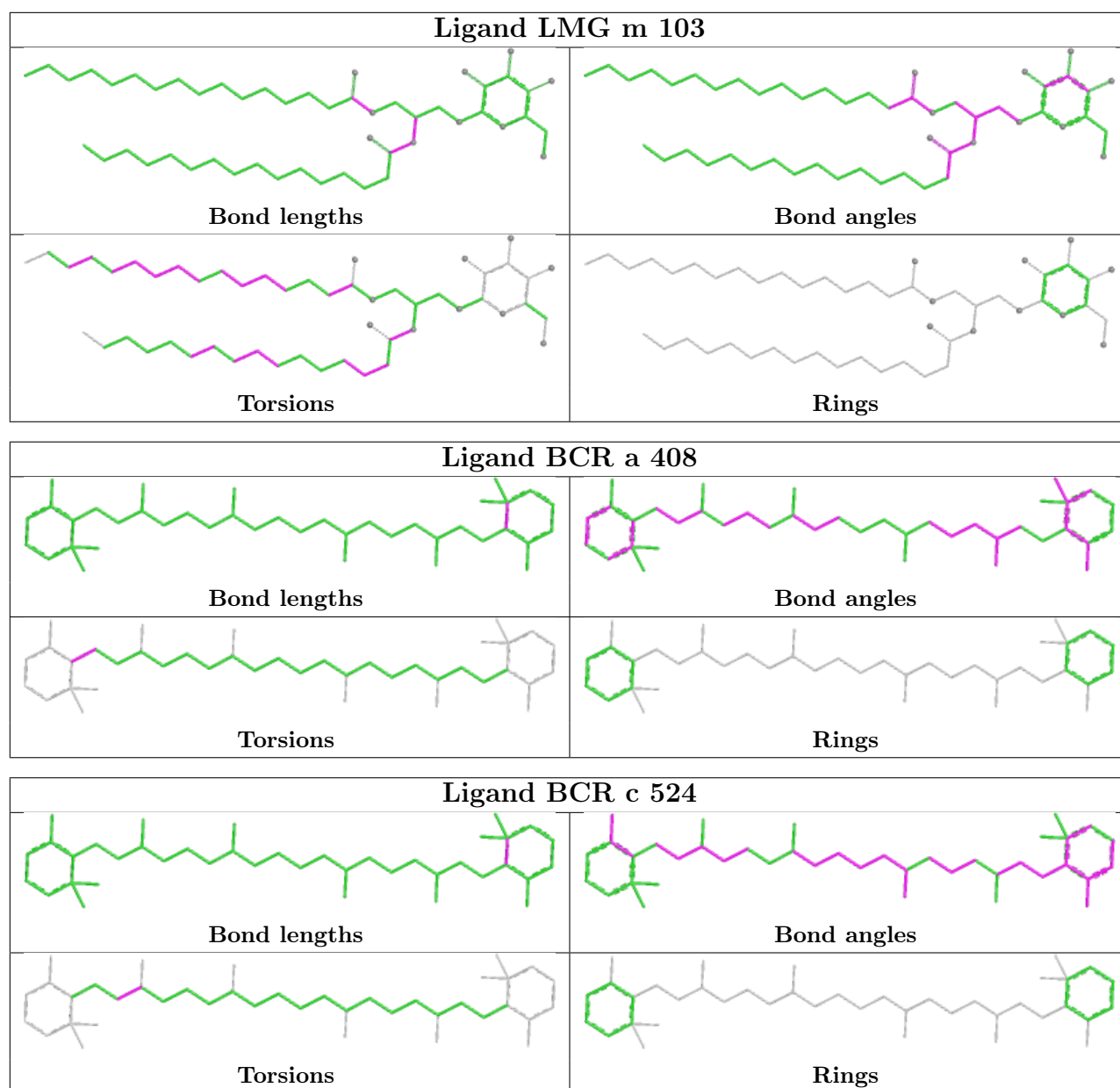


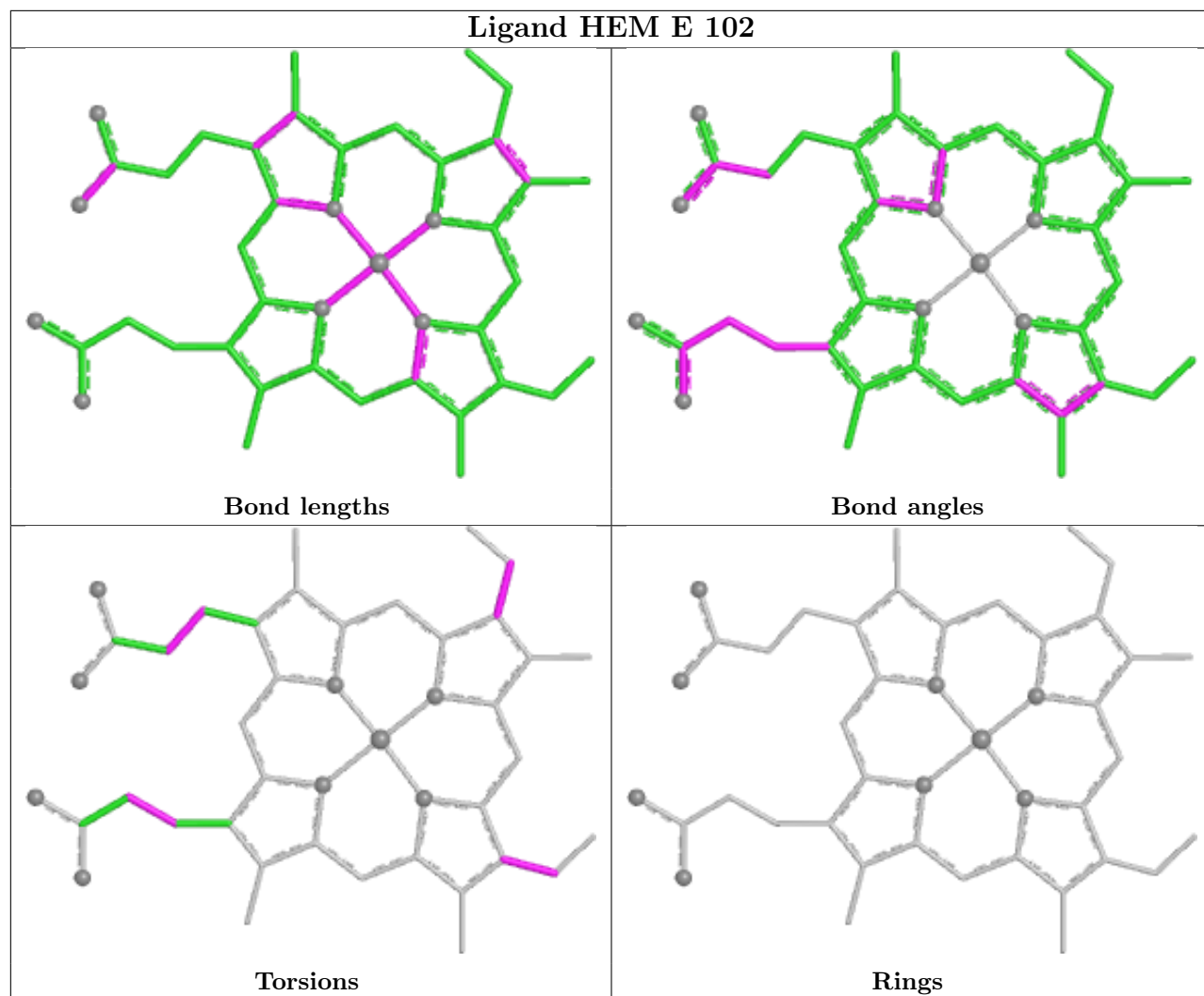


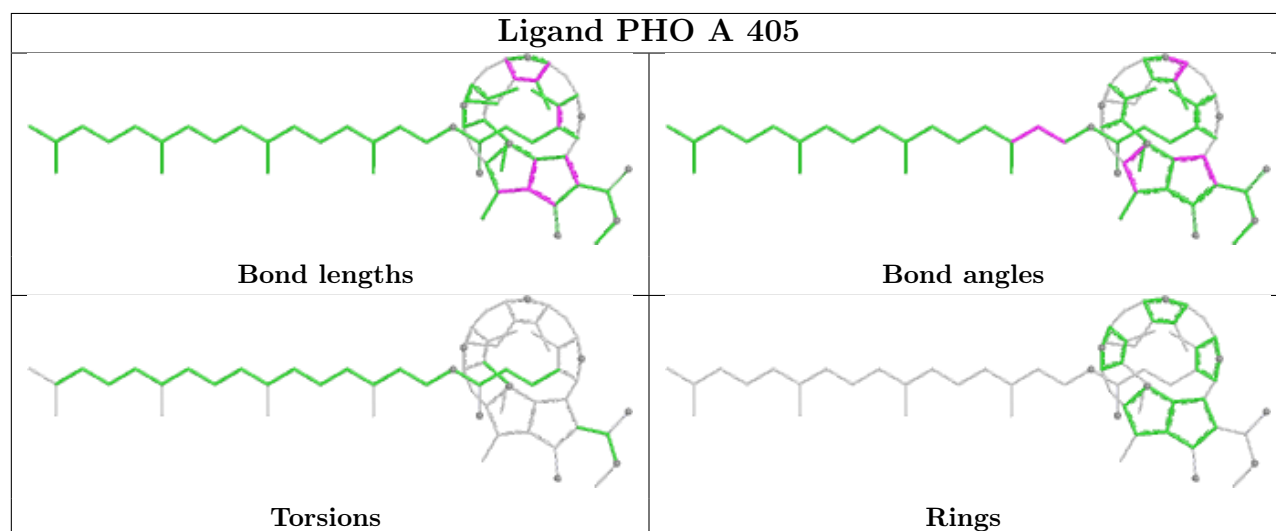
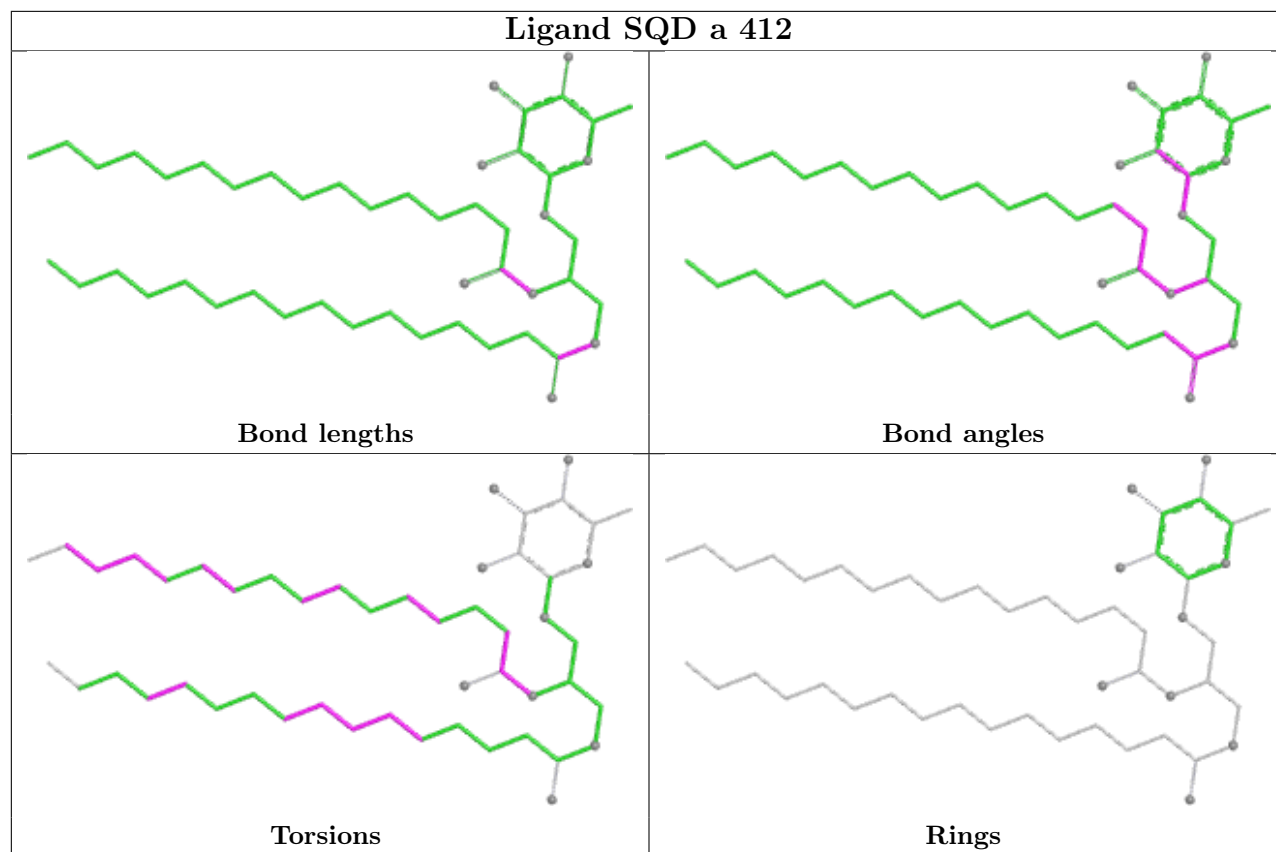


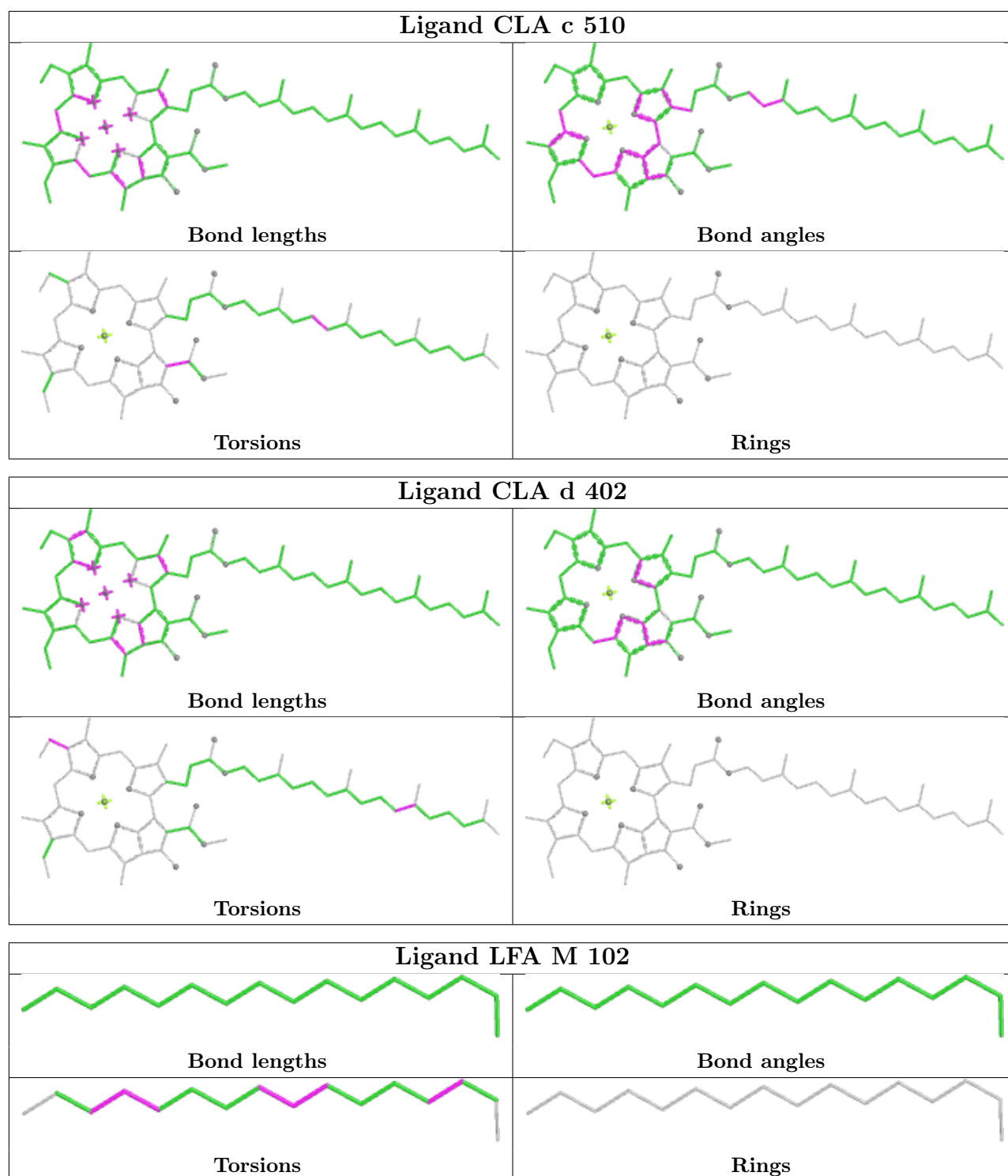


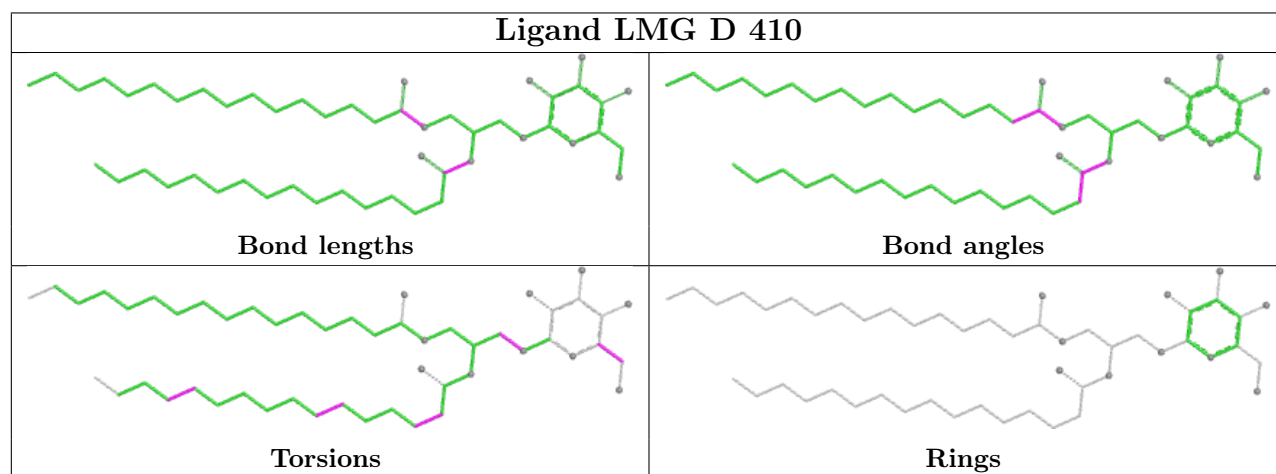
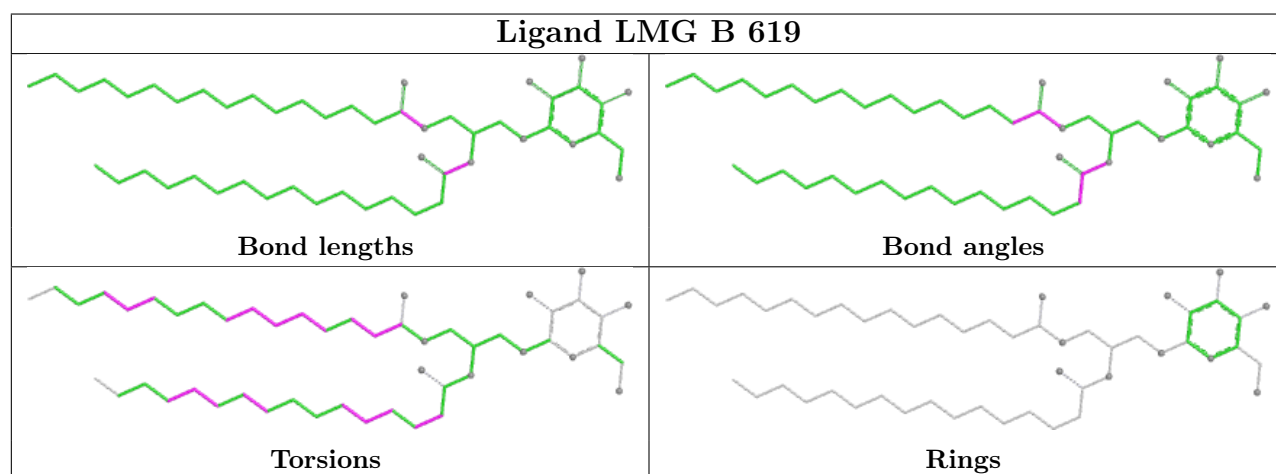
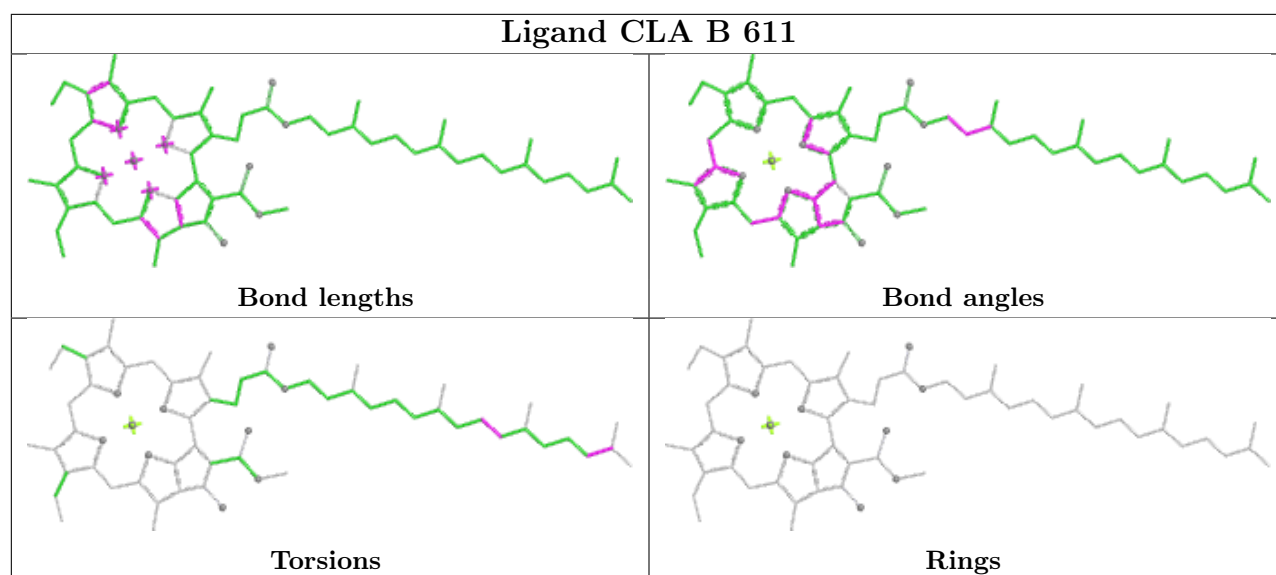


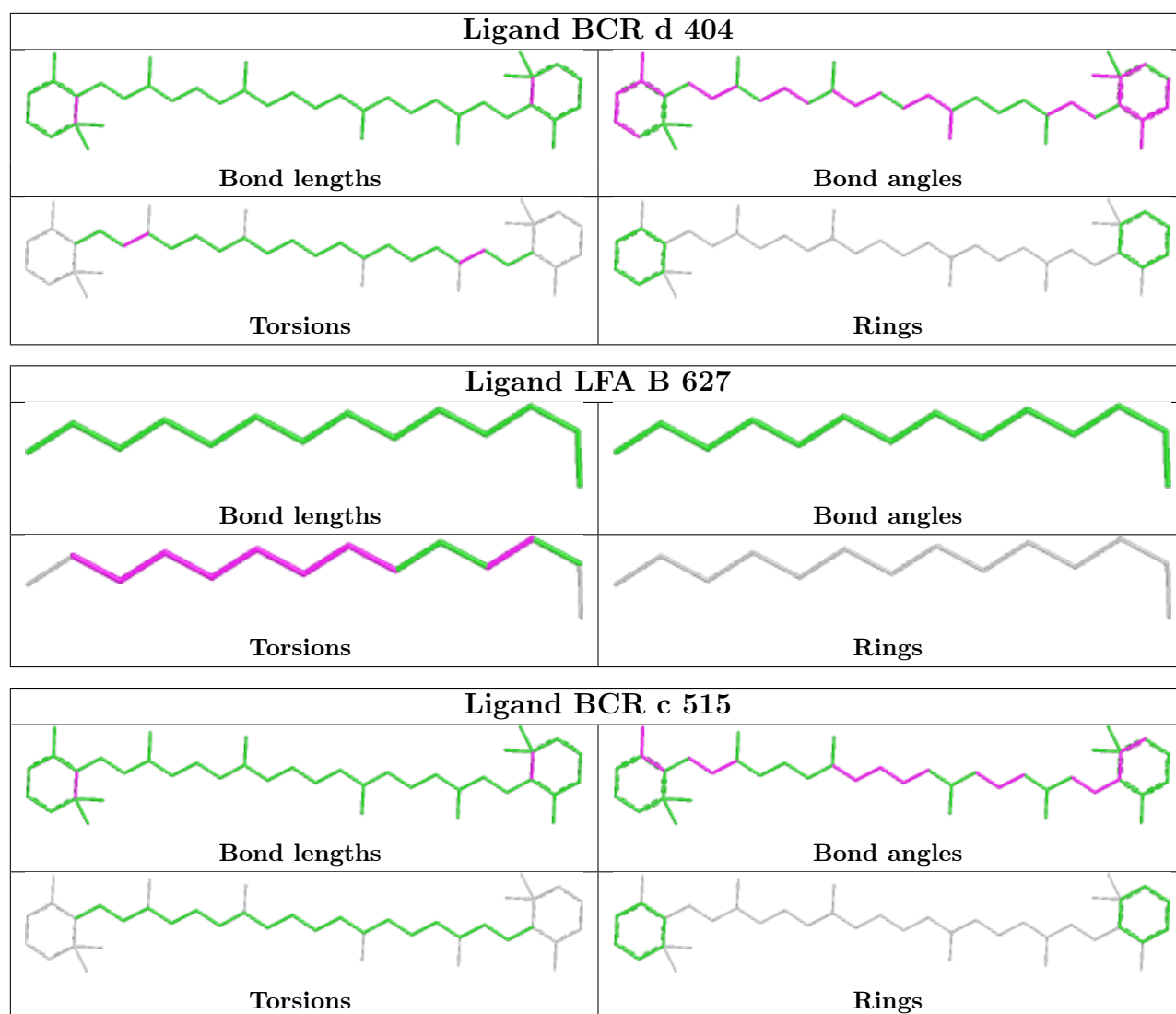


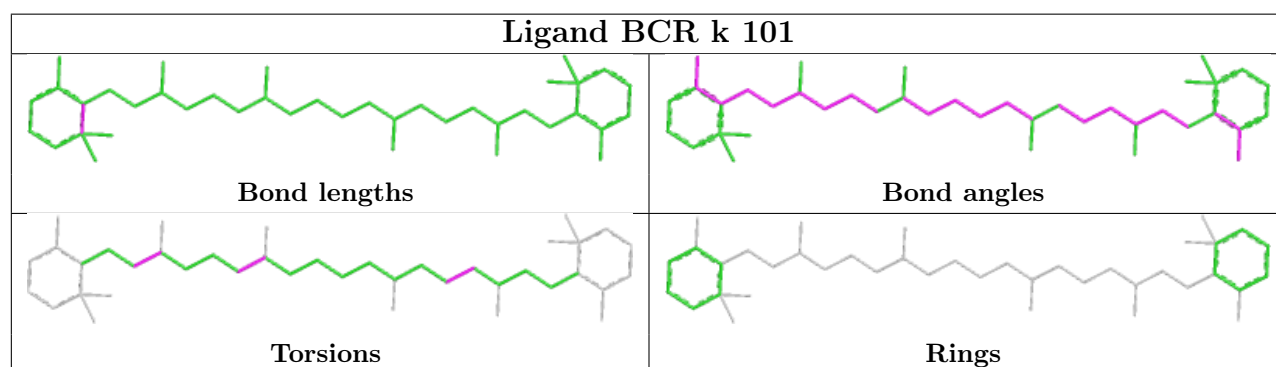
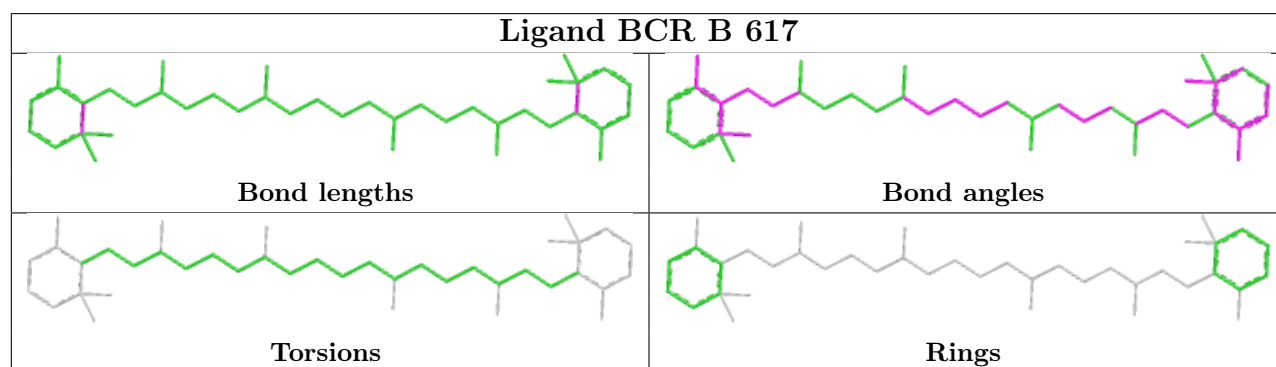
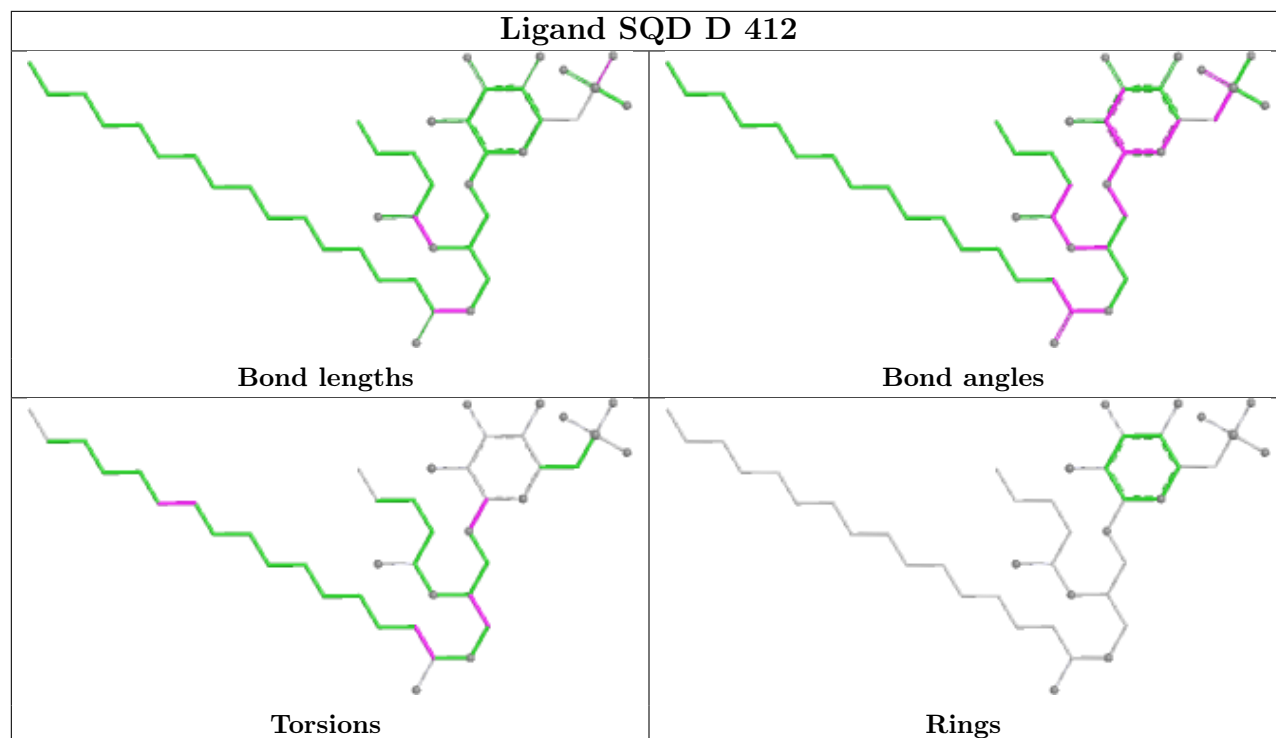


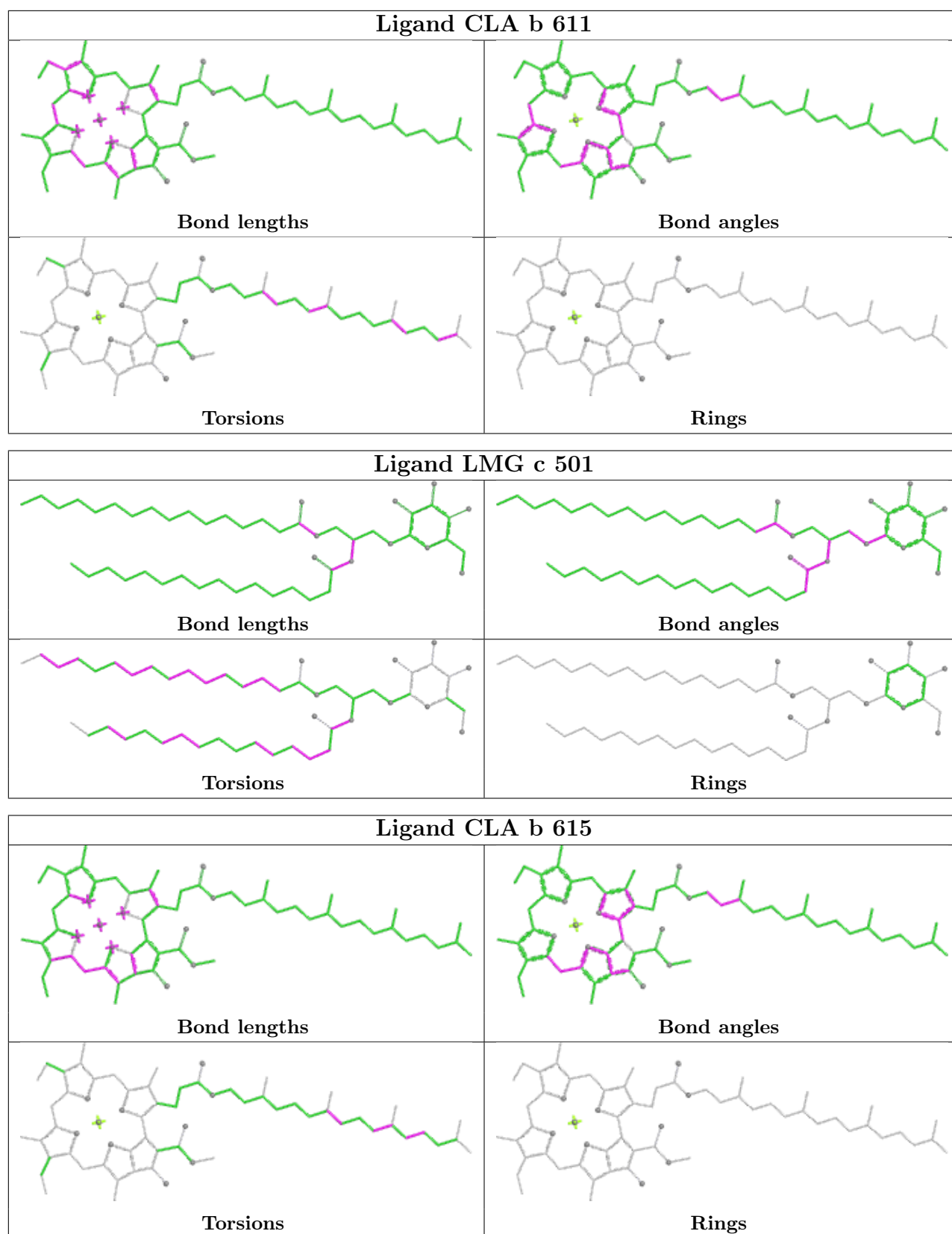


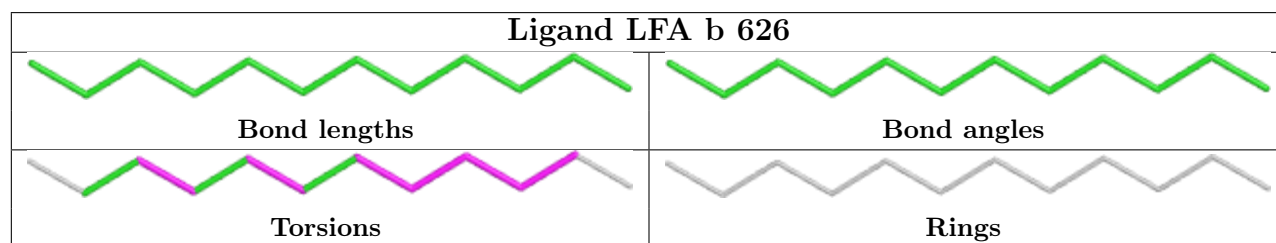
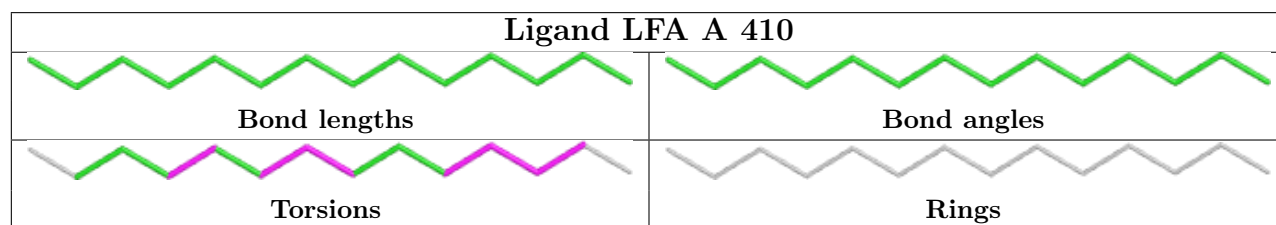
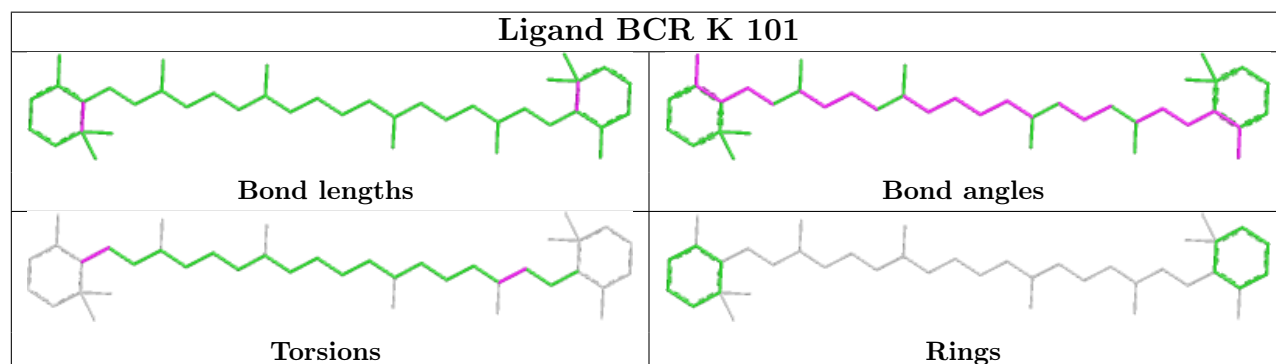
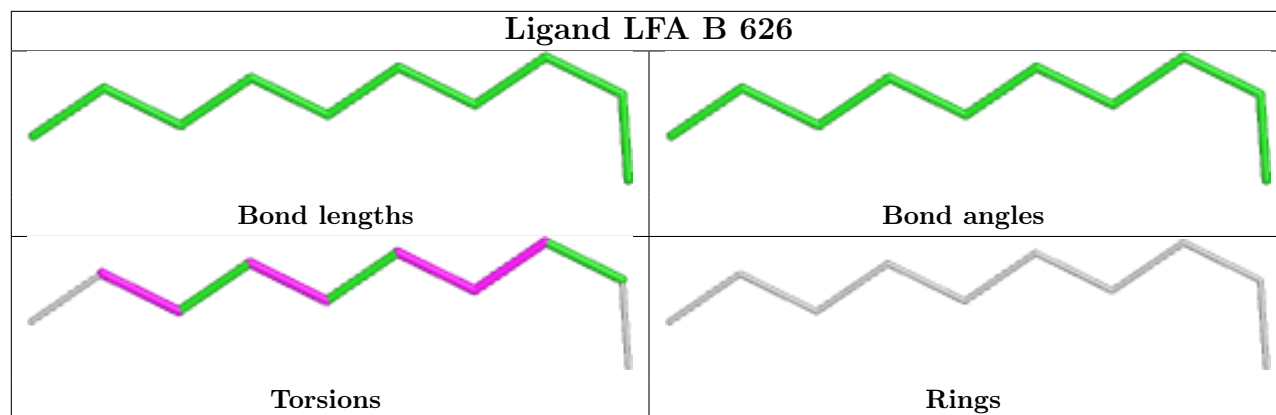


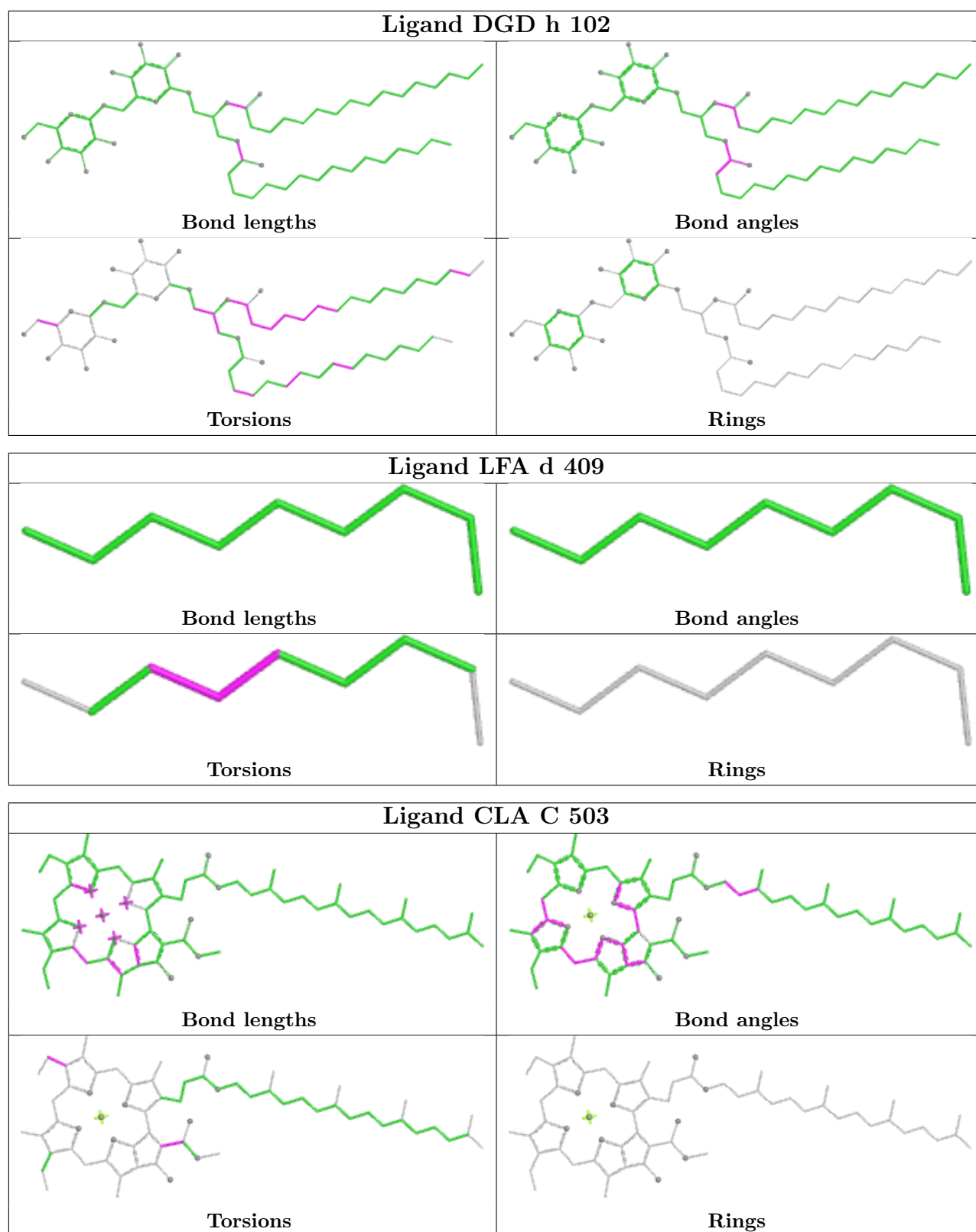


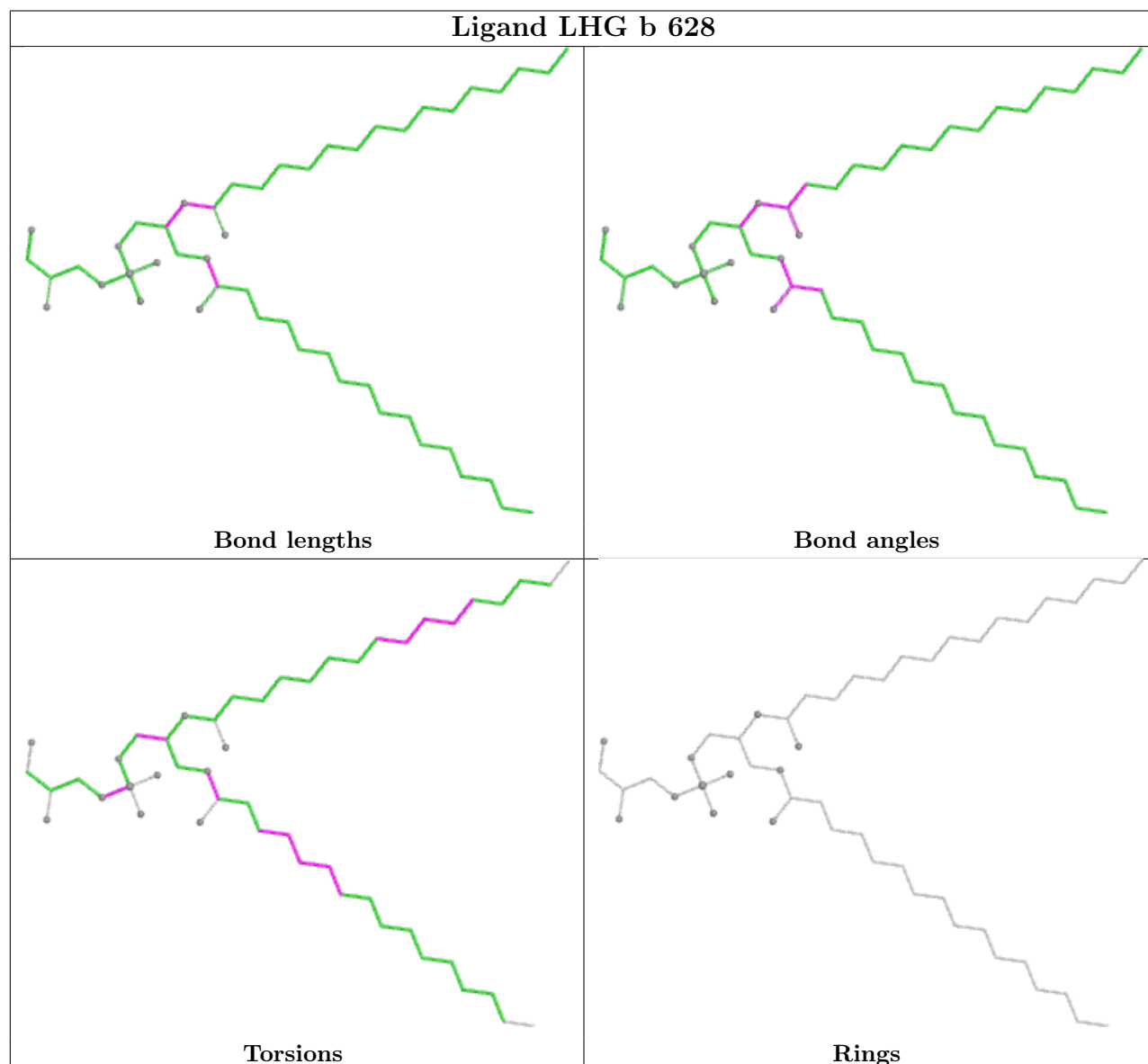
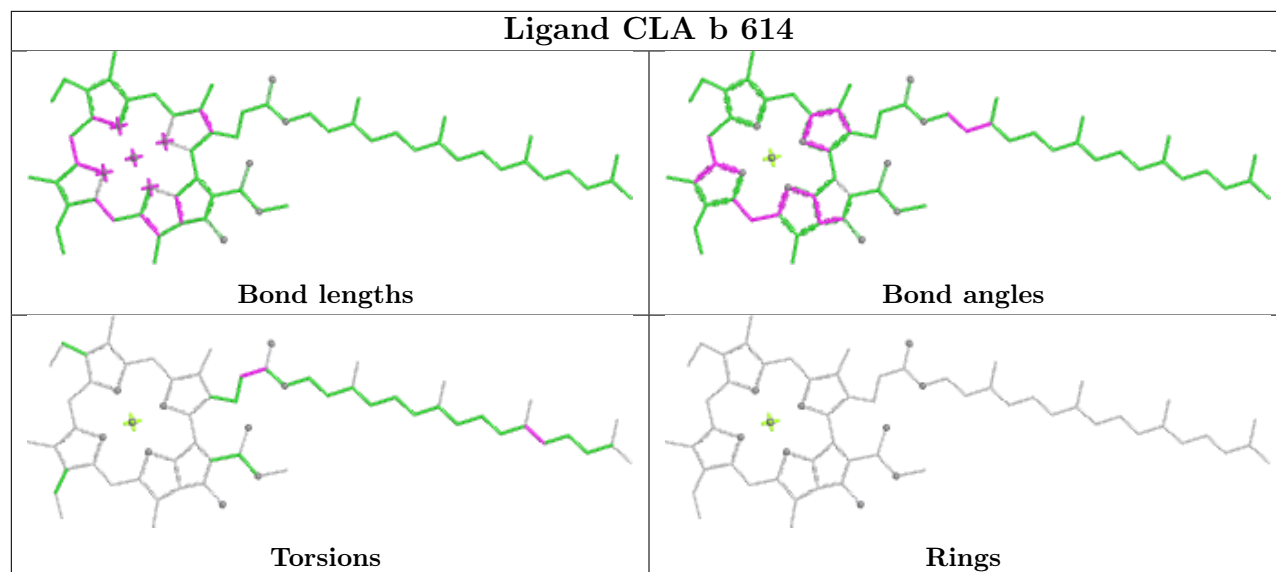


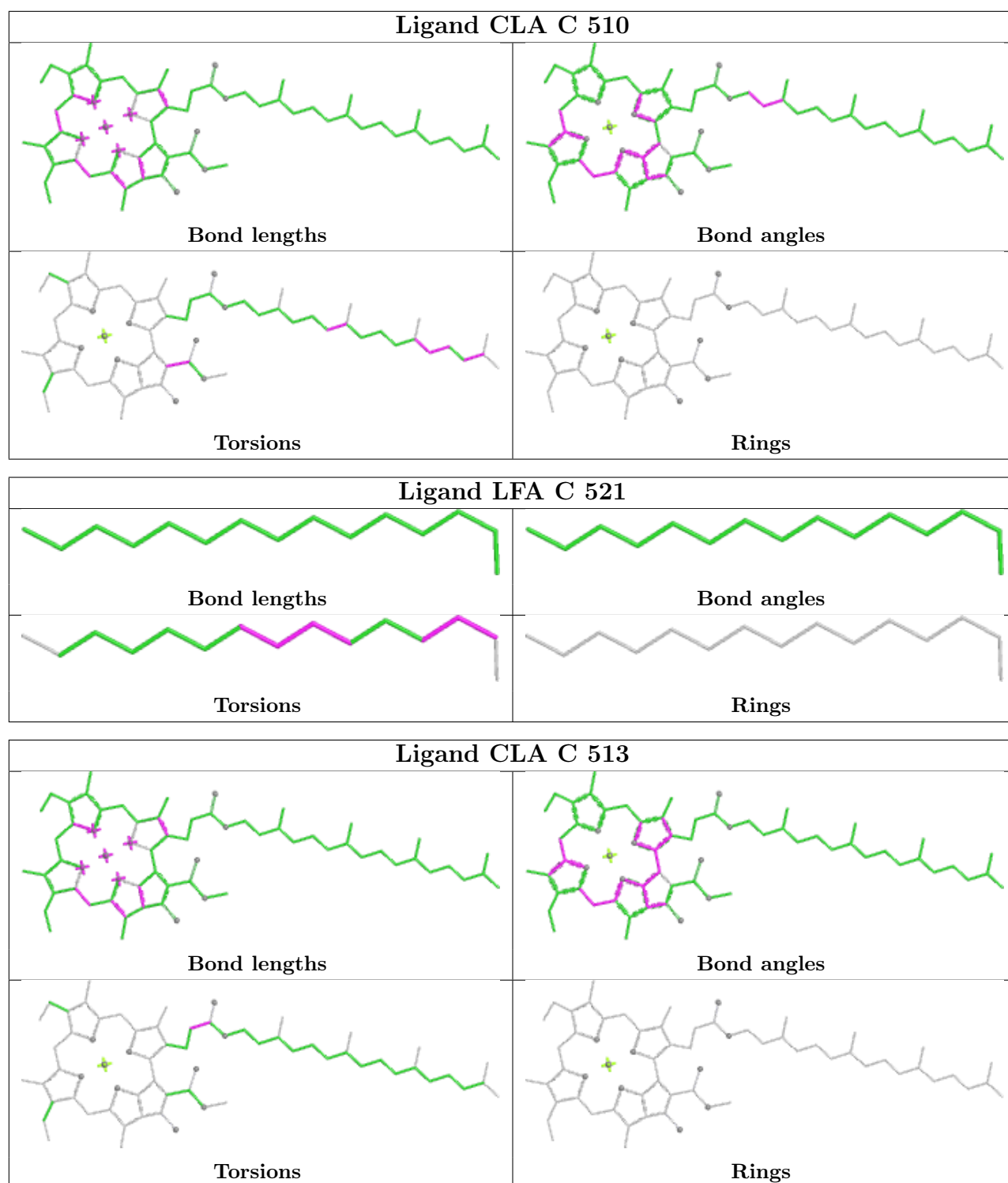


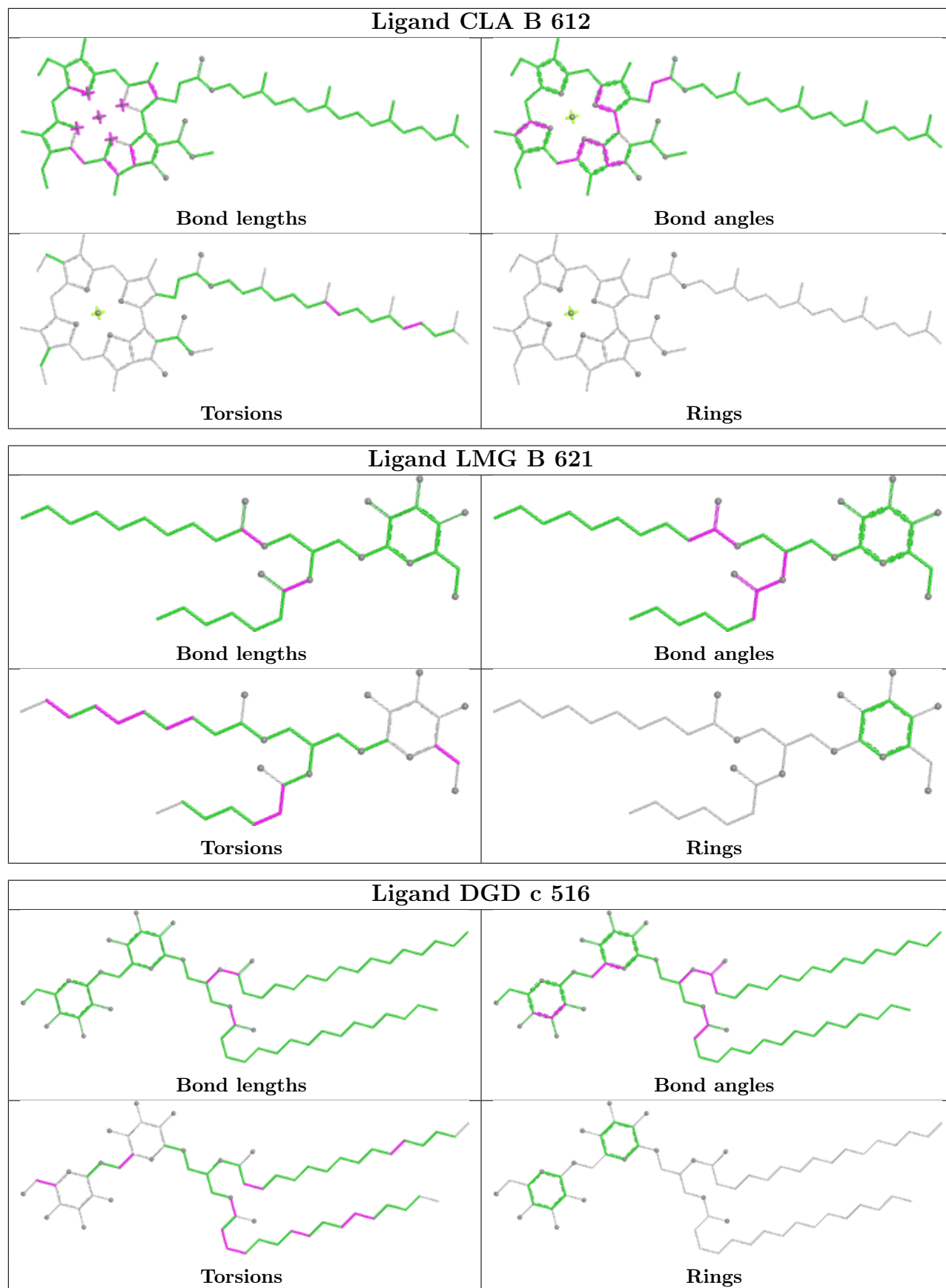


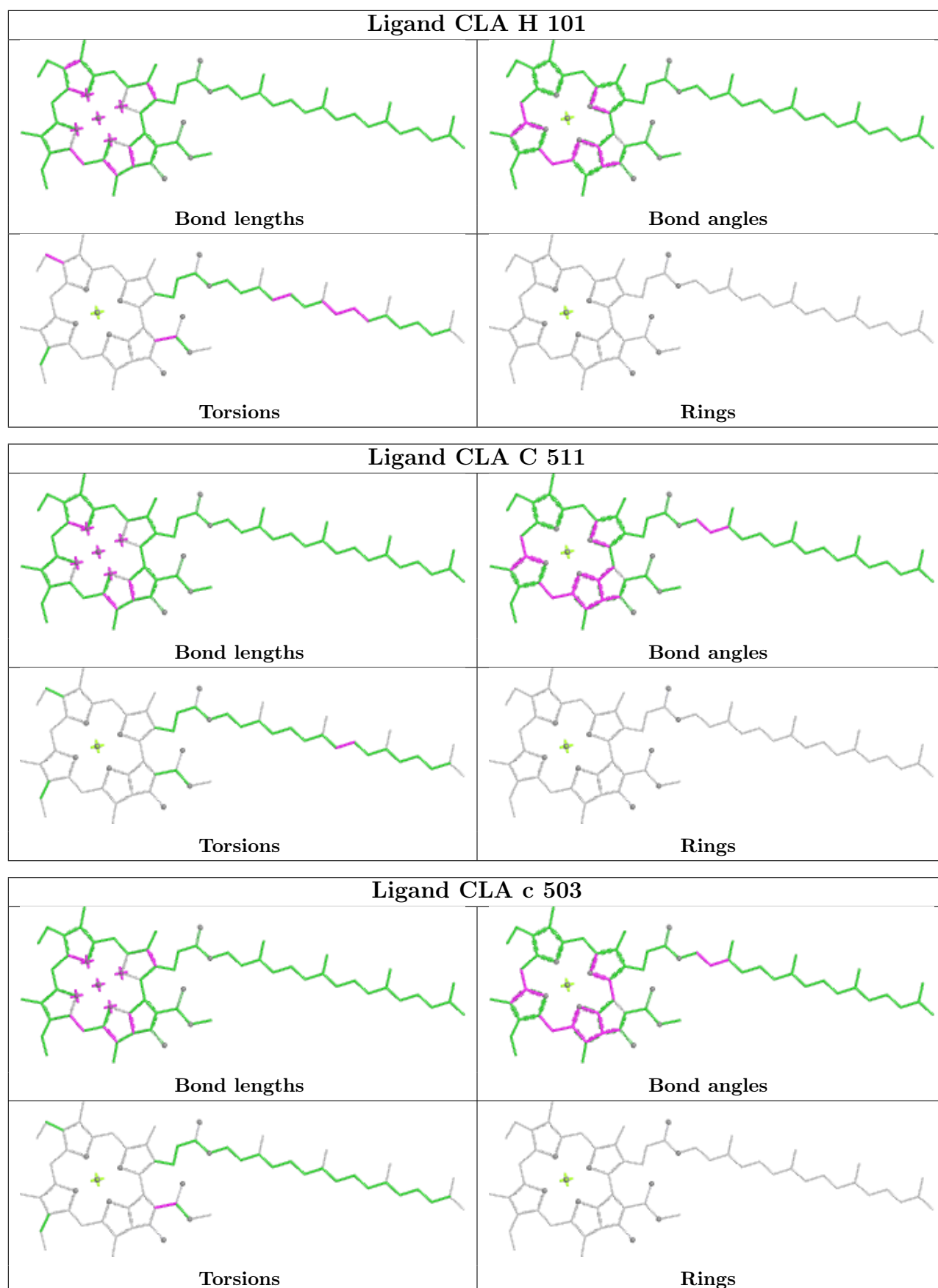


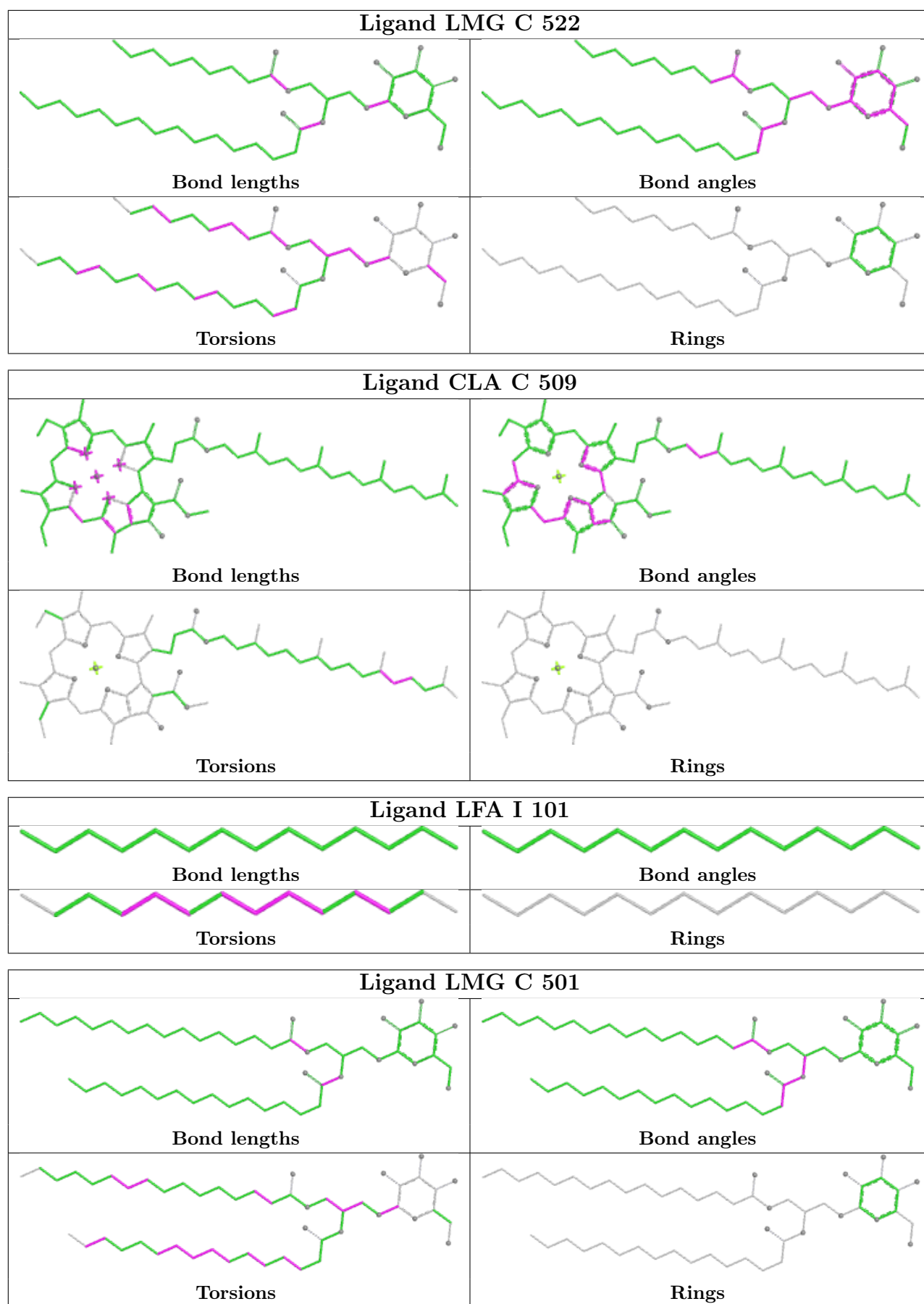


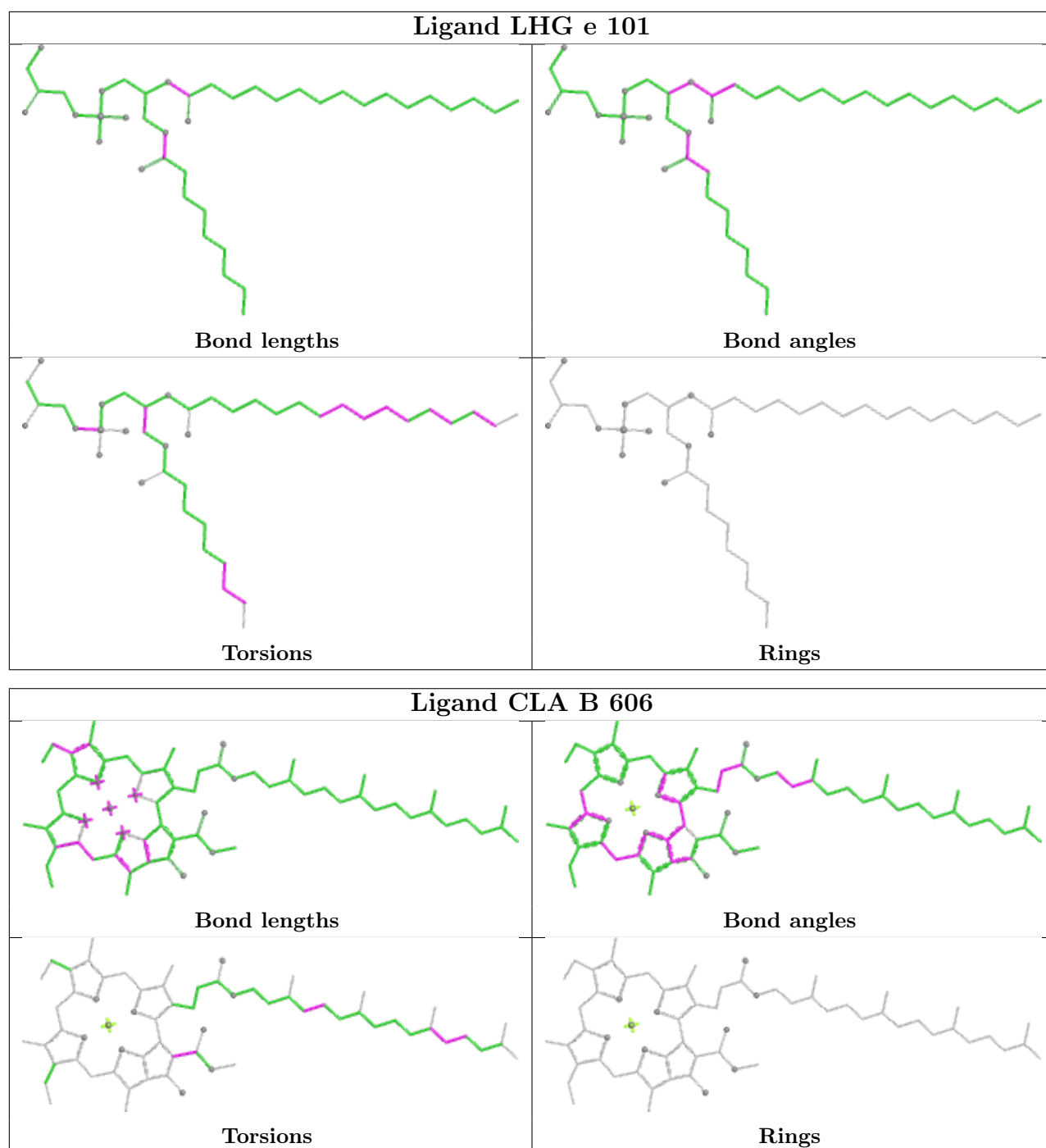


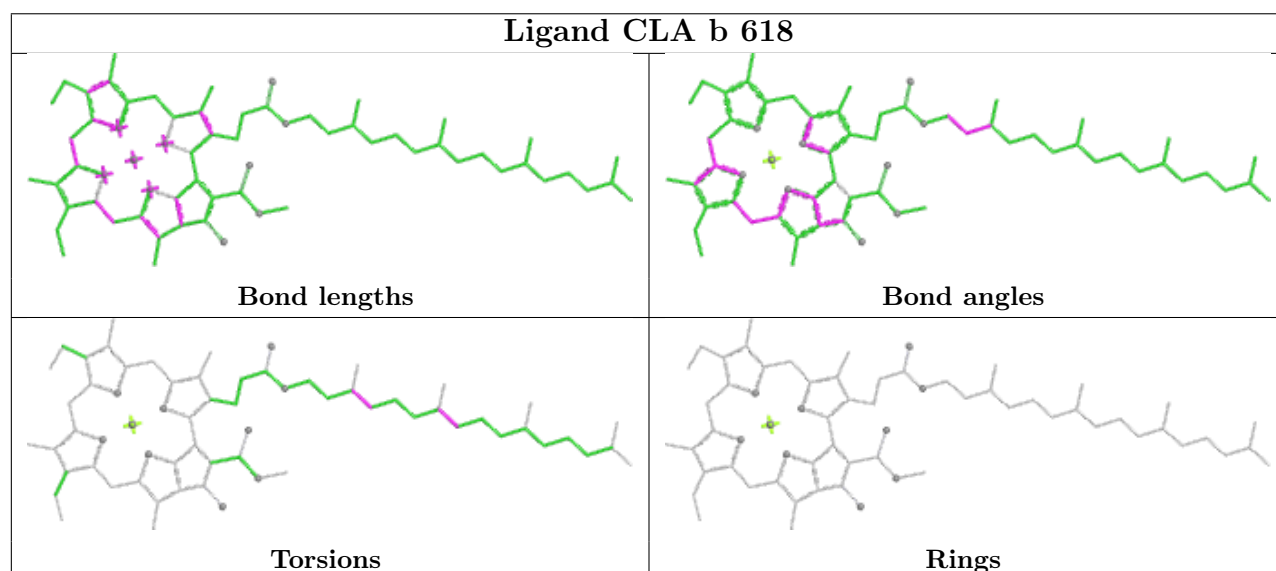
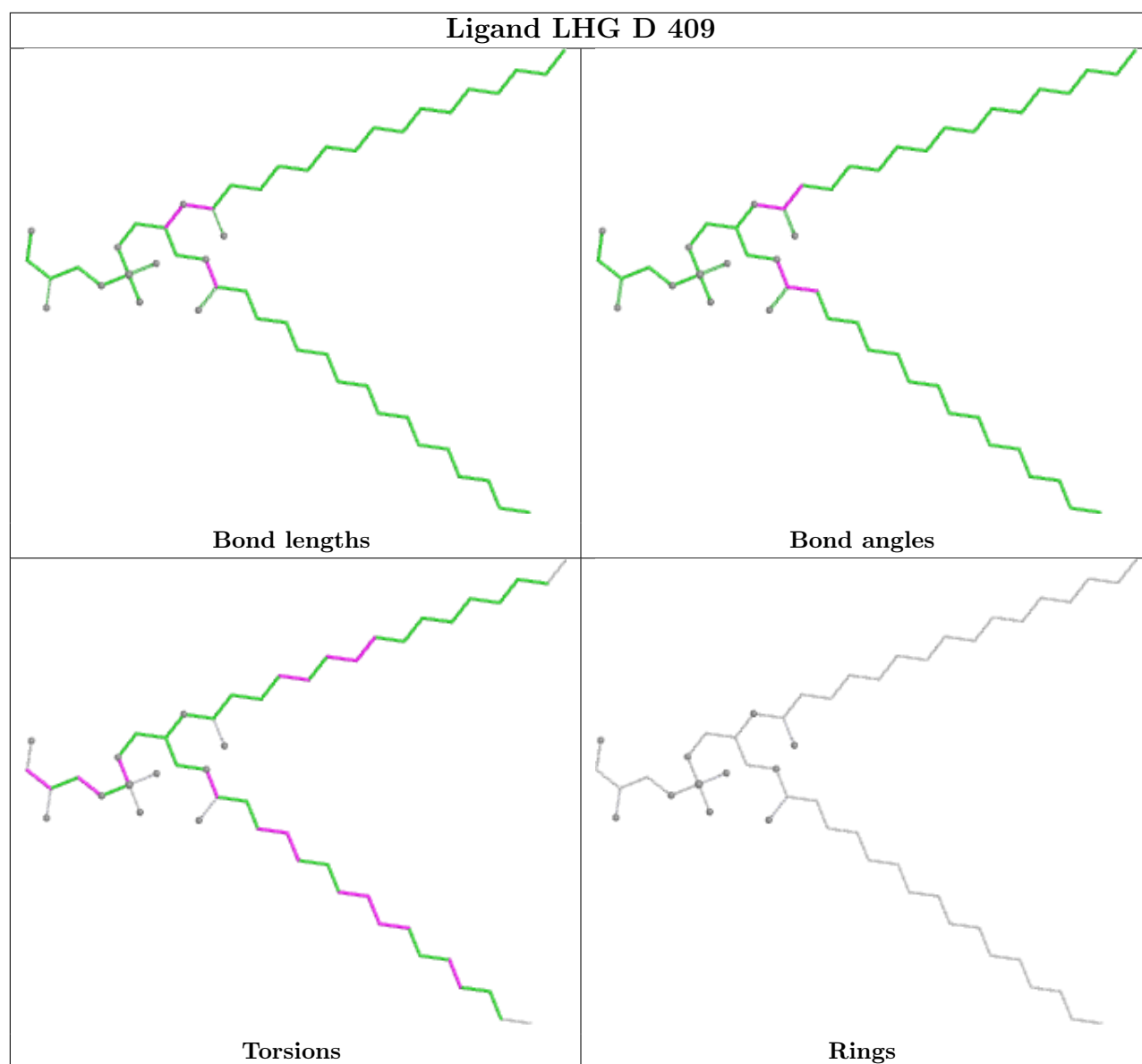


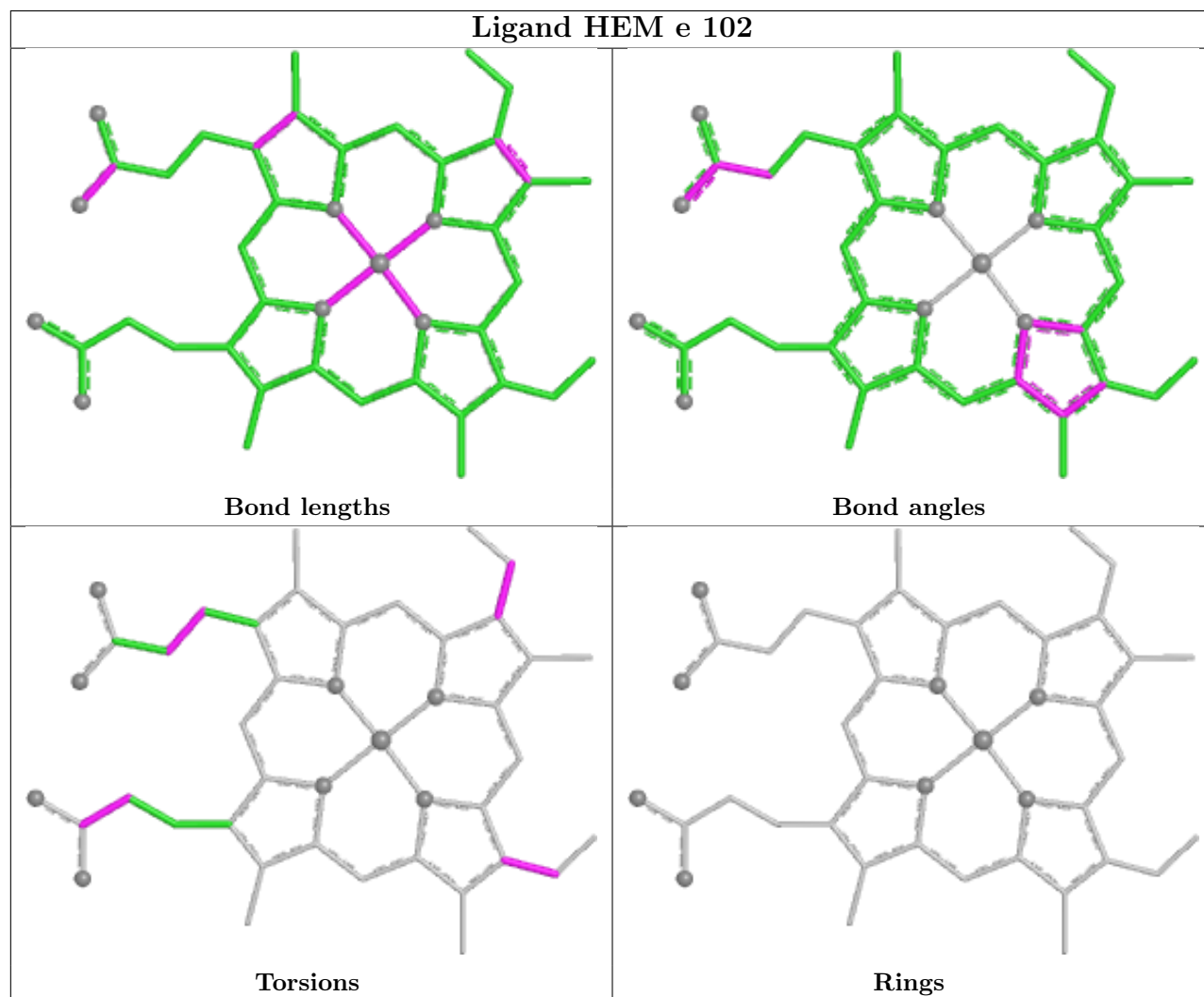
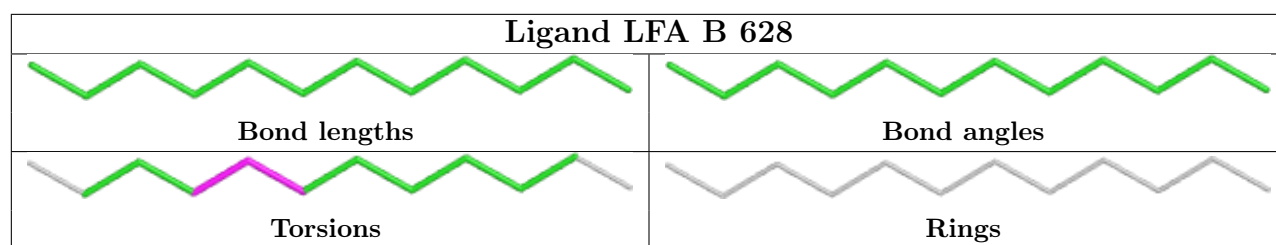


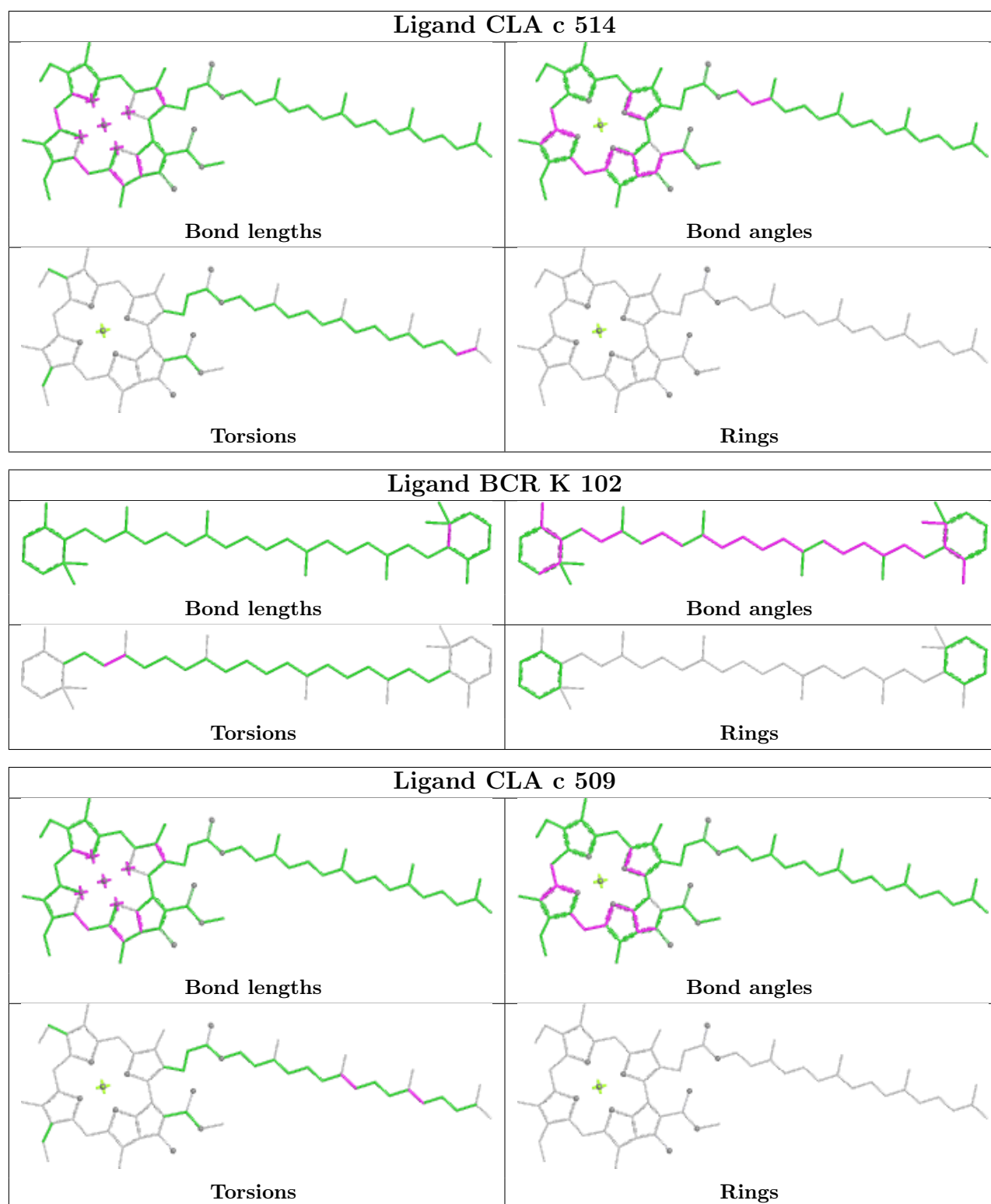


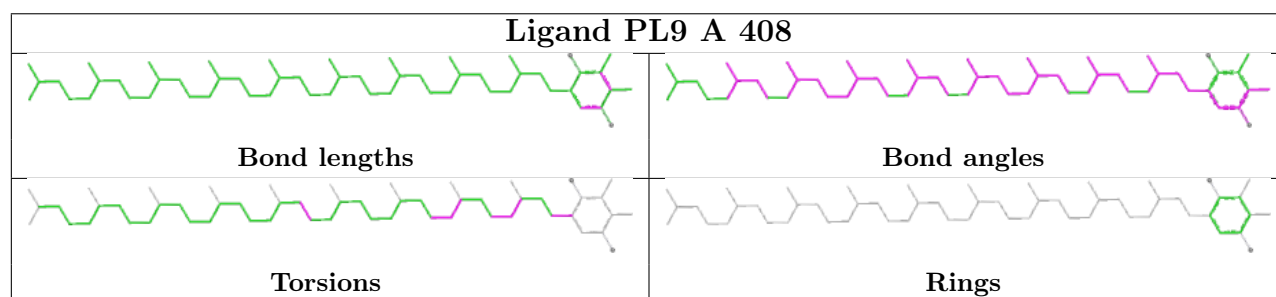
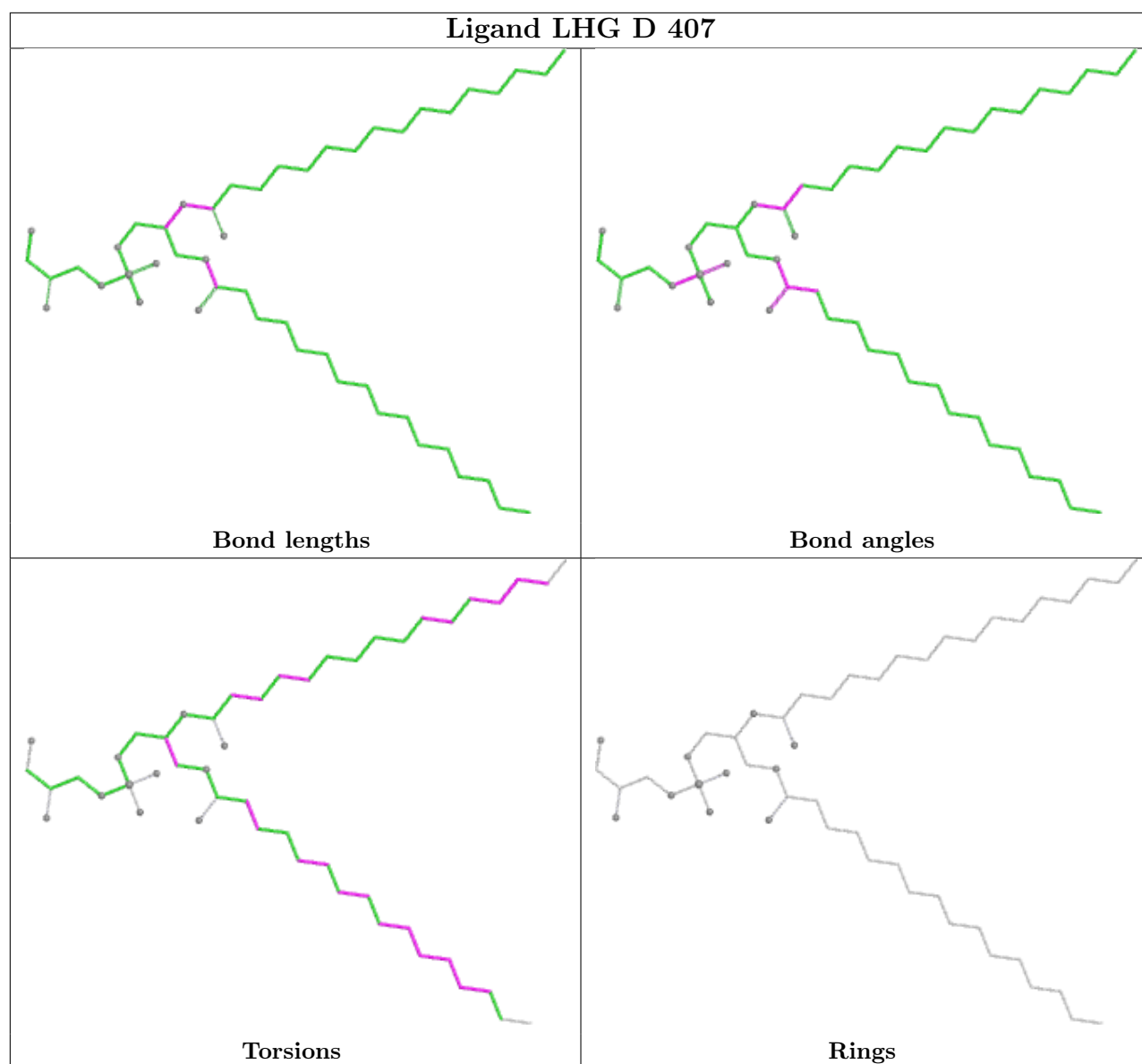


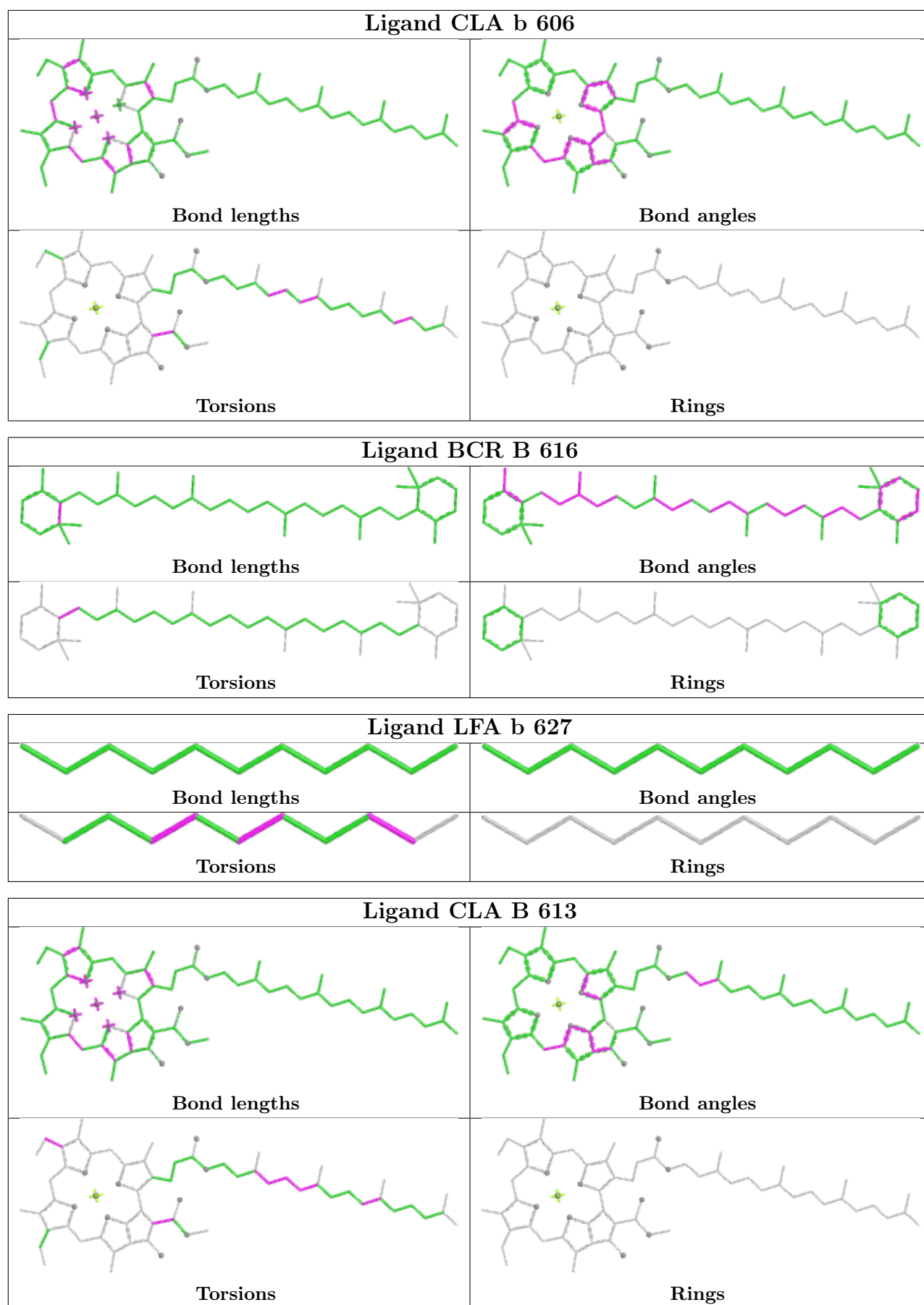


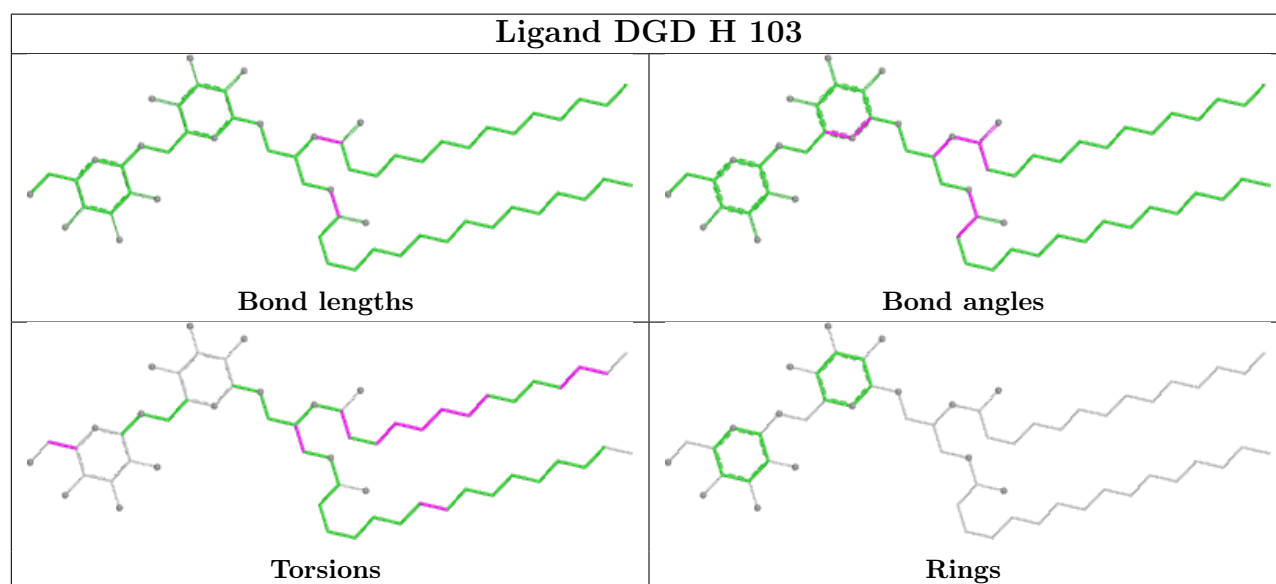
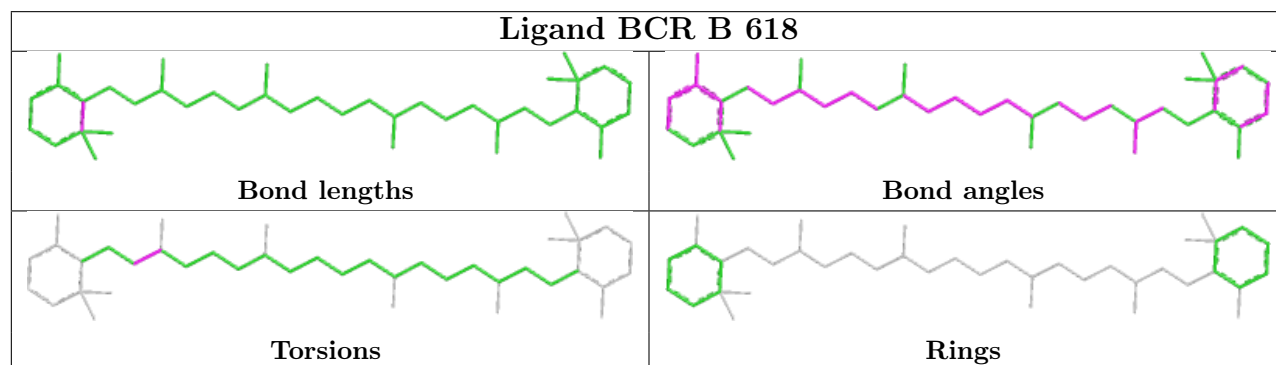
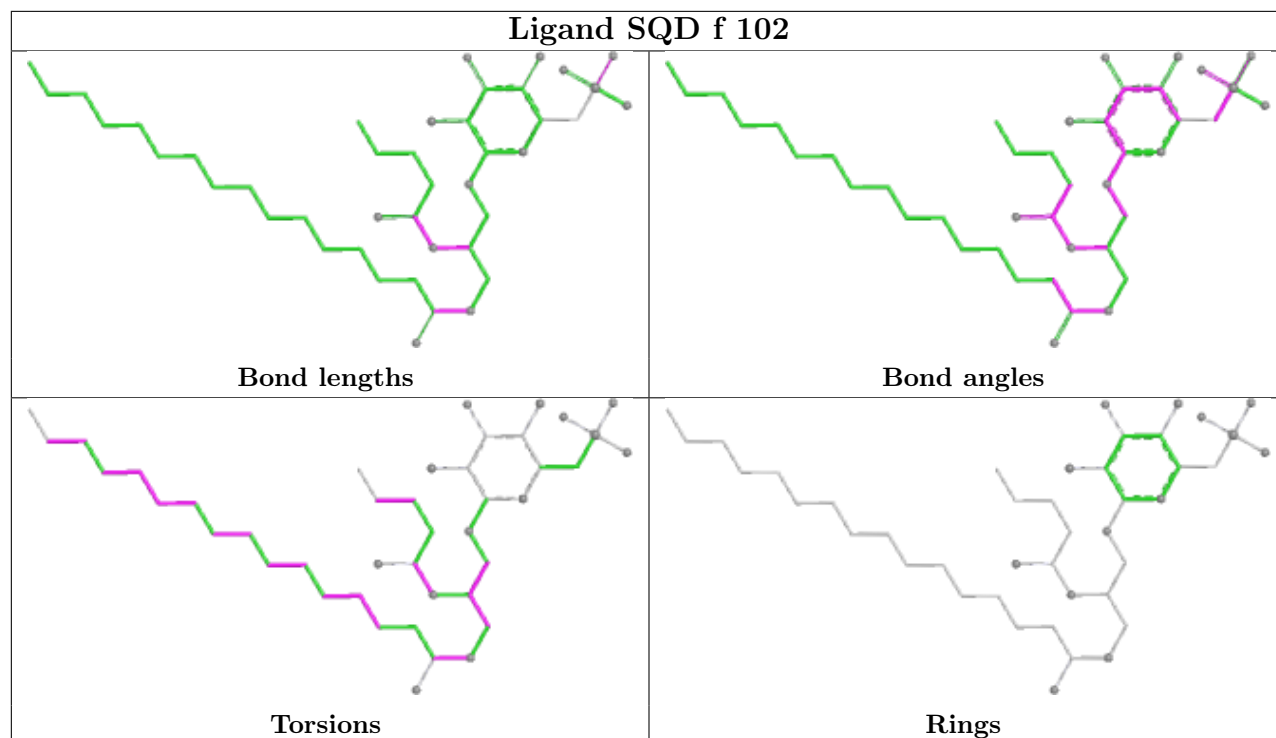


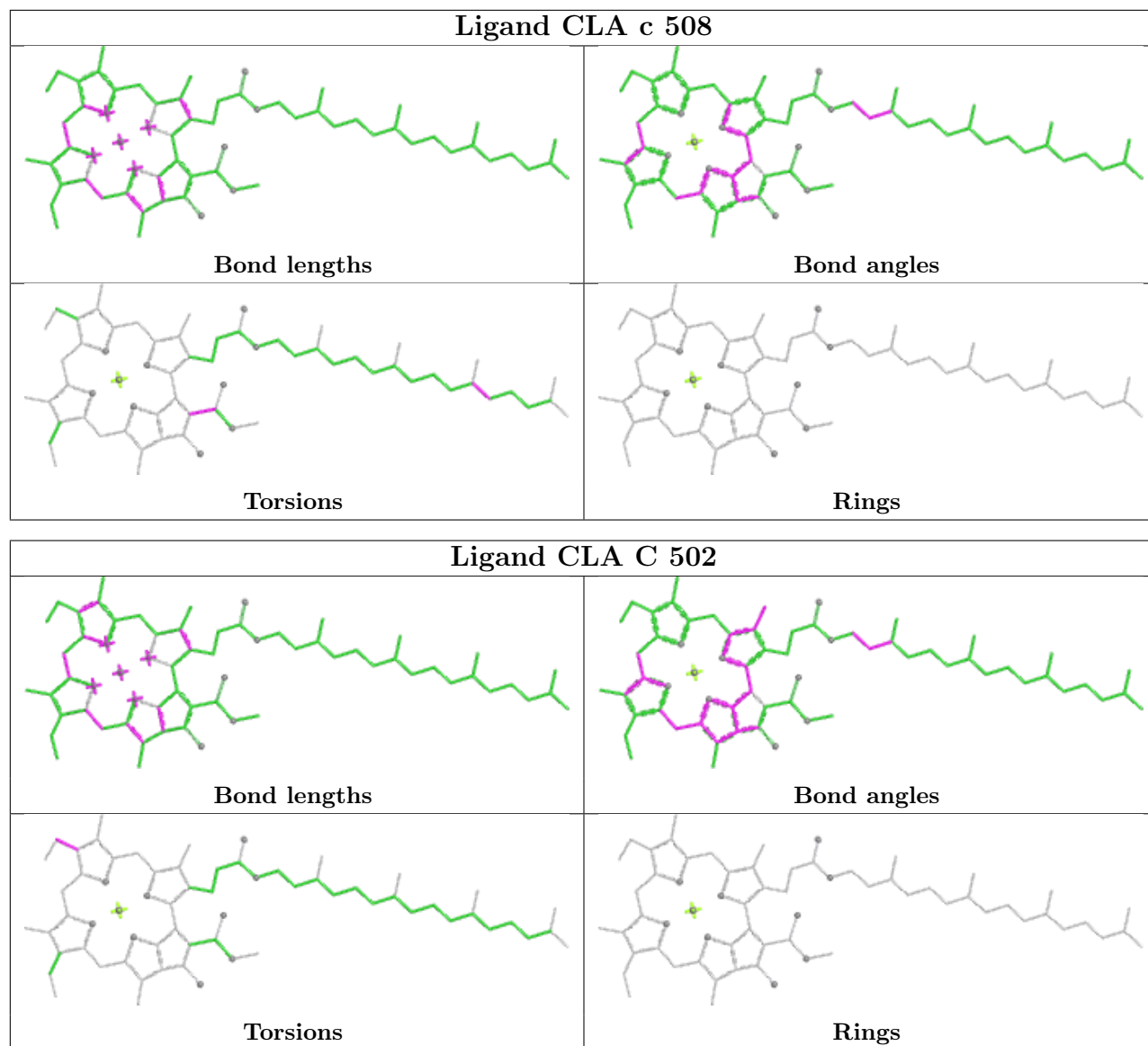


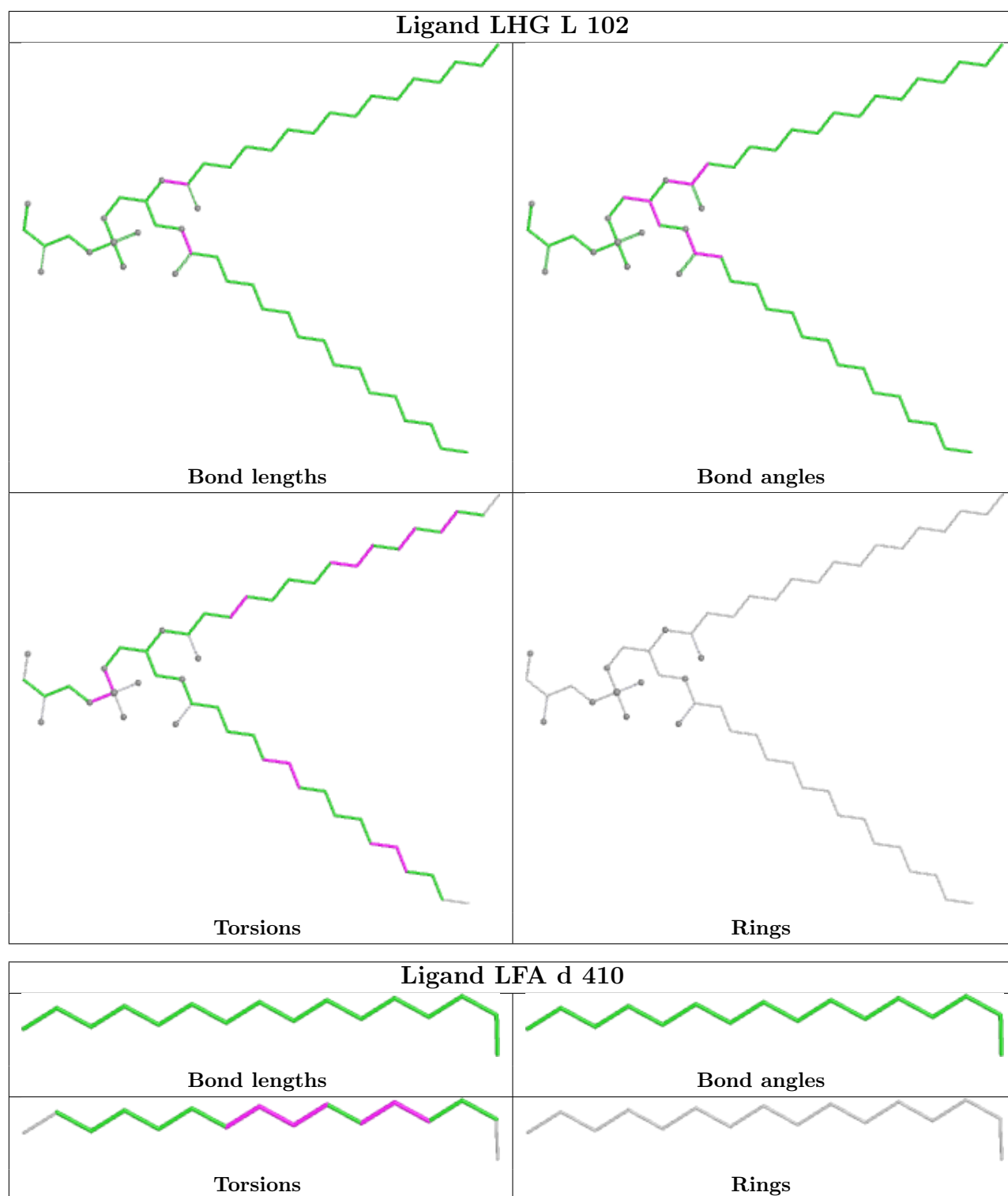


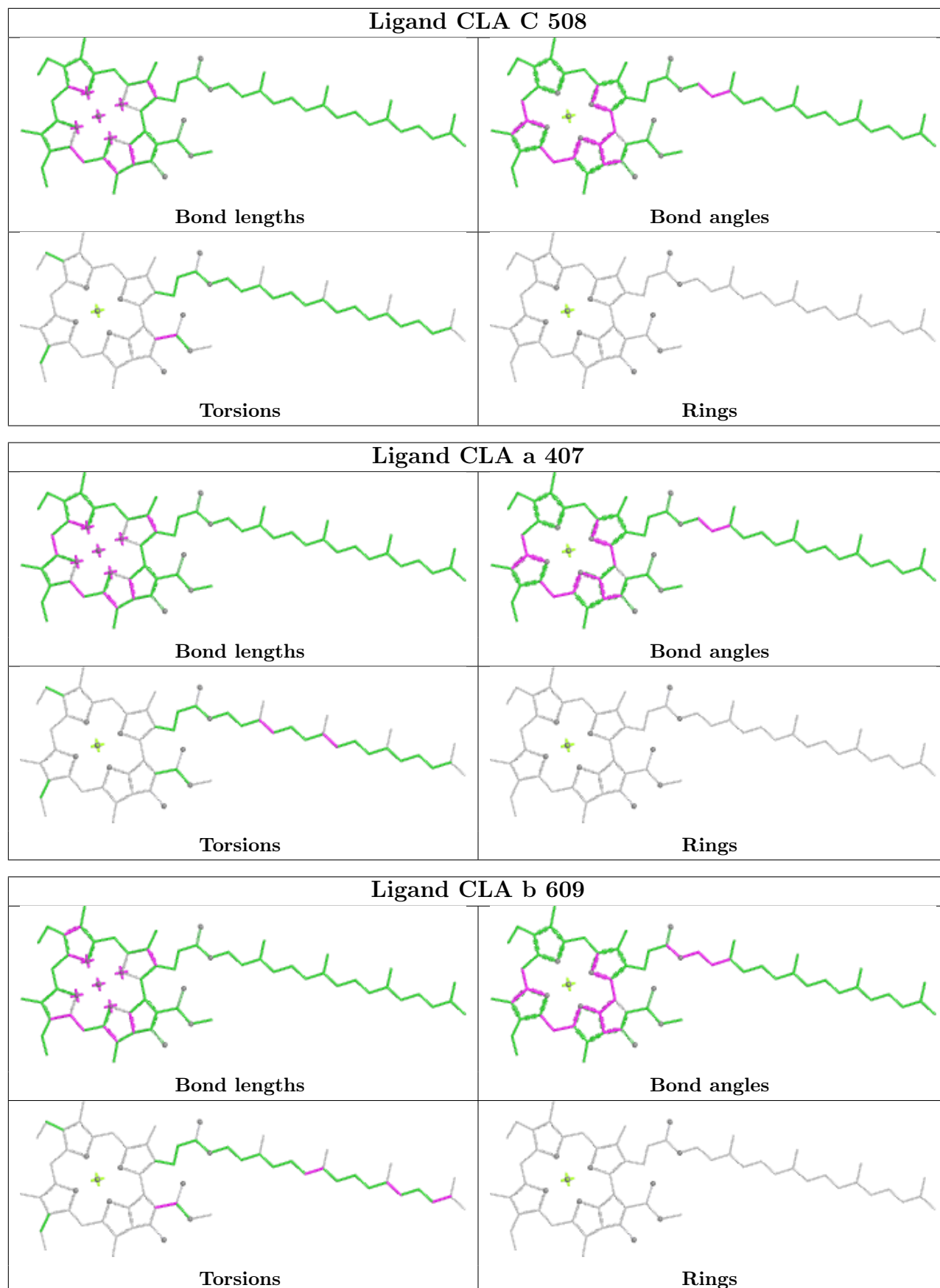


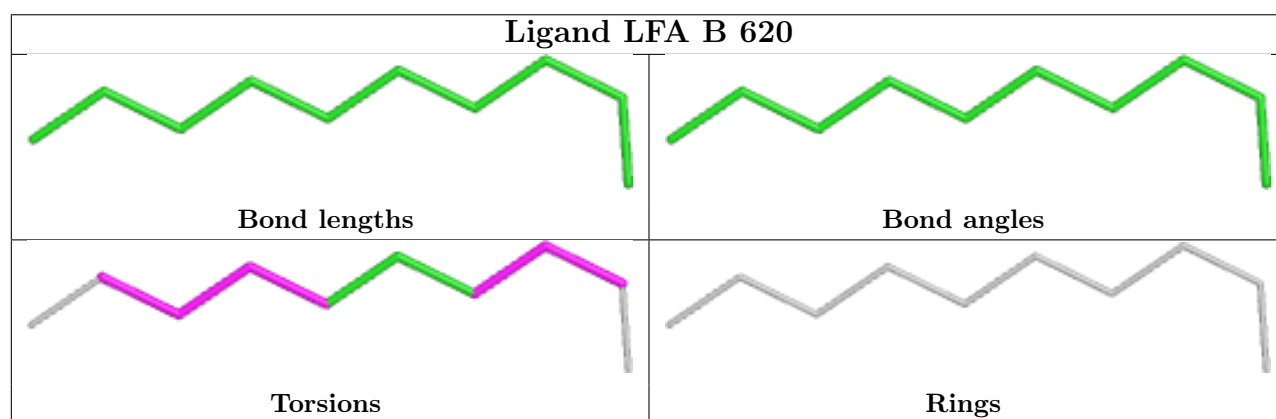
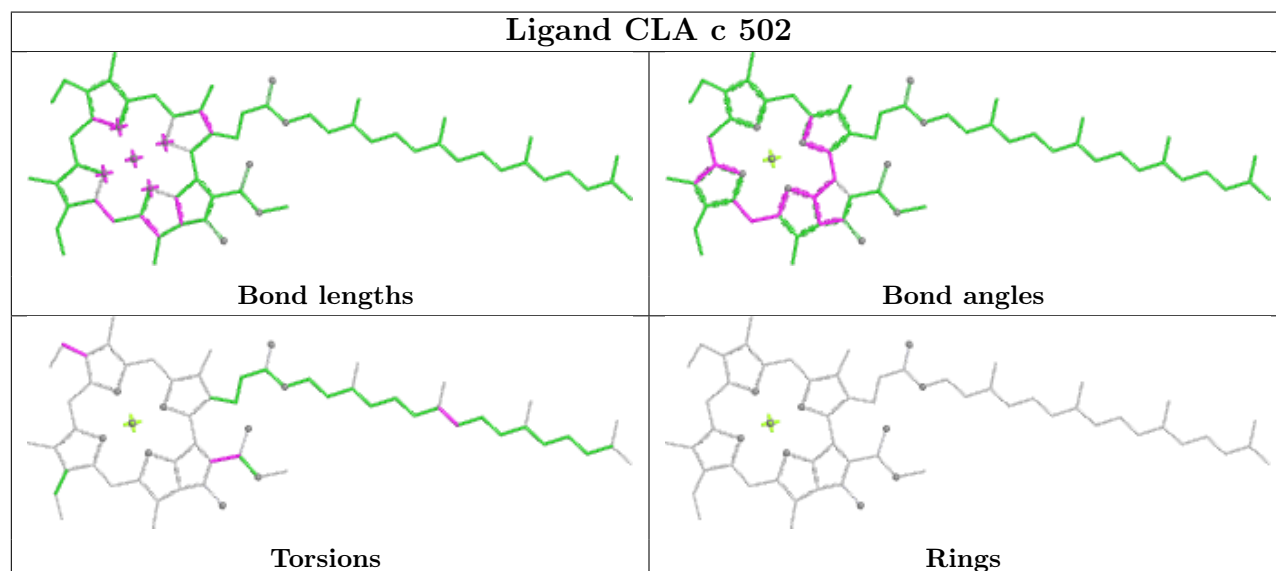
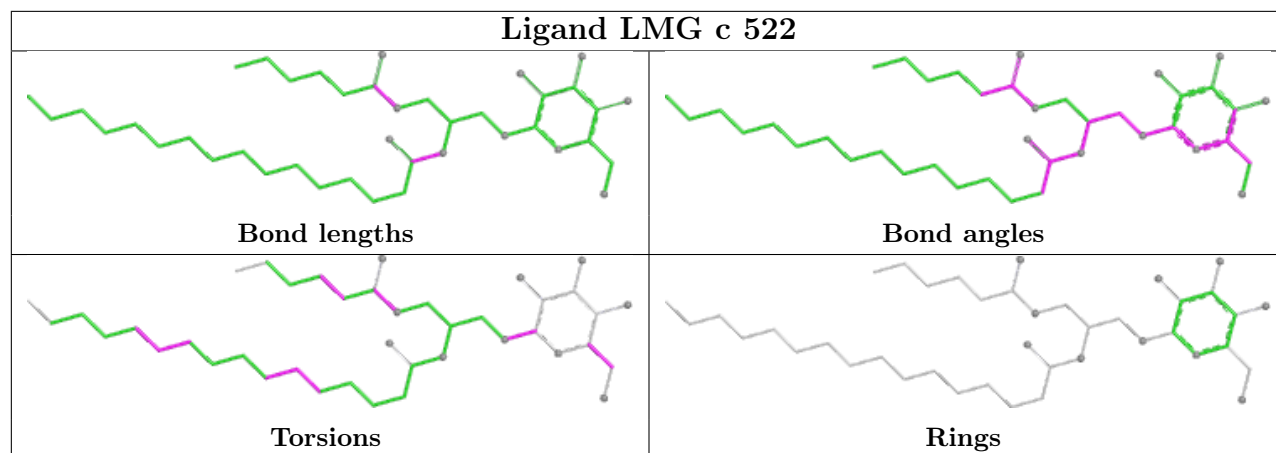


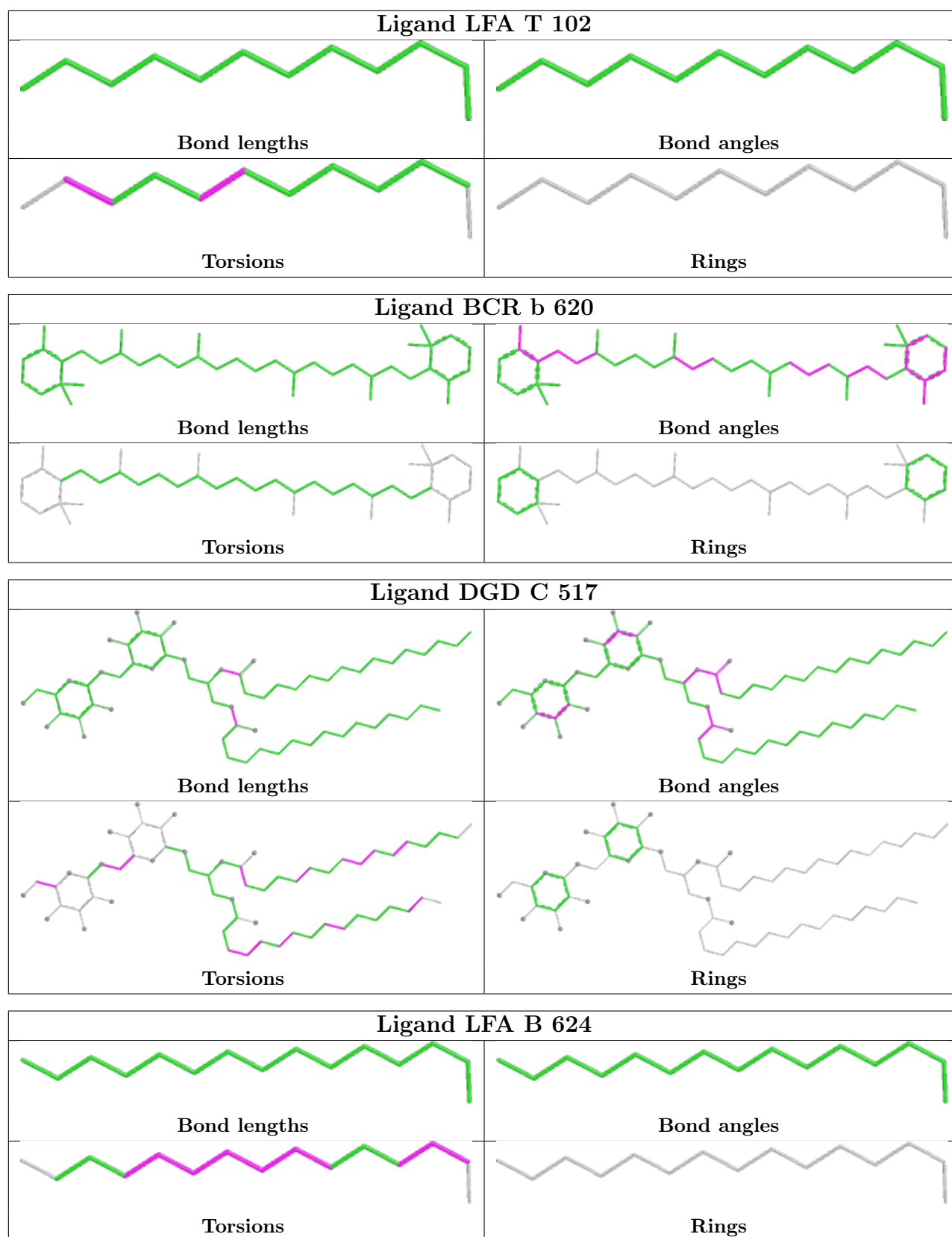


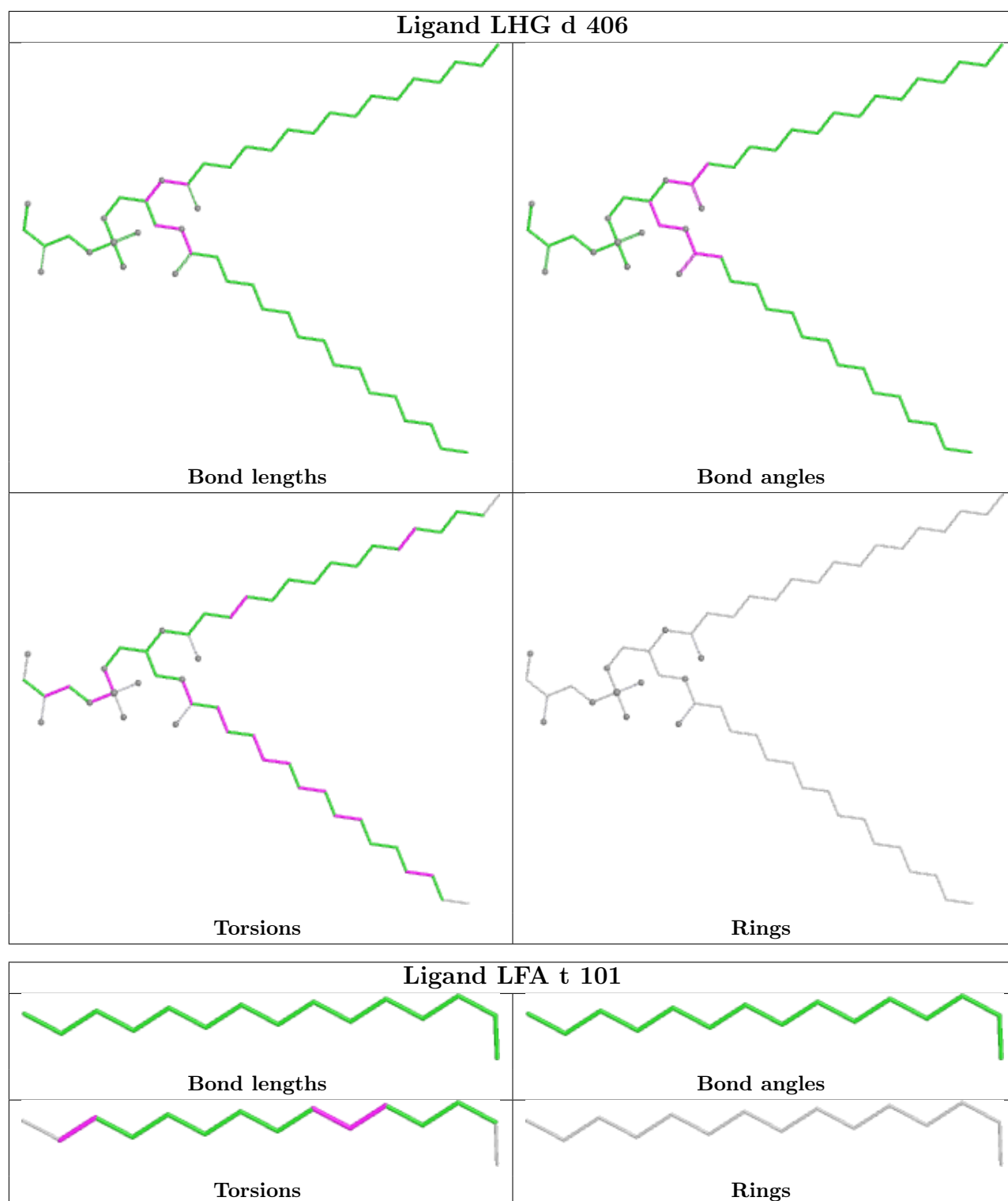


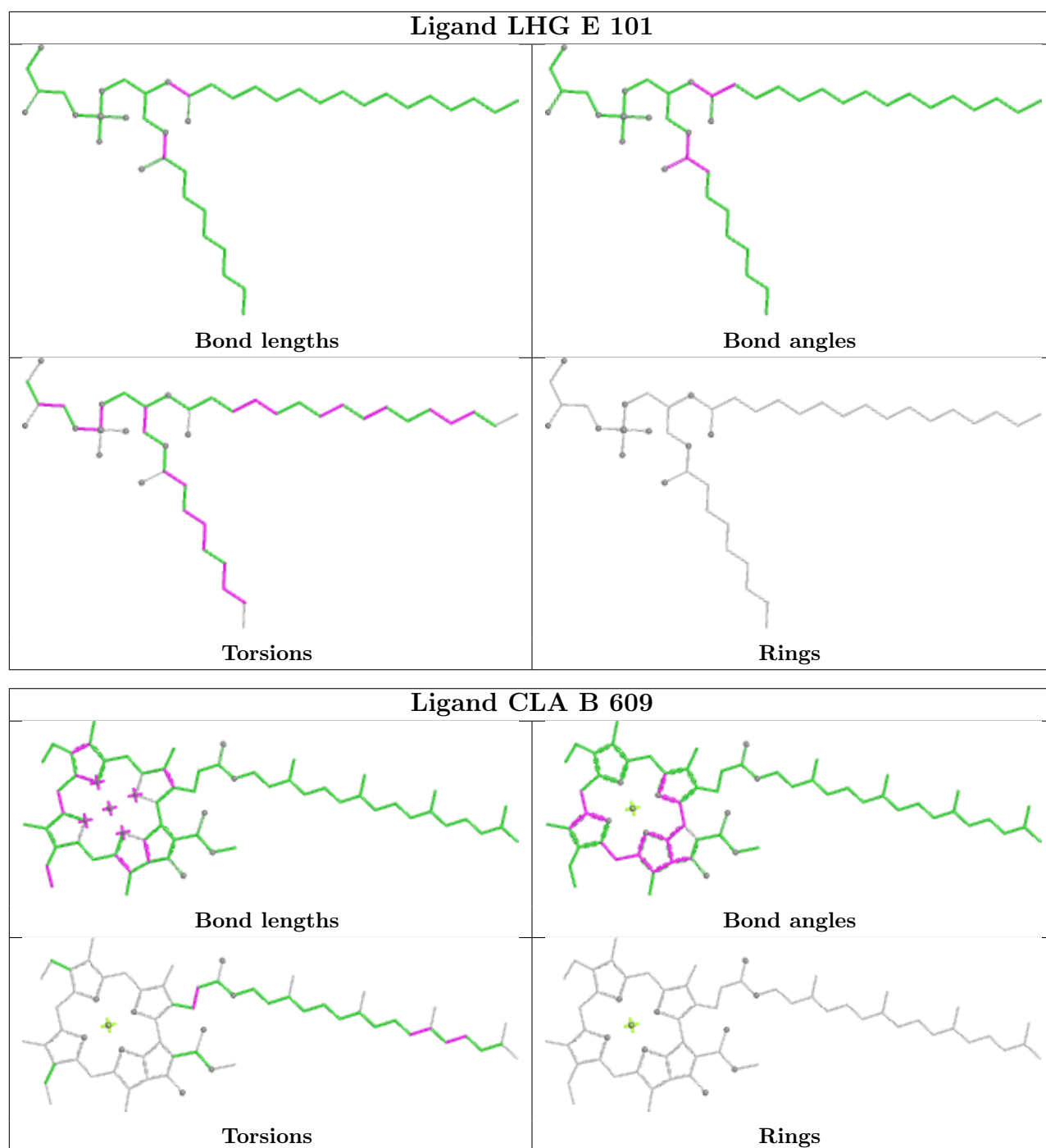


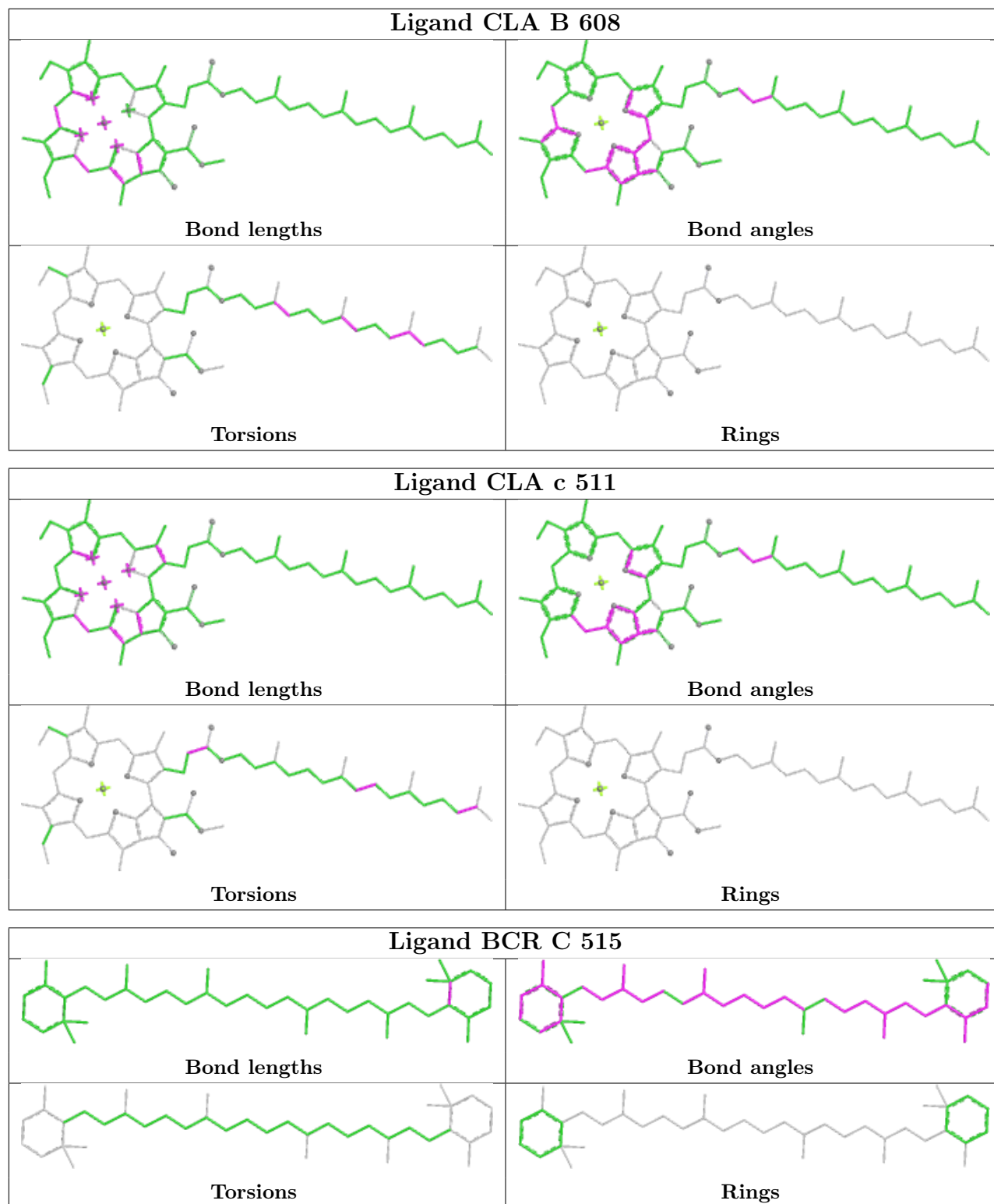


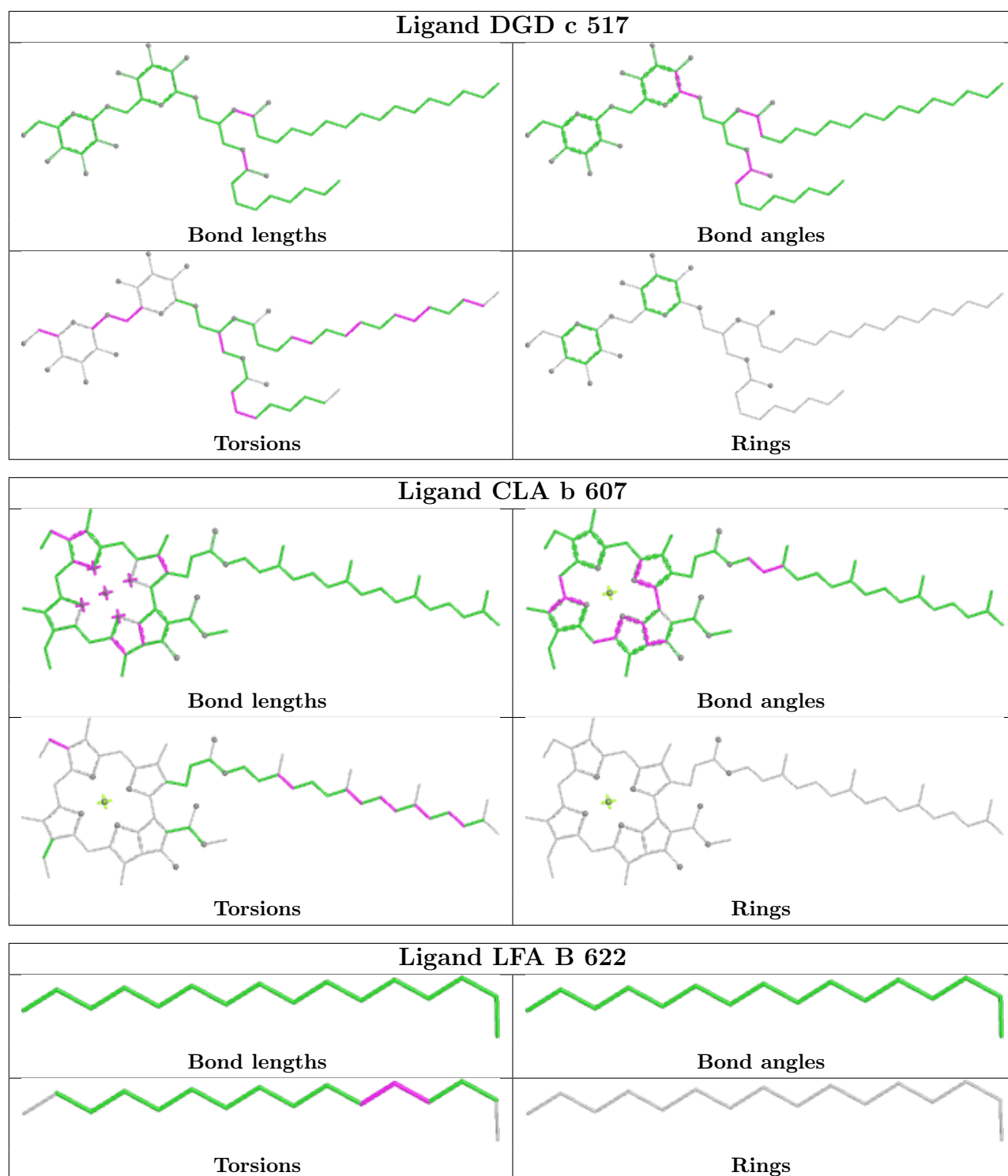


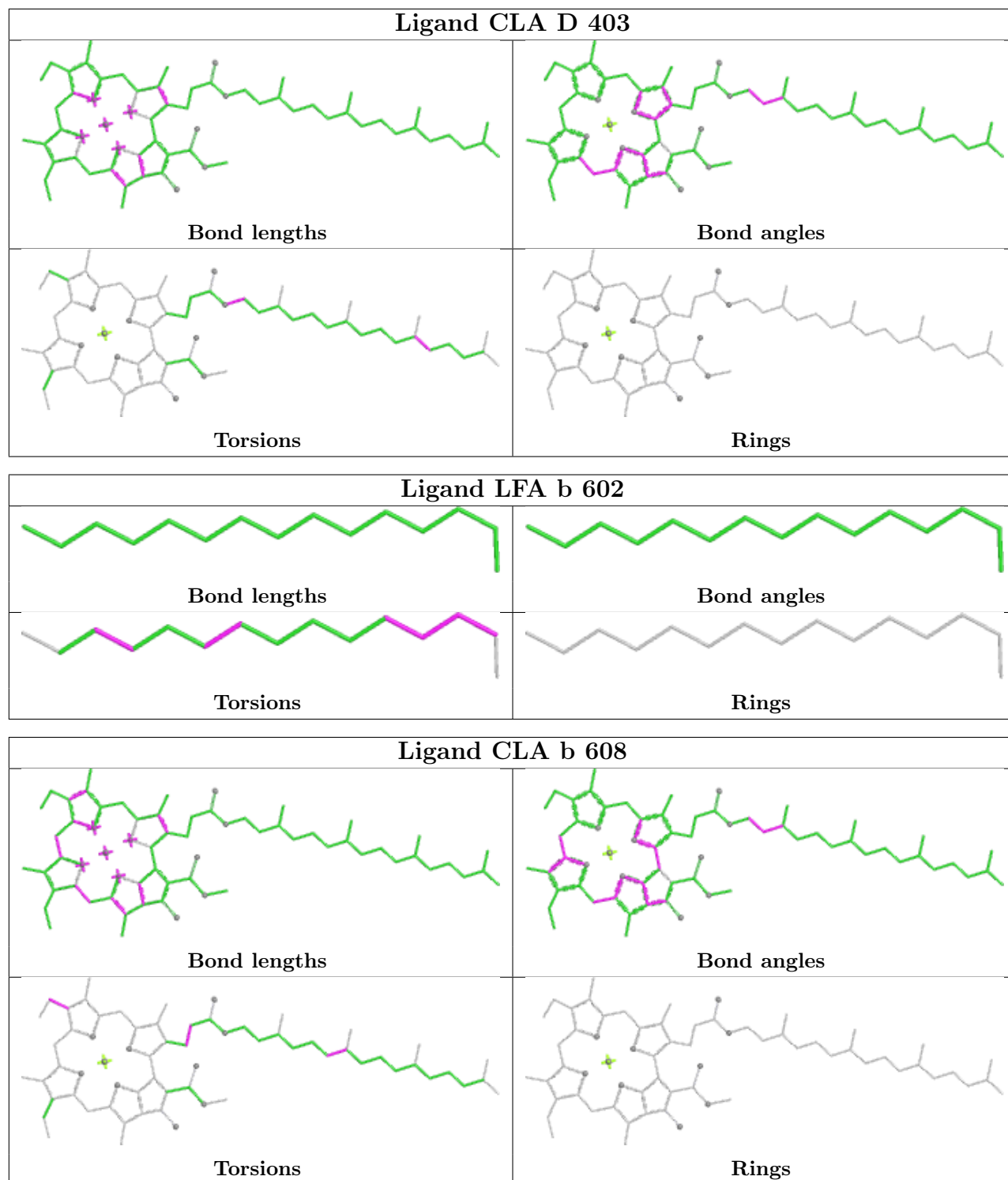


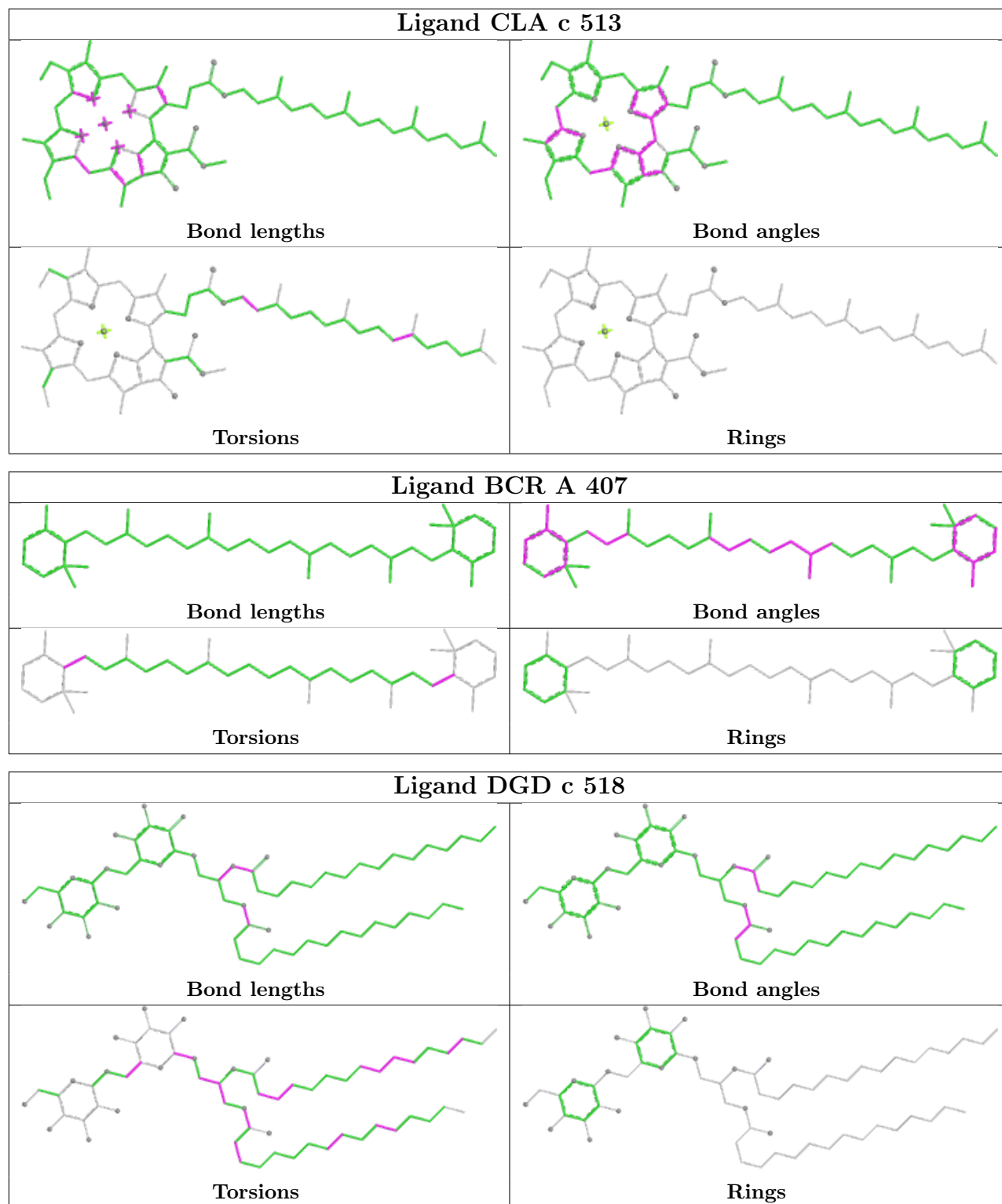


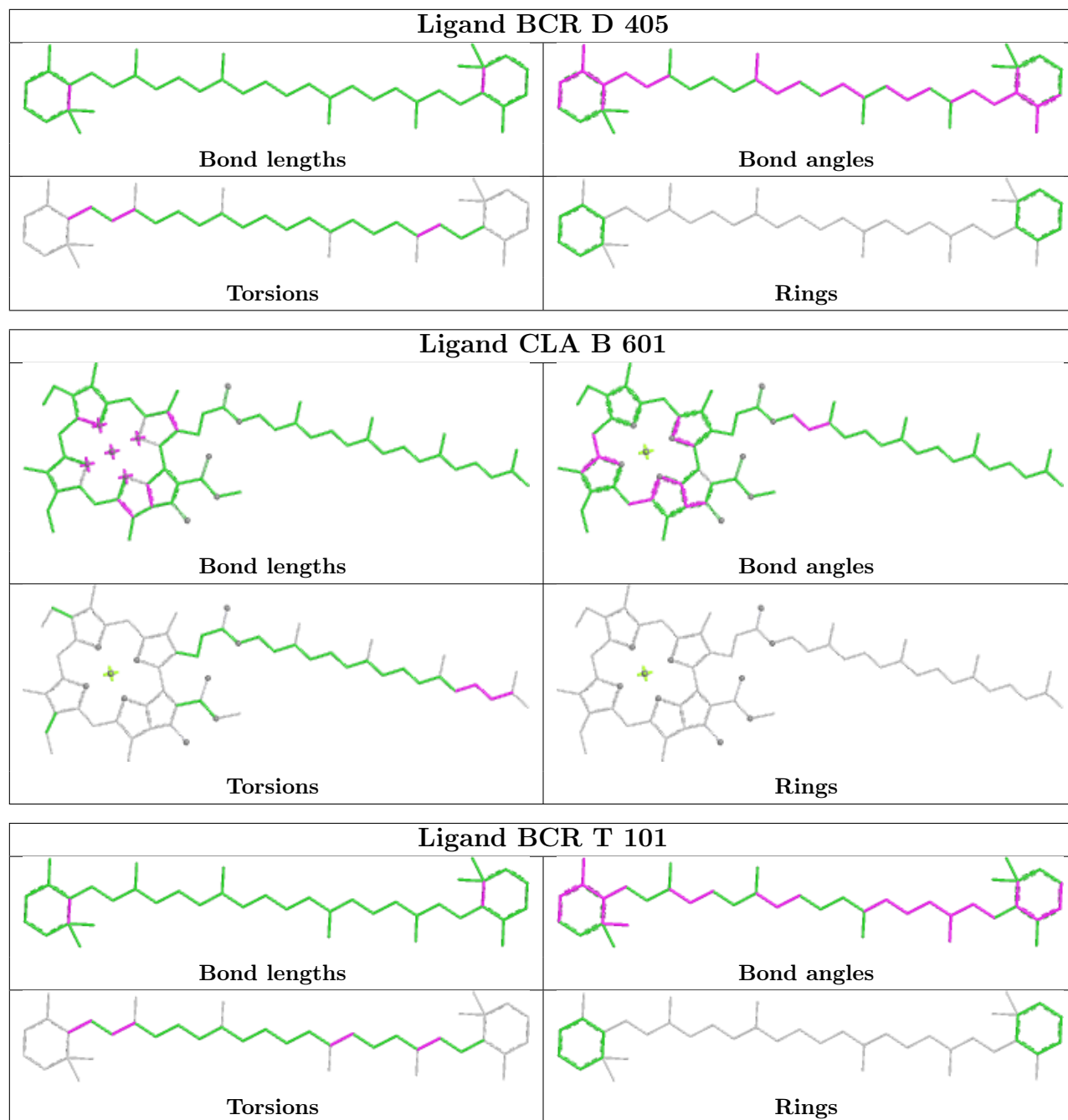


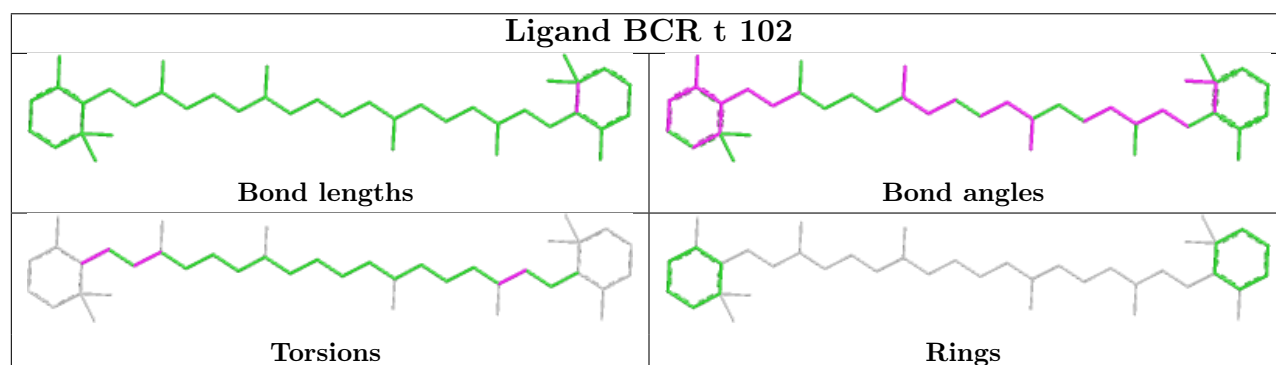
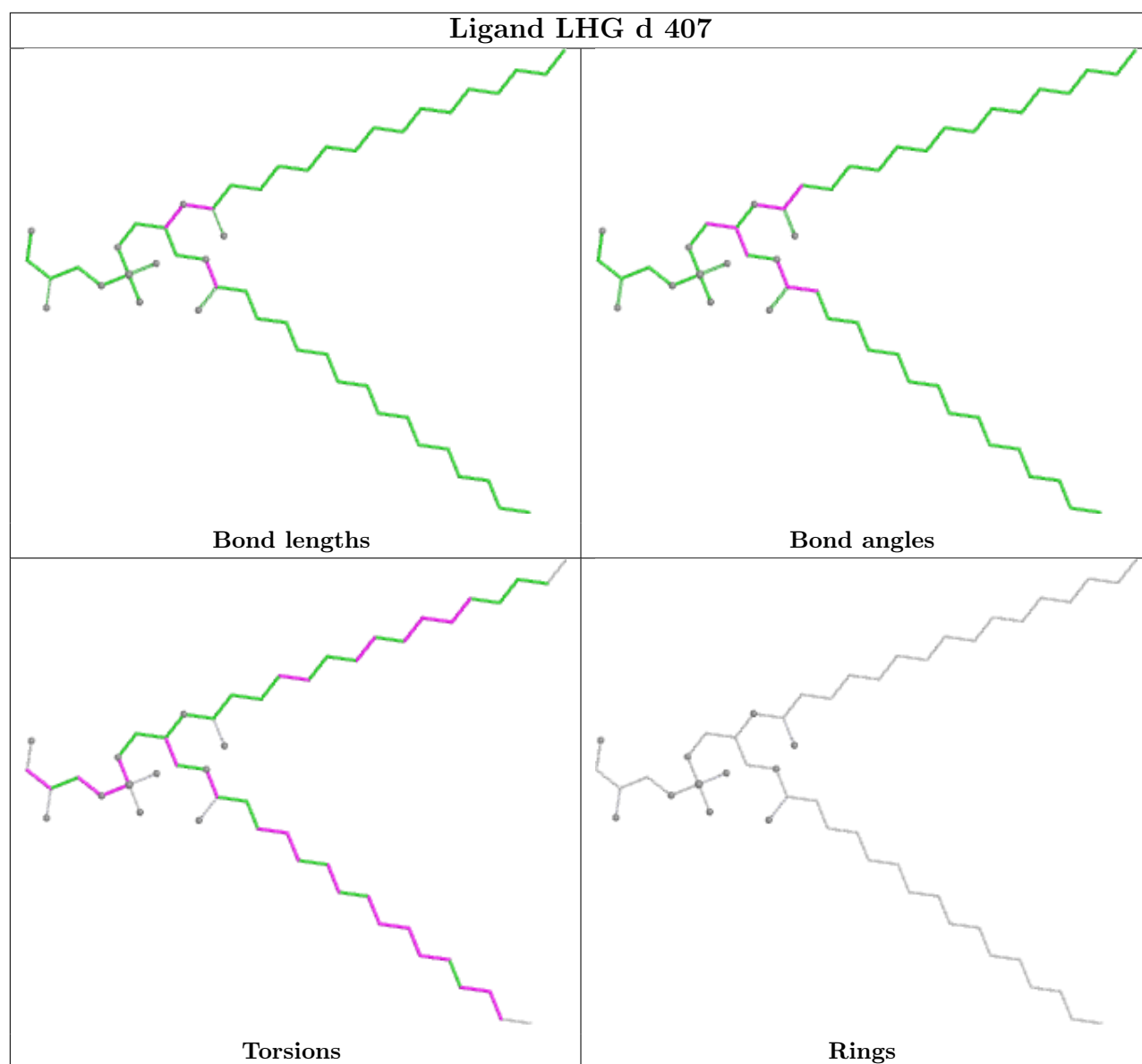


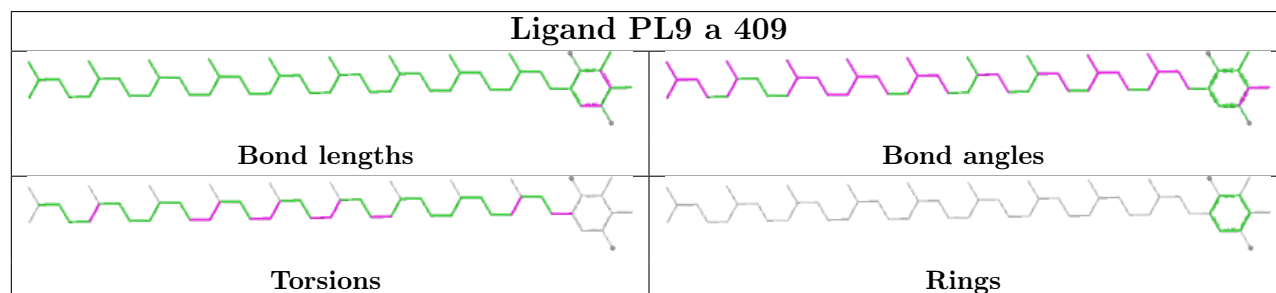
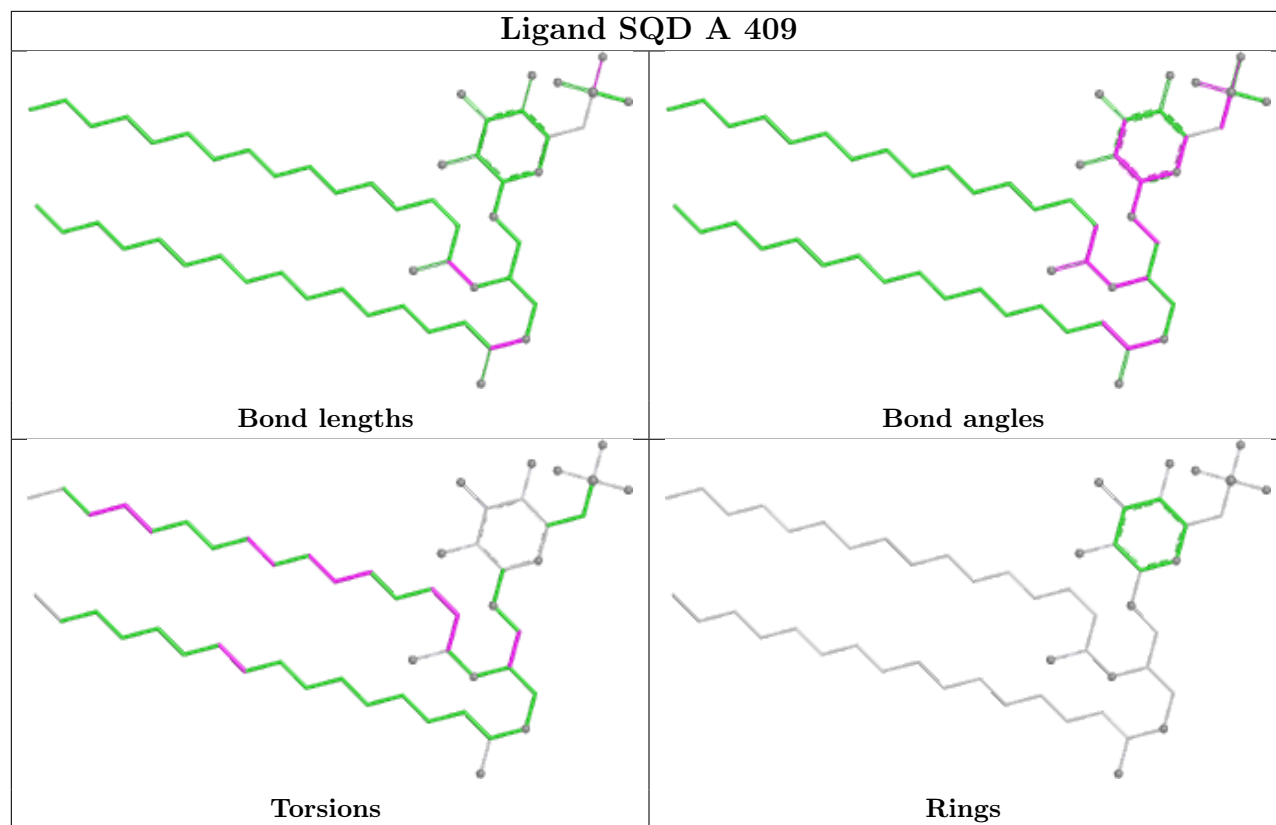


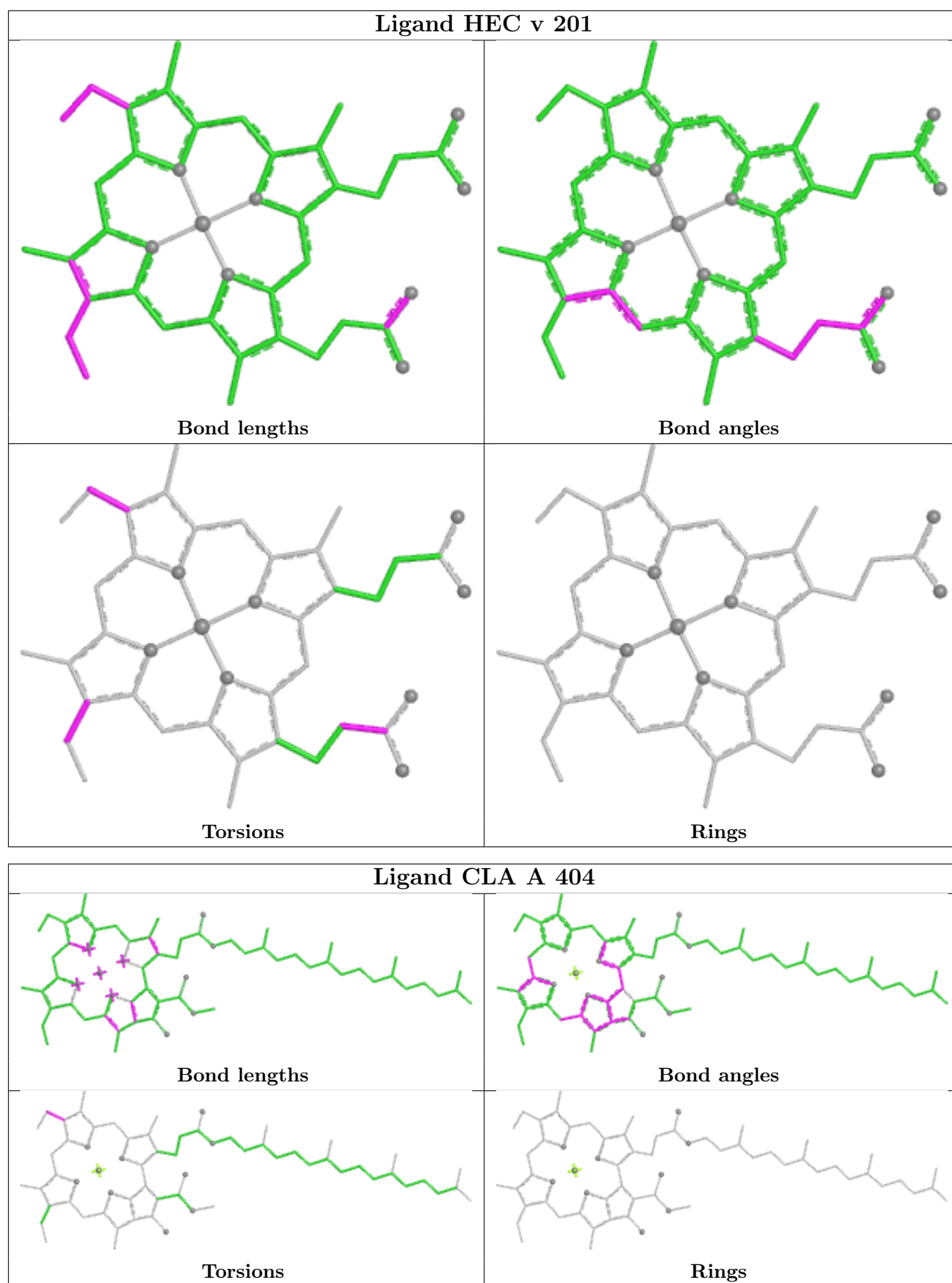


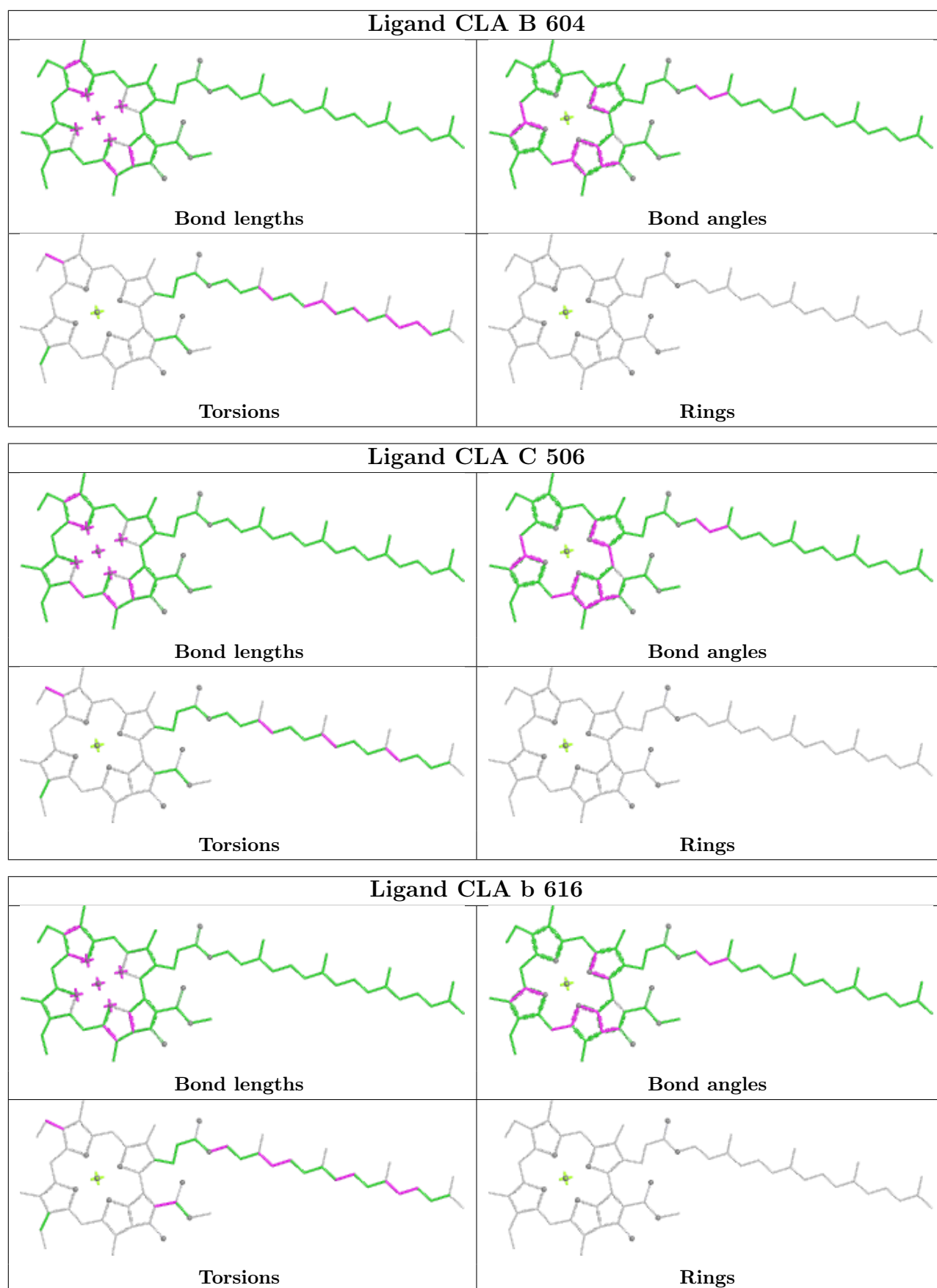


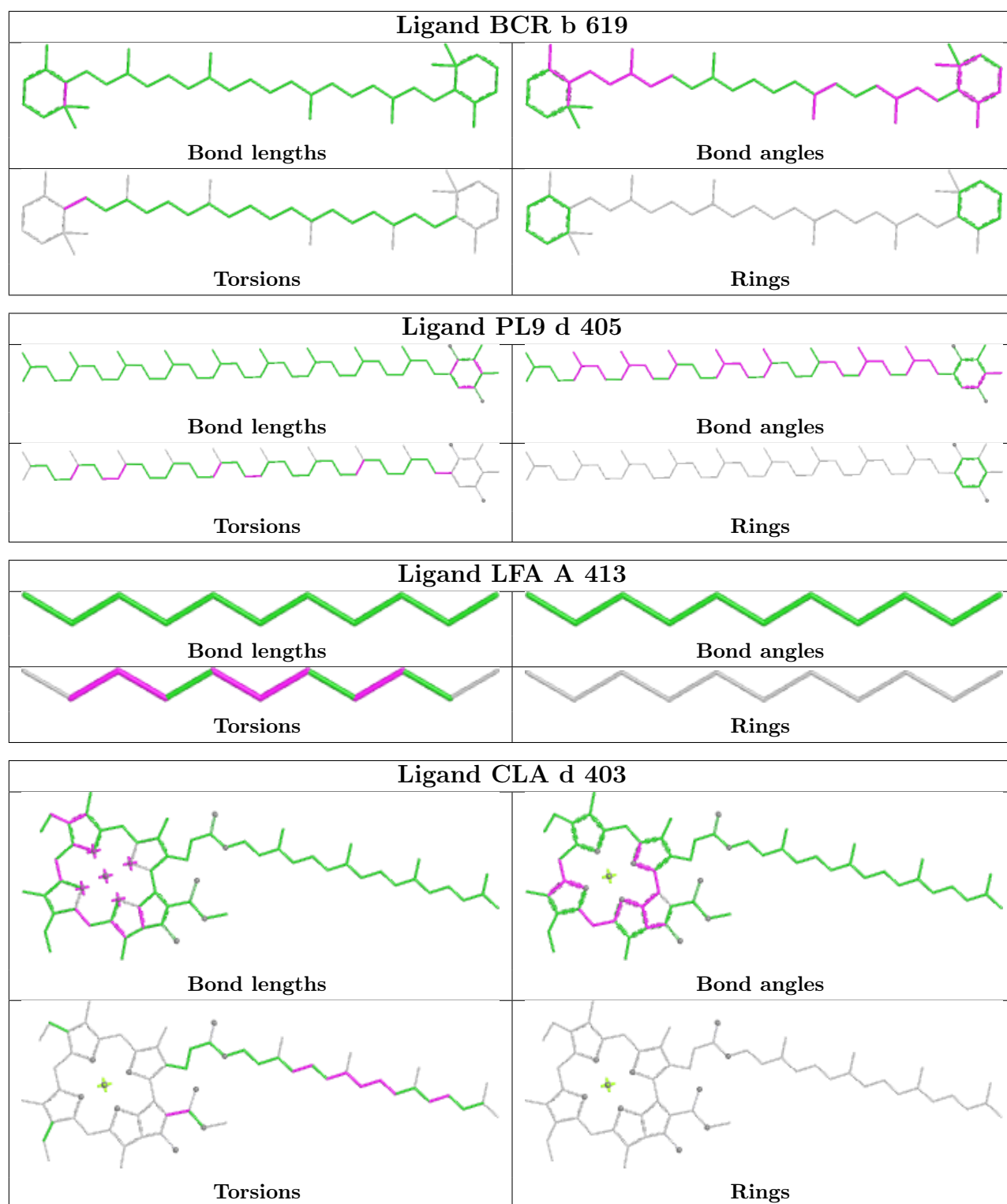


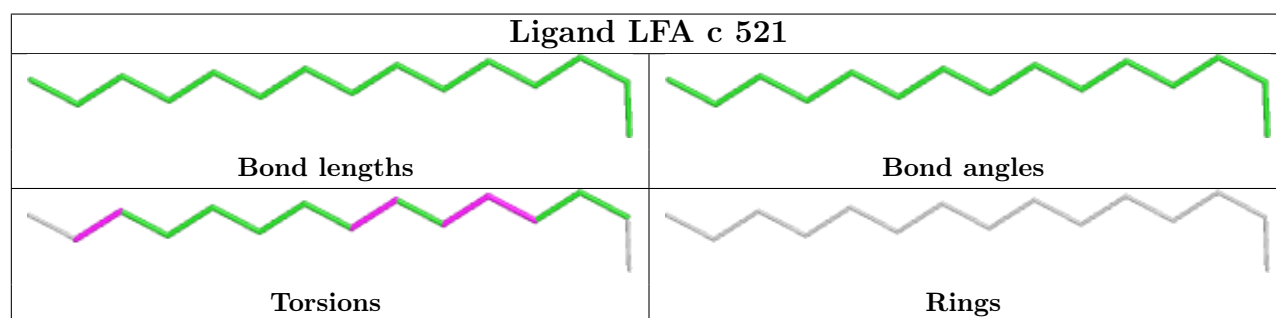
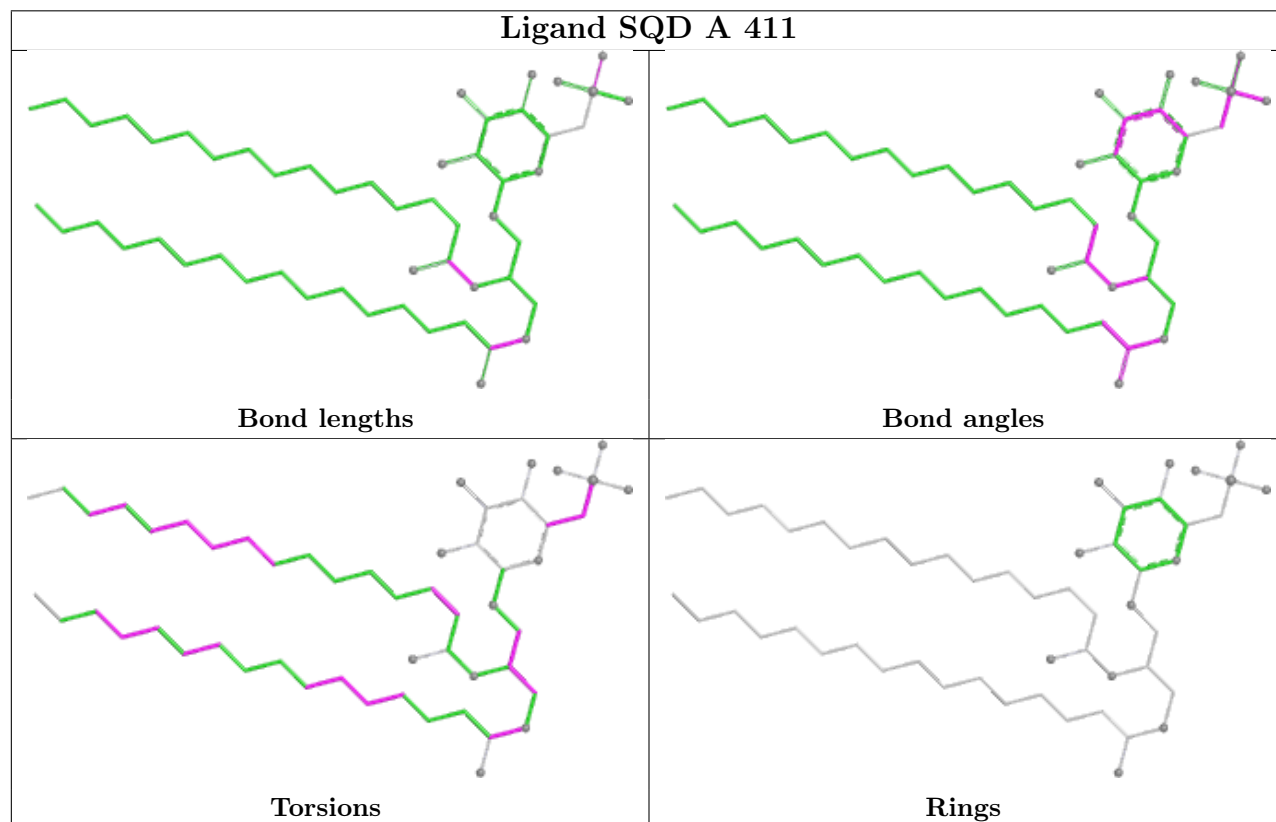
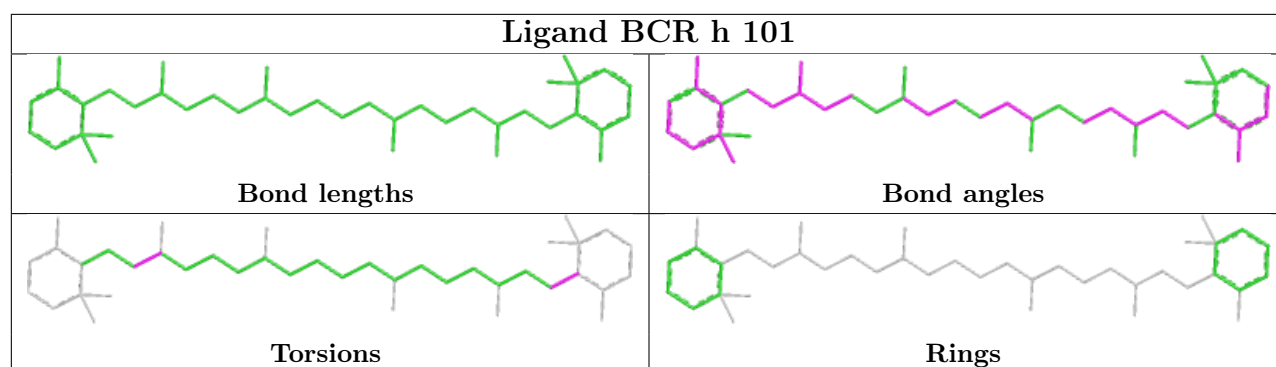


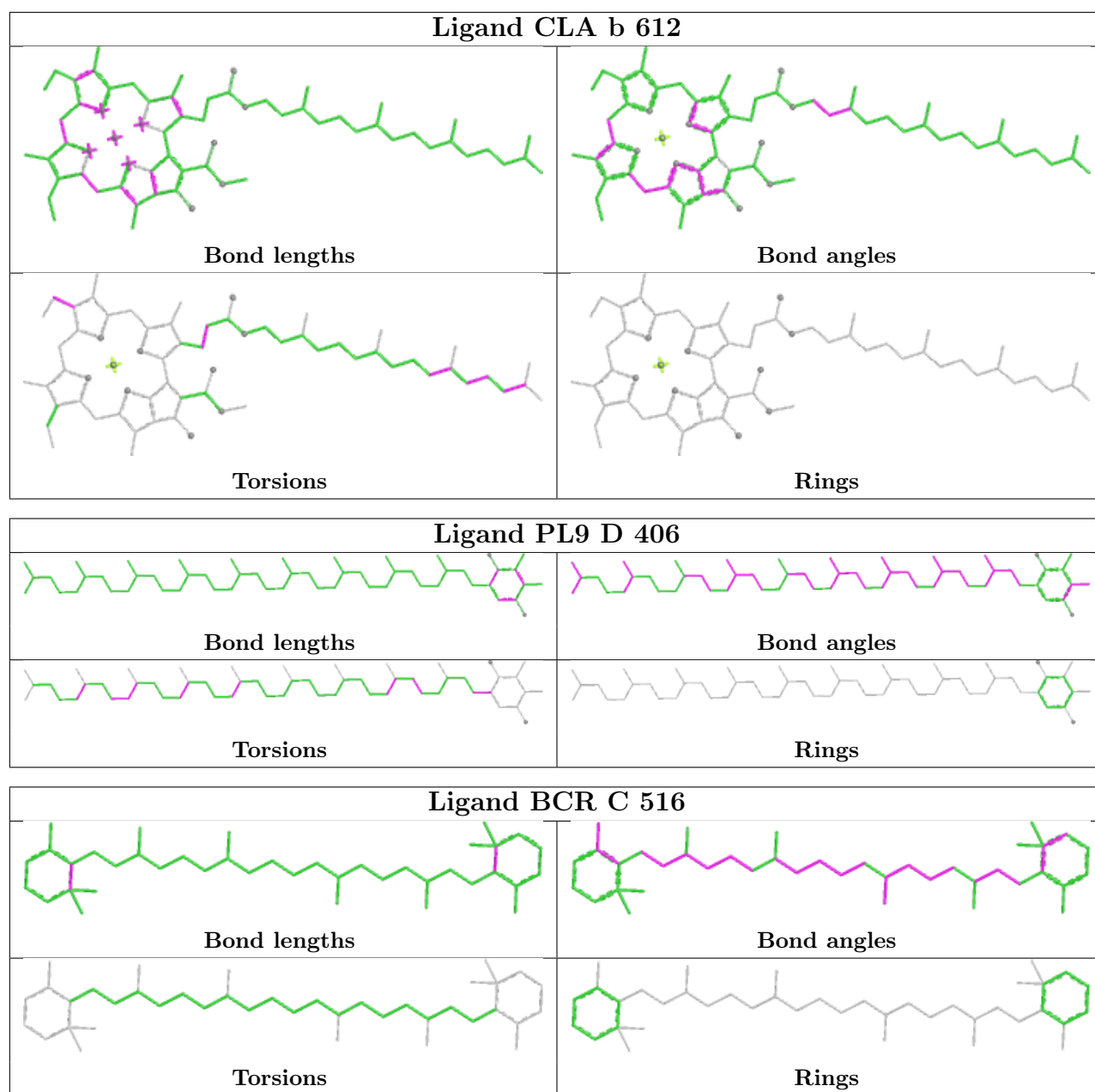


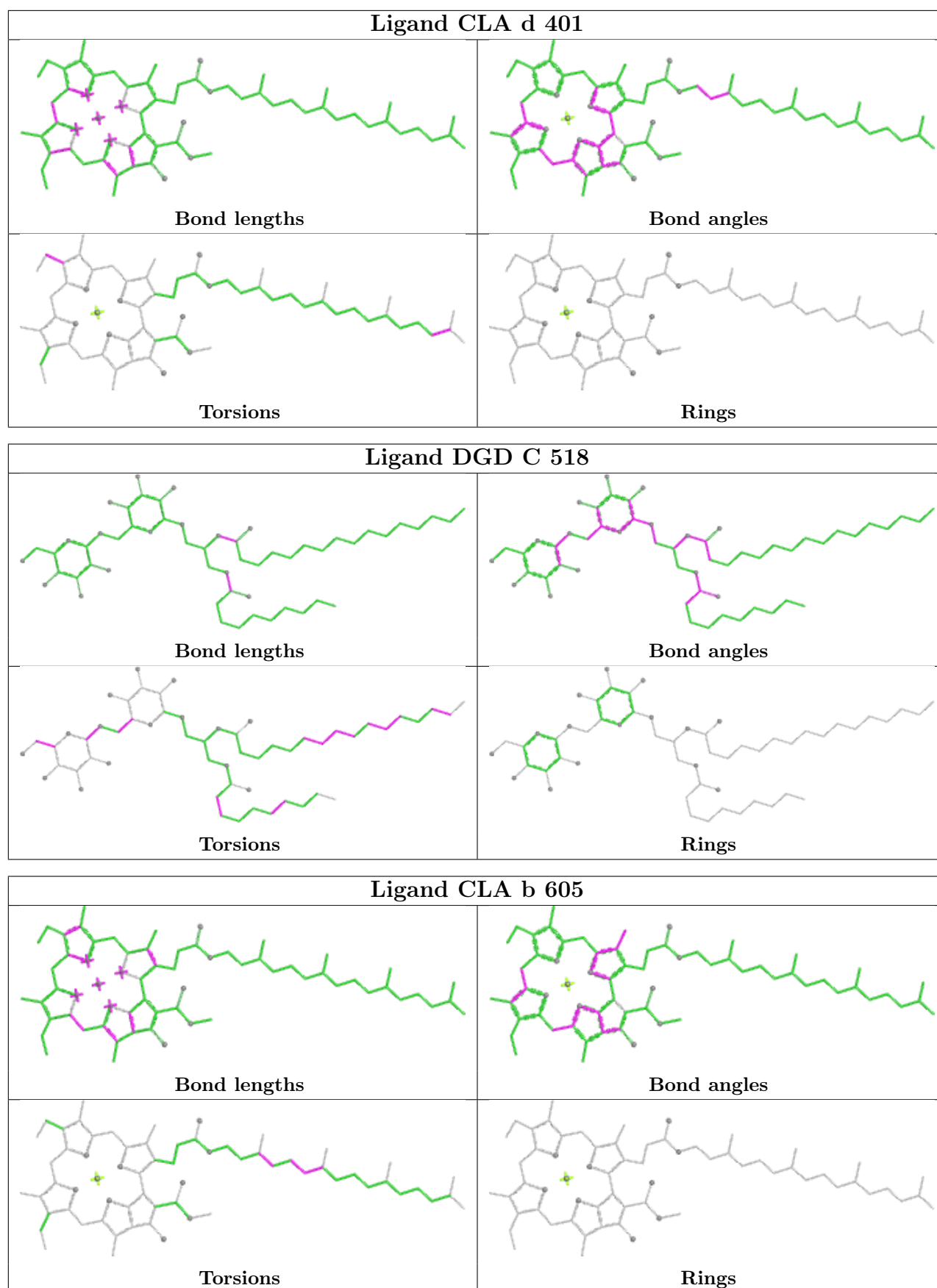


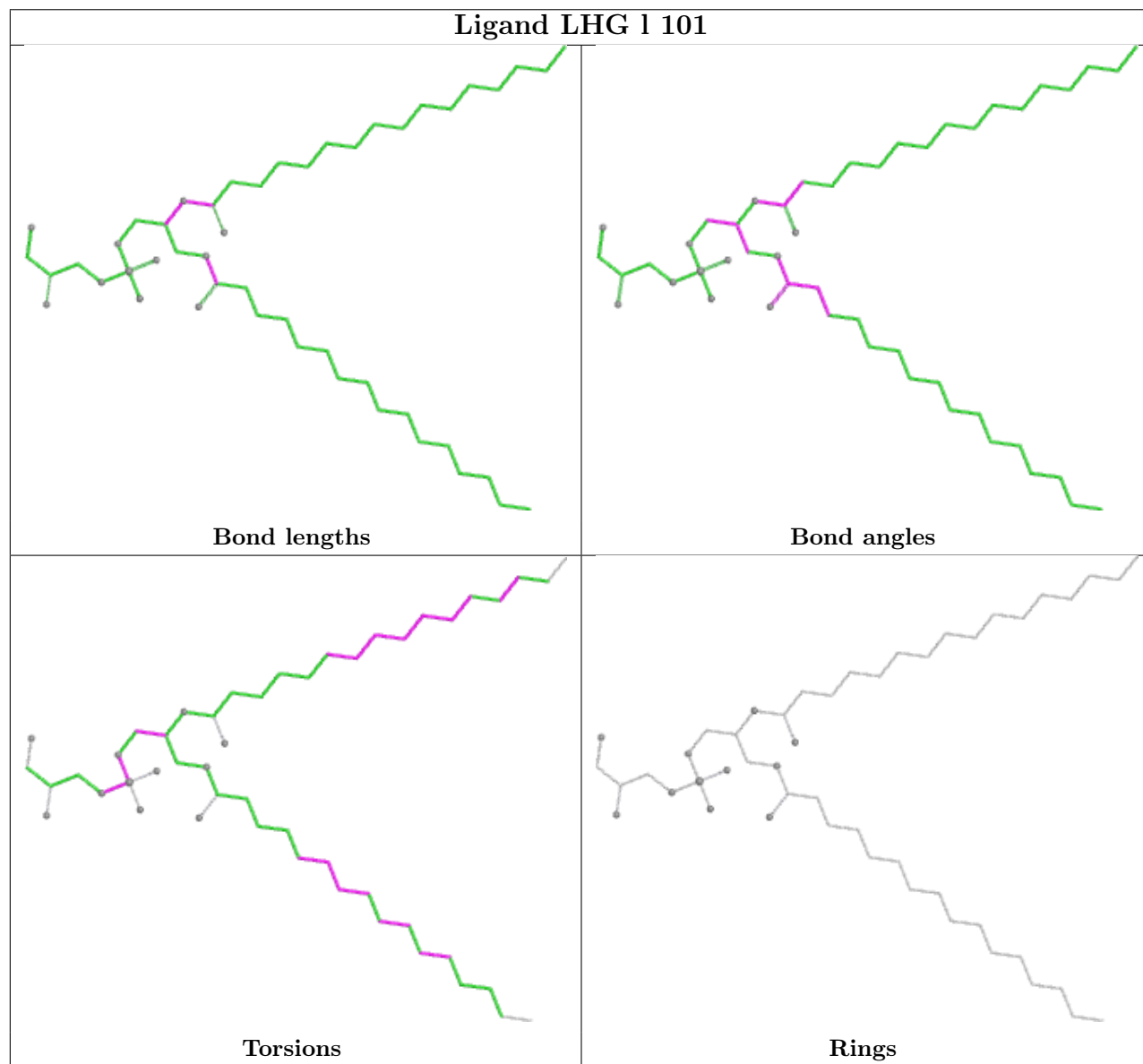
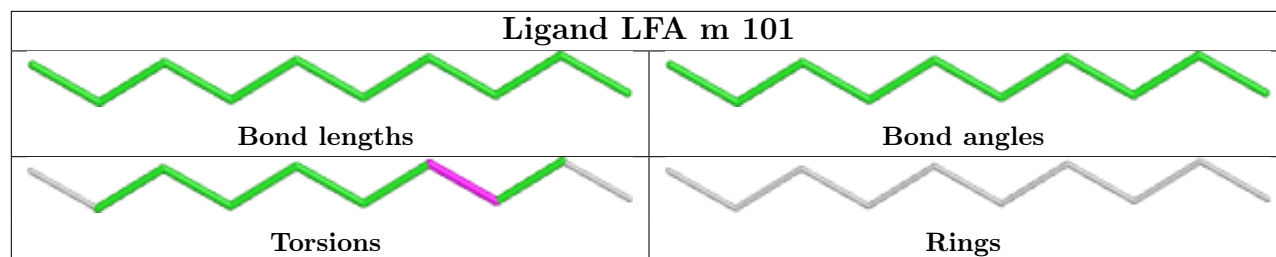


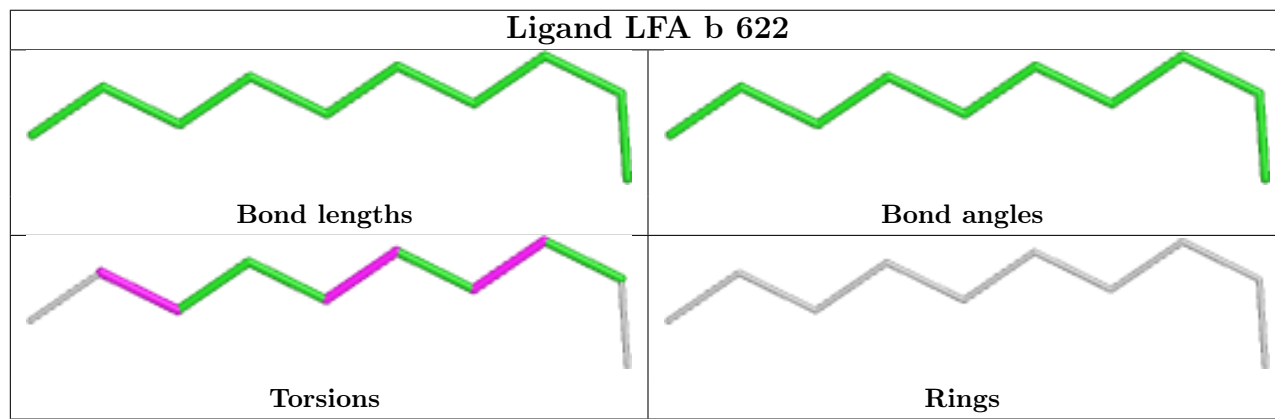
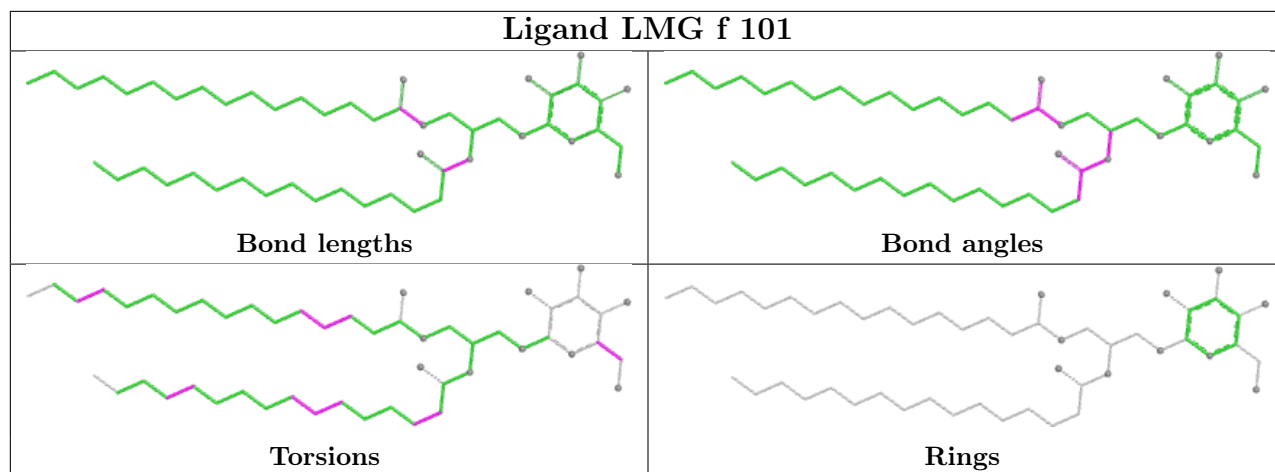












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	c	1
5	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	399:ALA	C	400:PRO	N	1.19
1	e	63:ILE	C	64:PRO	N	1.13

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	333/344 (96%)	-0.18	10 (3%) 52 49	17, 24, 47, 70	0
1	a	333/344 (96%)	-0.23	4 (1%) 76 74	16, 24, 48, 66	0
2	B	505/510 (99%)	-0.16	12 (2%) 59 56	16, 25, 55, 73	0
2	b	503/510 (98%)	-0.05	10 (1%) 65 62	19, 30, 59, 90	0
3	C	447/461 (96%)	-0.01	6 (1%) 75 73	20, 32, 50, 83	0
3	c	448/461 (97%)	-0.10	0 100 100	21, 32, 46, 67	0
4	D	340/352 (96%)	-0.28	3 (0%) 81 79	16, 25, 42, 62	0
4	d	340/352 (96%)	-0.15	2 (0%) 85 83	17, 28, 48, 67	0
5	E	81/84 (96%)	0.48	1 (1%) 76 74	29, 46, 59, 76	0
5	e	79/84 (94%)	0.74	5 (6%) 26 23	34, 50, 68, 87	0
6	F	33/45 (73%)	0.23	0 100 100	32, 39, 49, 58	0
6	f	33/45 (73%)	0.50	1 (3%) 52 49	39, 44, 61, 63	0
7	H	62/66 (93%)	-0.16	1 (1%) 70 67	25, 30, 36, 45	0
7	h	63/66 (95%)	0.35	2 (3%) 50 47	34, 39, 50, 55	0
8	I	33/38 (86%)	-0.24	0 100 100	23, 28, 35, 43	0
8	i	33/38 (86%)	-0.32	1 (3%) 52 49	21, 28, 39, 45	0
9	J	33/40 (82%)	0.27	1 (3%) 52 49	33, 41, 49, 54	0
9	j	33/40 (82%)	0.53	1 (3%) 52 49	33, 41, 49, 56	0
10	K	35/46 (76%)	0.72	4 (11%) 10 7	41, 47, 69, 76	0
10	k	36/46 (78%)	0.56	2 (5%) 30 27	35, 45, 66, 77	0
11	L	36/37 (97%)	-0.44	0 100 100	18, 22, 46, 54	0
11	l	36/37 (97%)	-0.53	0 100 100	17, 23, 43, 55	0
12	M	32/36 (88%)	-0.38	0 100 100	19, 24, 45, 51	0
12	m	32/36 (88%)	-0.22	0 100 100	20, 25, 48, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/272 (88%)	0.39	14 (5%) 29 25	24, 43, 69, 124	0
13	o	241/272 (88%)	0.31	10 (4%) 41 38	25, 39, 68, 122	0
14	T	28/32 (87%)	-0.39	0 100 100	19, 23, 42, 72	0
14	t	29/32 (90%)	-0.15	2 (6%) 23 20	20, 24, 46, 57	0
15	U	96/134 (71%)	1.07	11 (11%) 9 7	45, 61, 83, 90	0
15	u	96/134 (71%)	0.13	0 100 100	32, 40, 51, 54	0
16	V	137/163 (84%)	0.14	2 (1%) 72 69	32, 40, 50, 61	0
16	v	137/163 (84%)	0.34	0 100 100	34, 43, 59, 75	0
17	Y	21/46 (45%)	1.49	6 (28%) 1 1	54, 65, 81, 85	0
17	y	23/46 (50%)	1.26	2 (8%) 16 13	50, 58, 79, 82	0
18	X	37/41 (90%)	-0.01	1 (2%) 56 53	32, 38, 53, 65	0
18	x	38/41 (92%)	0.65	1 (2%) 57 54	38, 49, 68, 84	0
19	Z	61/62 (98%)	1.64	18 (29%) 1 1	50, 64, 121, 133	0
19	z	61/62 (98%)	1.78	21 (34%) 1 0	51, 72, 114, 128	0
20	R	35/41 (85%)	1.29	7 (20%) 3 2	49, 61, 81, 84	0
20	r	32/41 (78%)	1.71	10 (31%) 1 1	56, 65, 90, 97	0
All	All	5253/5700 (92%)	0.08	171 (3%) 49 46	16, 33, 65, 133	0

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	33	TRP	5.7
1	A	344	ALA	5.6
3	C	29	GLU	4.9
19	z	39	LEU	4.8
13	O	59	LYS	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
27	LFA	A	410	14/20	0.68	0.17	37,39,43,45	0
27	LFA	B	624	15/20	0.70	0.20	28,37,47,48	0
27	LFA	b	623	12/20	0.73	0.16	25,36,38,39	0
27	LFA	b	626	12/20	0.75	0.15	29,36,43,47	0
27	LFA	m	101	10/20	0.76	0.14	28,36,44,50	0
27	LFA	i	102	7/20	0.78	0.13	26,32,34,39	0
27	LFA	b	629	9/20	0.78	0.14	29,31,33,39	0
27	LFA	b	627	11/20	0.79	0.15	36,46,49,53	0
29	LMG	c	522	41/55	0.79	0.14	21,46,54,60	0
29	LMG	B	621	36/55	0.80	0.14	28,50,59,63	0
27	LFA	b	630	15/20	0.80	0.15	31,39,42,42	0
29	LMG	C	522	44/55	0.81	0.14	32,42,53,58	0
29	LMG	C	520	48/55	0.81	0.15	38,53,67,71	0
27	LFA	B	626	10/20	0.82	0.13	20,29,38,40	0
27	LFA	a	411	7/20	0.82	0.13	26,32,35,35	0
27	LFA	A	413	11/20	0.82	0.14	27,32,46,47	0
27	LFA	d	409	9/20	0.82	0.14	24,35,40,46	0
29	LMG	b	624	39/55	0.82	0.14	34,53,60,66	0
22	CLA	b	603	65/65	0.82	0.14	33,57,78,85	0
25	PL9	A	408	55/55	0.83	0.13	34,43,53,56	0
26	SQD	A	411	54/54	0.83	0.14	27,47,71,83	0
27	LFA	b	625	16/20	0.83	0.12	27,32,41,45	0
27	LFA	D	411	15/20	0.83	0.12	23,28,40,47	0
27	LFA	D	413	8/20	0.83	0.14	25,30,37,40	0
27	LFA	B	623	13/20	0.84	0.12	21,31,34,36	0
29	LMG	C	501	51/55	0.84	0.12	26,40,50,53	0
27	LFA	B	628	12/20	0.84	0.11	23,28,37,37	0
27	LFA	i	101	16/20	0.84	0.12	23,32,40,41	0
27	LFA	b	622	10/20	0.84	0.11	27,31,37,38	0
26	SQD	b	601	54/54	0.84	0.11	25,39,62,65	0
27	LFA	B	627	14/20	0.85	0.12	20,31,36,39	0
27	LFA	j	101	15/20	0.85	0.15	41,45,51,56	0
29	LMG	c	519	51/55	0.85	0.15	38,52,64,67	0
26	SQD	L	101	48/54	0.85	0.11	21,42,66,69	0
32	LHG	E	101	42/49	0.85	0.12	31,54,67,71	0
32	LHG	e	101	42/49	0.85	0.14	40,62,80,94	0
27	LFA	d	408	15/20	0.86	0.11	25,32,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LFA	b	602	15/20	0.86	0.12	29,33,42,42	0
26	SQD	a	412	50/54	0.86	0.13	28,43,70,76	0
27	LFA	M	102	16/20	0.86	0.12	25,27,46,47	0
25	PL9	a	409	55/55	0.86	0.14	38,48,59,65	0
27	LFA	J	101	11/20	0.87	0.12	38,43,49,49	0
26	SQD	f	102	43/54	0.87	0.16	51,66,77,86	0
27	LFA	d	410	16/20	0.87	0.11	28,35,44,45	0
27	LFA	T	102	12/20	0.87	0.09	22,28,32,32	0
24	BCR	c	524	40/40	0.88	0.12	36,43,53,53	0
27	LFA	I	101	14/20	0.88	0.10	21,29,32,32	0
22	CLA	H	101	65/65	0.88	0.10	30,45,64,72	0
24	BCR	K	101	40/40	0.88	0.12	37,48,53,55	0
29	LMG	c	501	51/55	0.88	0.10	25,39,51,60	0
27	LFA	c	520	9/20	0.88	0.11	31,39,46,47	0
27	LFA	c	521	15/20	0.88	0.10	31,35,41,41	0
29	LMG	B	619	51/55	0.88	0.10	15,31,42,47	0
27	LFA	B	625	9/20	0.88	0.11	20,25,27,33	0
27	LFA	B	622	16/20	0.89	0.09	27,32,36,37	0
27	LFA	m	102	15/20	0.89	0.10	25,29,37,37	0
27	LFA	t	101	15/20	0.89	0.11	25,31,42,43	0
26	SQD	D	412	43/54	0.89	0.12	38,50,58,69	0
24	BCR	h	101	40/40	0.89	0.10	28,40,45,49	0
29	LMG	m	103	51/55	0.89	0.10	17,30,41,45	0
26	SQD	a	410	54/54	0.89	0.12	30,48,58,62	0
24	BCR	T	101	40/40	0.89	0.09	22,29,34,37	0
27	LFA	C	521	15/20	0.90	0.10	26,34,39,42	0
22	CLA	C	514	65/65	0.90	0.11	37,49,63,67	0
21	CL	A	401	1/1	0.90	0.11	57,57,57,57	0
27	LFA	D	414	10/20	0.90	0.09	22,23,26,28	0
22	CLA	C	511	65/65	0.90	0.09	25,34,41,49	0
24	BCR	C	515	40/40	0.90	0.10	36,45,52,55	0
30	DGD	h	102	62/66	0.90	0.10	23,33,40,45	0
27	LFA	B	620	10/20	0.90	0.10	22,24,28,33	0
22	CLA	C	513	65/65	0.90	0.10	34,41,54,63	0
24	BCR	c	523	40/40	0.91	0.10	39,46,52,55	0
22	CLA	c	514	65/65	0.91	0.11	33,45,61,67	0
30	DGD	C	518	56/66	0.91	0.10	29,38,48,53	0
24	BCR	d	404	40/40	0.91	0.10	25,36,53,56	0
22	CLA	c	513	65/65	0.91	0.10	36,42,55,62	0
24	BCR	k	101	40/40	0.91	0.10	29,43,51,54	0
24	BCR	C	516	40/40	0.92	0.08	21,30,37,38	0
24	BCR	D	405	40/40	0.92	0.09	23,33,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	t	102	40/40	0.92	0.09	21,26,38,40	0
22	CLA	b	608	65/65	0.92	0.09	22,29,42,53	0
25	PL9	D	406	55/55	0.92	0.09	12,21,26,28	0
24	BCR	K	102	40/40	0.92	0.10	39,44,47,48	0
29	LMG	f	101	51/55	0.92	0.10	31,38,55,61	0
26	SQD	A	409	54/54	0.92	0.11	24,42,54,56	0
22	CLA	b	618	65/65	0.92	0.11	23,32,58,64	0
30	DGD	H	103	60/66	0.92	0.09	22,29,40,45	0
22	CLA	C	507	65/65	0.92	0.09	22,30,55,57	0
32	LHG	D	409	49/49	0.92	0.11	16,33,53,57	0
22	CLA	C	503	65/65	0.92	0.08	24,32,36,38	0
22	CLA	C	504	65/65	0.92	0.08	20,35,38,42	0
29	LMG	D	410	51/55	0.93	0.10	25,36,51,54	0
24	BCR	B	616	40/40	0.93	0.07	19,25,31,32	0
24	BCR	B	617	40/40	0.93	0.07	15,24,30,30	0
24	BCR	B	618	40/40	0.93	0.07	18,26,34,36	0
22	CLA	C	512	65/65	0.93	0.09	35,44,52,56	0
22	CLA	c	504	65/65	0.93	0.08	26,34,39,40	0
22	CLA	c	507	65/65	0.93	0.09	25,32,52,58	0
24	BCR	H	102	40/40	0.93	0.08	22,28,42,43	0
30	DGD	C	519	62/66	0.93	0.09	27,33,46,60	0
22	CLA	c	510	65/65	0.93	0.09	22,31,38,40	0
30	DGD	c	517	55/66	0.93	0.09	25,34,50,63	0
30	DGD	c	518	62/66	0.93	0.09	26,32,52,58	0
22	CLA	B	615	65/65	0.93	0.10	19,25,70,79	0
22	CLA	C	505	65/65	0.93	0.09	28,35,48,61	0
24	BCR	b	619	40/40	0.93	0.08	18,28,34,35	0
32	LHG	d	407	49/49	0.93	0.12	21,37,60,63	0
24	BCR	b	620	40/40	0.93	0.07	18,25,30,32	0
22	CLA	b	611	65/65	0.94	0.08	23,30,40,52	0
22	CLA	b	616	65/65	0.94	0.08	20,26,39,42	0
22	CLA	C	508	65/65	0.94	0.07	21,26,35,45	0
22	CLA	c	502	65/65	0.94	0.08	17,28,35,38	0
22	CLA	C	509	65/65	0.94	0.09	22,31,62,66	0
25	PL9	d	405	55/55	0.94	0.07	16,23,27,30	0
22	CLA	c	505	65/65	0.94	0.09	21,33,49,53	0
22	CLA	C	510	65/65	0.94	0.08	25,31,39,40	0
22	CLA	c	508	65/65	0.94	0.07	22,30,34,37	0
30	DGD	C	517	62/66	0.94	0.09	20,26,49,52	0
22	CLA	B	605	65/65	0.94	0.07	17,25,38,44	0
22	CLA	c	511	65/65	0.94	0.07	27,32,38,44	0
22	CLA	c	512	65/65	0.94	0.08	28,39,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	DGD	c	516	62/66	0.94	0.09	23,28,49,52	0
27	LFA	M	101	10/20	0.94	0.08	26,31,41,42	0
24	BCR	b	621	40/40	0.94	0.08	23,34,42,47	0
24	BCR	c	515	40/40	0.94	0.07	19,29,38,41	0
31	BCT	D	401	4/4	0.94	0.08	25,29,31,32	0
32	LHG	D	407	49/49	0.94	0.08	17,24,30,33	0
22	CLA	b	604	65/65	0.94	0.08	25,30,41,46	0
22	CLA	C	502	65/65	0.94	0.08	18,24,33,35	0
32	LHG	b	628	49/49	0.94	0.08	22,27,35,49	0
22	CLA	d	403	65/65	0.94	0.09	22,30,57,63	0
22	CLA	b	610	65/65	0.94	0.08	22,28,37,45	0
32	LHG	l	101	49/49	0.94	0.07	17,25,34,39	0
33	HEM	E	102	43/43	0.94	0.11	34,43,52,54	0
33	HEM	e	102	43/43	0.94	0.11	37,48,57,60	0
22	CLA	a	404	65/65	0.95	0.07	14,20,27,36	0
22	CLA	a	405	65/65	0.95	0.07	14,19,25,31	0
22	CLA	c	506	65/65	0.95	0.07	21,26,37,40	0
22	CLA	B	613	65/65	0.95	0.08	18,25,46,57	0
24	BCR	a	408	40/40	0.95	0.06	18,22,29,31	0
22	CLA	A	412	65/65	0.95	0.06	16,20,25,27	0
22	CLA	c	509	65/65	0.95	0.09	24,30,59,66	0
22	CLA	b	606	65/65	0.95	0.07	16,23,38,45	0
22	CLA	b	607	65/65	0.95	0.07	18,23,30,32	0
22	CLA	B	602	65/65	0.95	0.07	18,21,35,38	0
22	CLA	B	604	65/65	0.95	0.06	15,21,25,29	0
22	CLA	A	404	65/65	0.95	0.08	15,23,61,72	0
22	CLA	d	401	65/65	0.95	0.09	18,27,63,69	0
22	CLA	d	402	65/65	0.95	0.07	17,20,37,40	0
22	CLA	b	613	65/65	0.95	0.07	18,23,29,31	0
31	BCT	a	413	4/4	0.95	0.08	31,33,34,40	0
23	PHO	A	405	64/64	0.95	0.06	15,21,28,31	0
23	PHO	a	406	64/64	0.95	0.06	13,17,25,27	0
24	BCR	A	407	40/40	0.95	0.06	14,23,30,31	0
32	LHG	L	102	49/49	0.95	0.07	18,24,31,34	0
22	CLA	b	614	65/65	0.95	0.07	16,23,28,32	0
22	CLA	b	615	65/65	0.95	0.07	16,21,36,39	0
22	CLA	B	610	65/65	0.95	0.06	12,18,24,29	0
22	CLA	b	617	65/65	0.95	0.07	21,27,39,50	0
22	CLA	C	506	65/65	0.95	0.07	17,27,32,40	0
22	CLA	B	611	65/65	0.95	0.07	14,19,25,28	0
22	CLA	D	403	65/65	0.96	0.06	13,18,26,35	0
22	CLA	D	404	65/65	0.96	0.09	17,24,62,66	0

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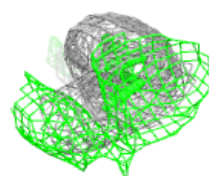
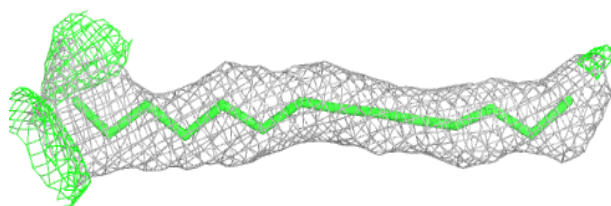
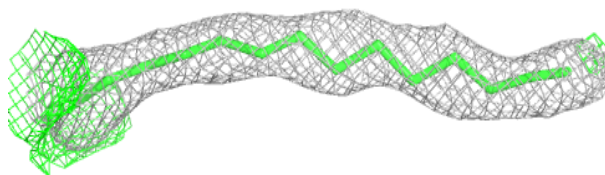
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	609	65/65	0.96	0.06	15,20,27,29	0
21	CL	A	402	1/1	0.96	0.12	57,57,57,57	0
22	CLA	B	603	65/65	0.96	0.06	14,21,35,44	0
22	CLA	a	407	65/65	0.96	0.08	13,19,56,60	0
23	PHO	D	402	64/64	0.96	0.06	14,18,25,28	0
22	CLA	B	612	65/65	0.96	0.06	13,18,40,43	0
23	PHO	a	414	64/64	0.96	0.06	21,28,33,39	0
22	CLA	c	503	65/65	0.96	0.06	23,30,38,39	0
32	LHG	D	408	49/49	0.96	0.07	18,24,30,37	0
22	CLA	A	403	65/65	0.96	0.06	12,18,23,30	0
22	CLA	b	605	65/65	0.96	0.07	18,22,37,49	0
22	CLA	B	614	65/65	0.96	0.06	15,22,32,47	0
22	CLA	B	601	65/65	0.96	0.07	17,26,32,36	0
32	LHG	d	406	49/49	0.96	0.07	18,24,32,36	0
22	CLA	B	606	65/65	0.96	0.06	10,18,33,37	0
22	CLA	b	609	65/65	0.96	0.06	11,21,29,32	0
22	CLA	B	607	65/65	0.96	0.06	13,19,26,34	0
22	CLA	B	608	65/65	0.96	0.06	15,24,33,36	0
22	CLA	b	612	65/65	0.96	0.07	16,25,31,33	0
34	HEC	V	201	43/43	0.96	0.09	28,36,41,45	0
22	CLA	A	406	65/65	0.97	0.08	11,20,54,60	0
21	CL	a	402	1/1	0.97	0.08	52,52,52,52	0
21	CL	a	403	1/1	0.97	0.11	40,40,40,40	0
34	HEC	v	201	43/43	0.97	0.07	28,34,38,41	0
28	FE	A	414	1/1	0.98	0.03	26,26,26,26	0
28	FE	a	401	1/1	0.99	0.05	39,39,39,39	0

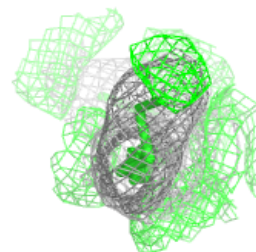
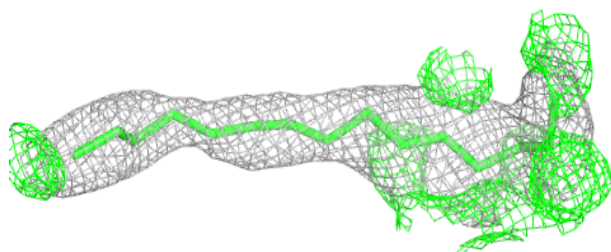
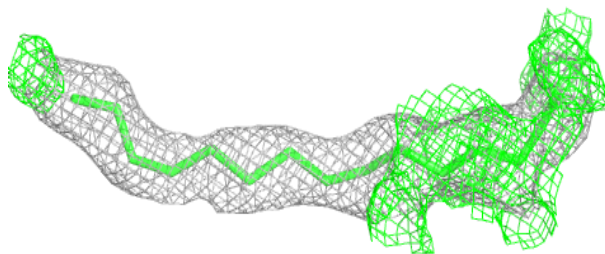
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA 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)

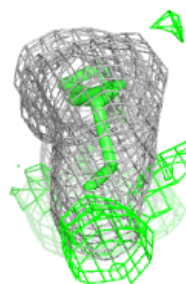
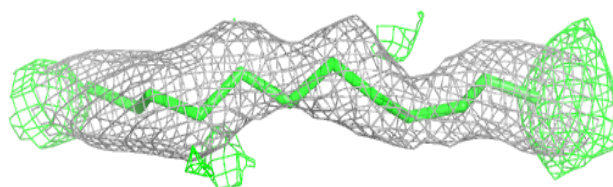
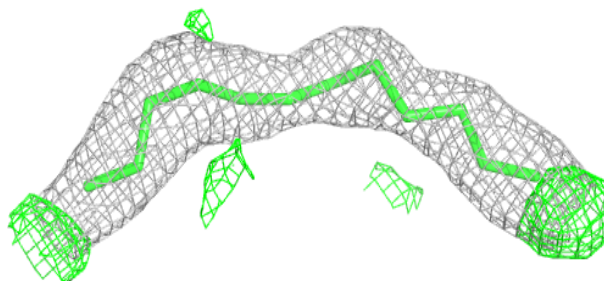
**Electron density around LFA B 624:**

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

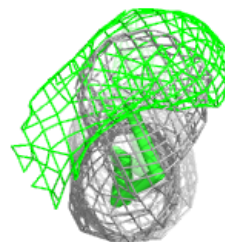
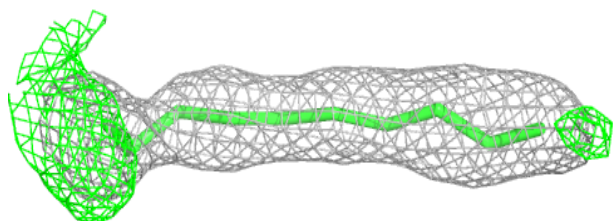
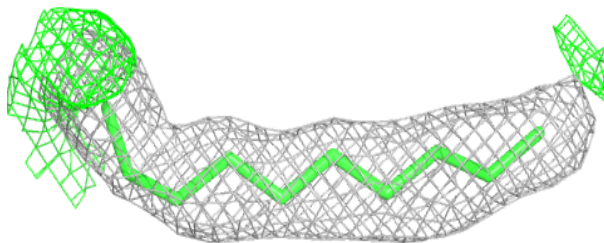


Electron density around LFA b 626:

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

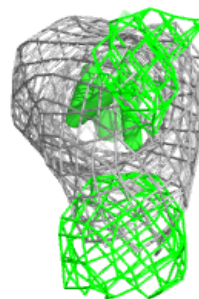
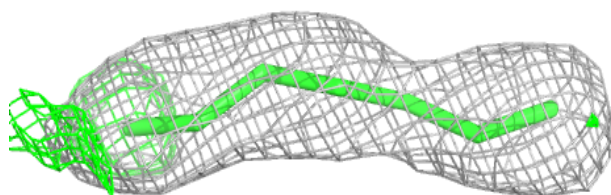
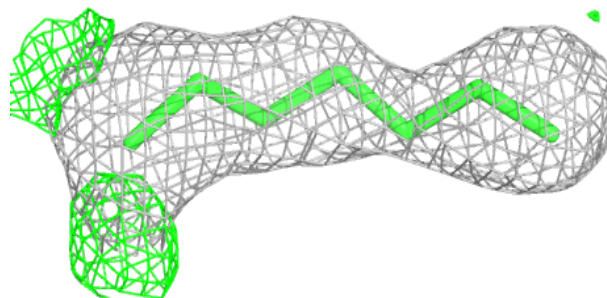
**Electron density around LFA m 101:**

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

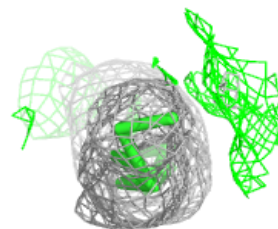
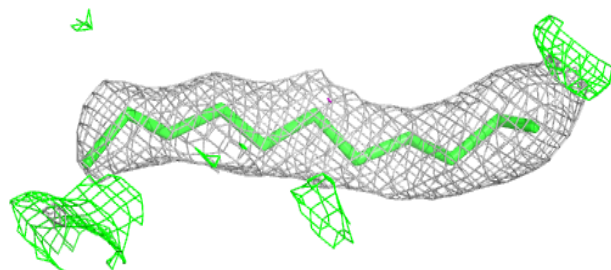
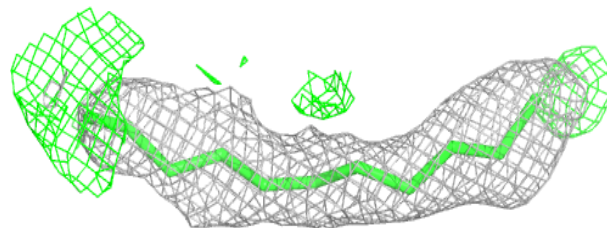


Electron density around LFA i 102:

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

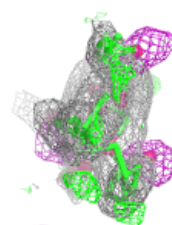
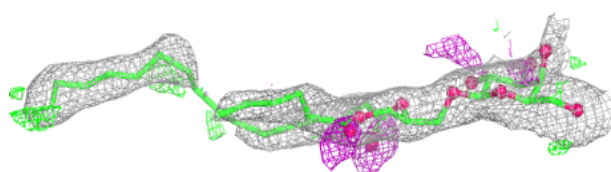
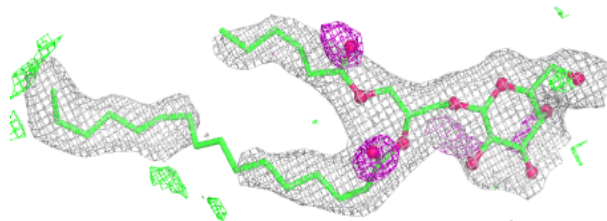
**Electron density around LFA b 627:**

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

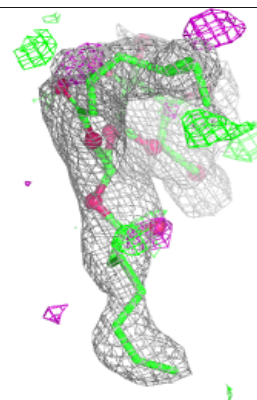
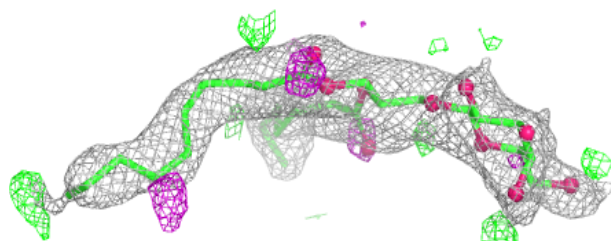
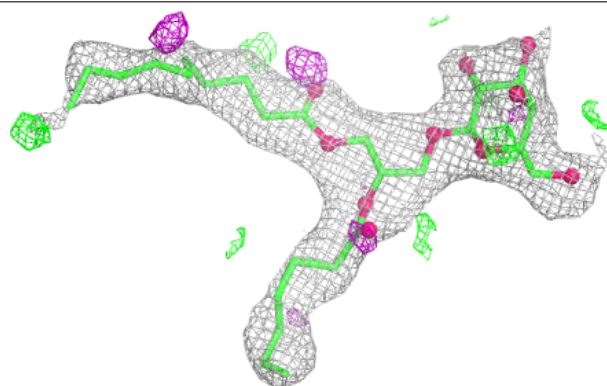


Electron density around LMG c 522:

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

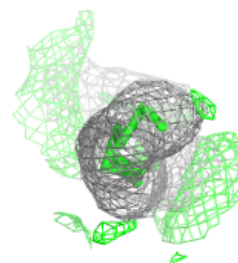
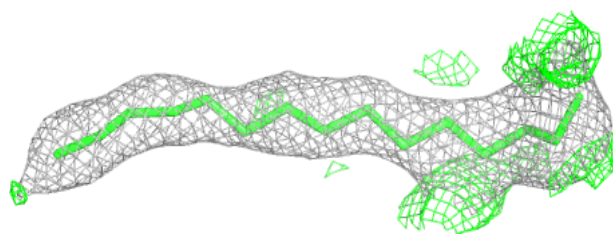
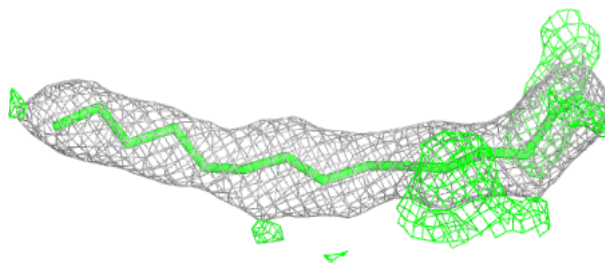
**Electron density around LMG B 621:**

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

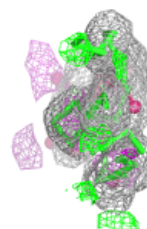
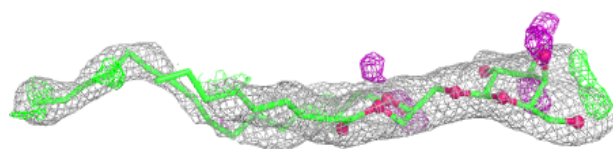
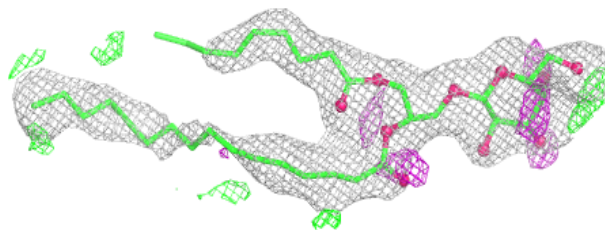


Electron density around LFA b 630:

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

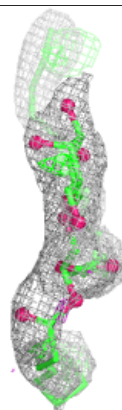
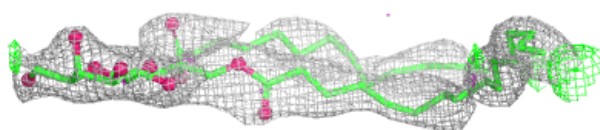
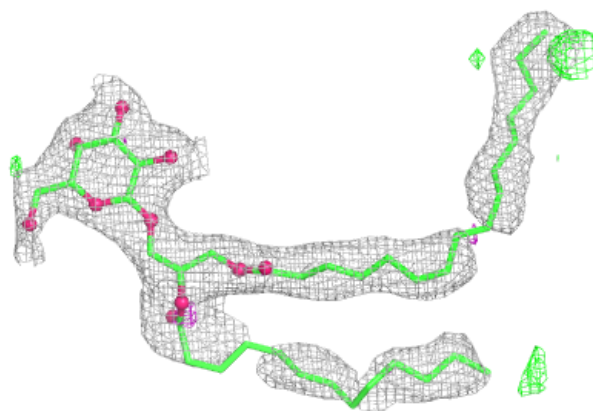
**Electron density around LMG C 522:**

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

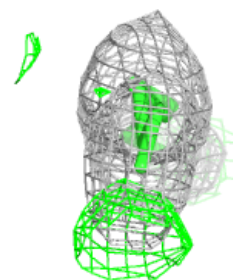
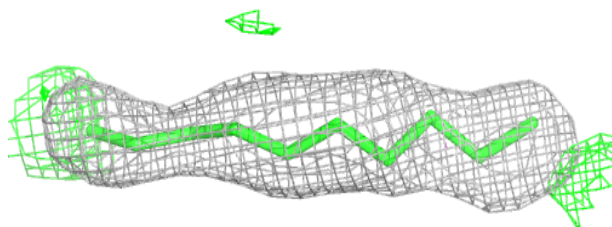
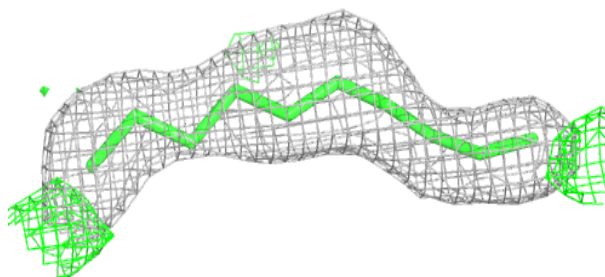


Electron density around LMG C 520:

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

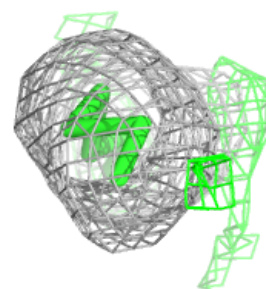
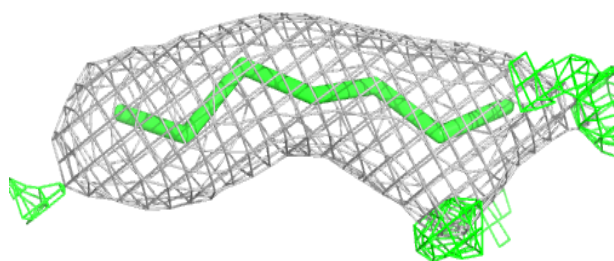
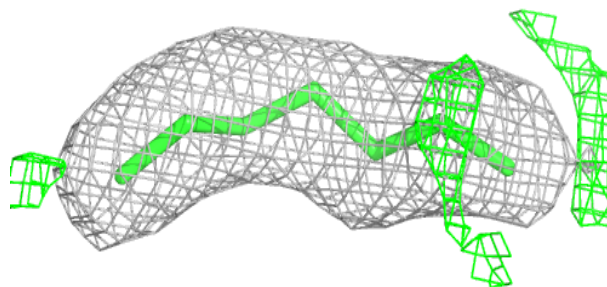
**Electron density around LFA B 626:**

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

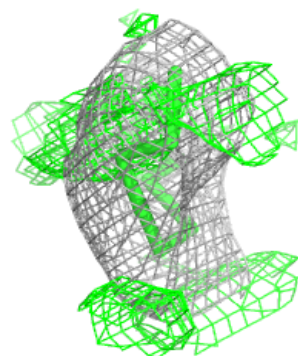
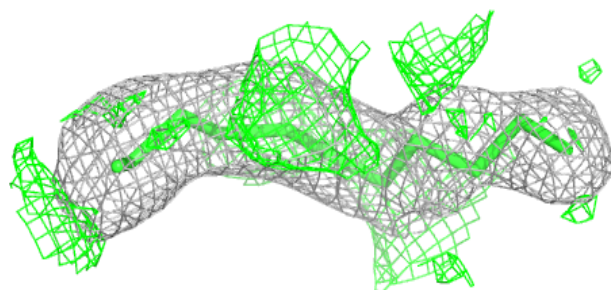
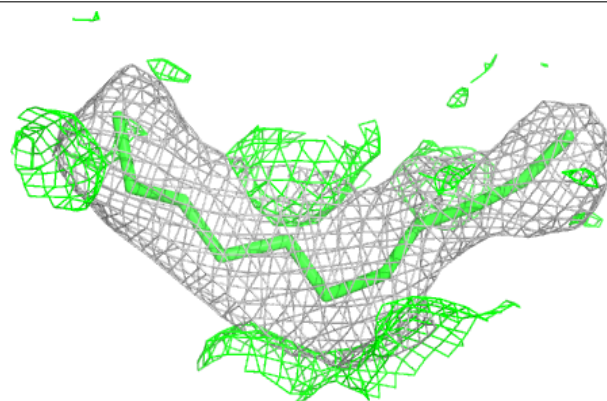


Electron density around LFA a 411:

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

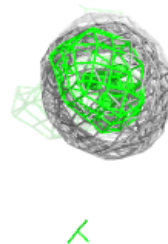
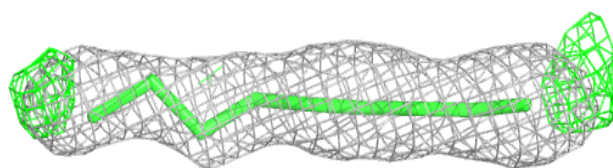
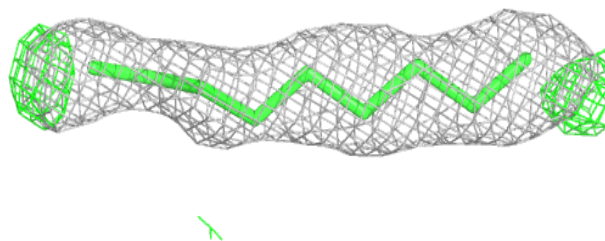
**Electron density around LFA A 413:**

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

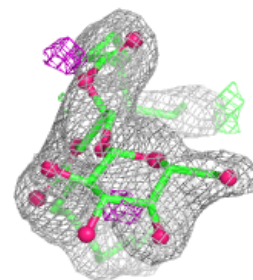
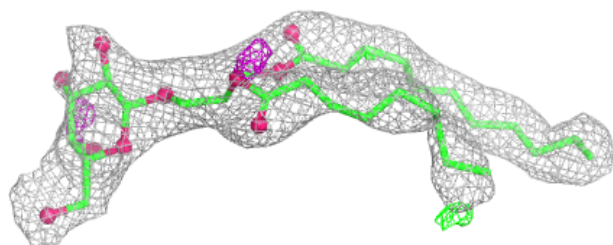
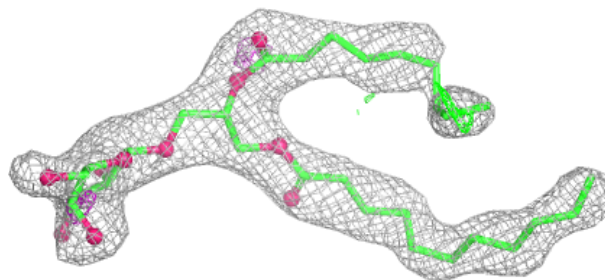


Electron density around LFA d 409:

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

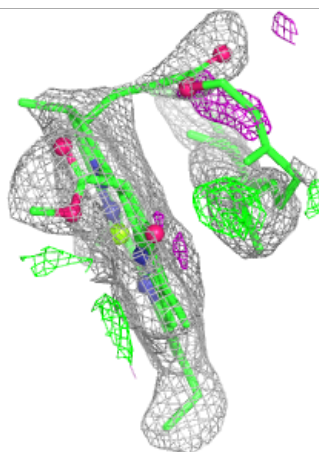
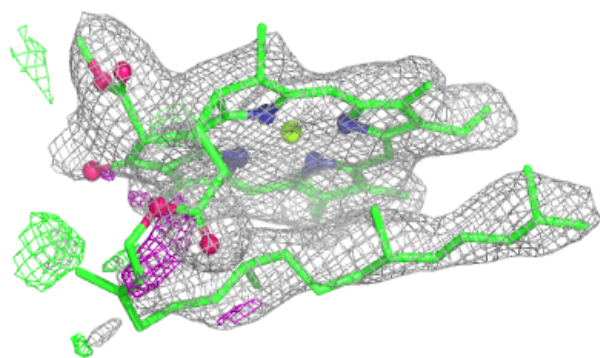
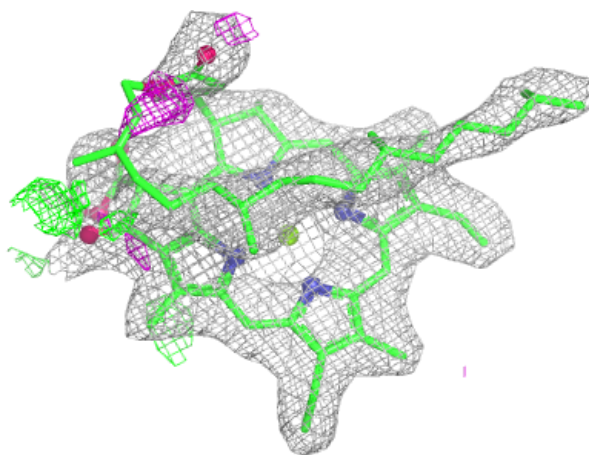
**Electron density around LMG b 624:**

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



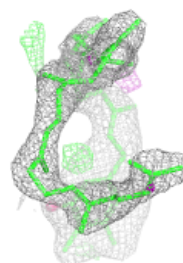
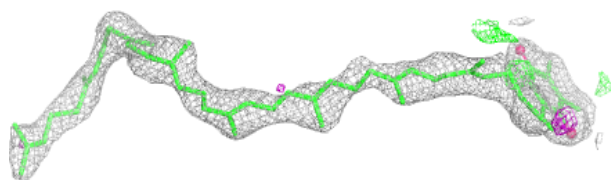
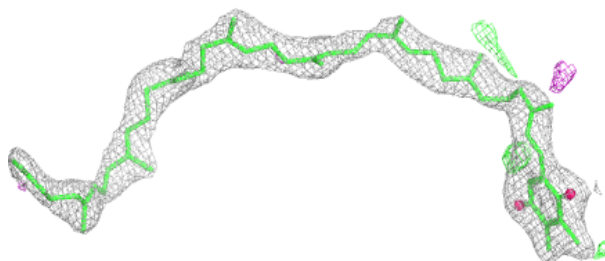
Electron density around CLA b 603:

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

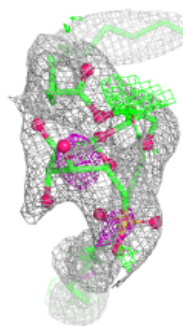
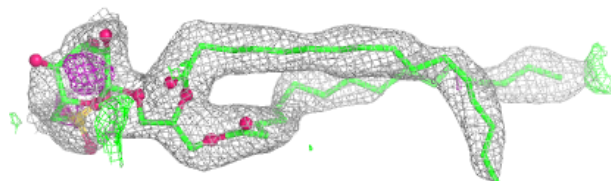
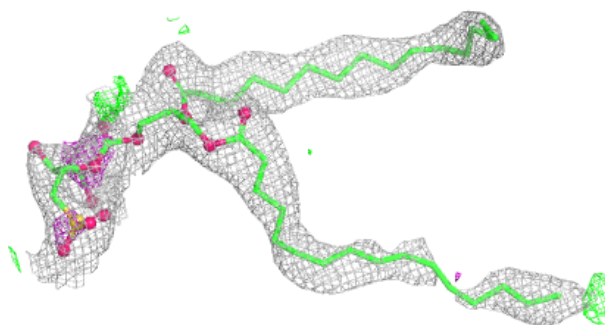


Electron density around PL9 A 408:

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

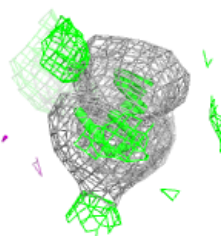
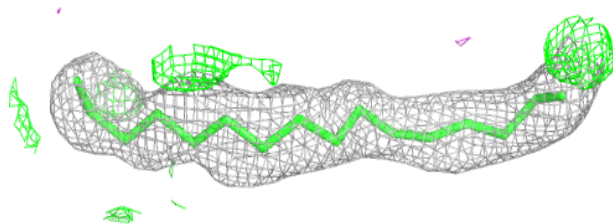
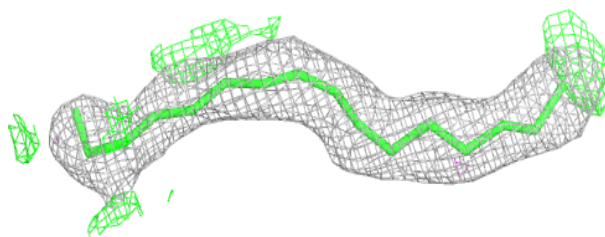
**Electron density around SQD A 411:**

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

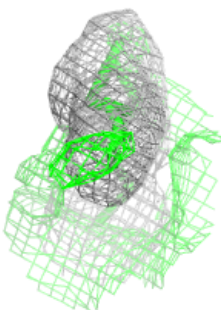
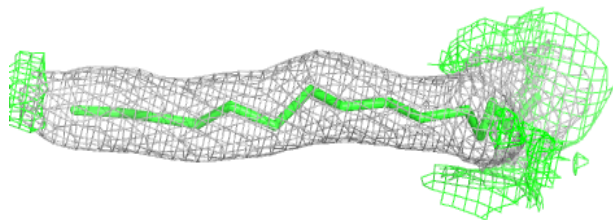
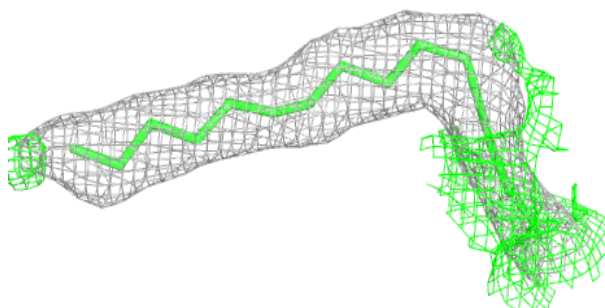


Electron density around LFA b 625:

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

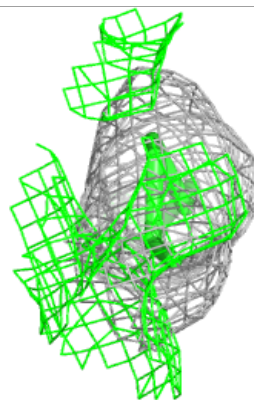
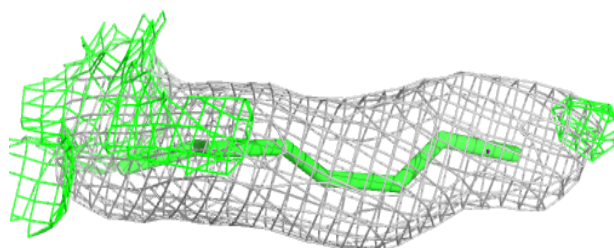
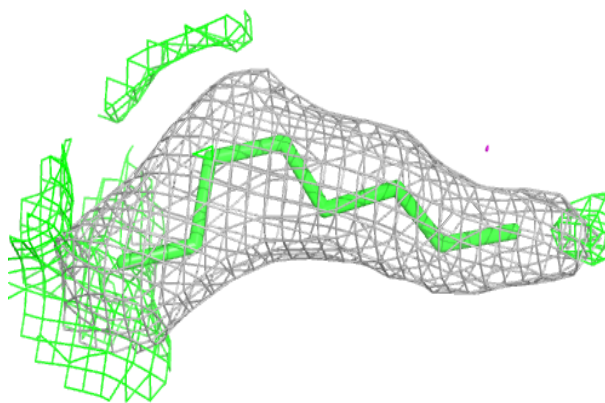
**Electron density around LFA D 411:**

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

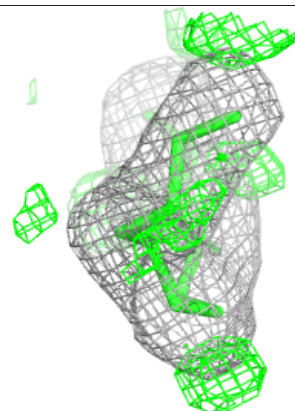
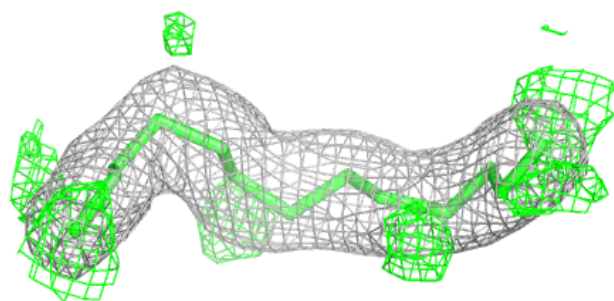
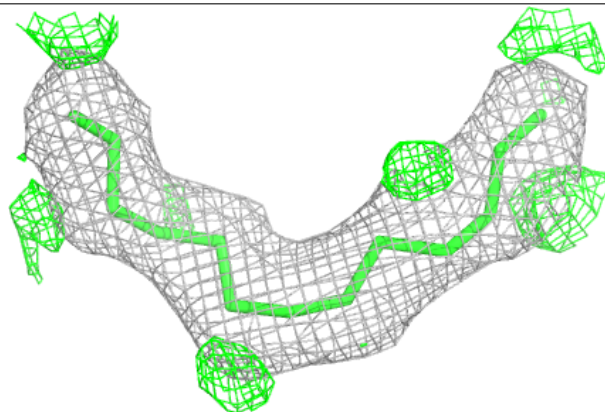


Electron density around LFA D 413:

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

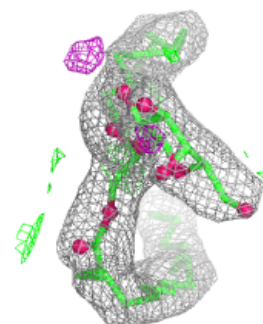
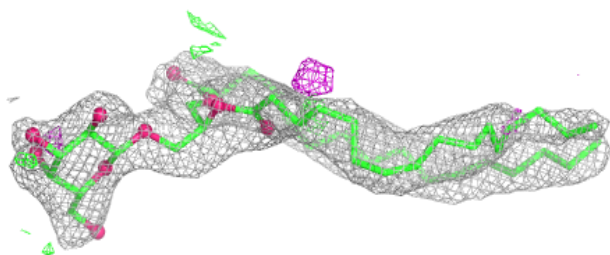
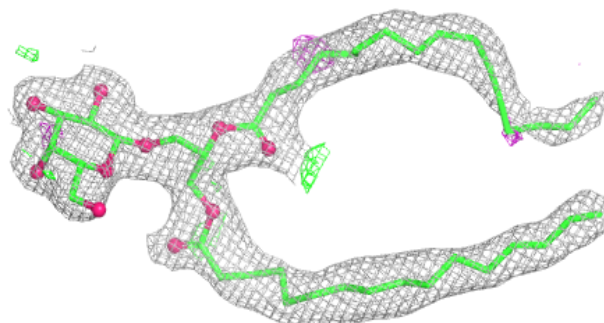
**Electron density around LFA B 623:**

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

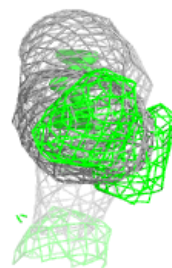
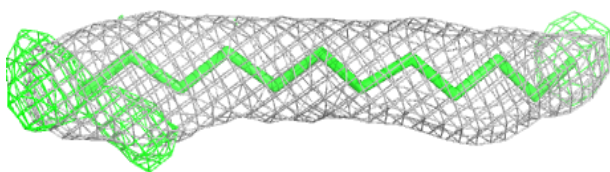
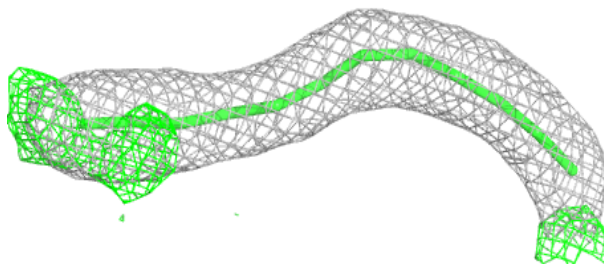


Electron density around LMG C 501:

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

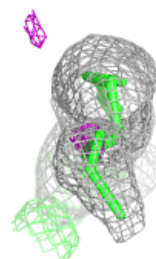
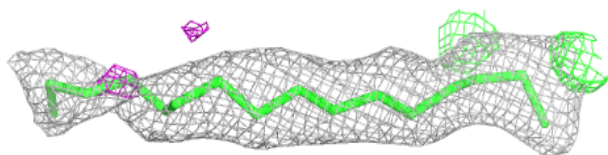
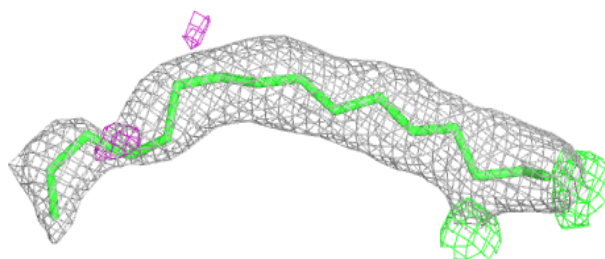
**Electron density around LFA B 628:**

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

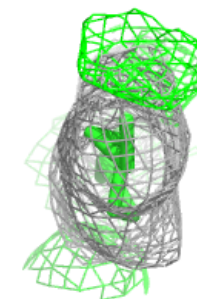
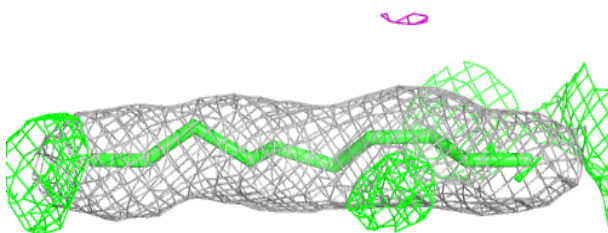
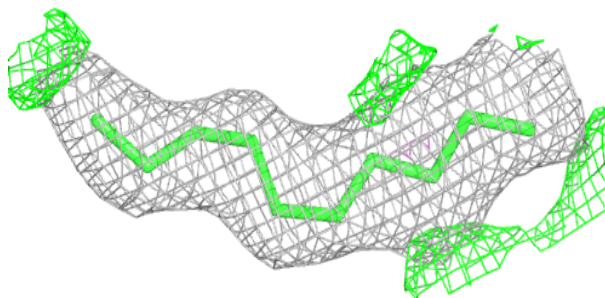


Electron density around LFA i 101:

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

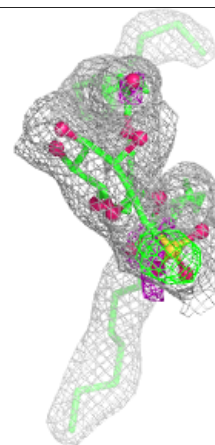
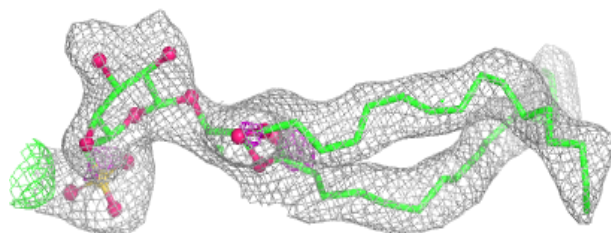
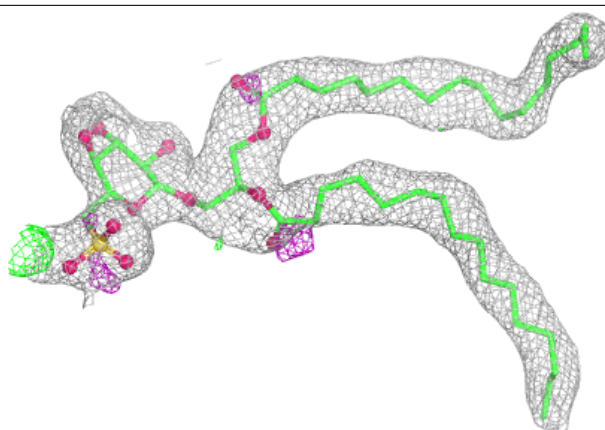
**Electron density around LFA b 622:**

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

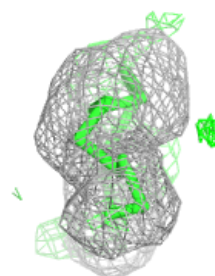
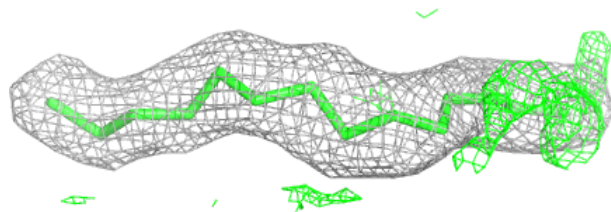


Electron density around SQD b 601:

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

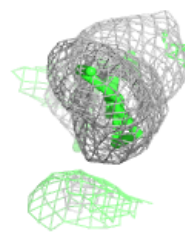
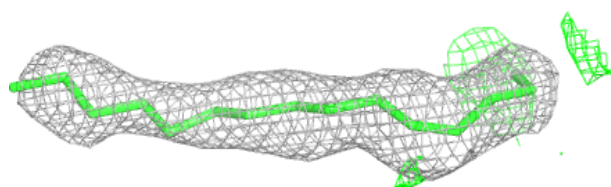
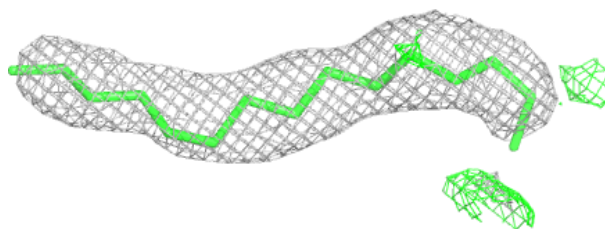
**Electron density around LFA B 627:**

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



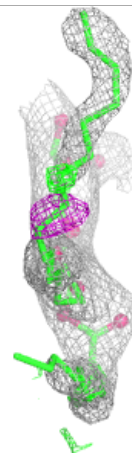
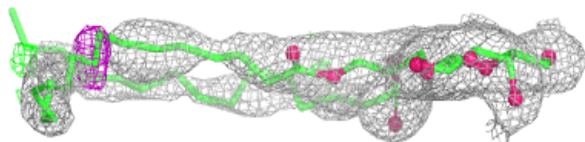
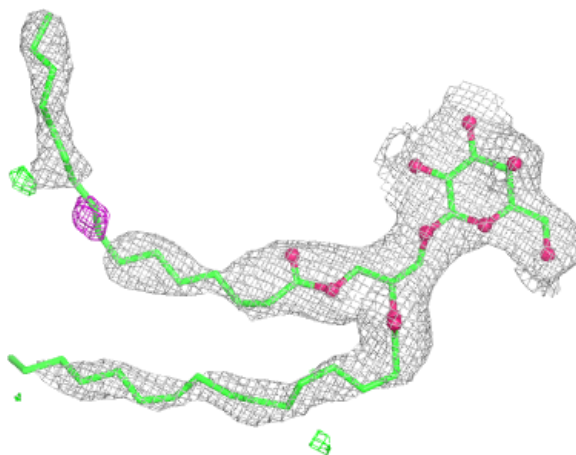
Electron density around LFA j 101:

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



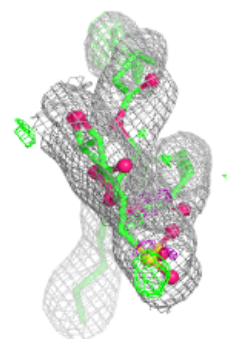
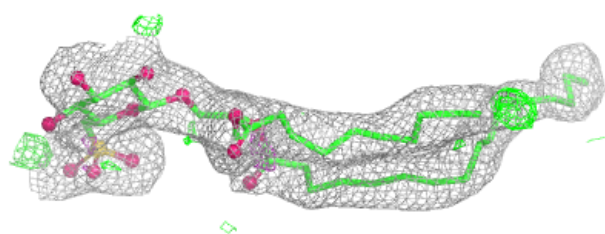
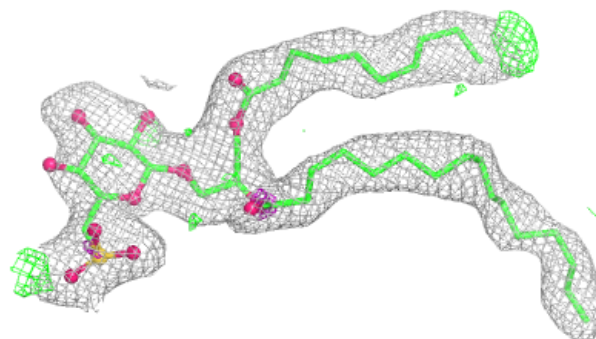
Electron density around LMG c 519:

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

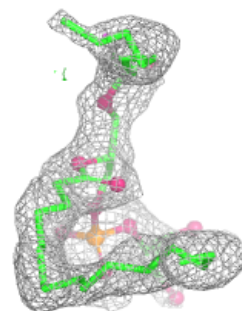
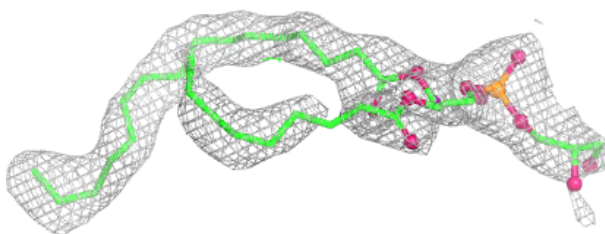
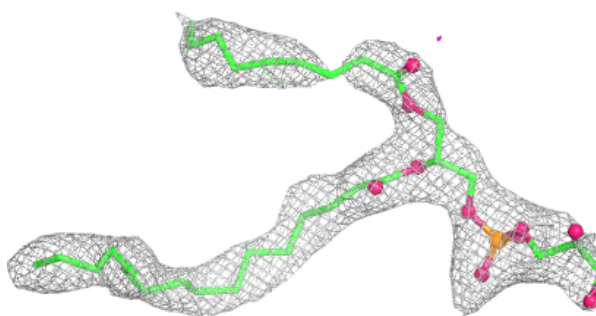


Electron density around SQD L 101:

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

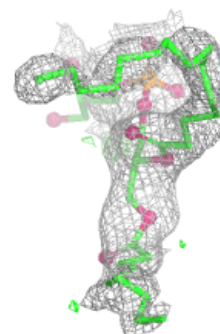
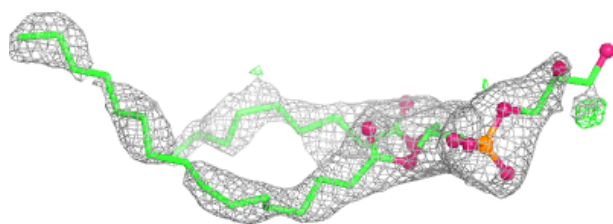
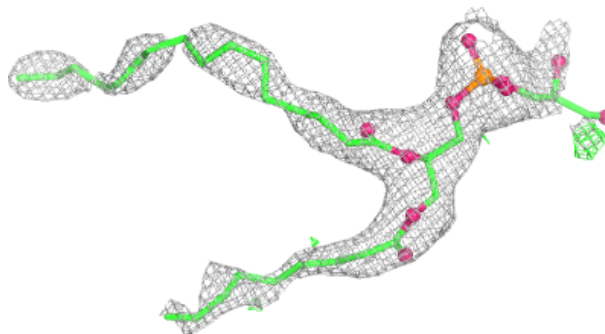
**Electron density around LHG E 101:**

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

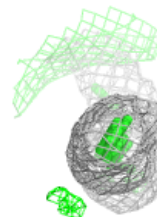
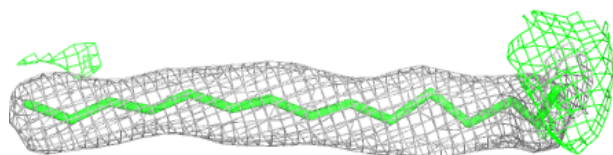
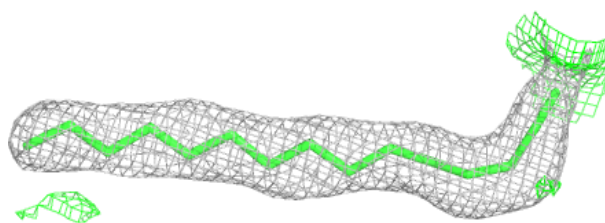


Electron density around LHG e 101:

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

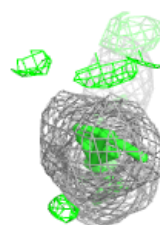
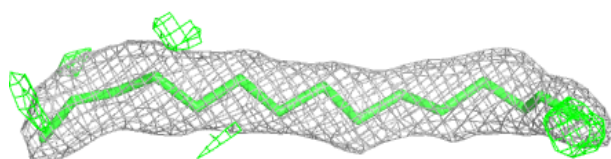
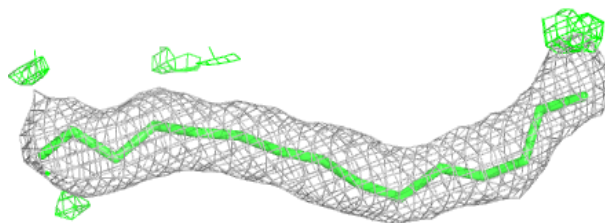
**Electron density around LFA d 408:**

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

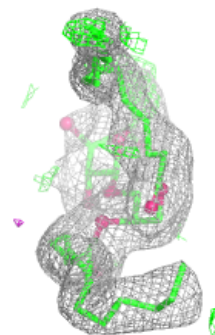
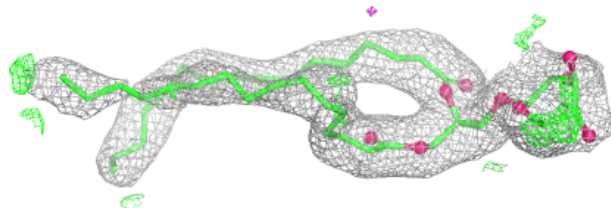
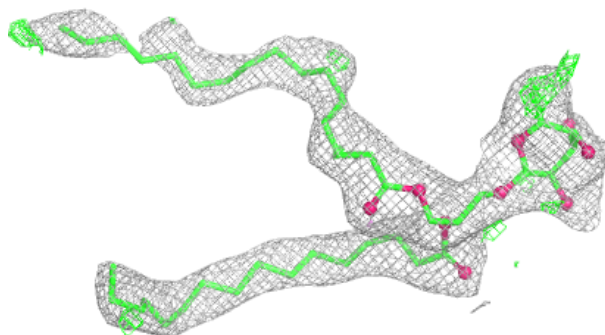


Electron density around LFA b 602:

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

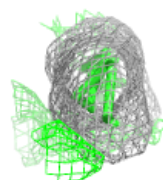
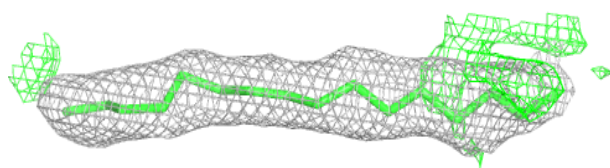
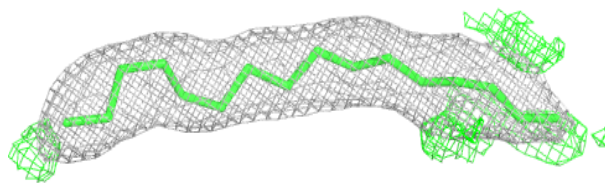
**Electron density around SQD a 412:**

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

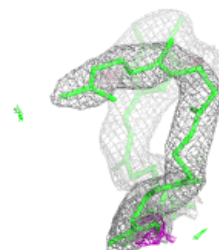
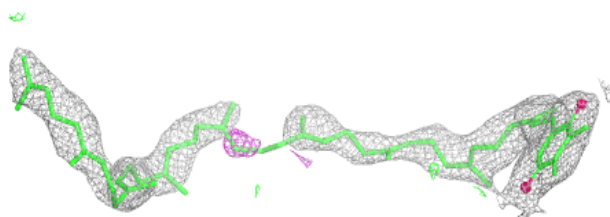
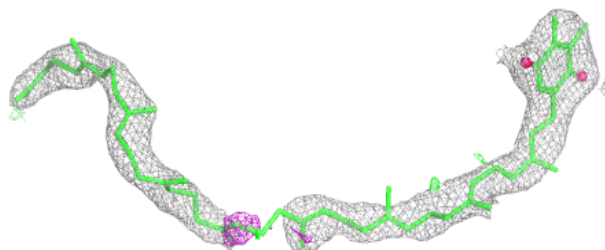


Electron density around LFA M 102:

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

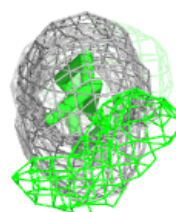
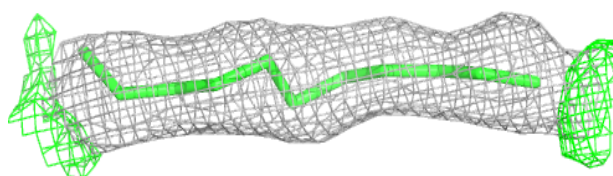
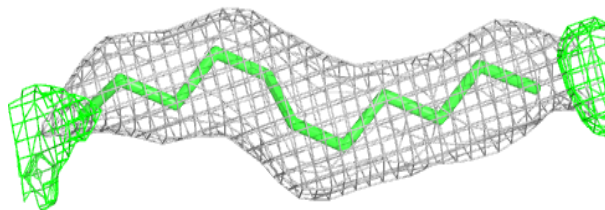
**Electron density around PL9 a 409:**

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

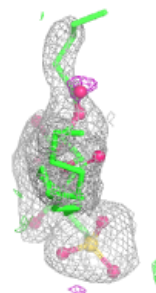
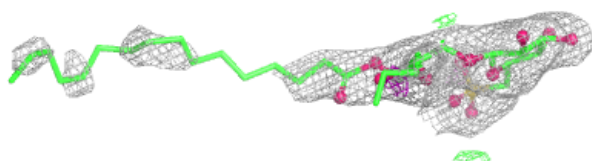
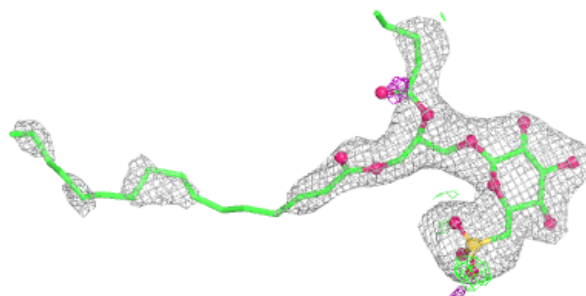


Electron density around LFA J 101:

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

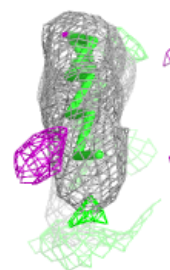
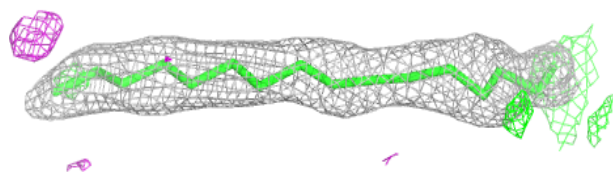
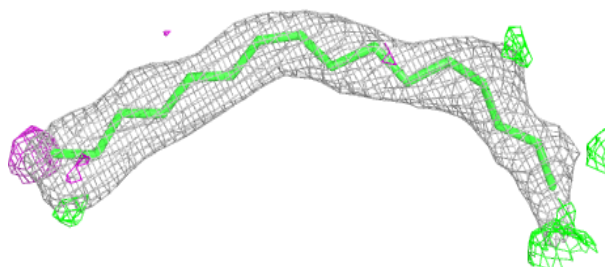
**Electron density around SQD f 102:**

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

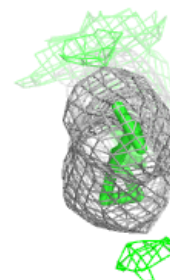
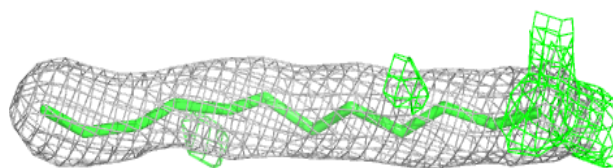
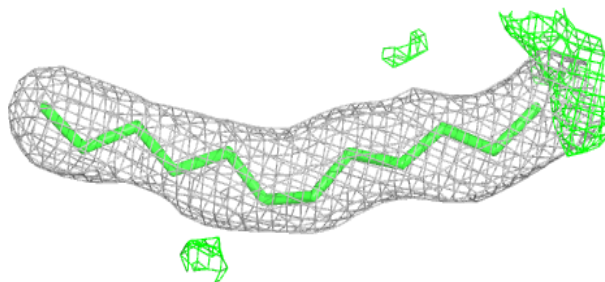


Electron density around LFA d 410:

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

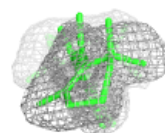
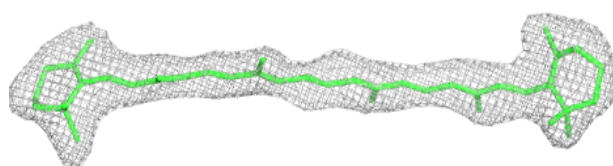
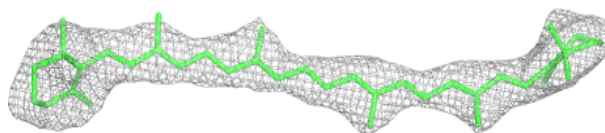
**Electron density around LFA T 102:**

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

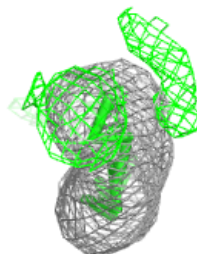
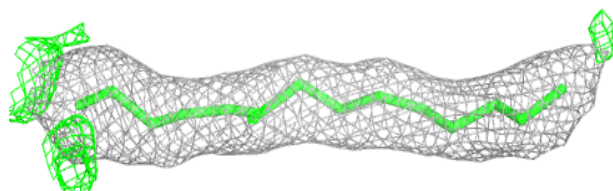
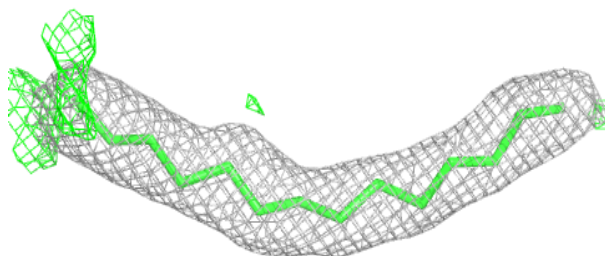


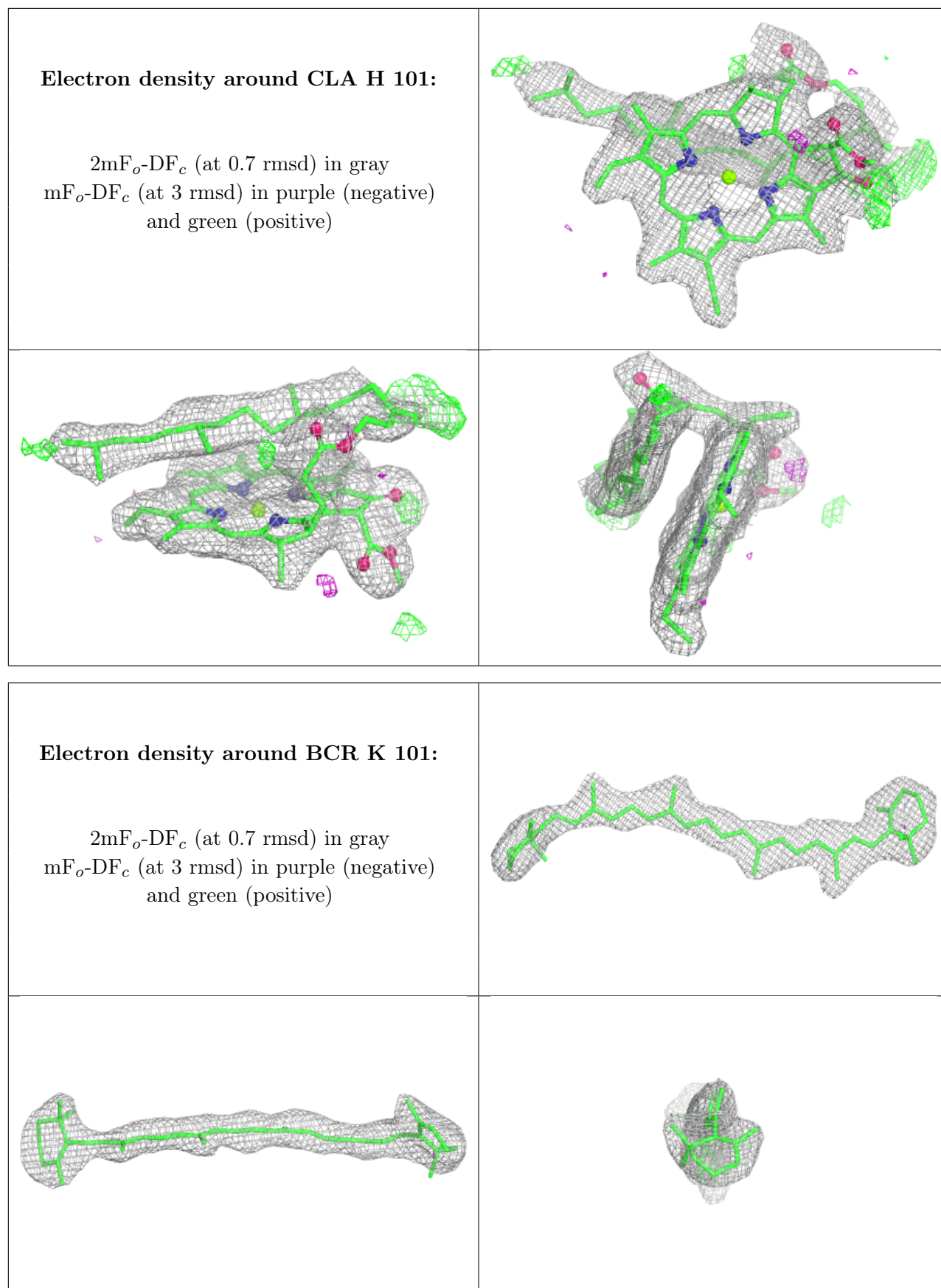
Electron density around BCR c 524:

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

**Electron density around LFA I 101:**

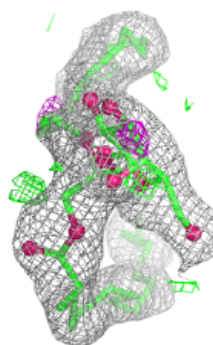
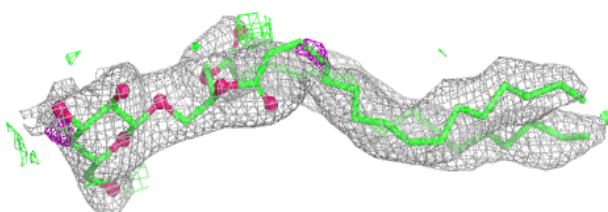
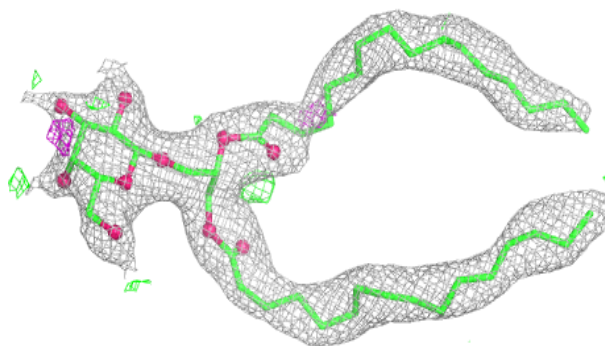
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



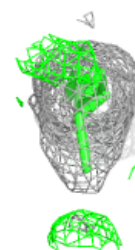
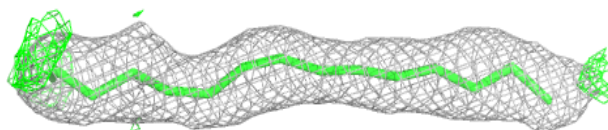
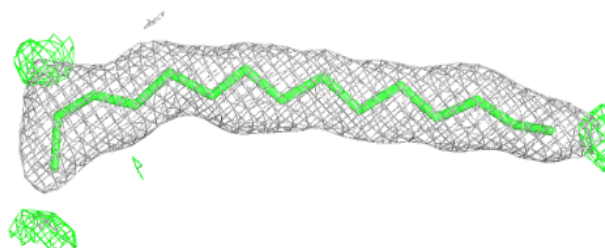


Electron density around LMG c 501:

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

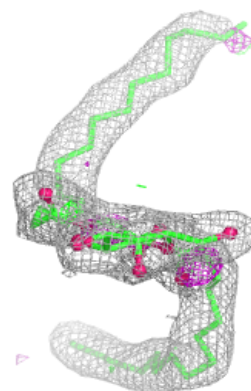
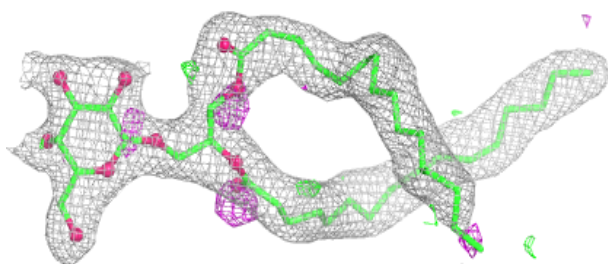
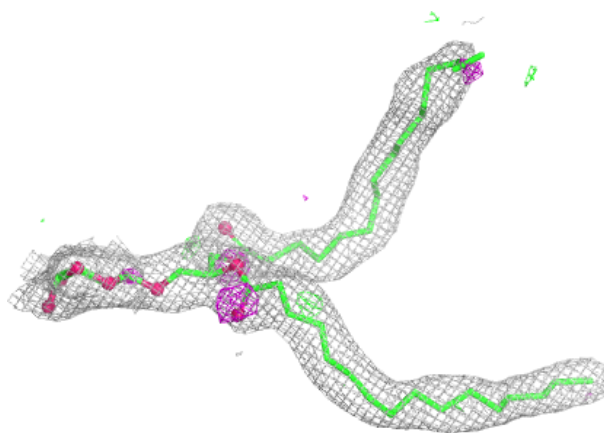
**Electron density around LFA c 521:**

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

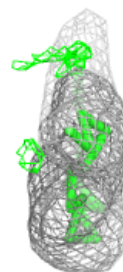
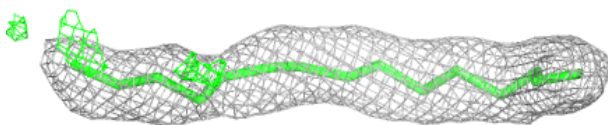
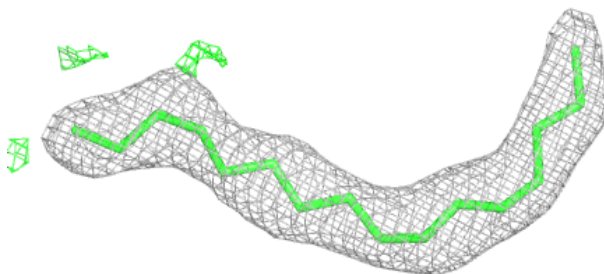


Electron density around LMG B 619:

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

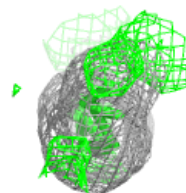
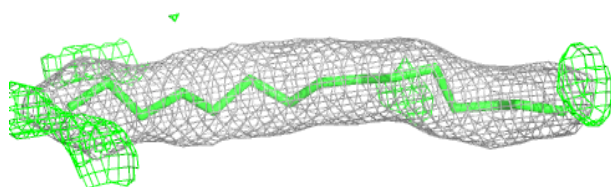
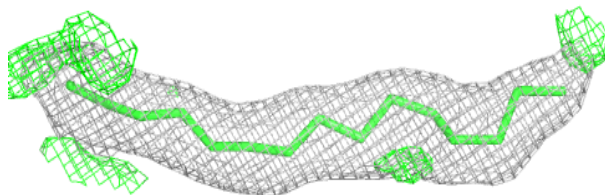
**Electron density around LFA B 622:**

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

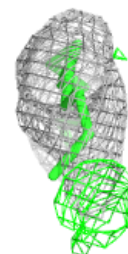
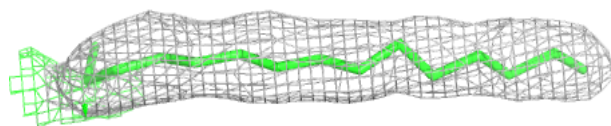
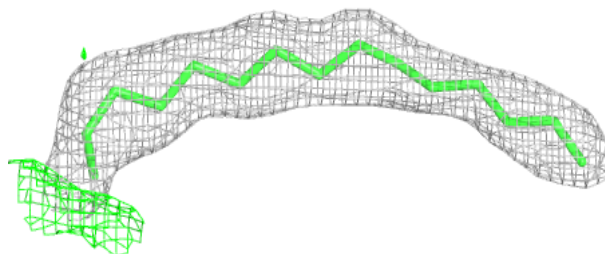


Electron density around LFA m 102:

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

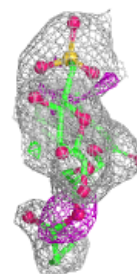
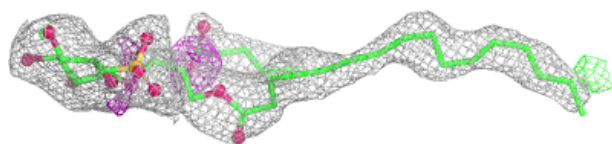
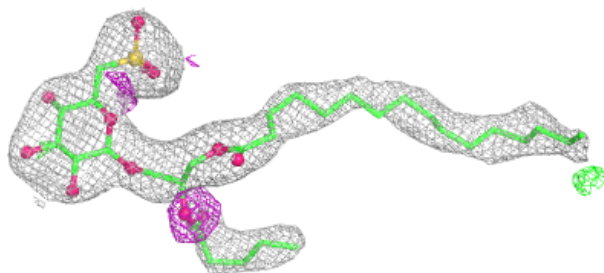
**Electron density around LFA t 101:**

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

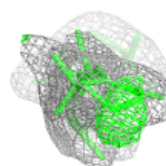
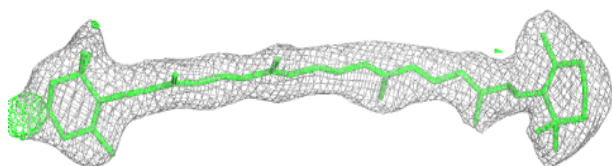
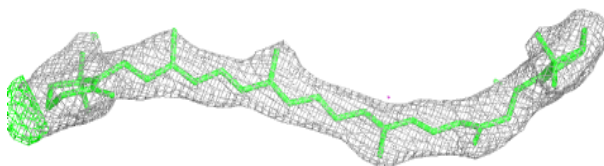


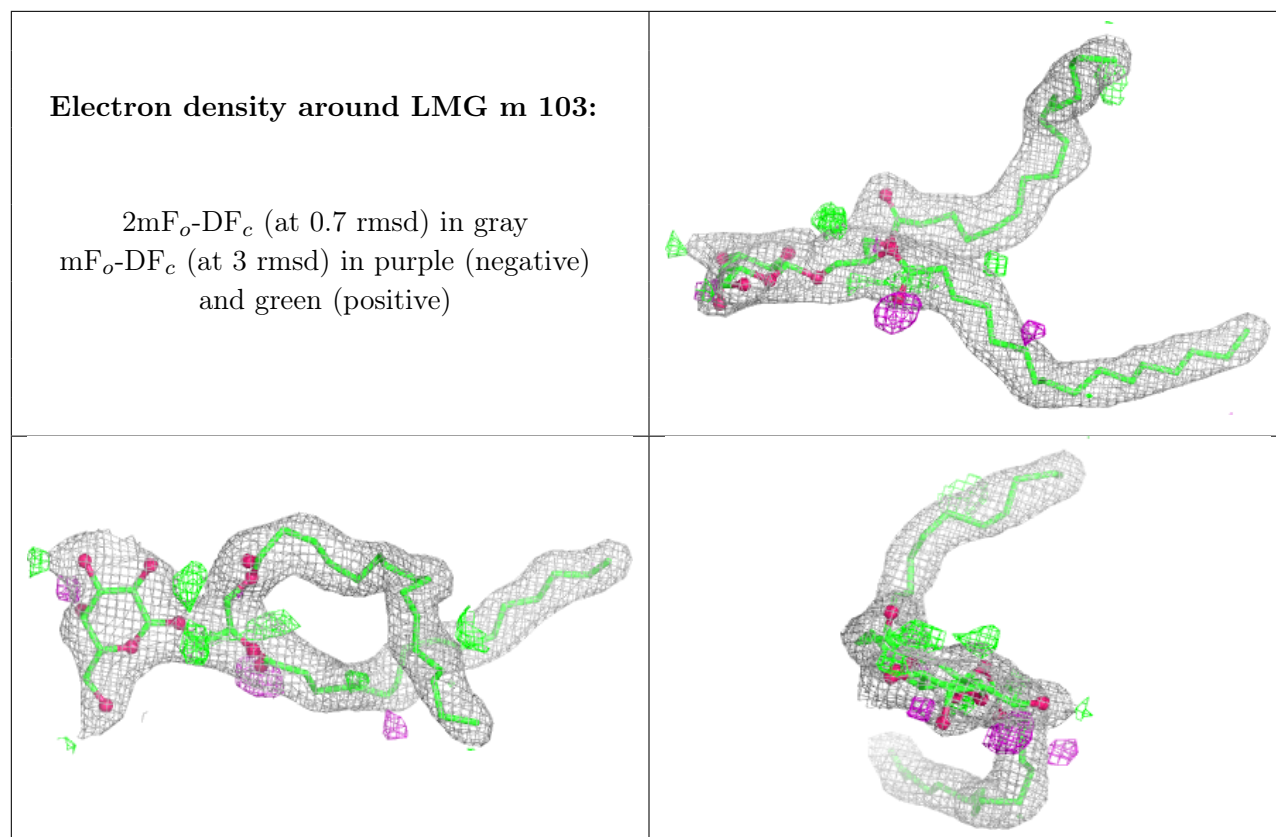
Electron density around SQD D 412:

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

**Electron density around BCR h 101:**

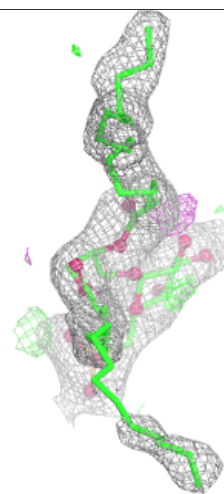
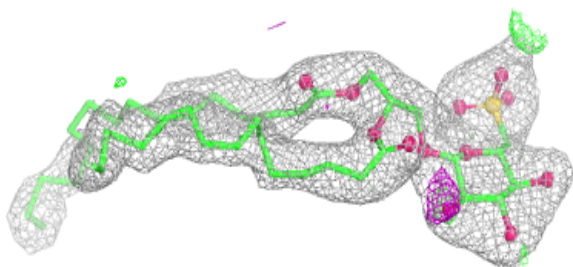
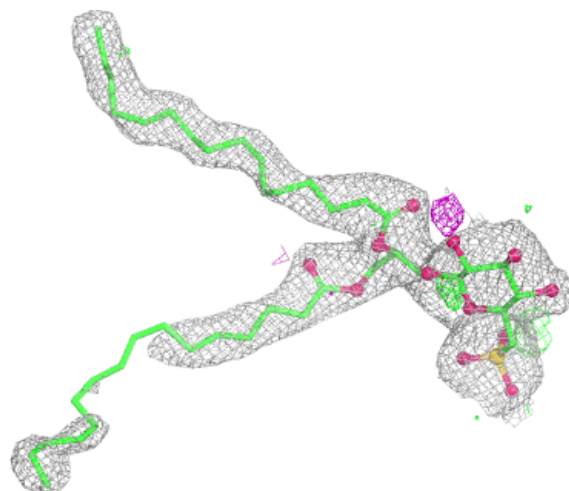
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

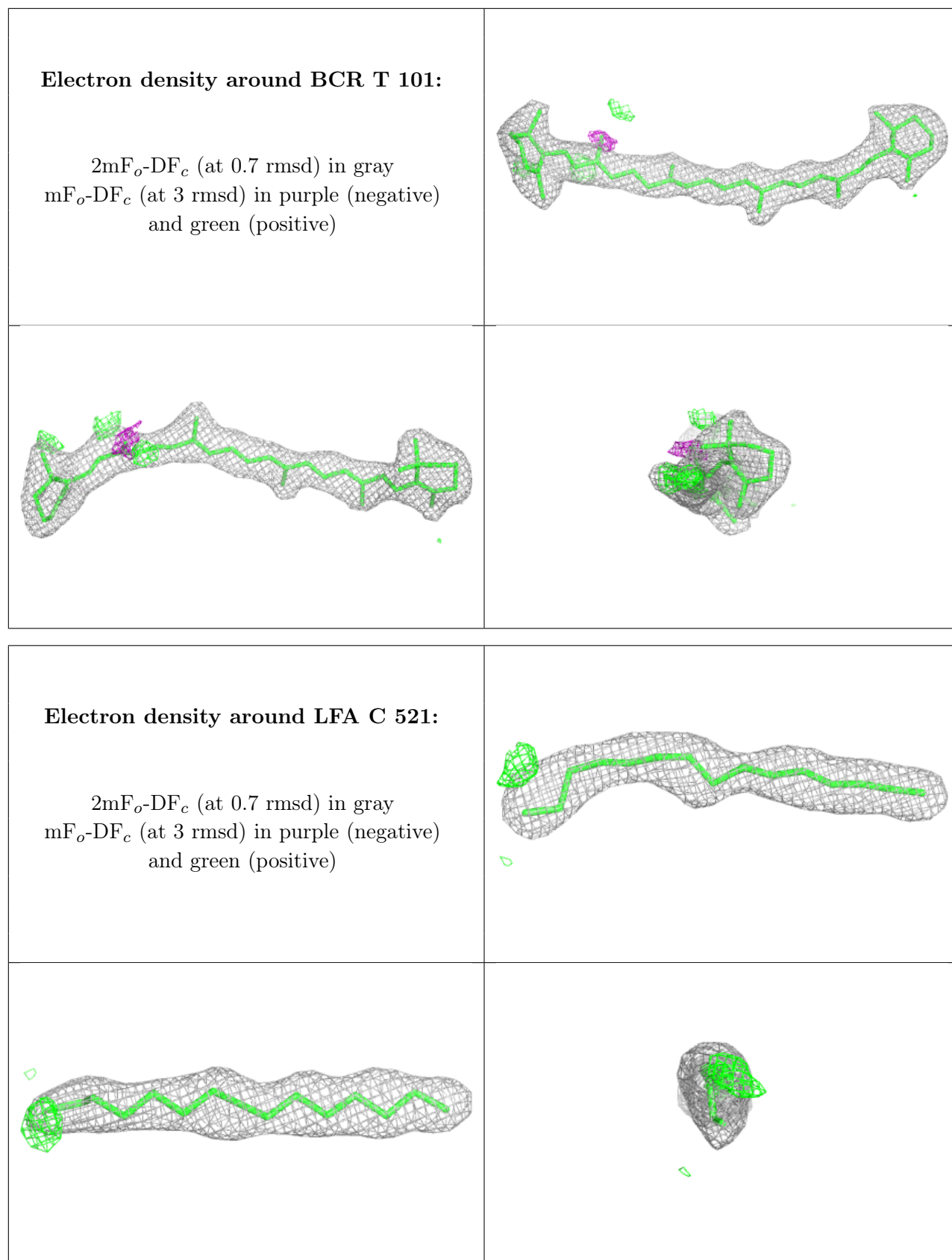


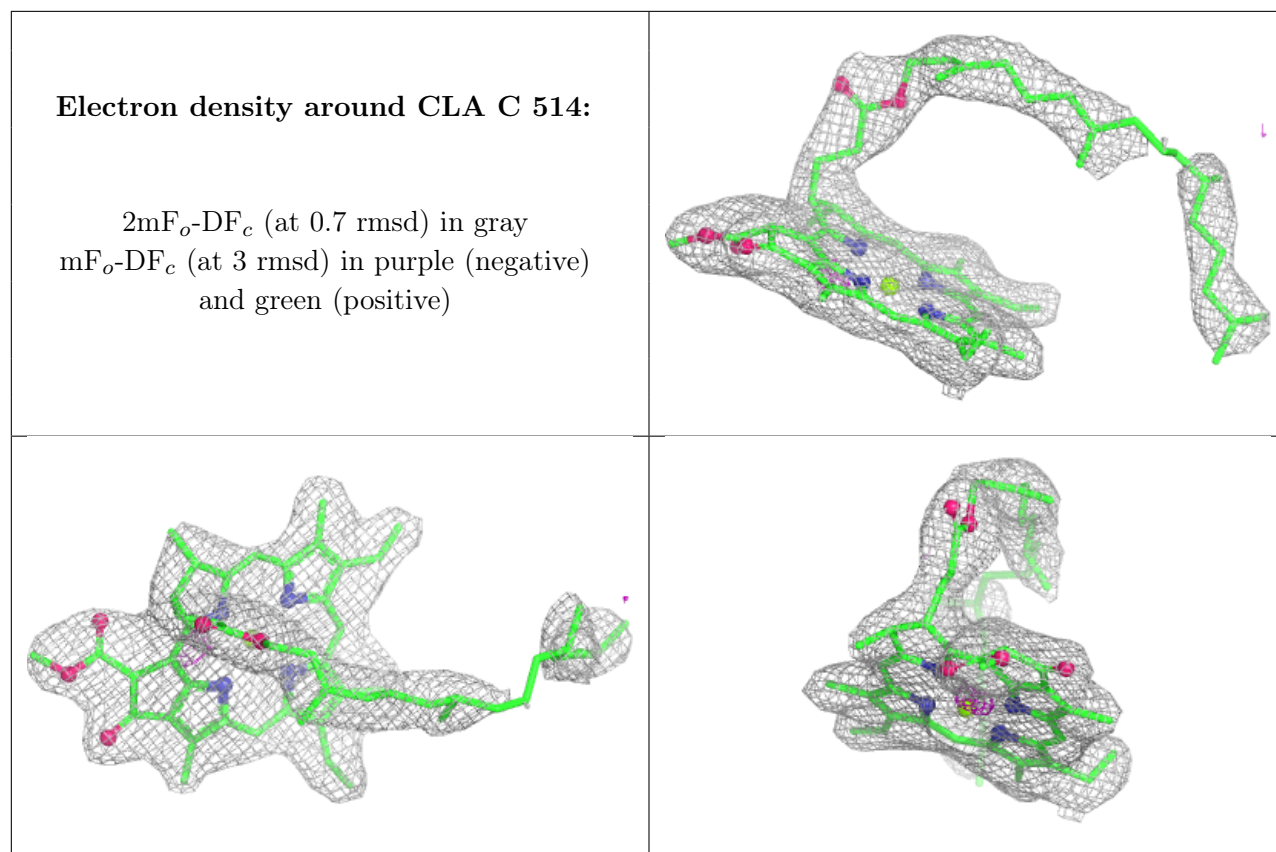


Electron density around SQD a 410:

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

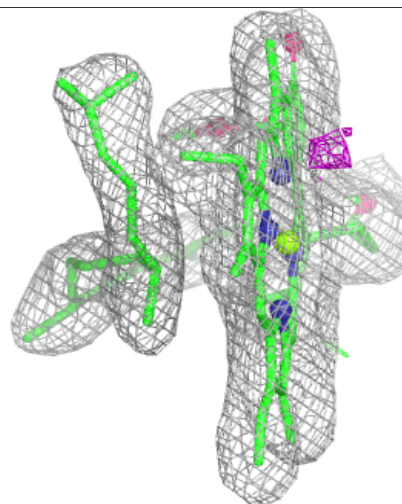
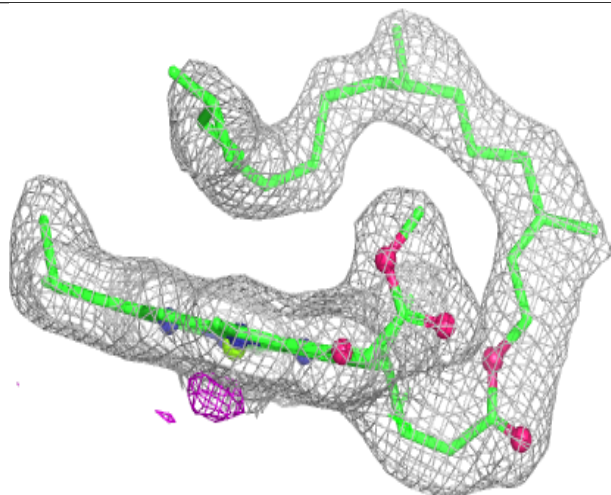
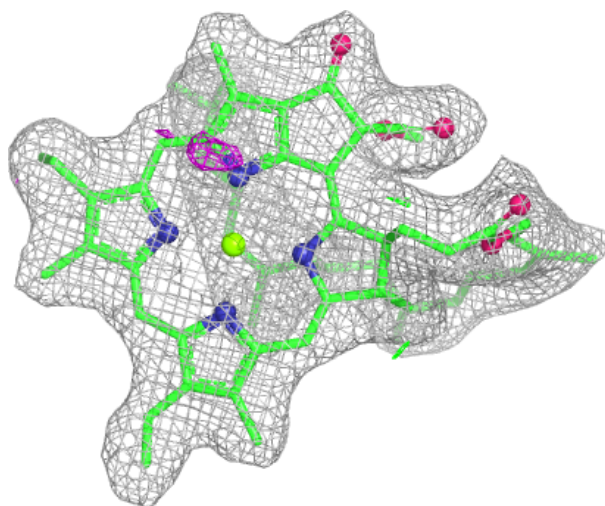


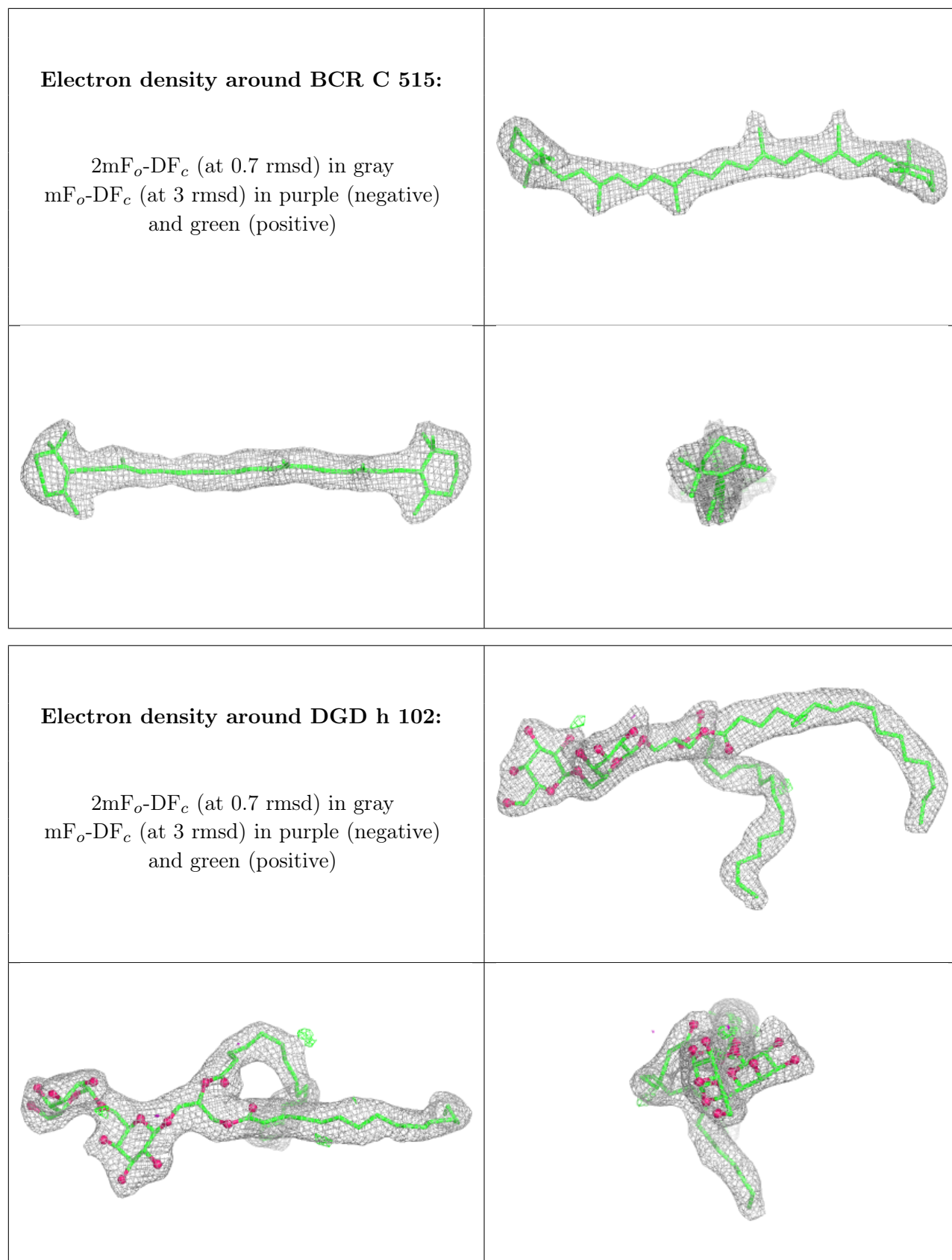




Electron density around CLA C 511:

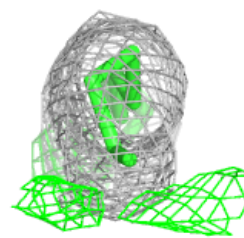
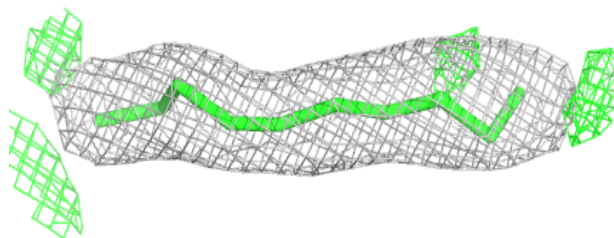
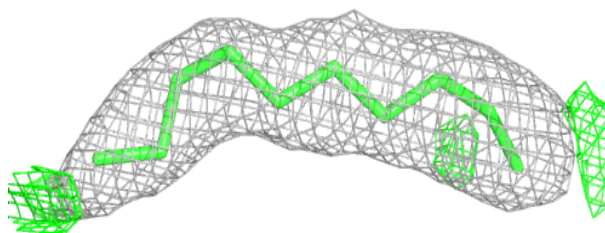
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





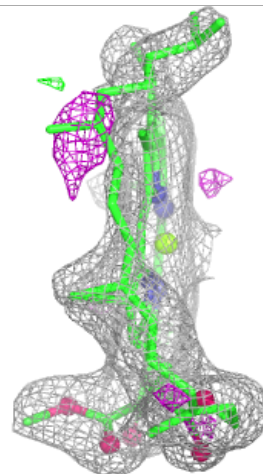
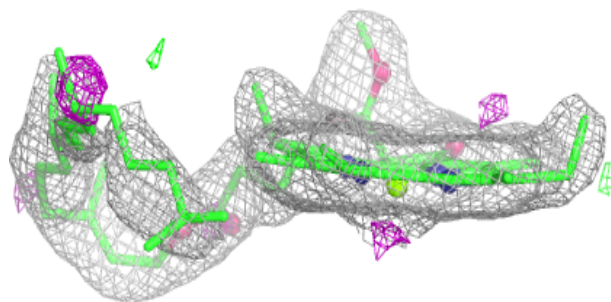
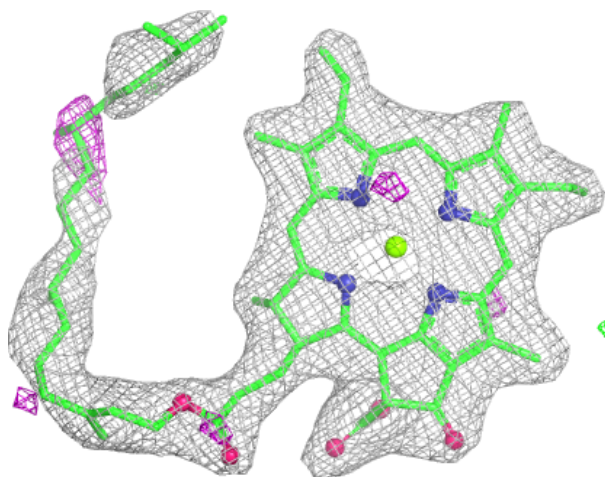
Electron density around LFA B 620:

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



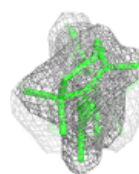
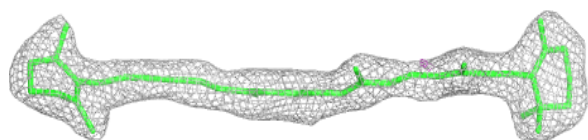
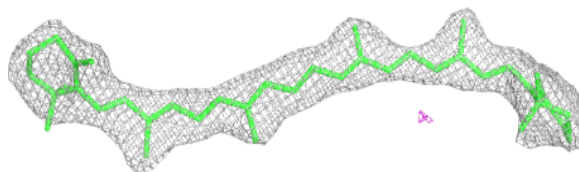
Electron density around CLA C 513:

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

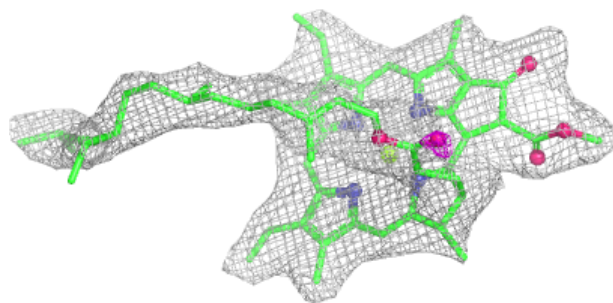
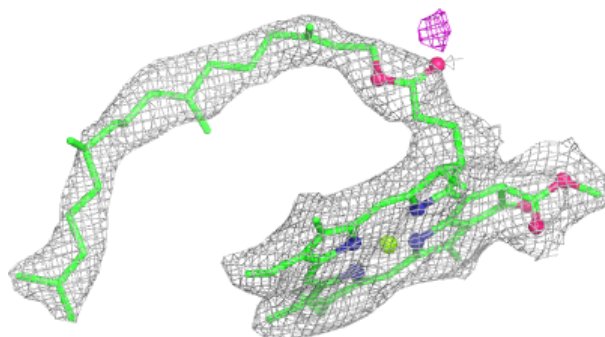


Electron density around BCR c 523:

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

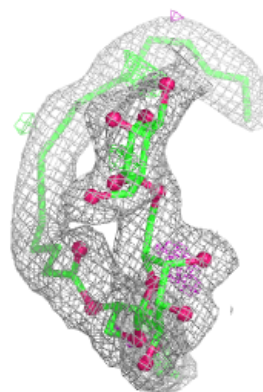
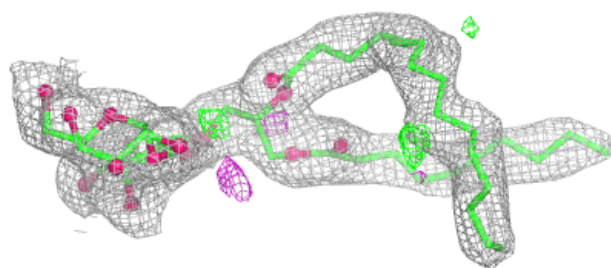
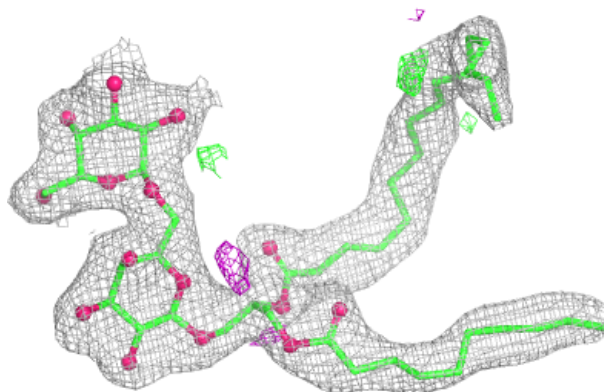
**Electron density around CLA c 514:**

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

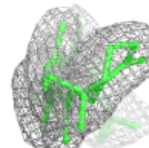
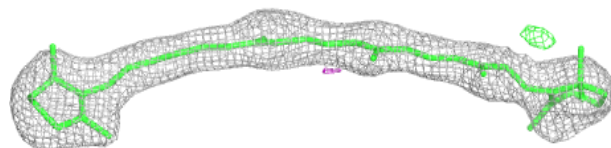


Electron density around DGD C 518:

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

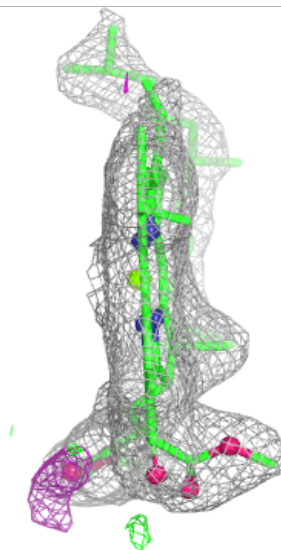
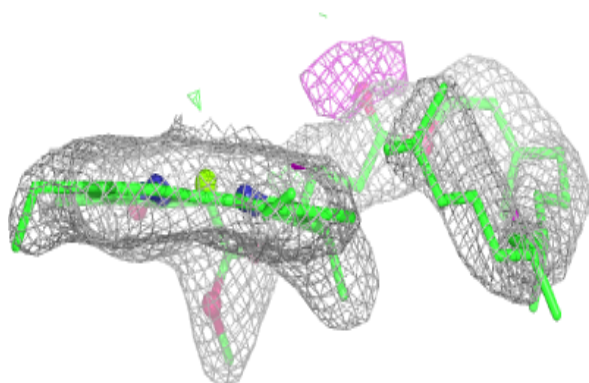
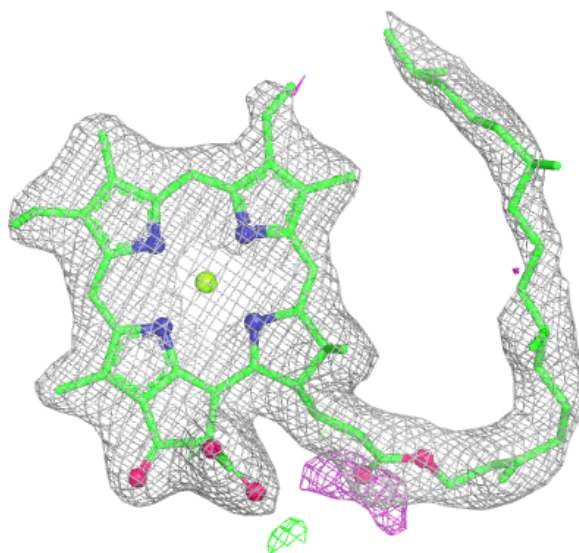
**Electron density around BCR d 404:**

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



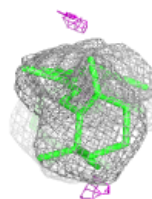
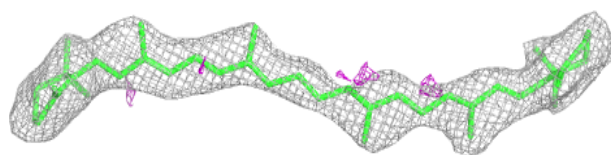
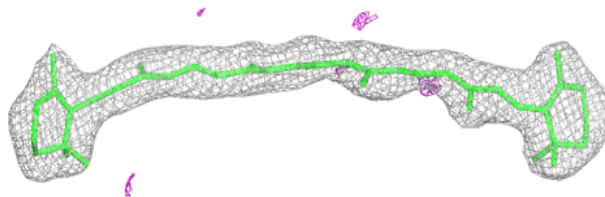
Electron density around CLA c 513:

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

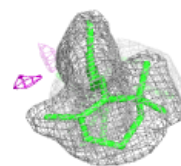
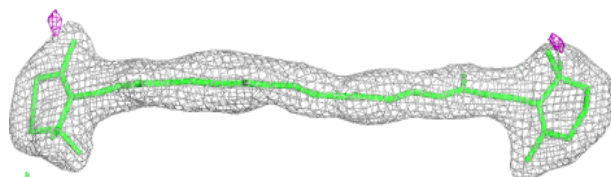
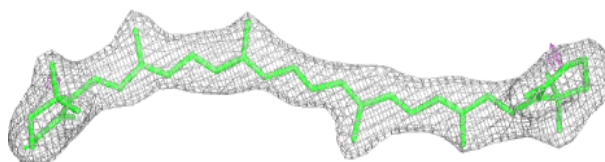


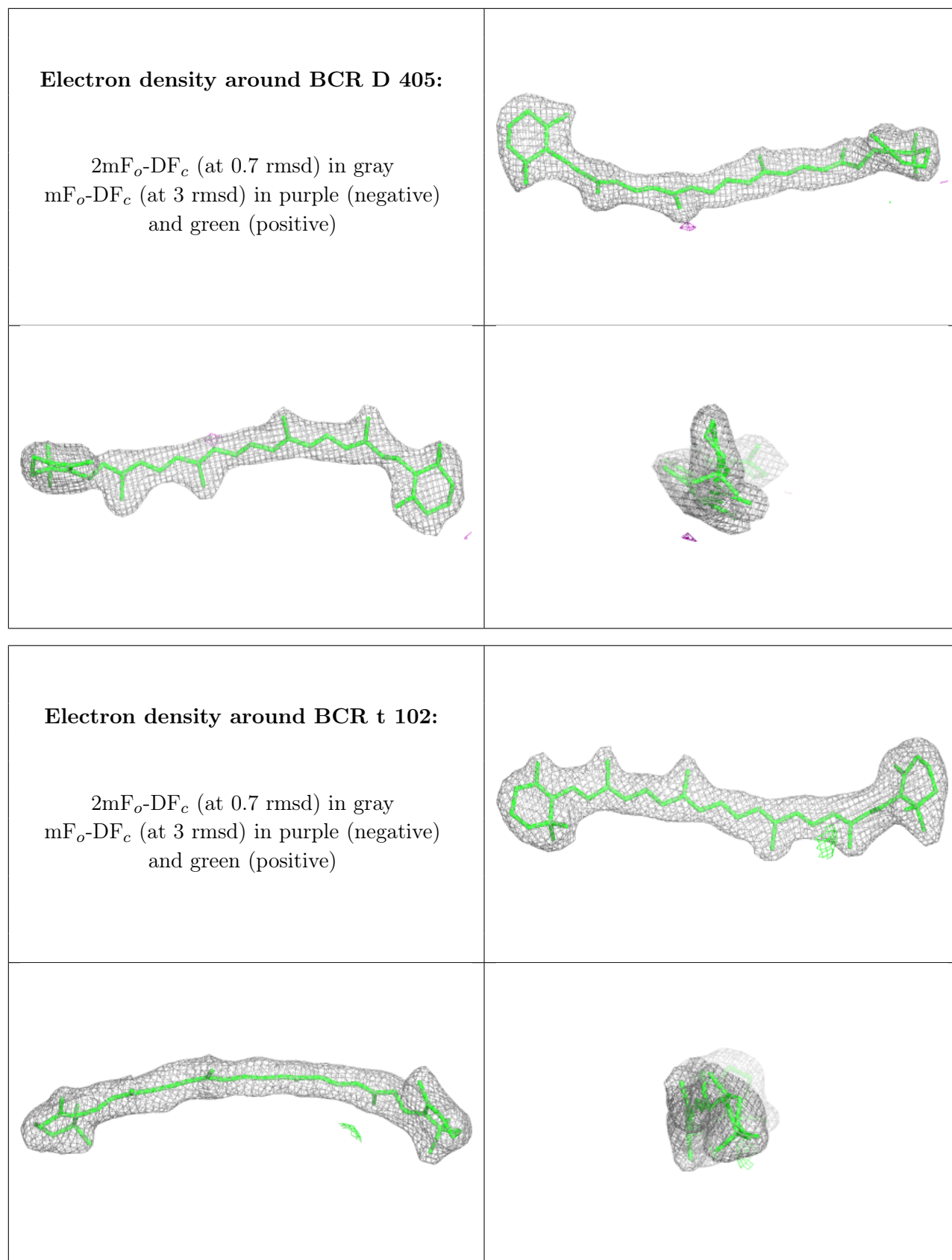
Electron density around BCR k 101:

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

**Electron density around BCR C 516:**

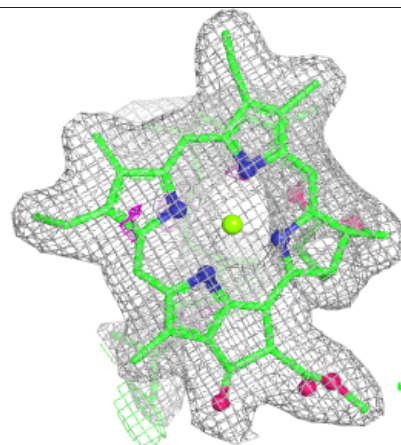
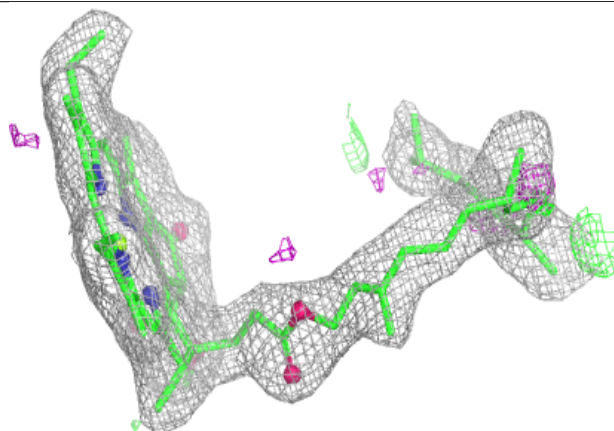
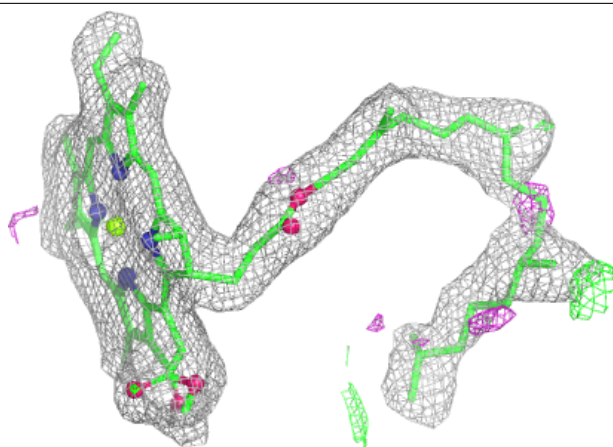
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



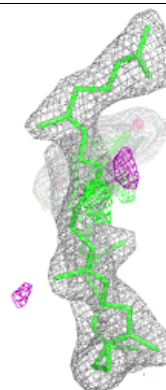
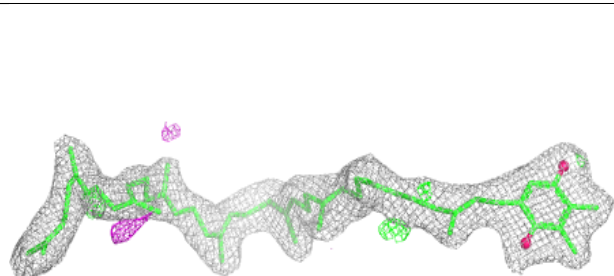
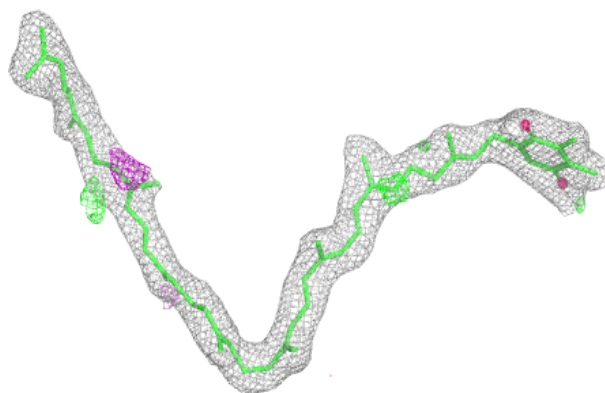


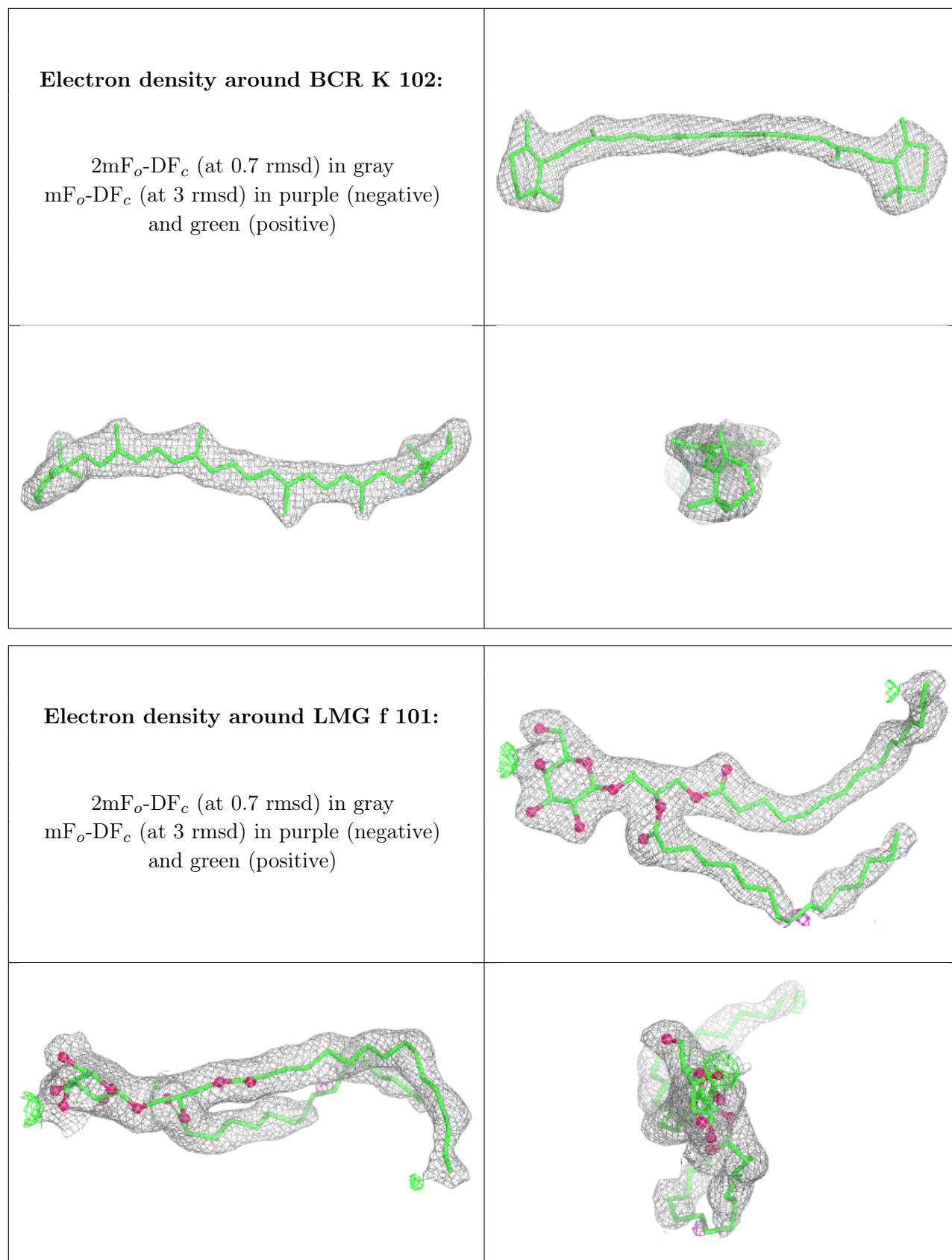
Electron density around CLA b 608:

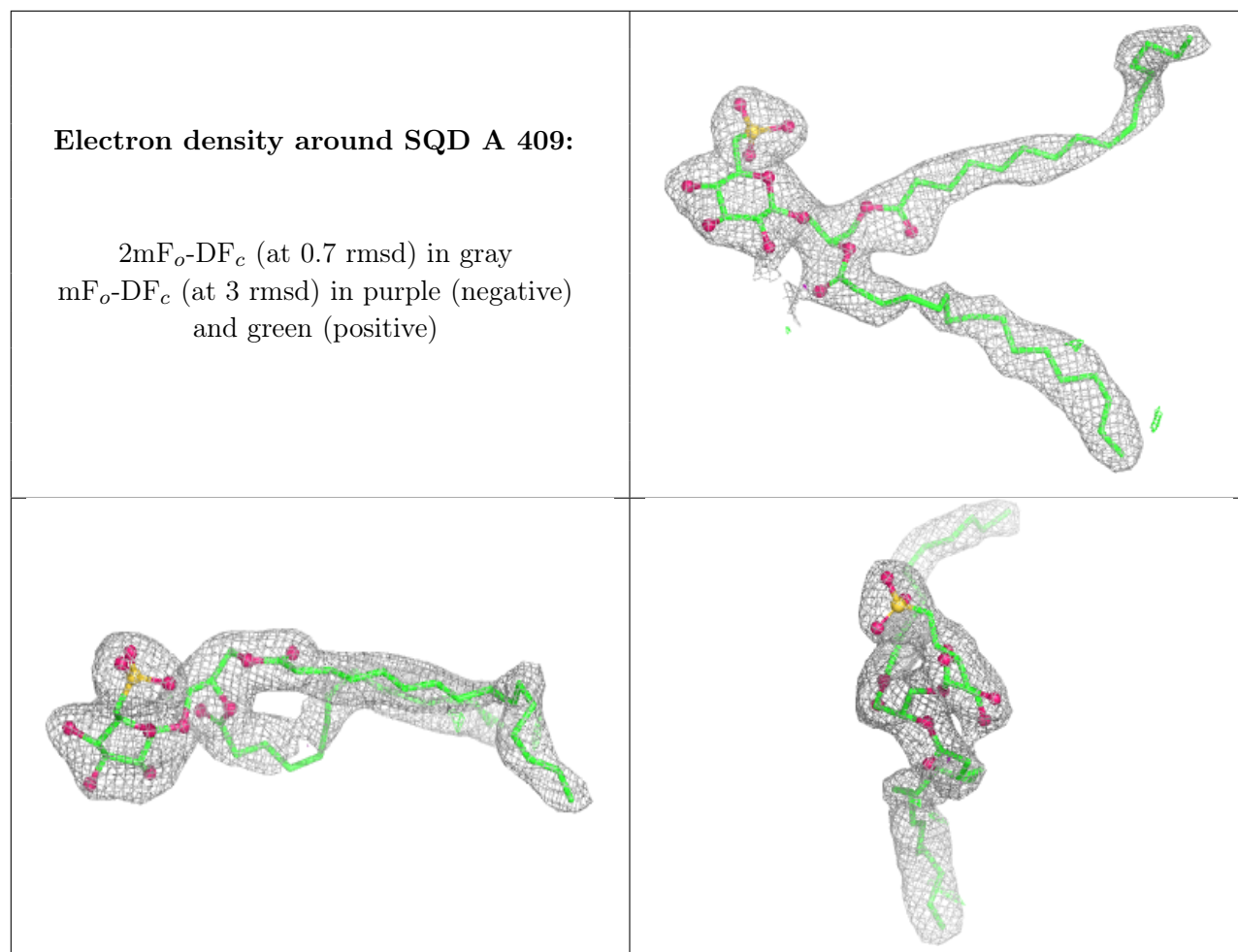
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PL9 D 406:**

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

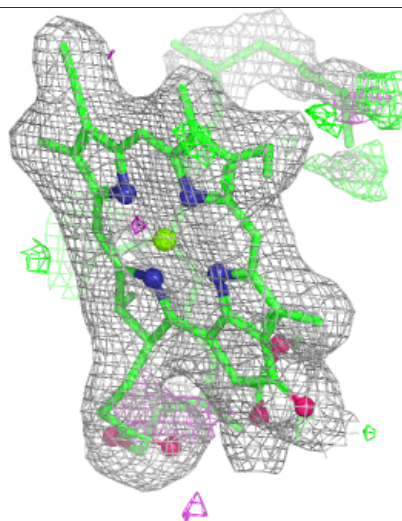
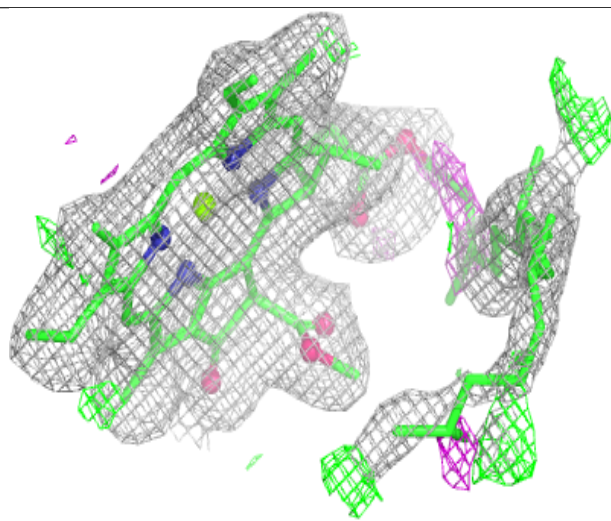
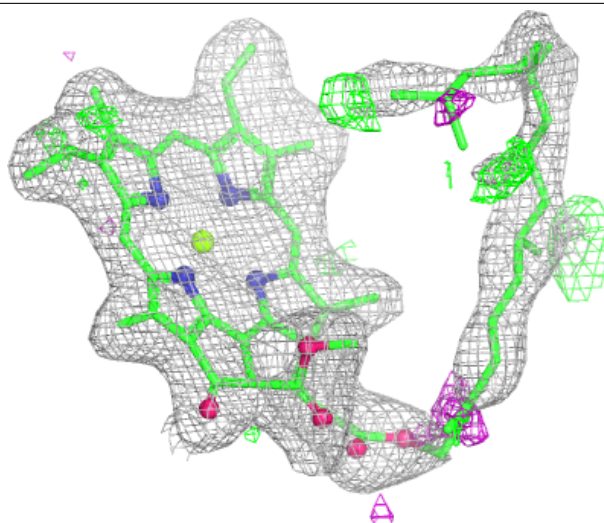






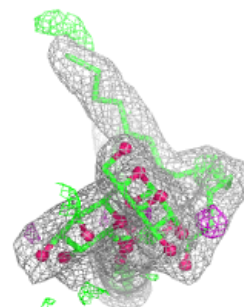
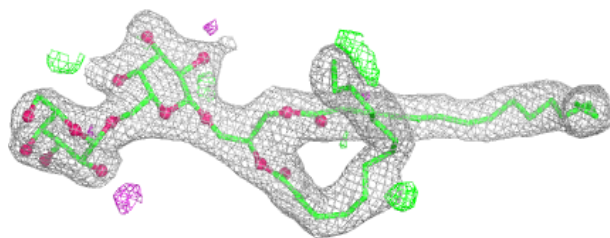
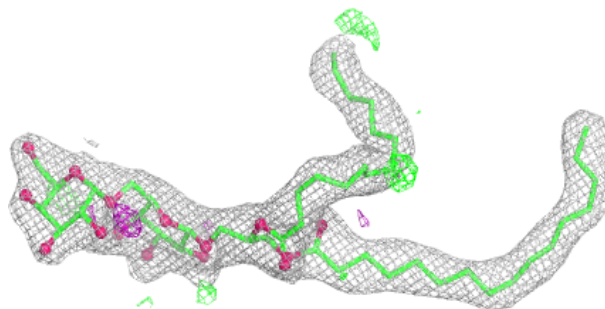
Electron density around CLA b 618:

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

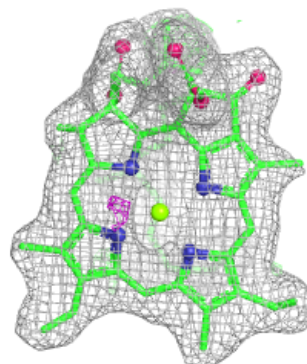
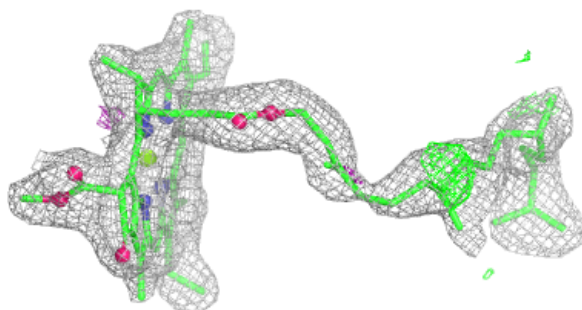
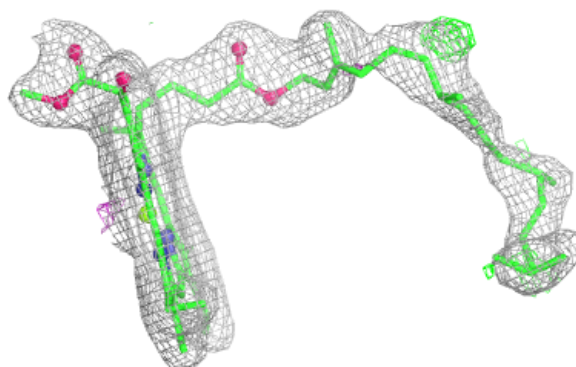


Electron density around DGD H 103:

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

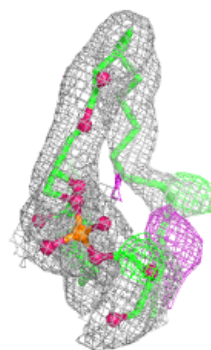
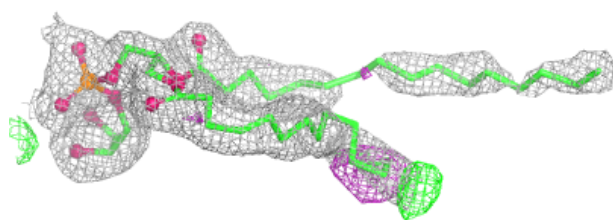
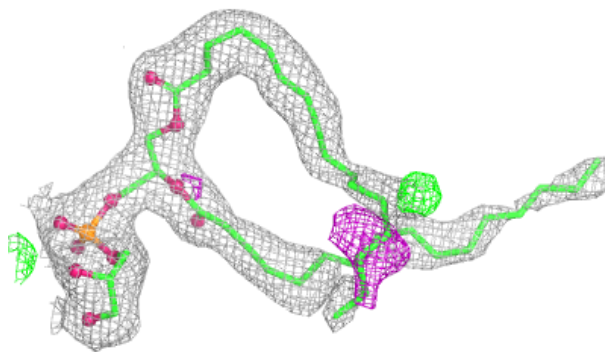
**Electron density around CLA C 507:**

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

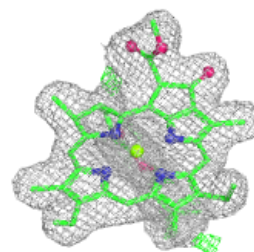
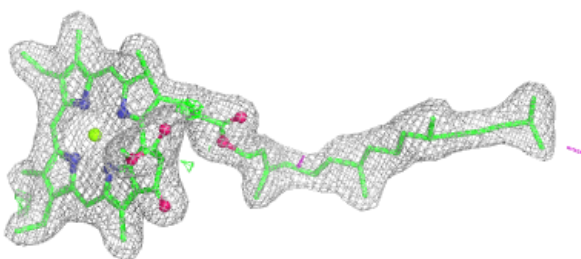
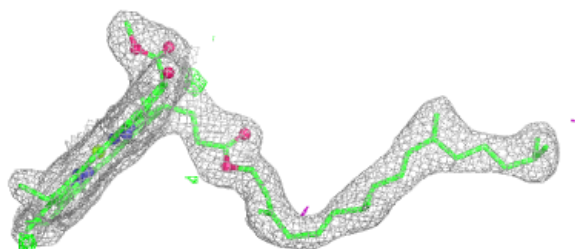


Electron density around LHG D 409:

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

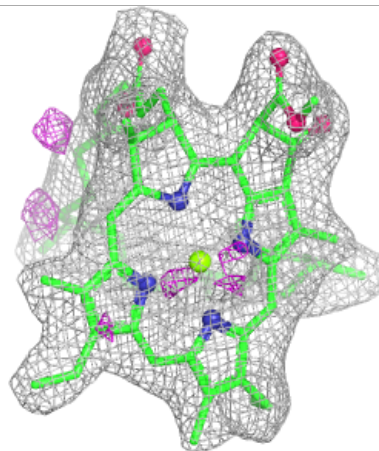
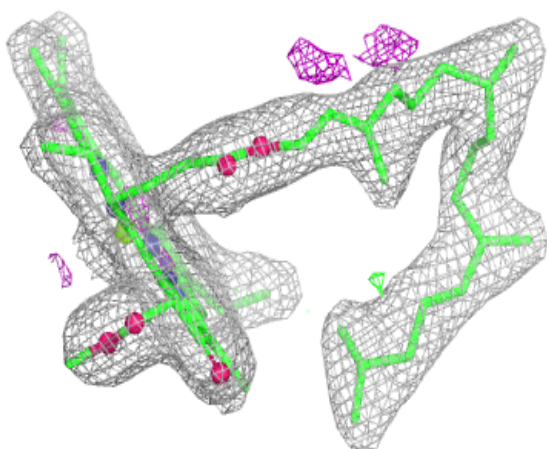
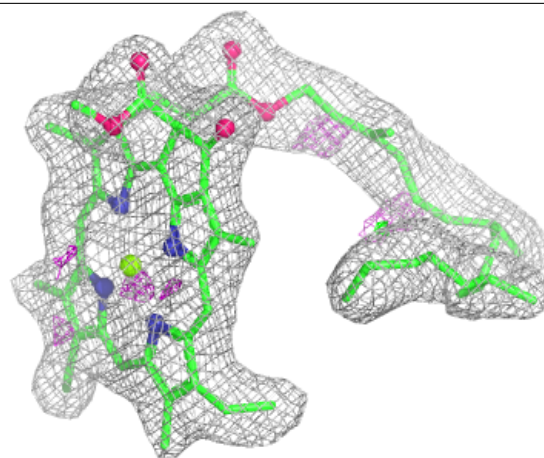
**Electron density around CLA C 503:**

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



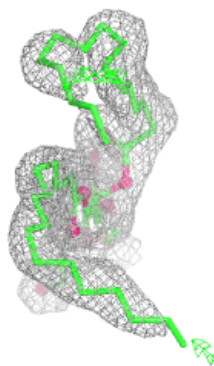
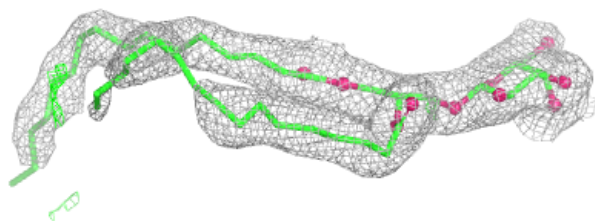
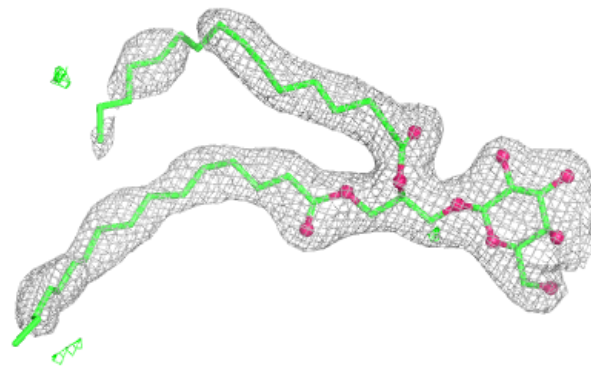
Electron density around CLA C 504:

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

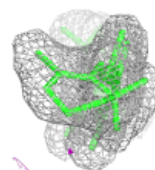
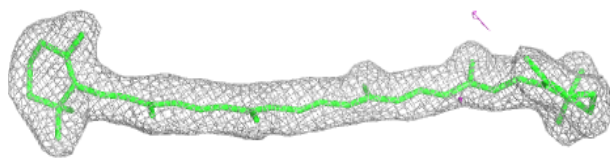
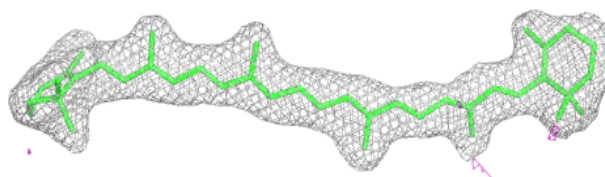


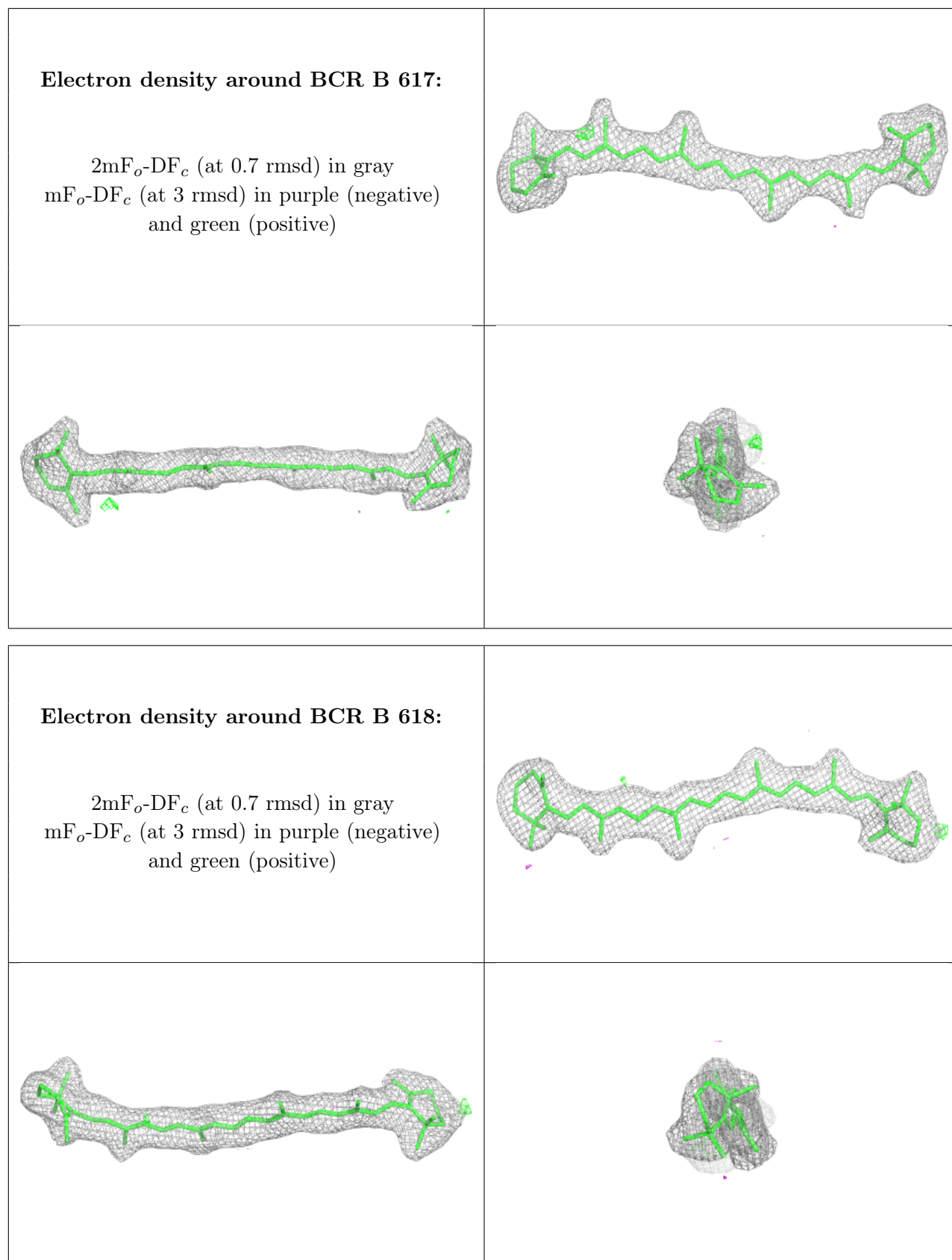
Electron density around LMG D 410:

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

**Electron density around BCR B 616:**

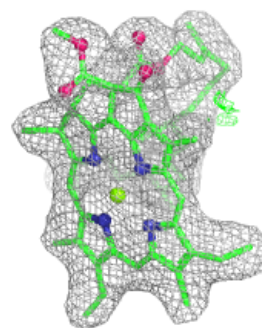
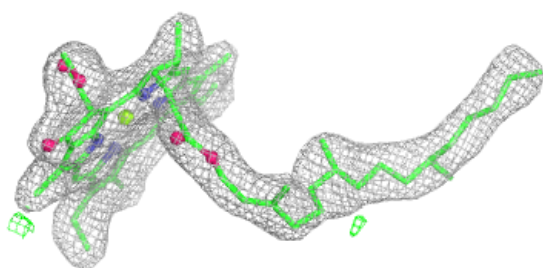
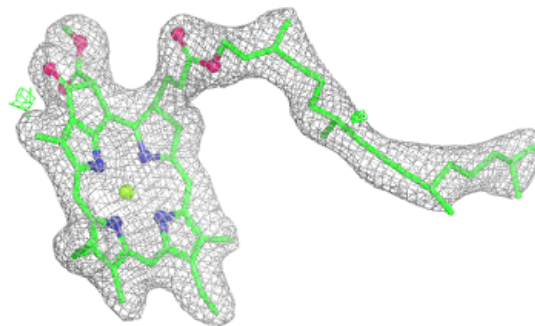
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





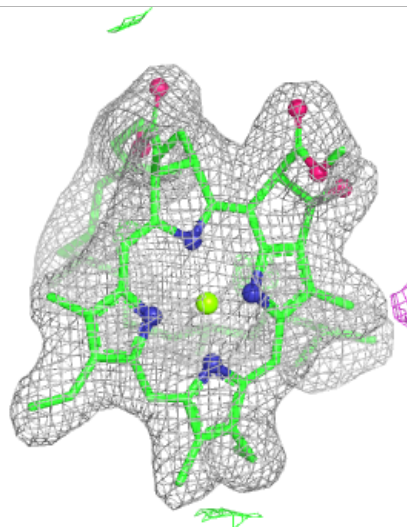
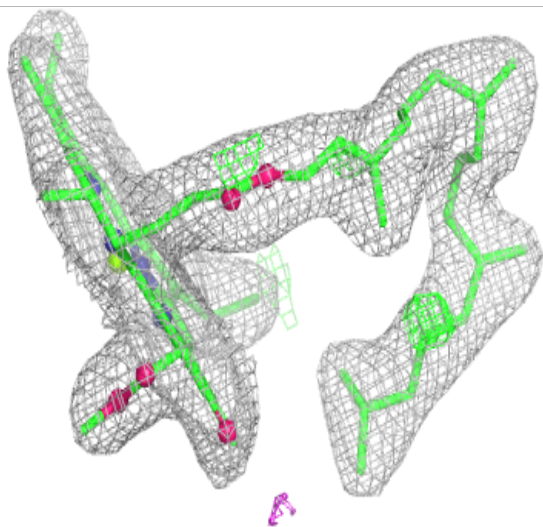
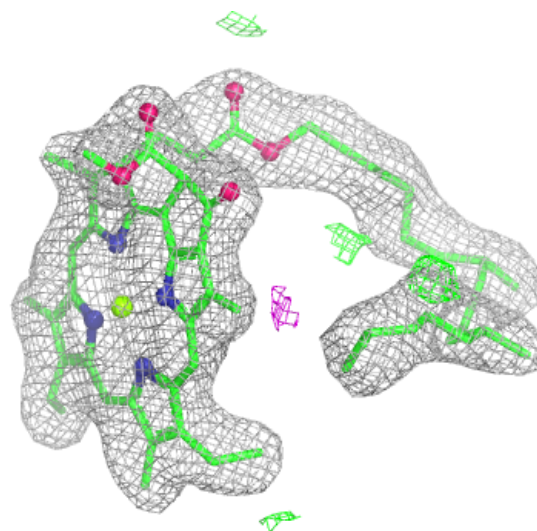
Electron density around CLA C 512:

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



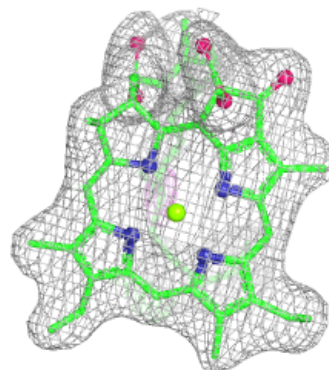
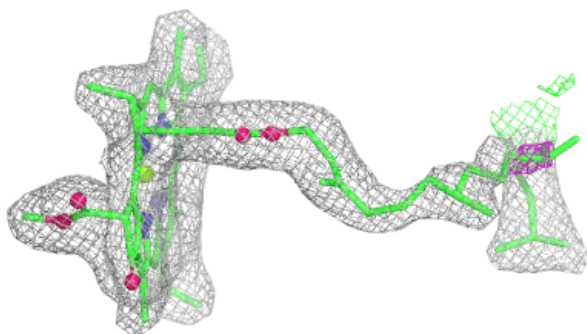
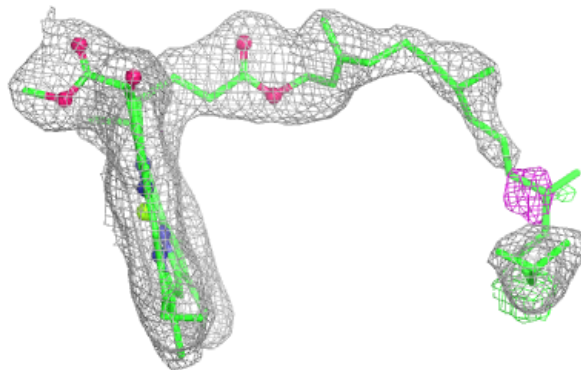
Electron density around CLA c 504:

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

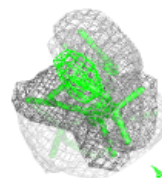
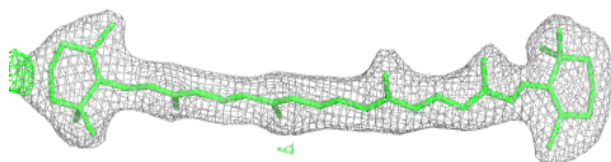
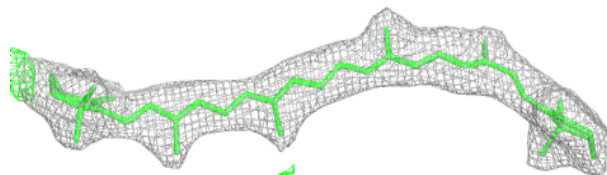


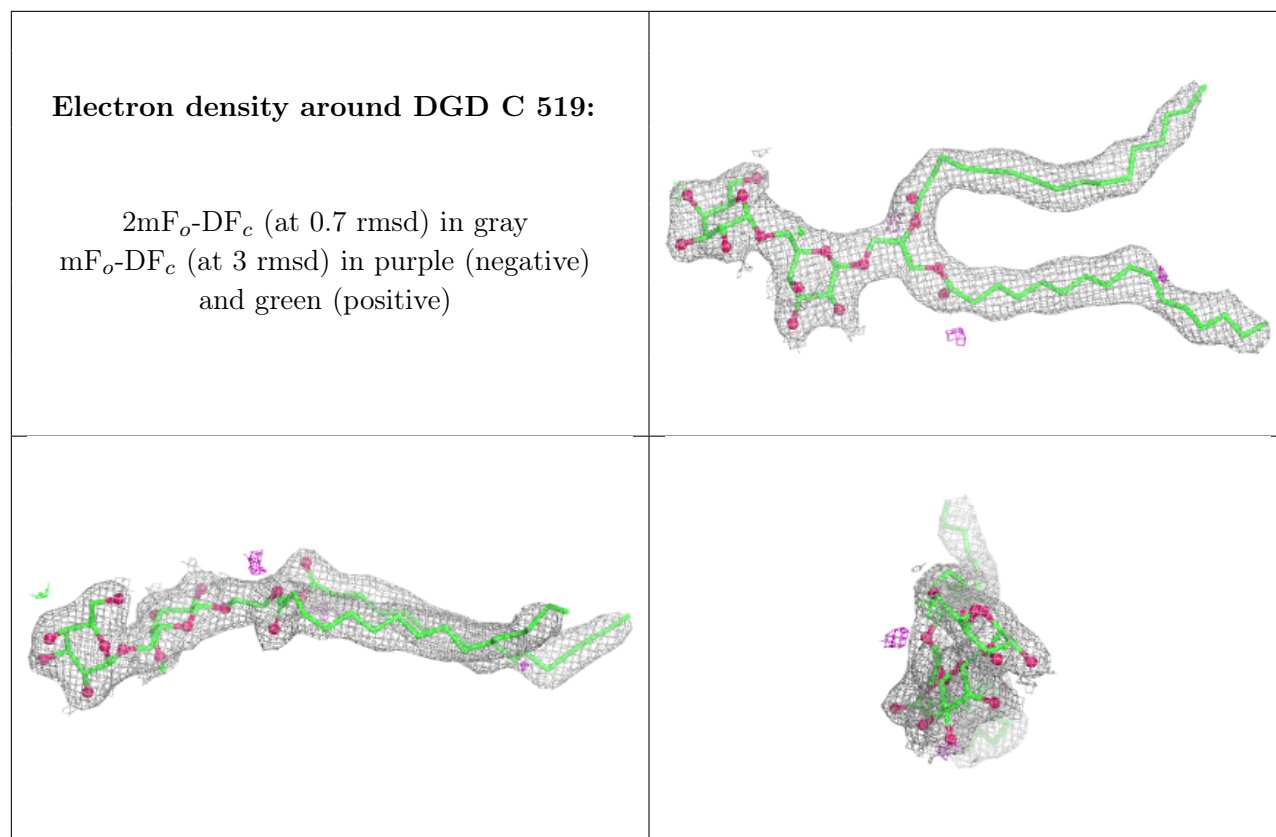
Electron density around CLA c 507:

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

**Electron density around BCR H 102:**

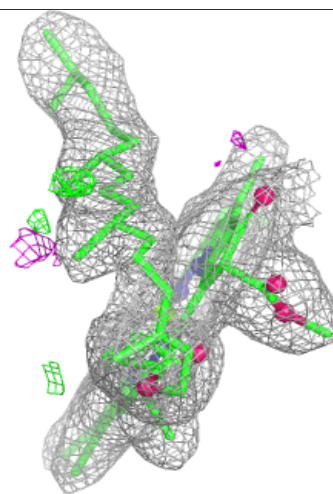
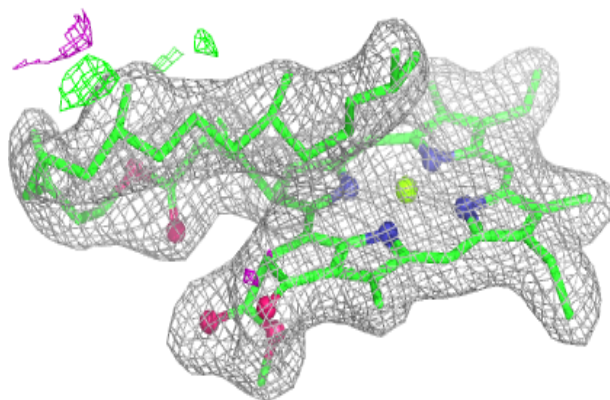
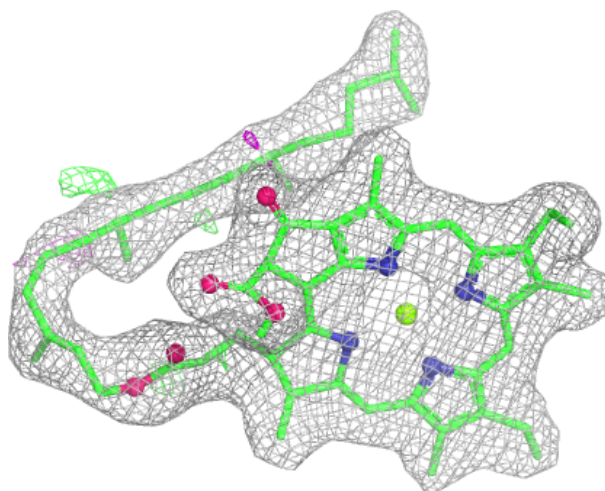
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





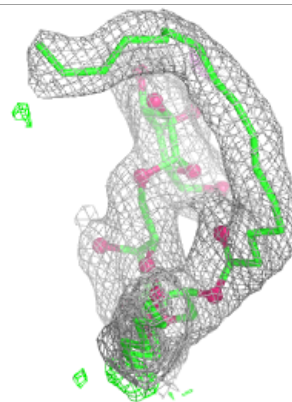
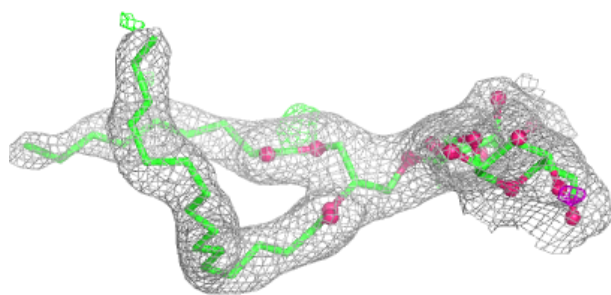
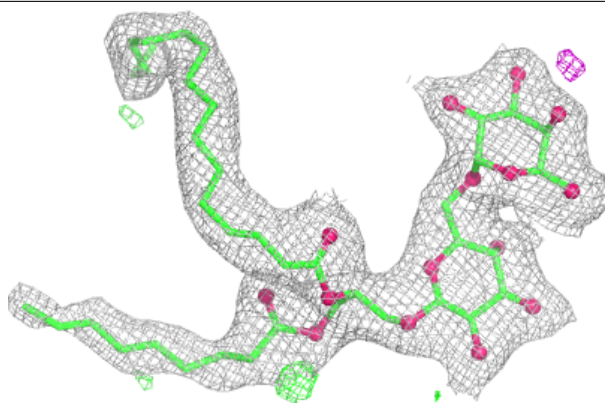
Electron density around CLA c 510:

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

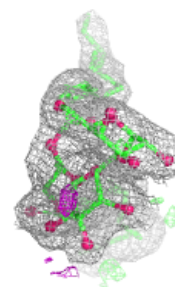
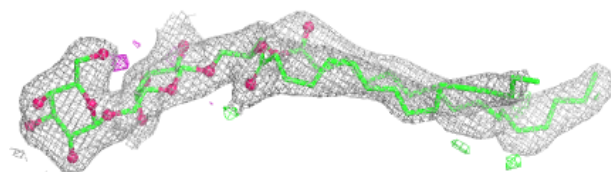
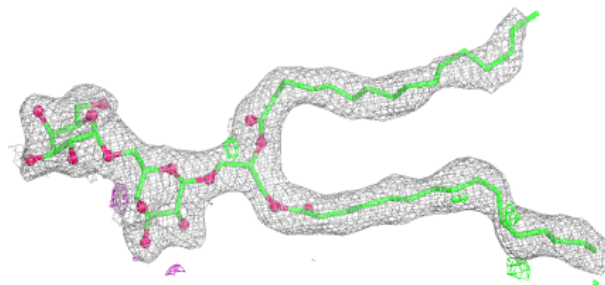


Electron density around DGD c 517:

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

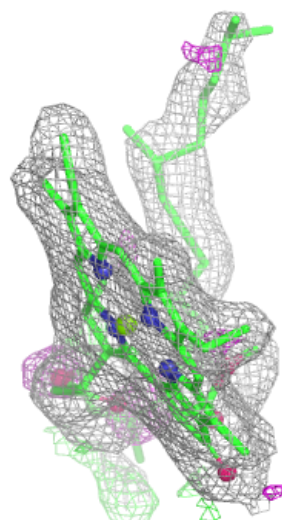
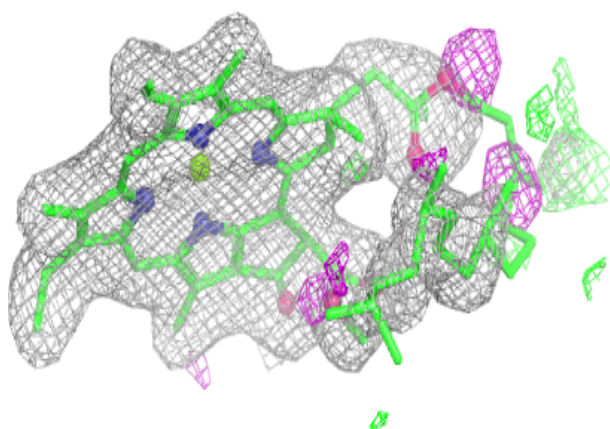
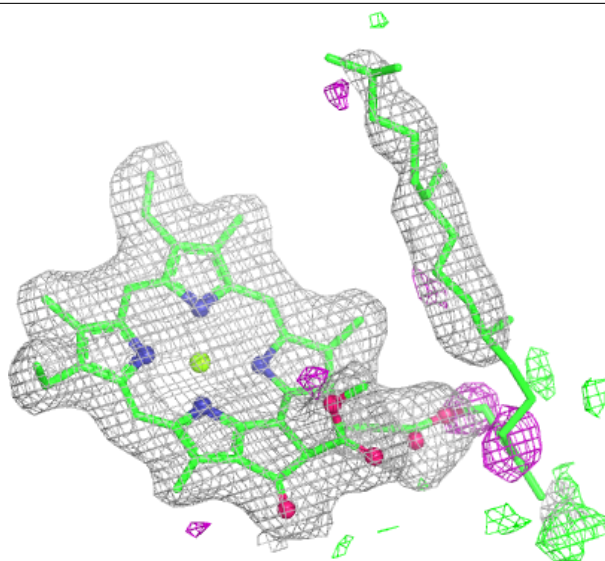
**Electron density around DGD c 518:**

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



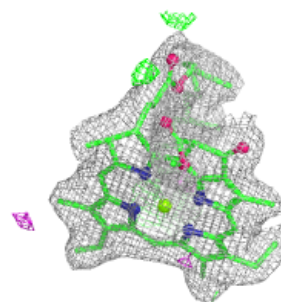
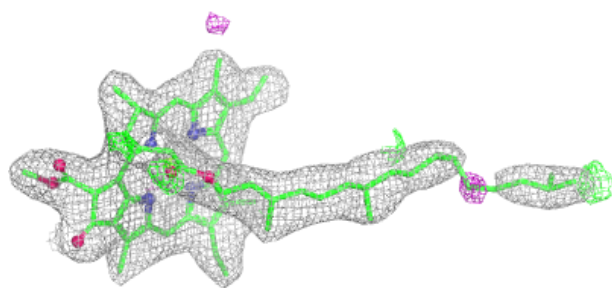
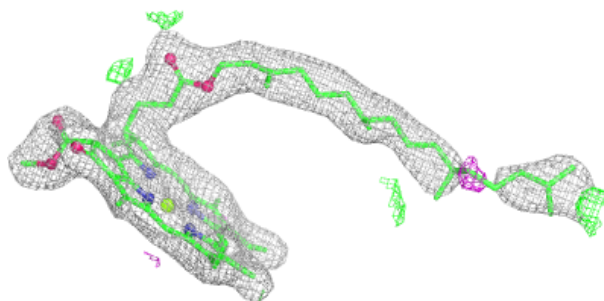
Electron density around CLA B 615:

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

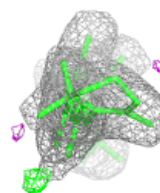
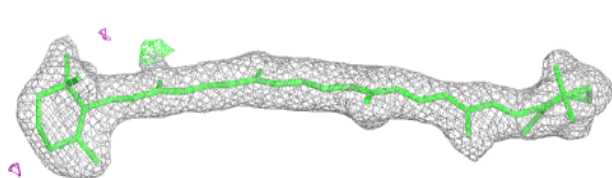
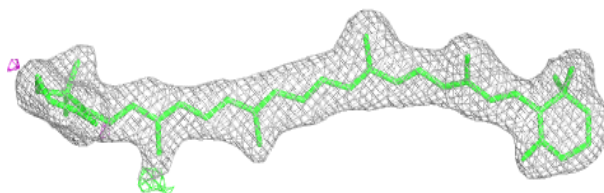


Electron density around CLA C 505:

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

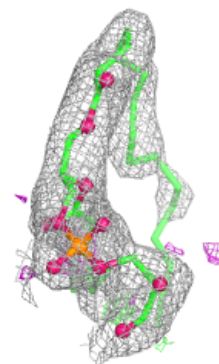
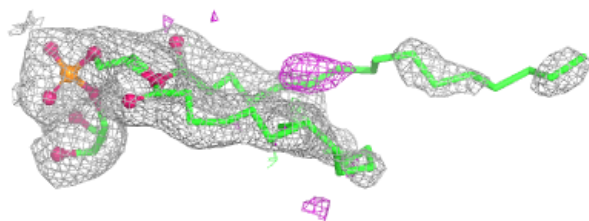
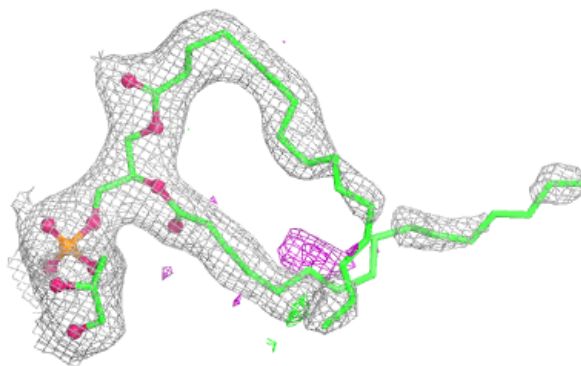
**Electron density around BCR b 619:**

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

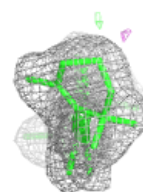
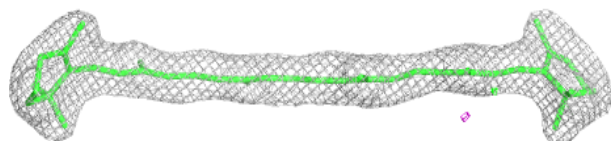
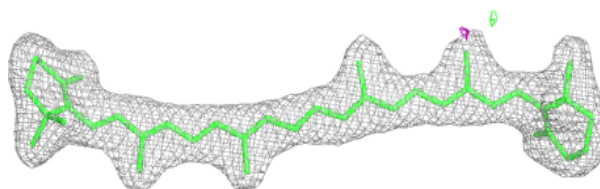


Electron density around LHG d 407:

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

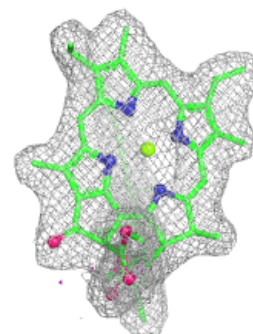
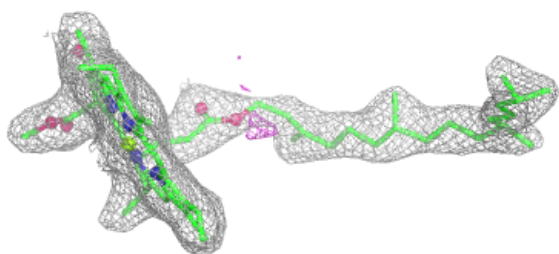
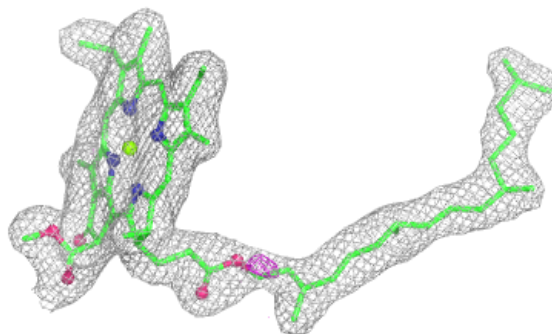
**Electron density around BCR b 620:**

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

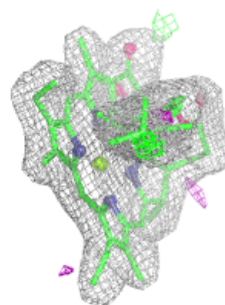
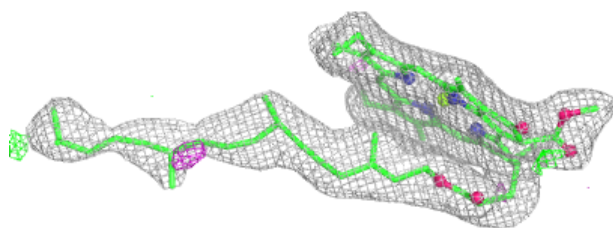
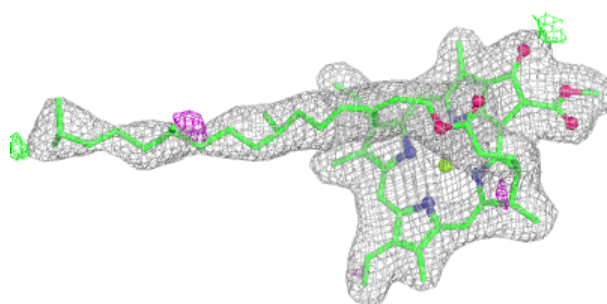


Electron density around CLA b 611:

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

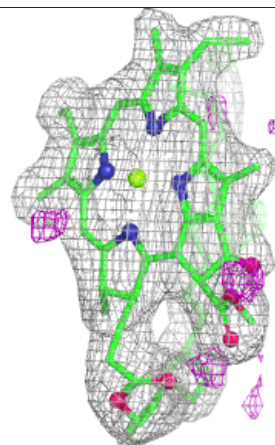
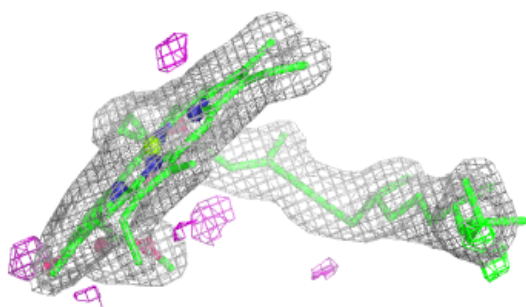
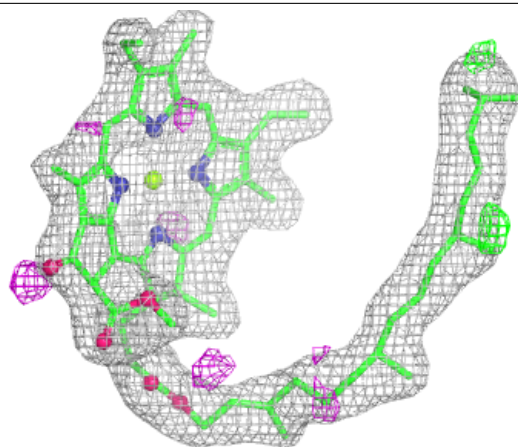
**Electron density around CLA b 616:**

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



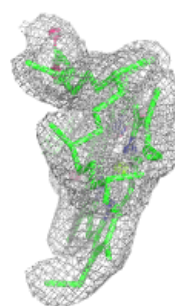
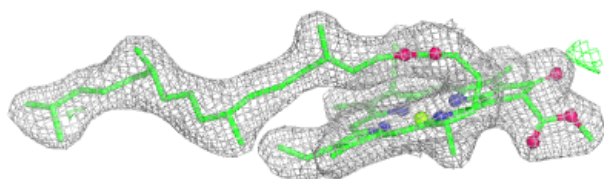
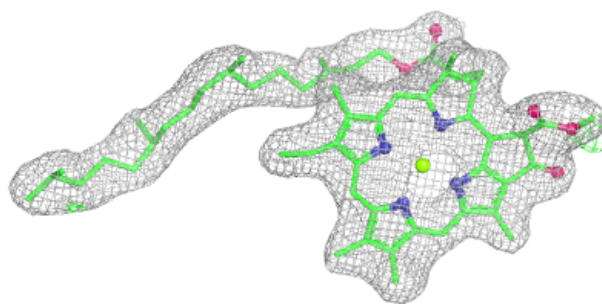
Electron density around CLA C 508:

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

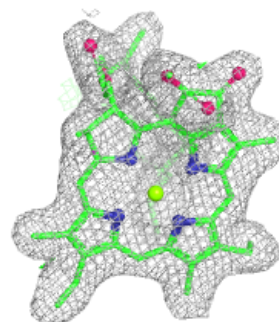
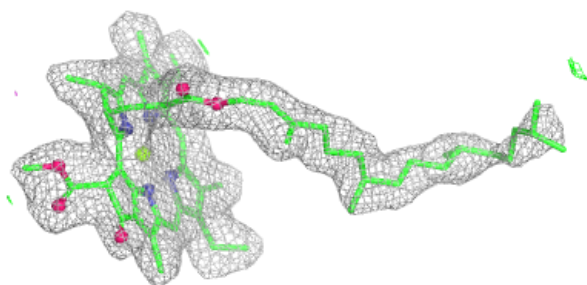
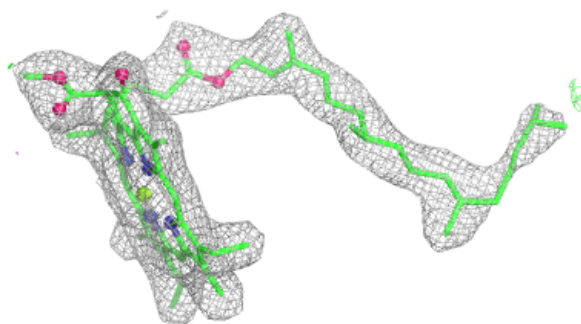


Electron density around CLA c 502:

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

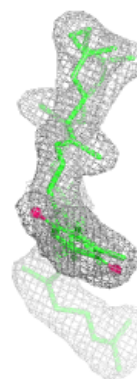
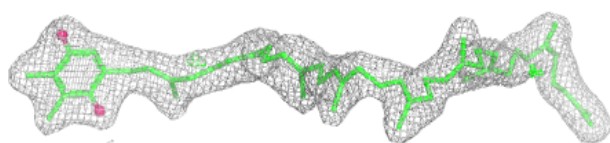
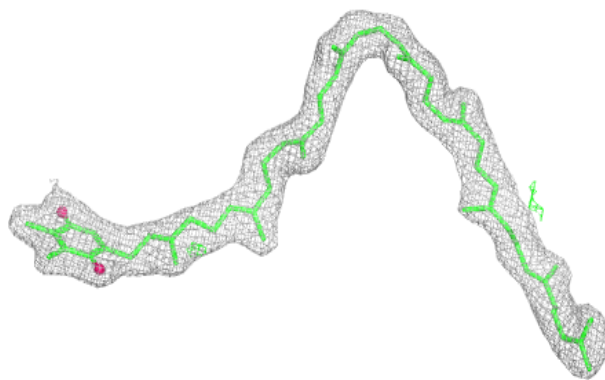
**Electron density around CLA C 509:**

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

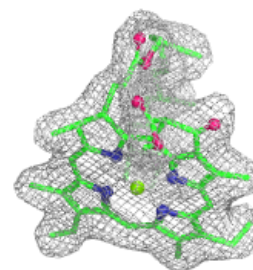
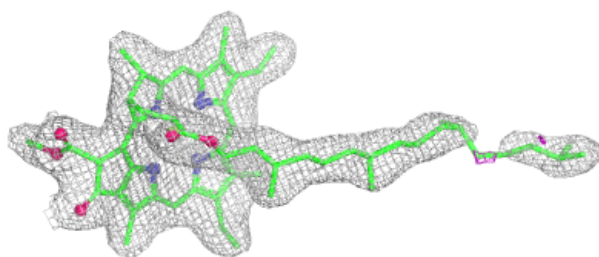
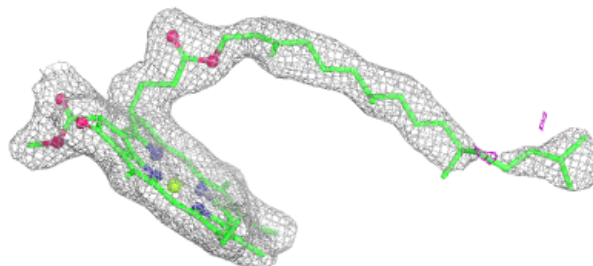


Electron density around PL9 d 405:

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

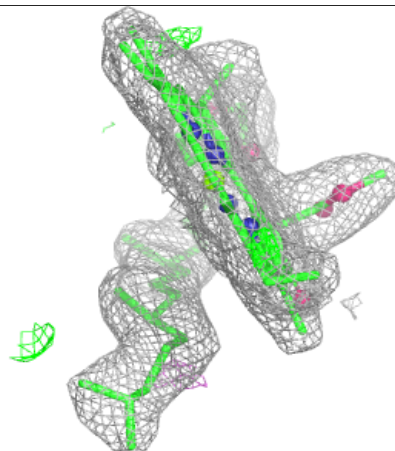
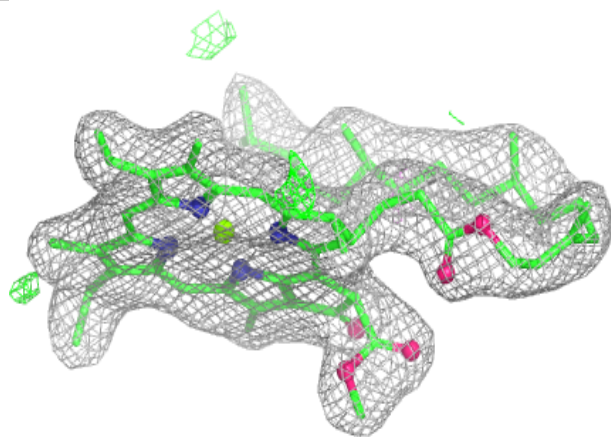
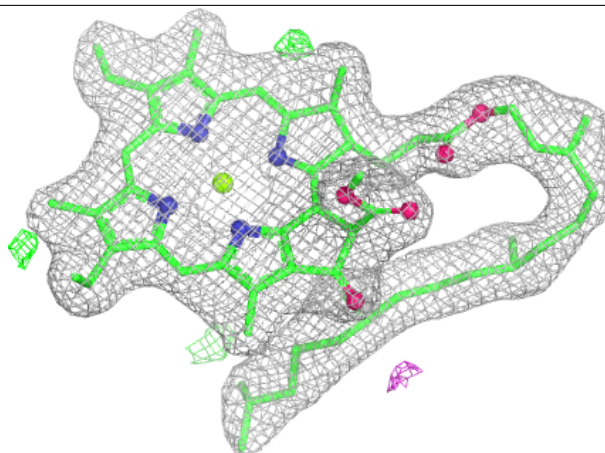
**Electron density around CLA c 505:**

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



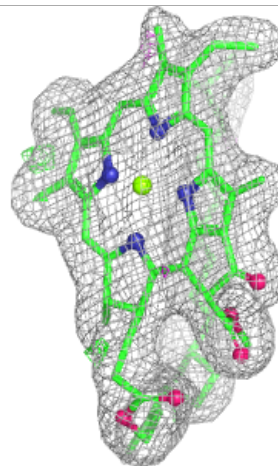
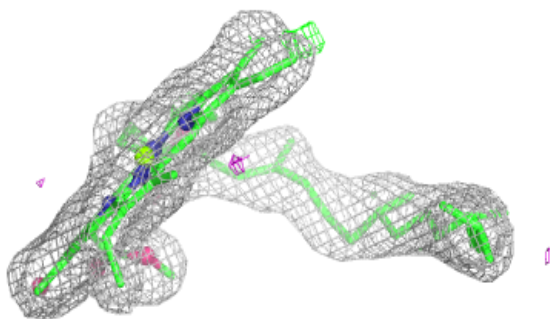
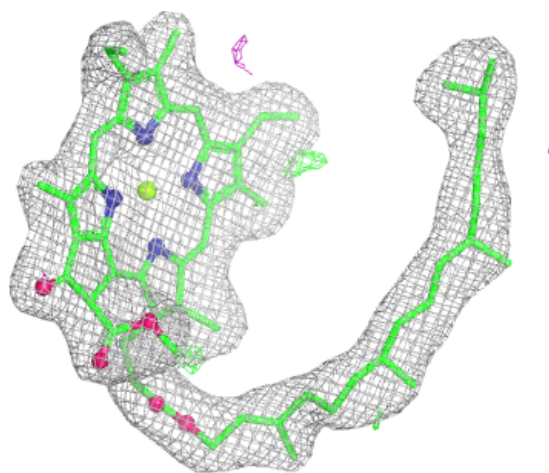
Electron density around CLA C 510:

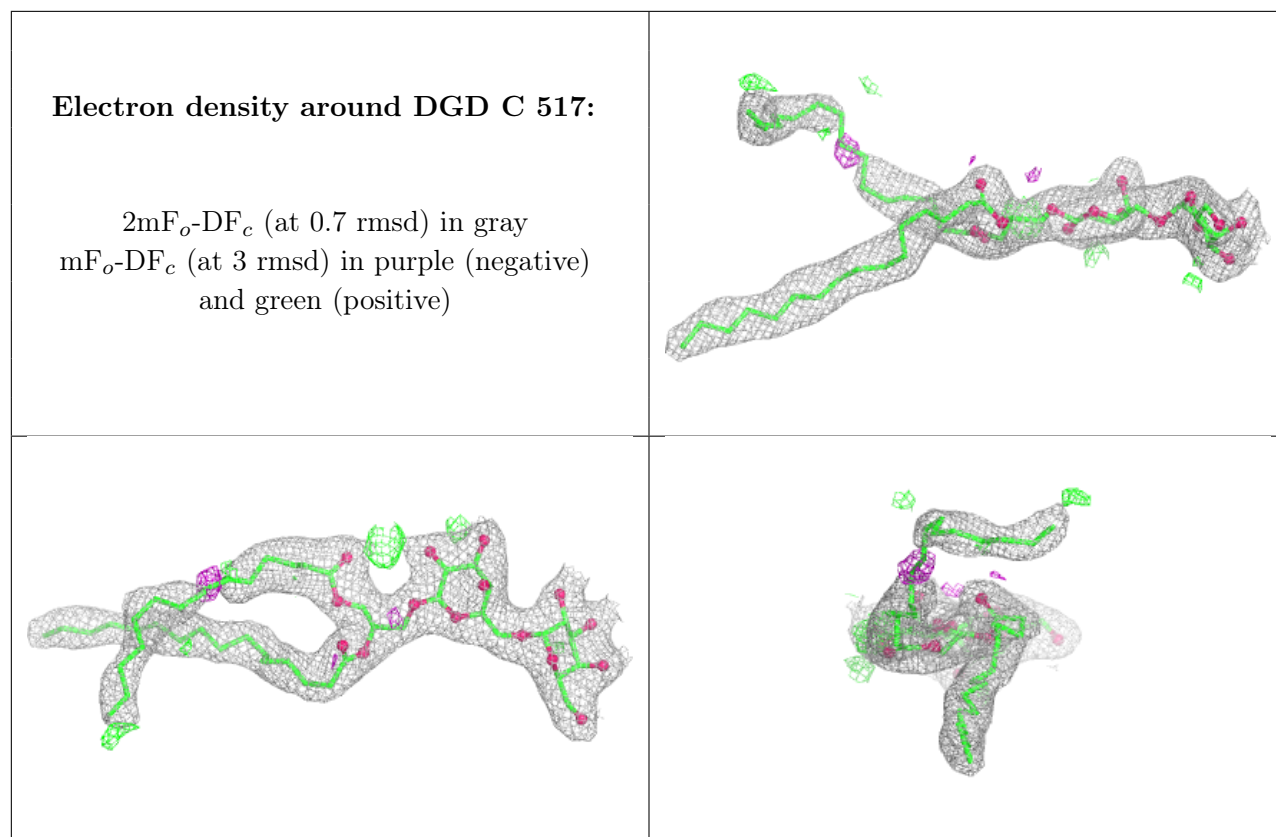
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 508:

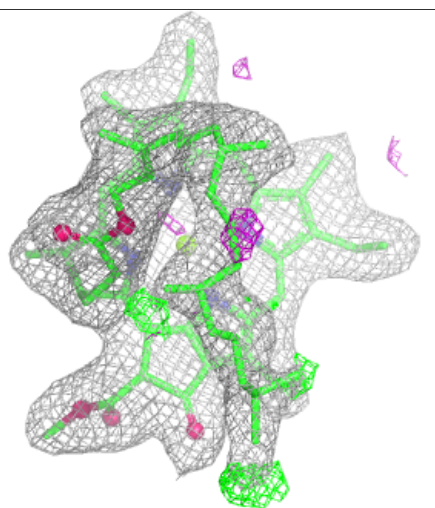
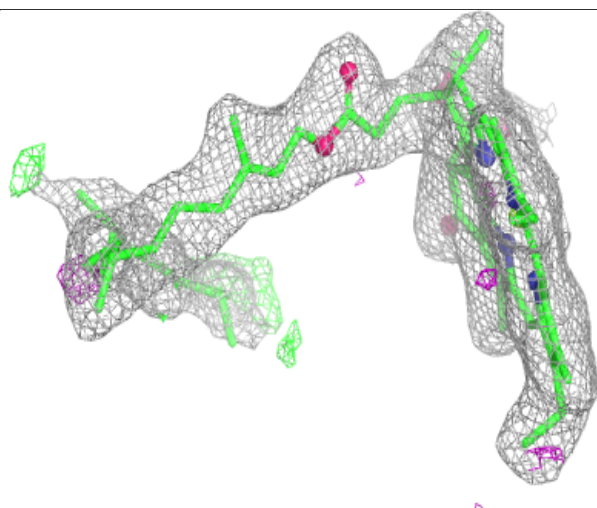
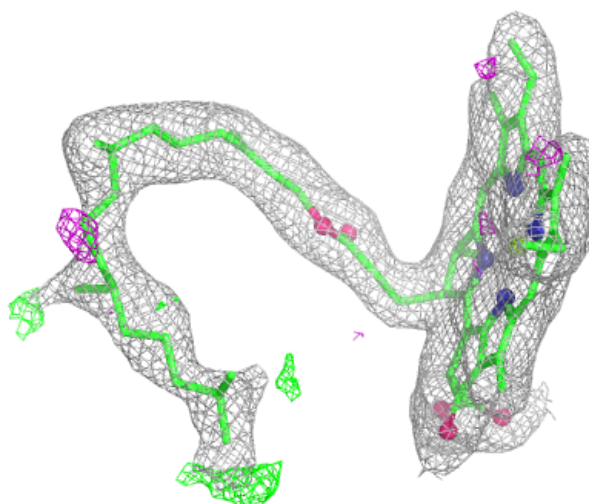
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





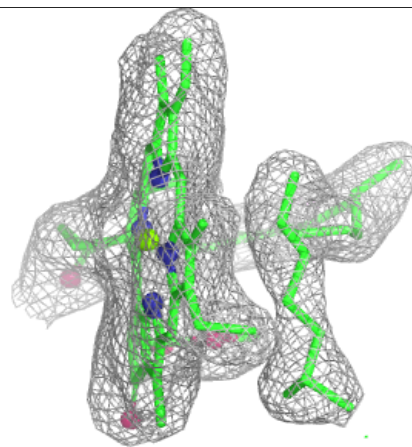
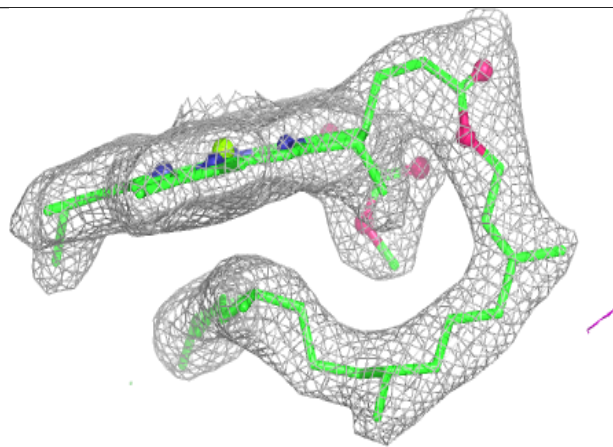
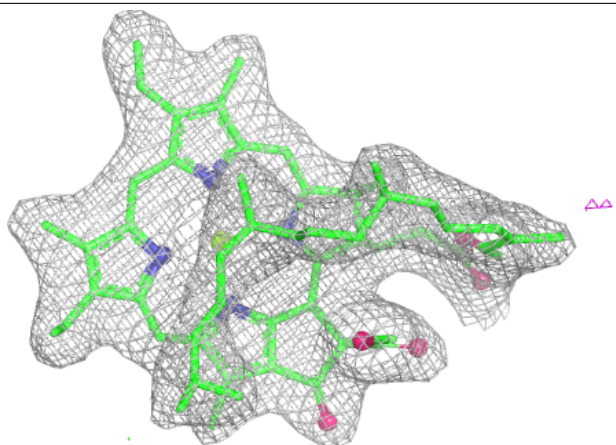
Electron density around CLA B 605:

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



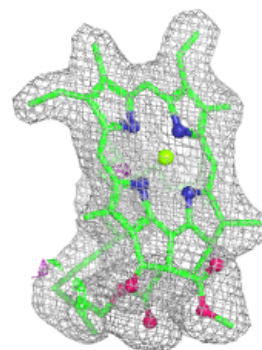
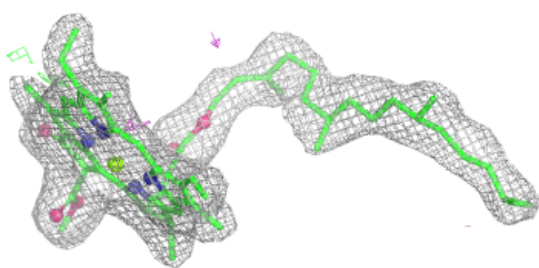
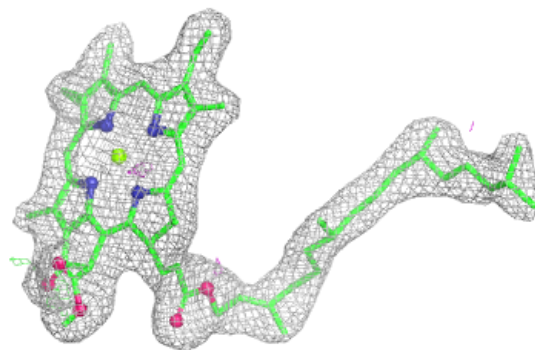
Electron density around CLA c 511:

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

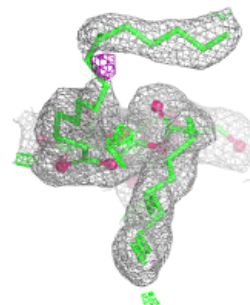
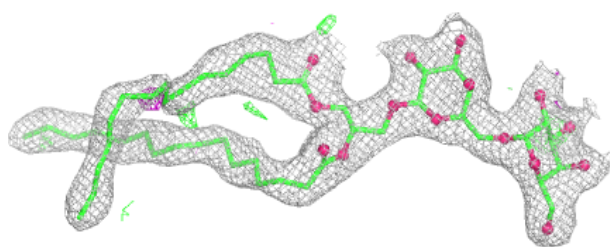
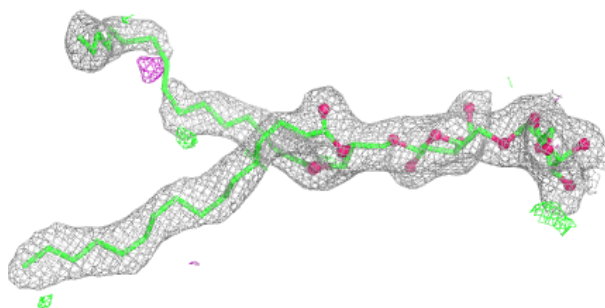


Electron density around CLA c 512:

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

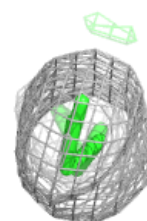
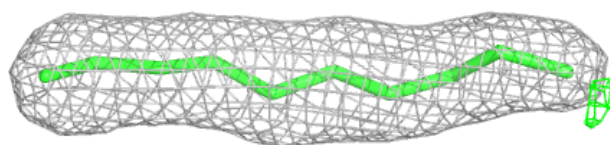
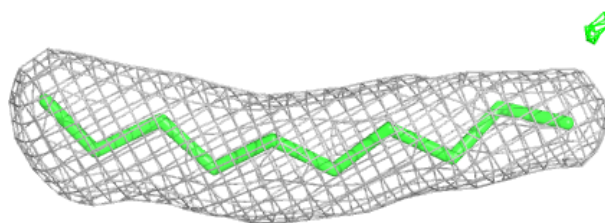
**Electron density around DGD c 516:**

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

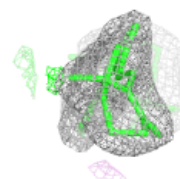
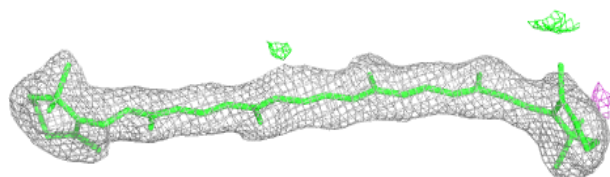
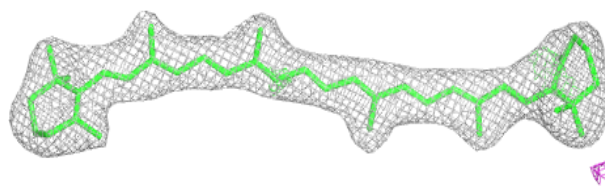


Electron density around LFA M 101:

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

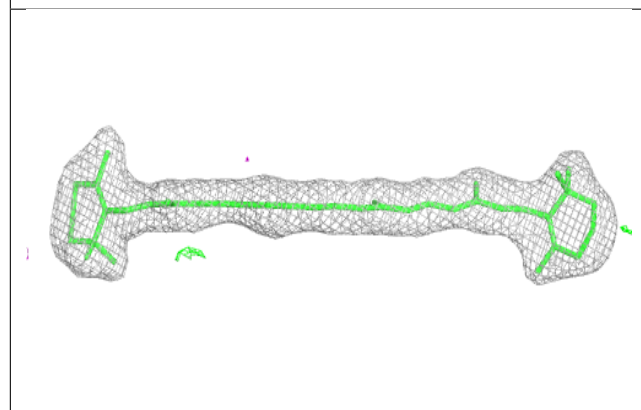
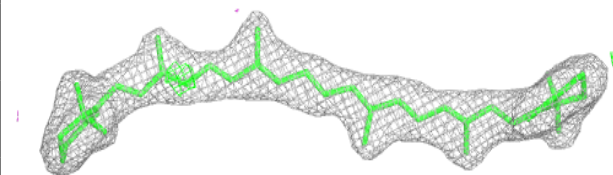
**Electron density around BCR b 621:**

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

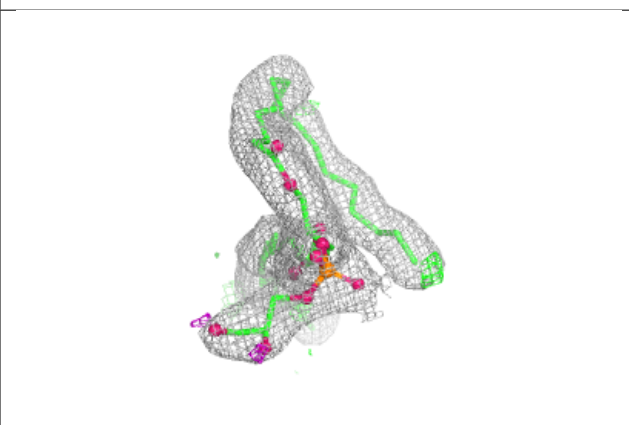
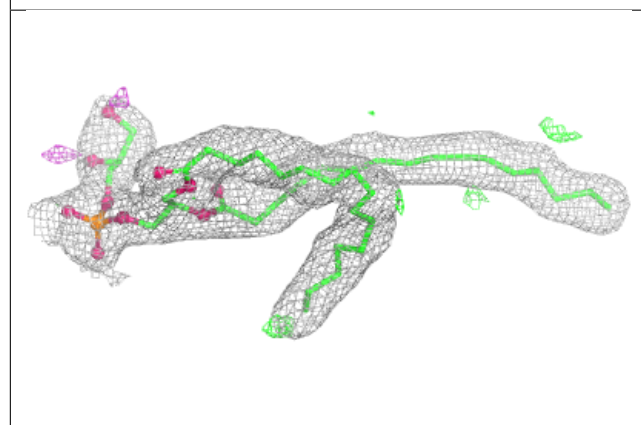
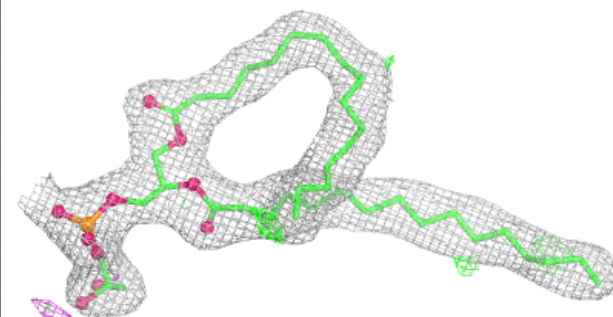


Electron density around BCR c 515:

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

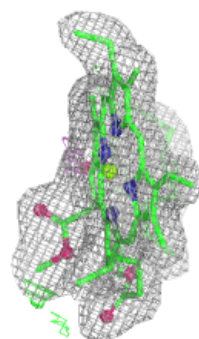
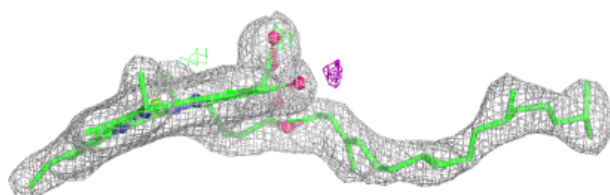
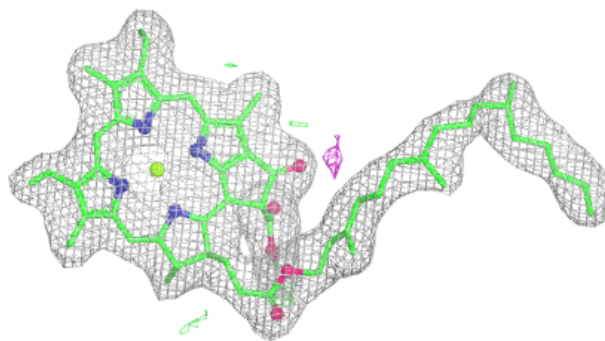
**Electron density around LHG D 407:**

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

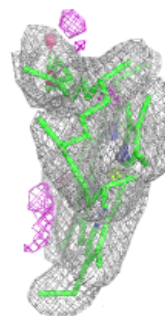
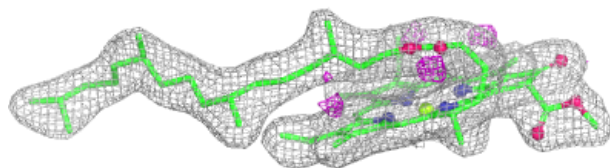
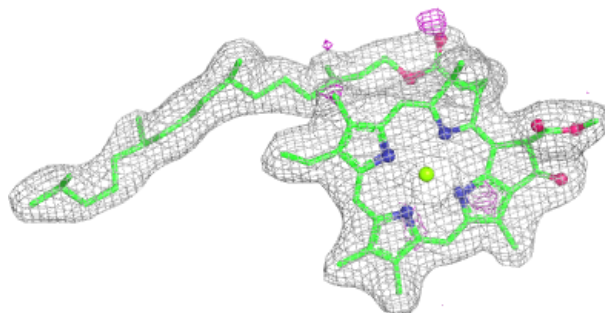


Electron density around CLA b 604:

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

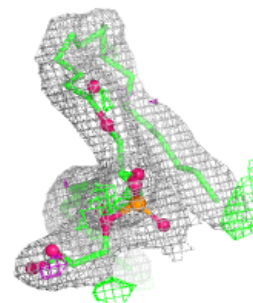
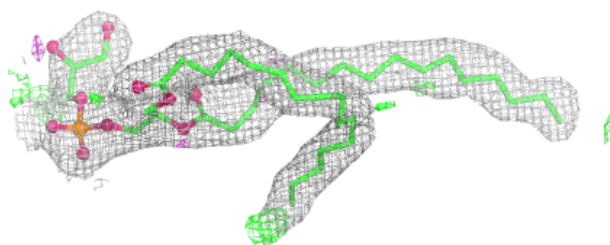
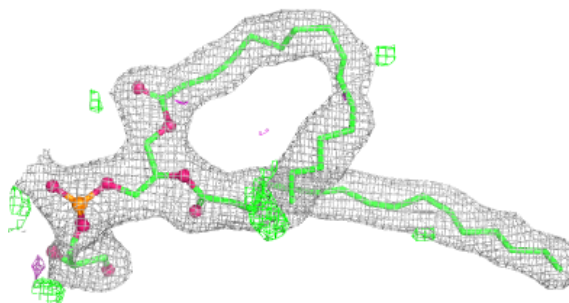
**Electron density around CLA C 502:**

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

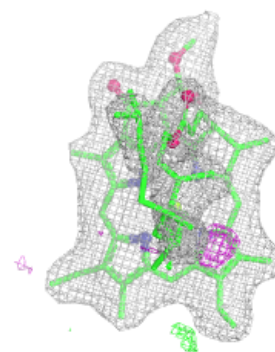
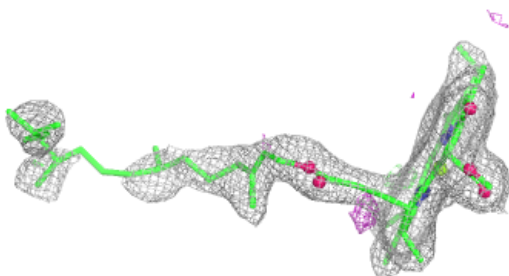
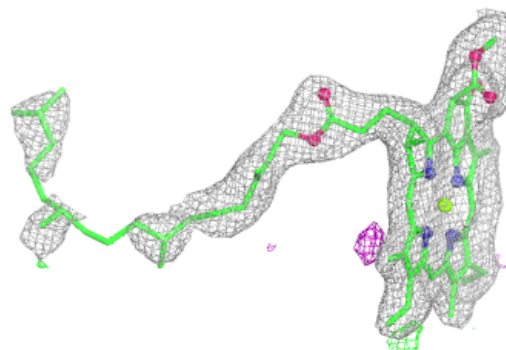


Electron density around LHG b 628:

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

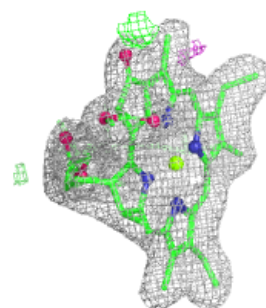
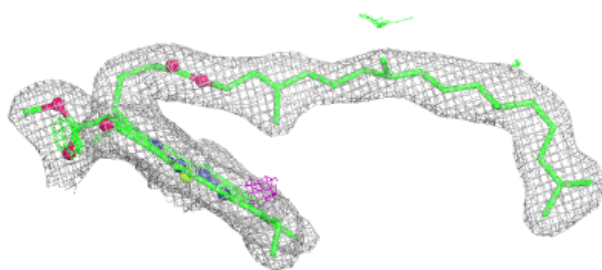
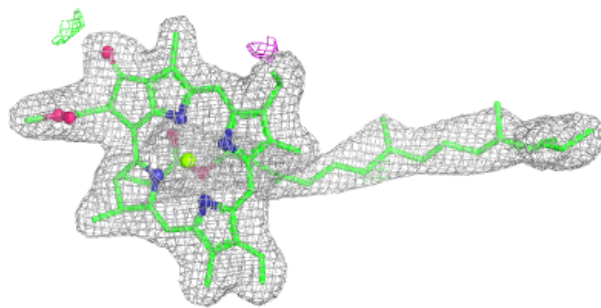
**Electron density around CLA d 403:**

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



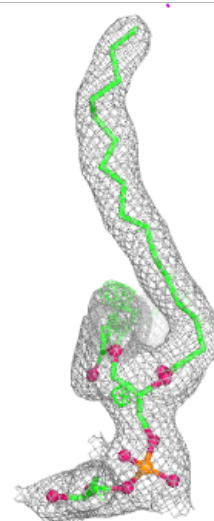
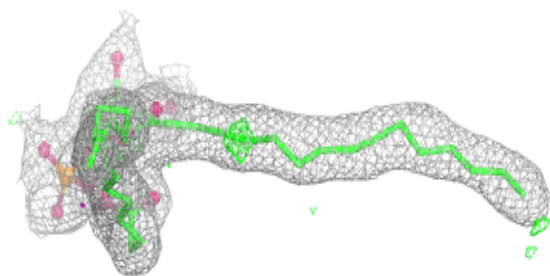
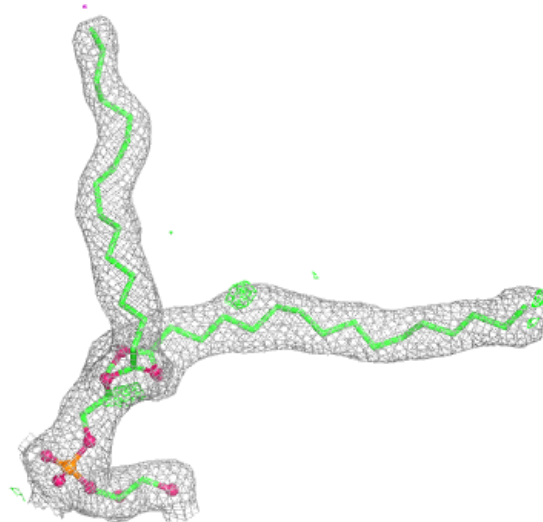
Electron density around CLA b 610:

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



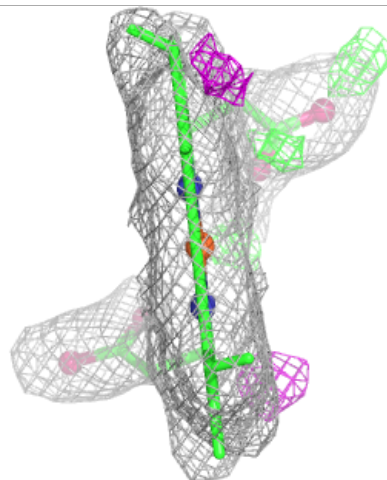
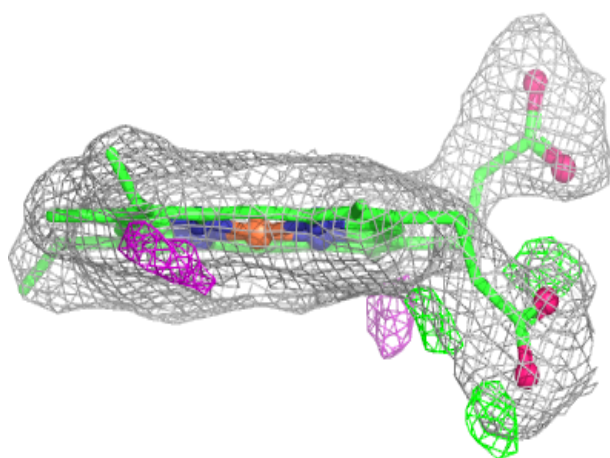
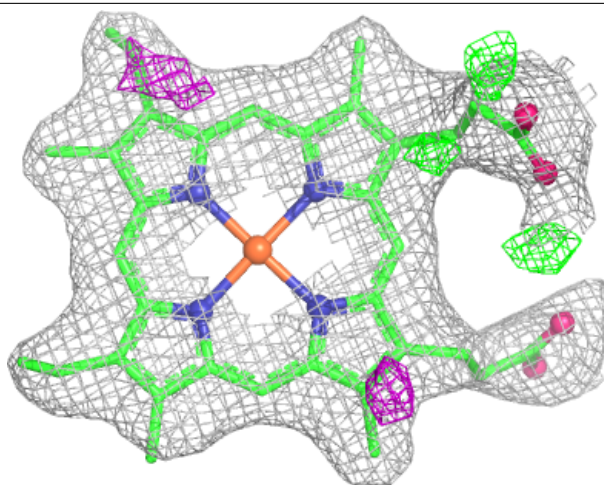
Electron density around LHG 1 101:

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



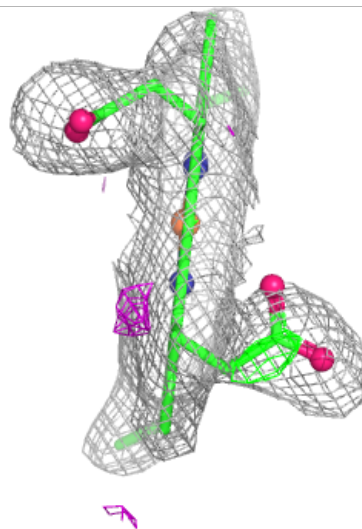
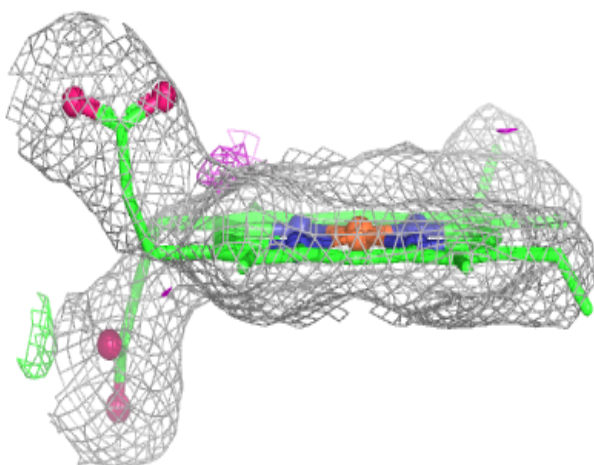
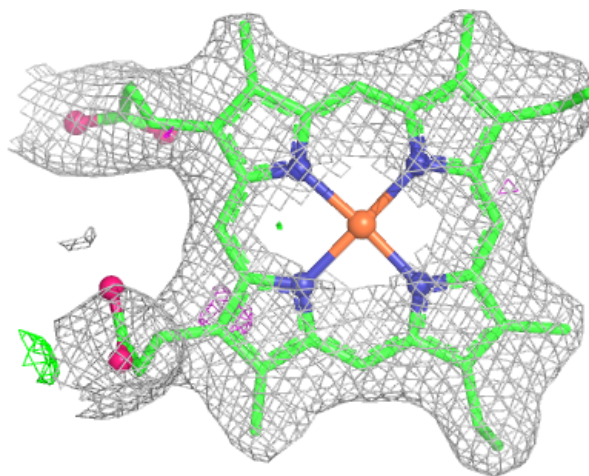
Electron density around HEM E 102:

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



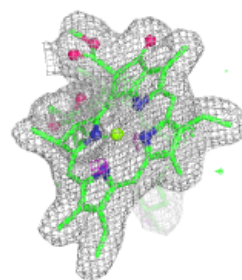
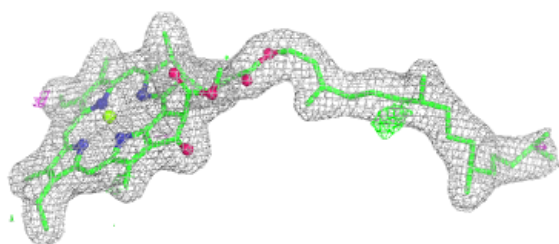
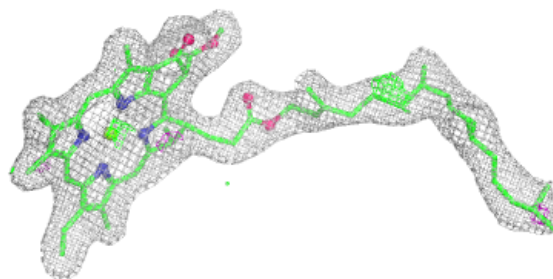
Electron density around HEM e 102:

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

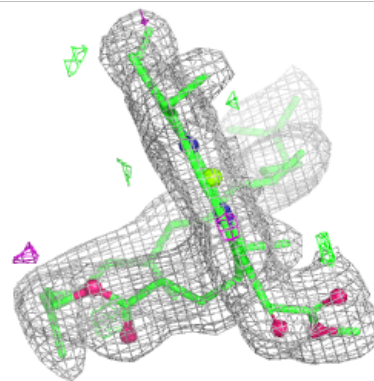
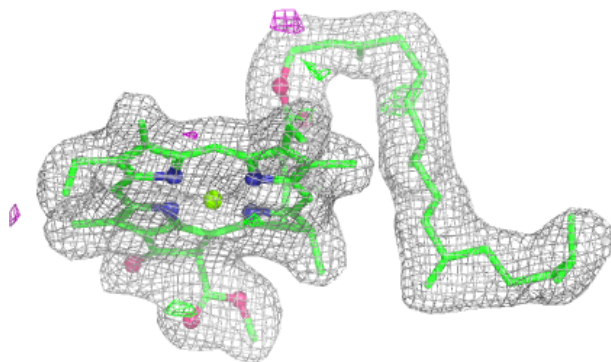
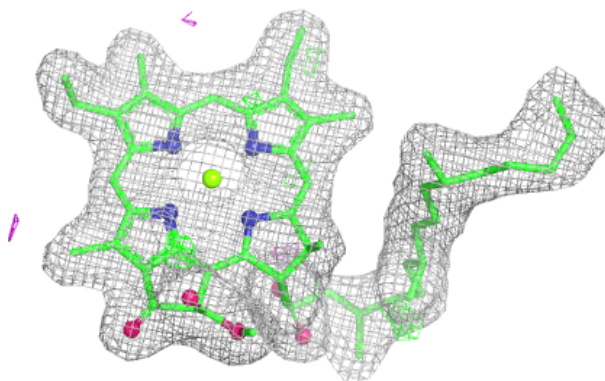


Electron density around CLA a 404:

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

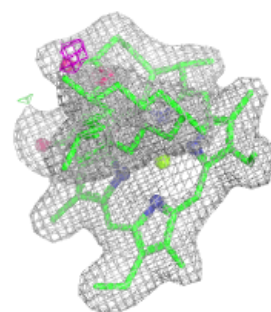
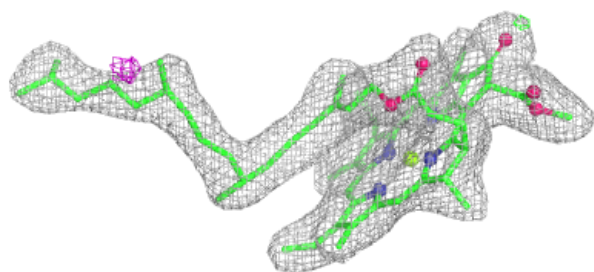
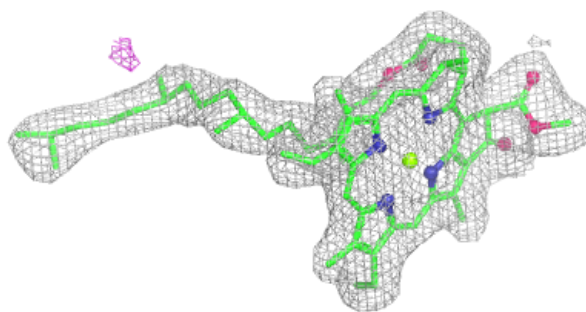
**Electron density around CLA a 405:**

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

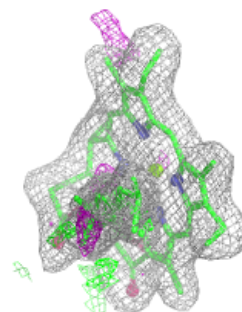
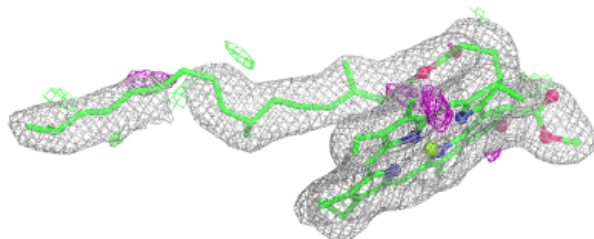
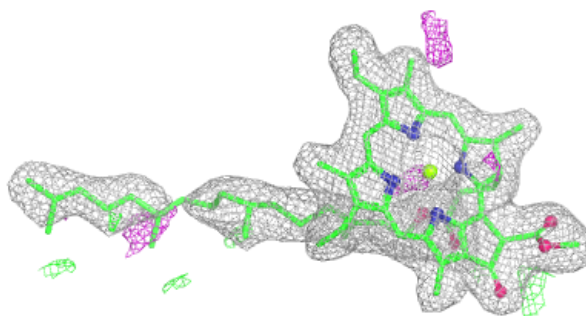


Electron density around CLA c 506:

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

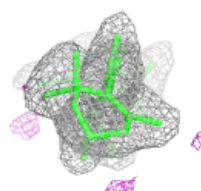
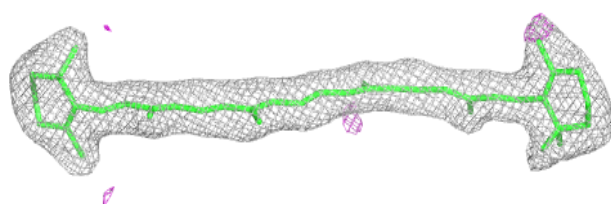
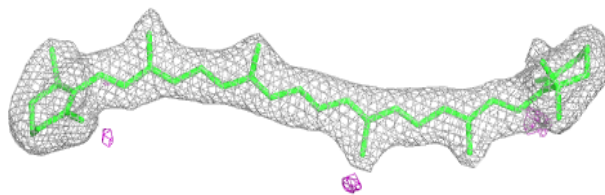
**Electron density around CLA B 613:**

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

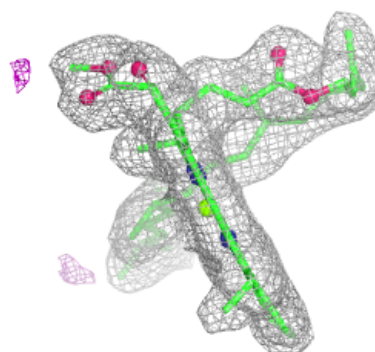
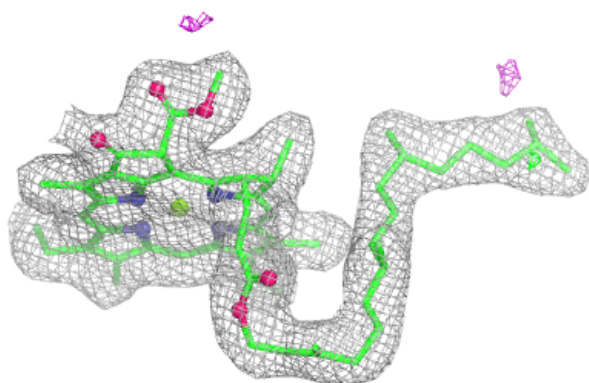
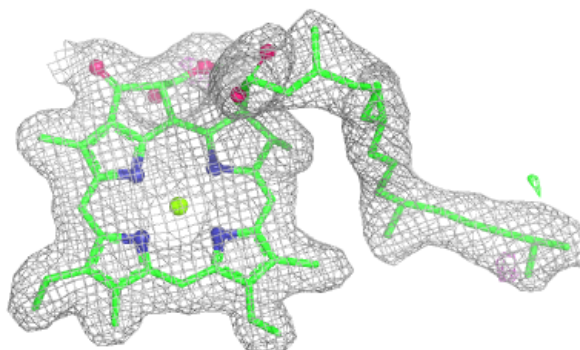


Electron density around BCR a 408:

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

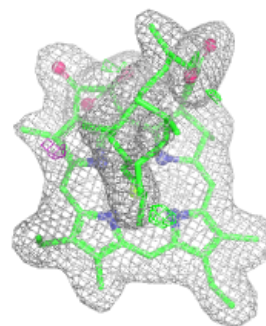
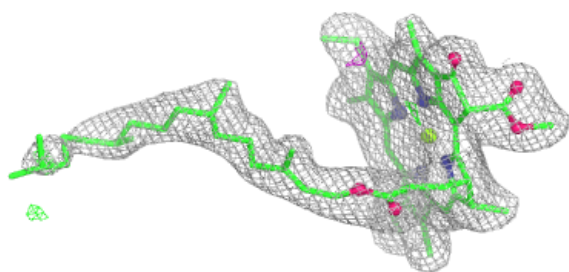
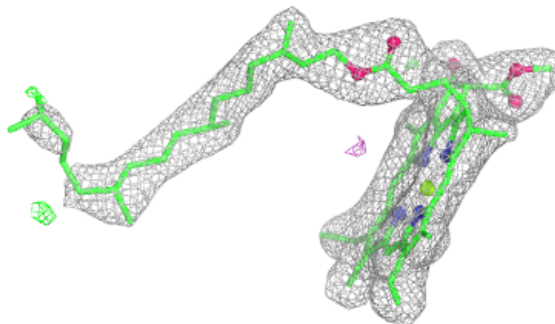
**Electron density around CLA A 412:**

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

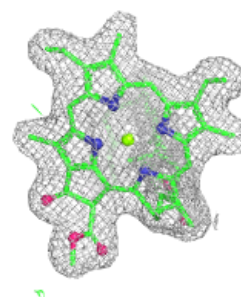
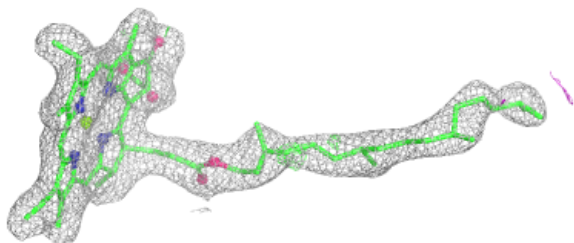
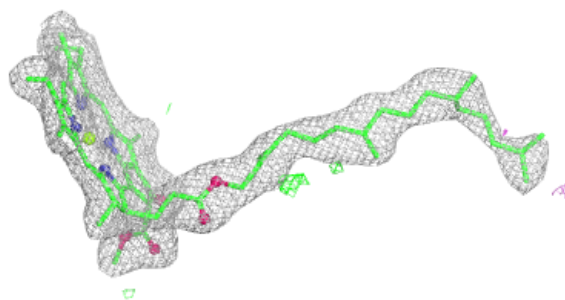


Electron density around CLA c 509:

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

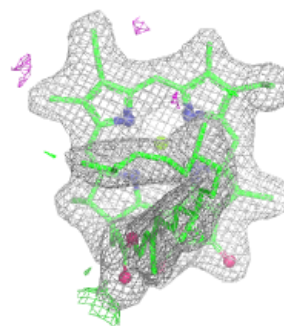
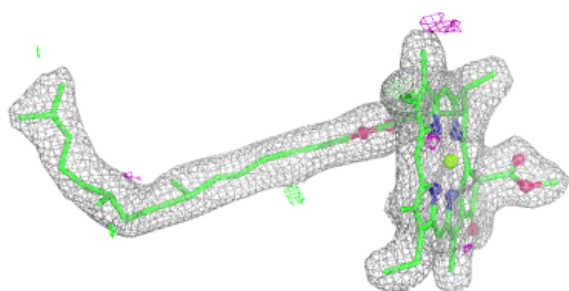
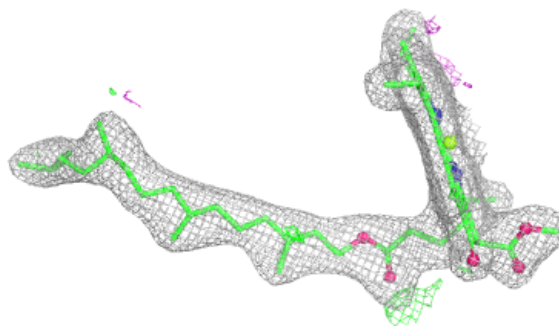
**Electron density around CLA b 606:**

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

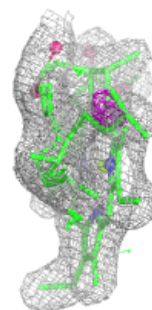
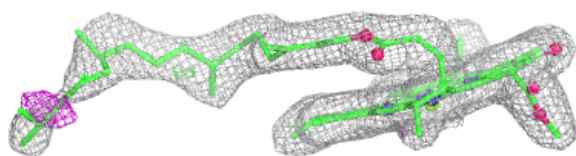
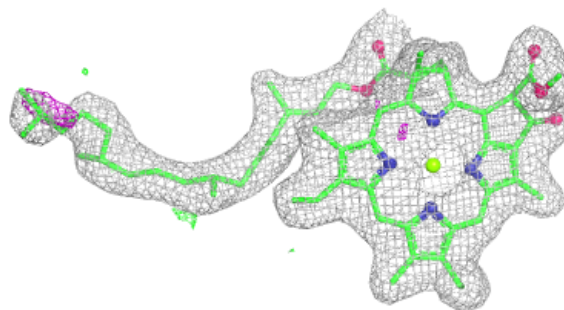


Electron density around CLA b 607:

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

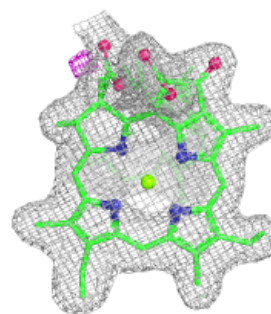
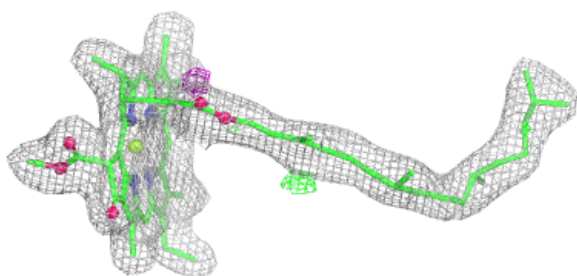
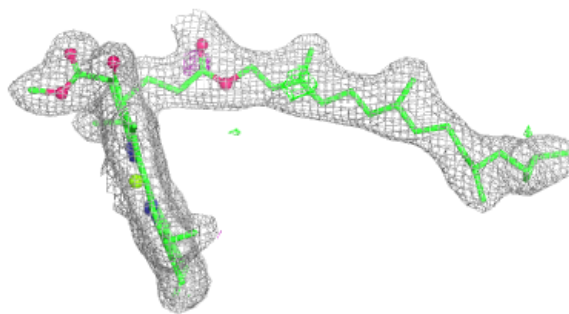
**Electron density around CLA B 602:**

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

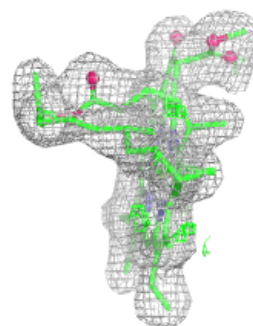
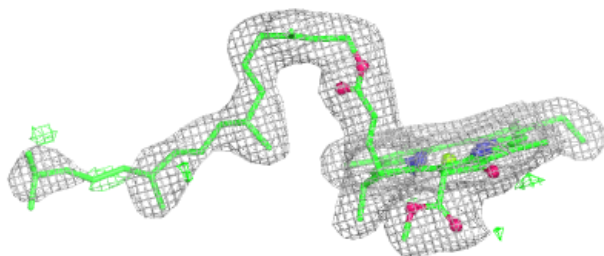
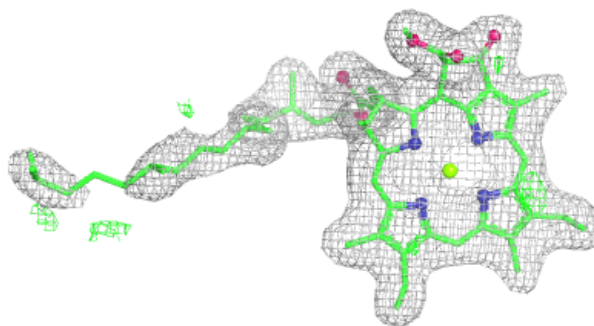


Electron density around CLA B 604:

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

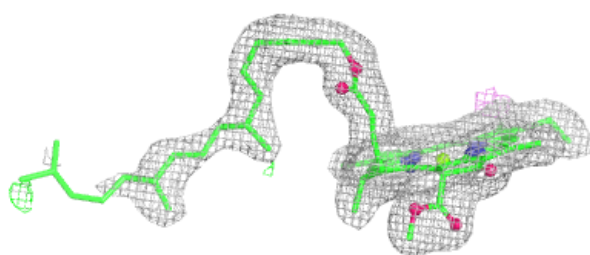
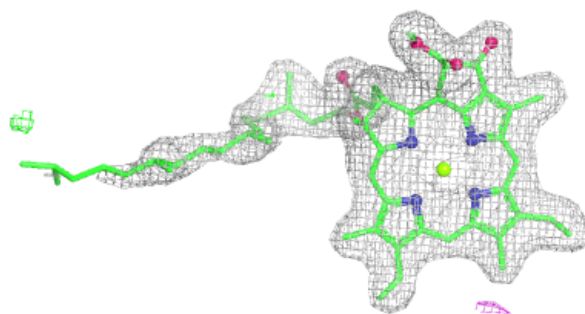
**Electron density around CLA A 404:**

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

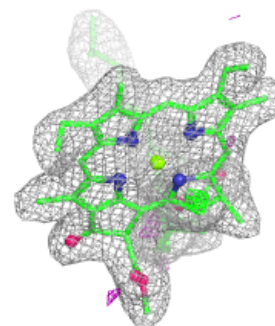
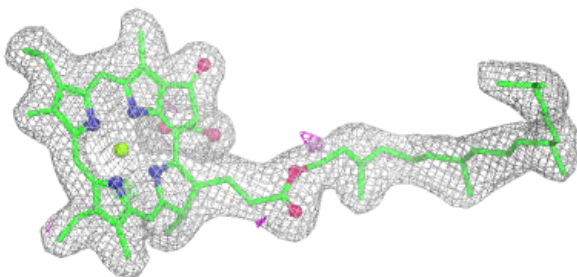
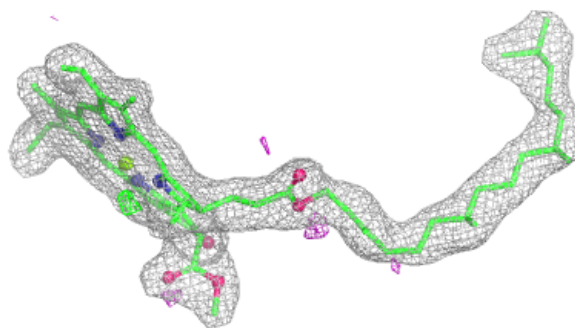


Electron density around CLA d 401:

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

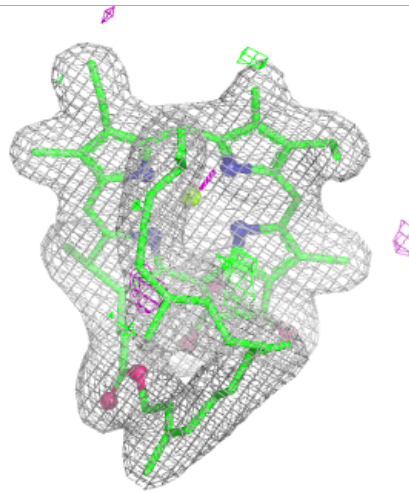
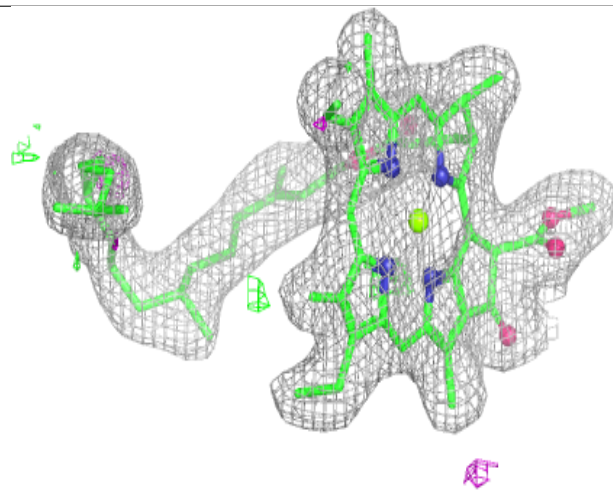
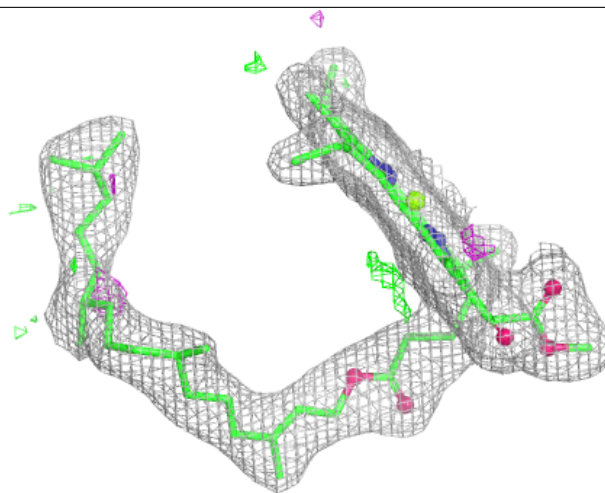
**Electron density around CLA d 402:**

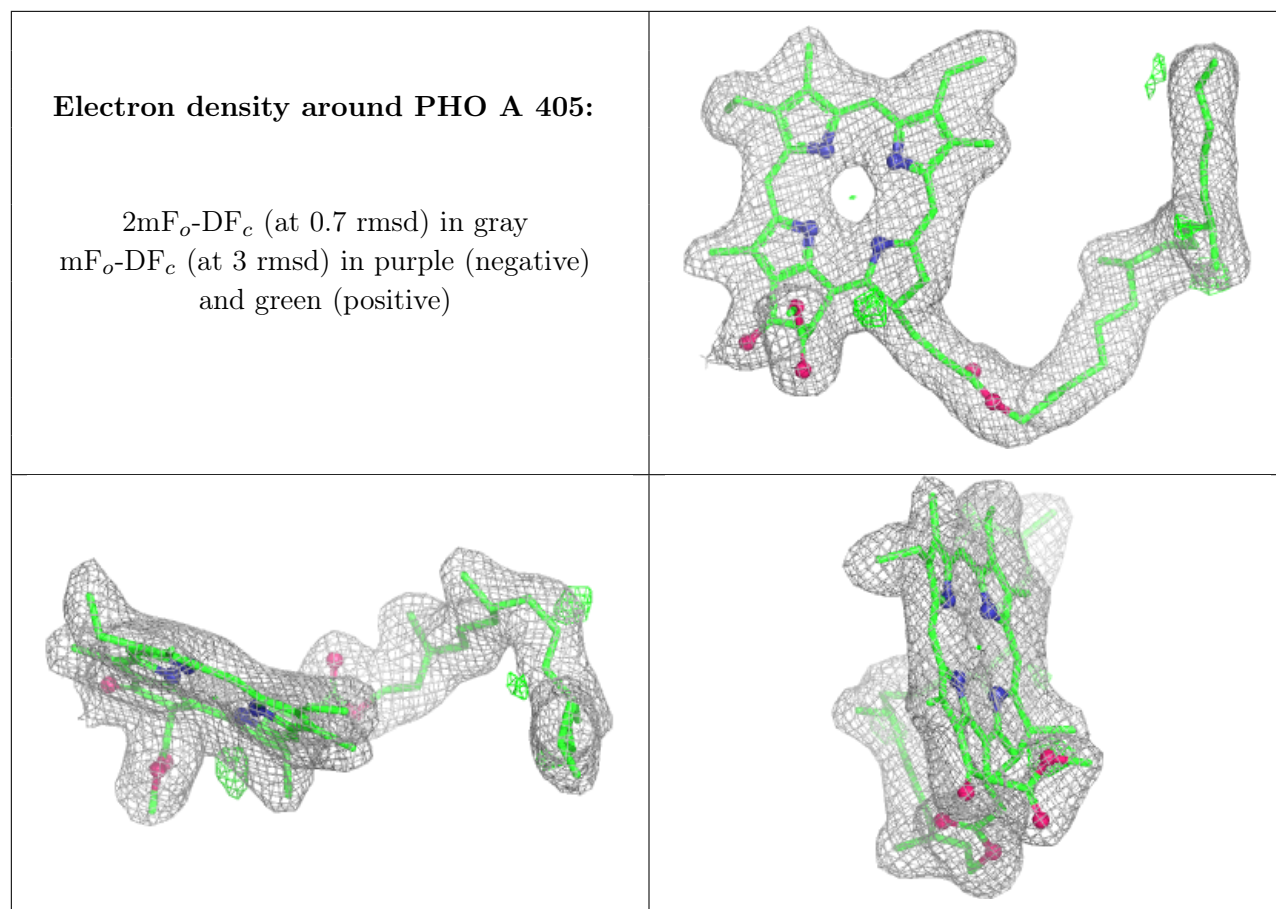
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 613:

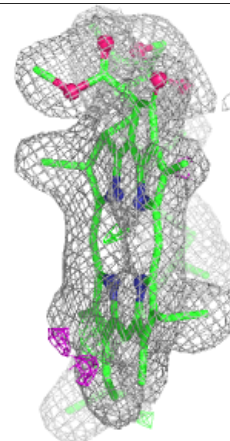
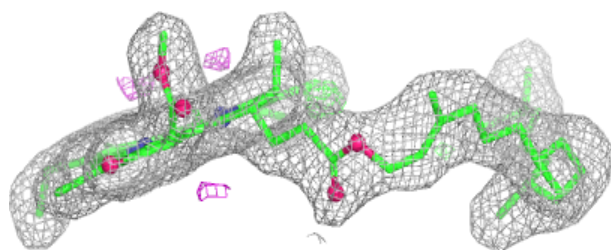
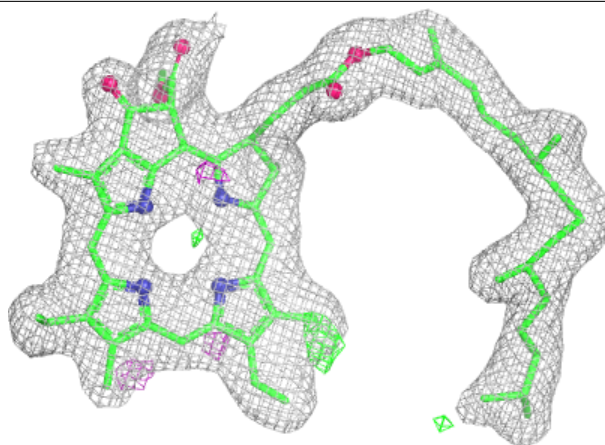
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



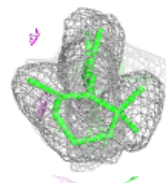
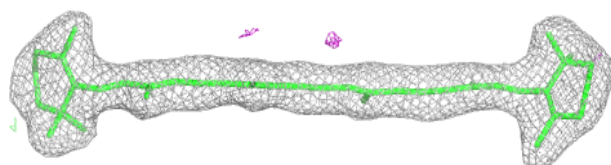
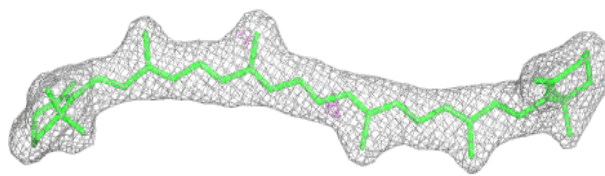


Electron density around PHO a 406:

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

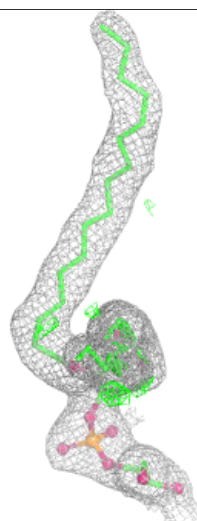
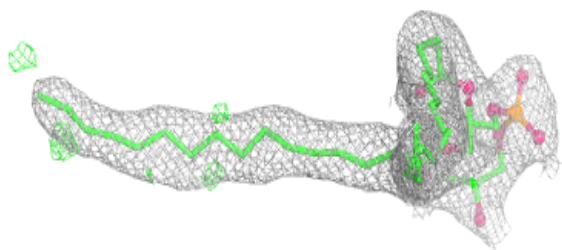
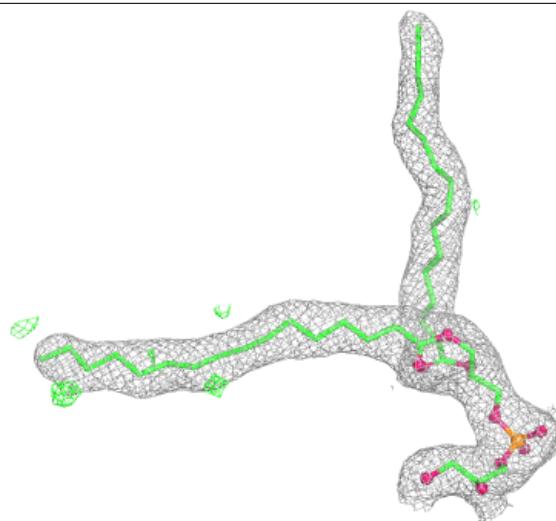
**Electron density around BCR A 407:**

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



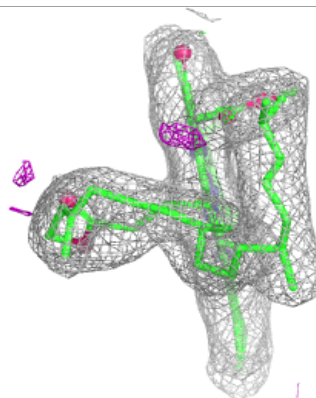
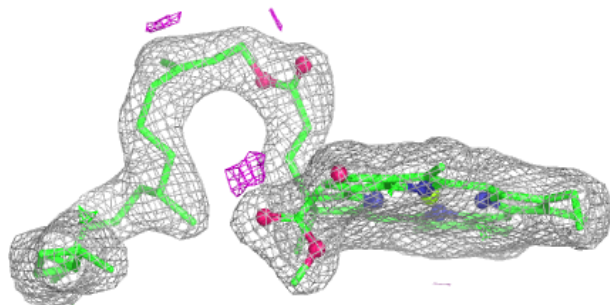
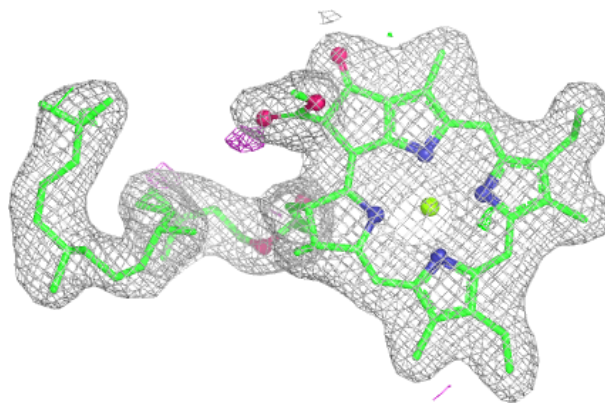
Electron density around LHG L 102:

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



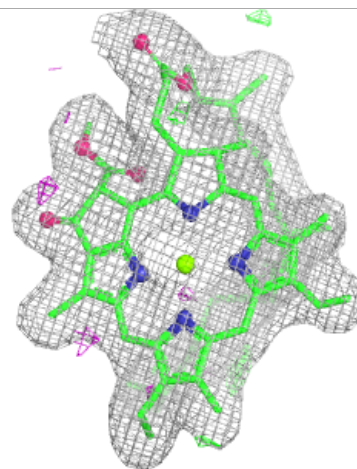
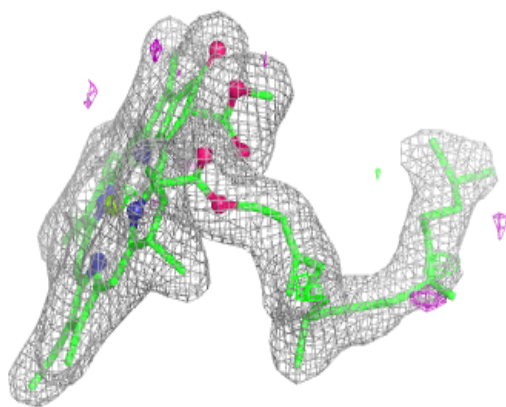
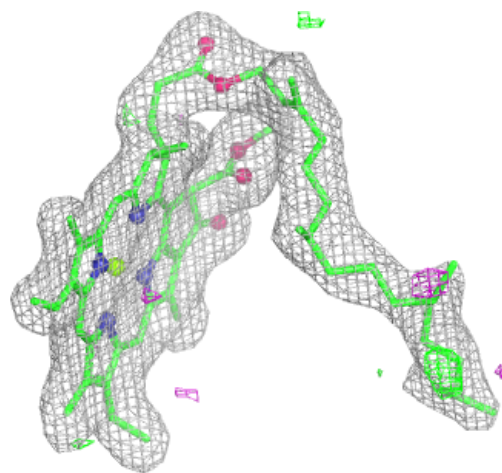
Electron density around CLA b 614:

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



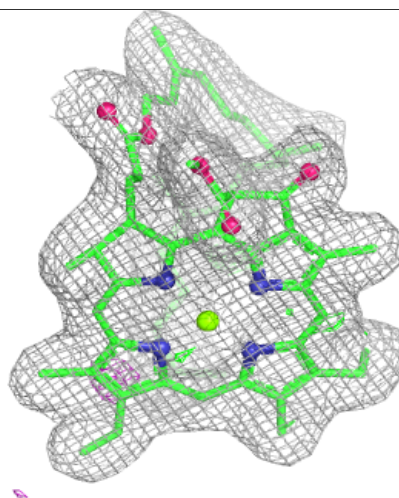
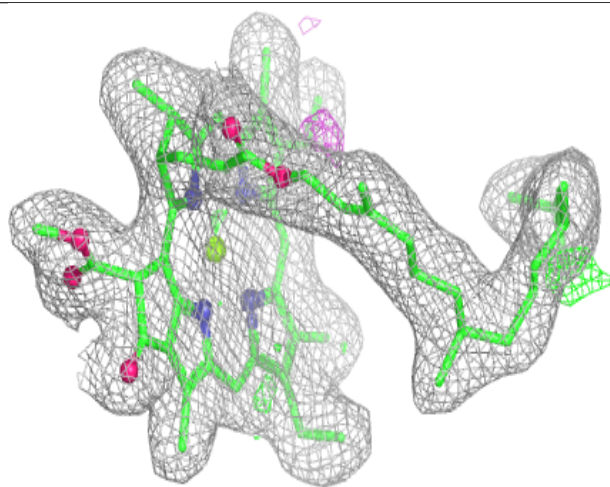
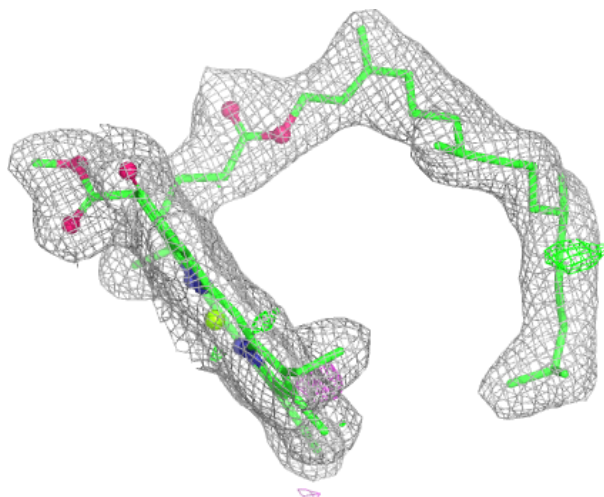
Electron density around CLA b 615:

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



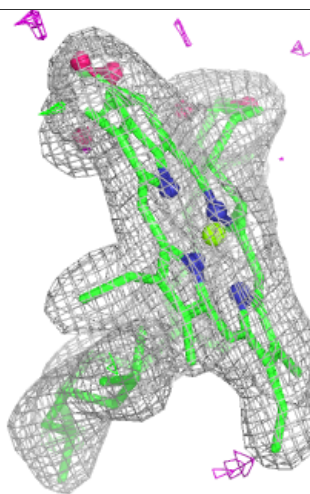
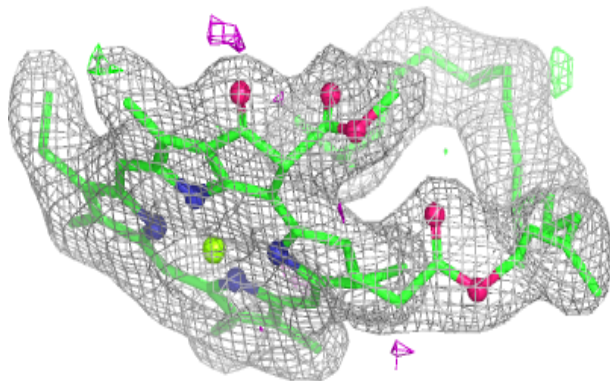
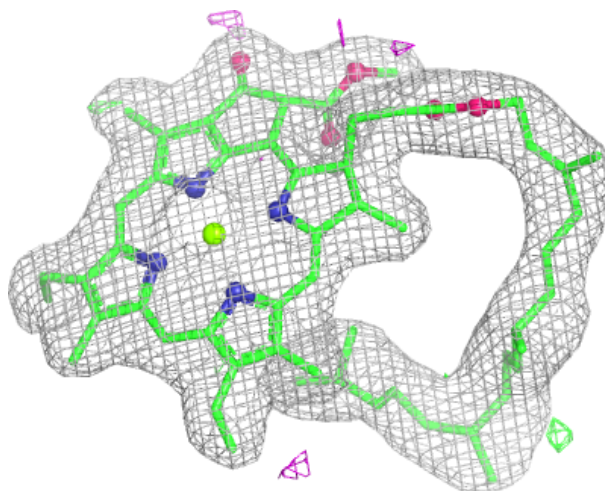
Electron density around CLA B 610:

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



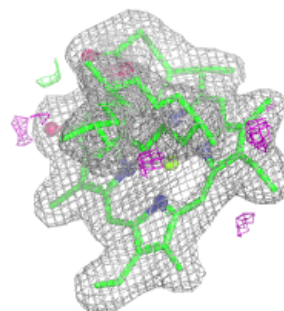
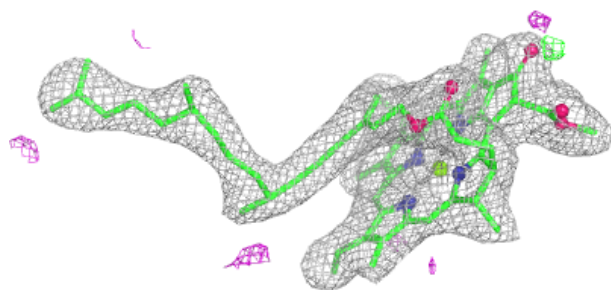
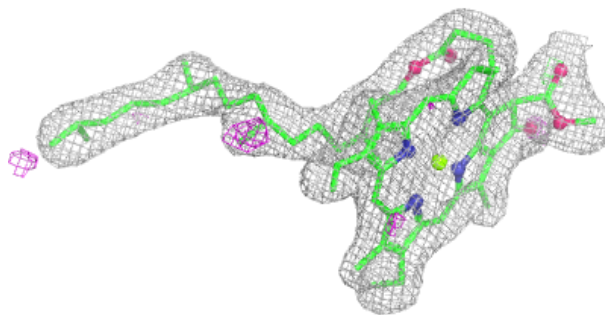
Electron density around CLA b 617:

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

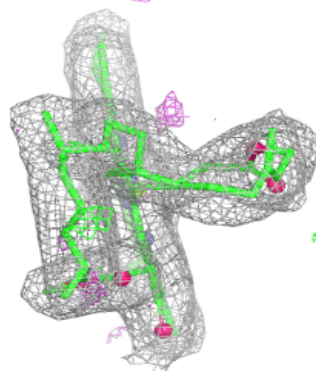
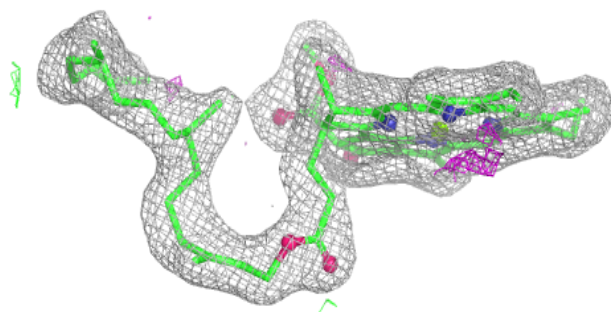
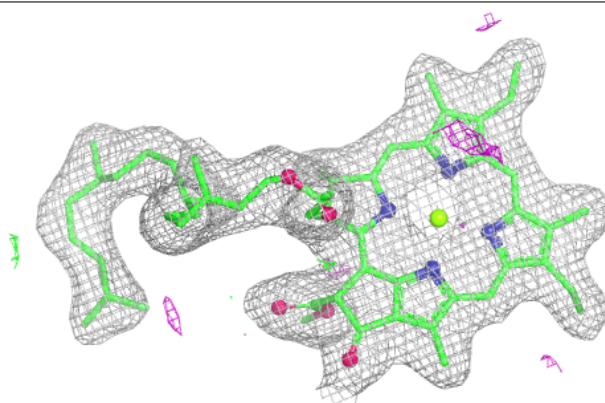


Electron density around CLA C 506:

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

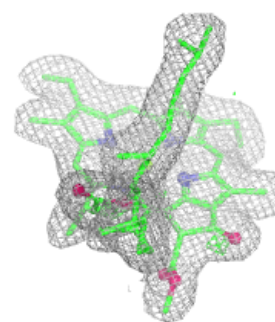
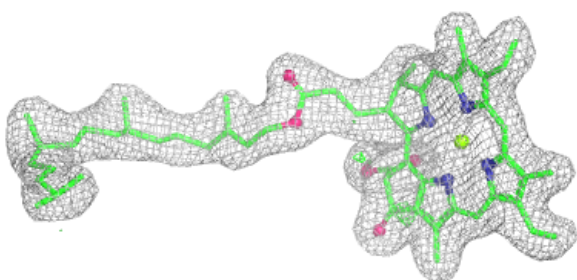
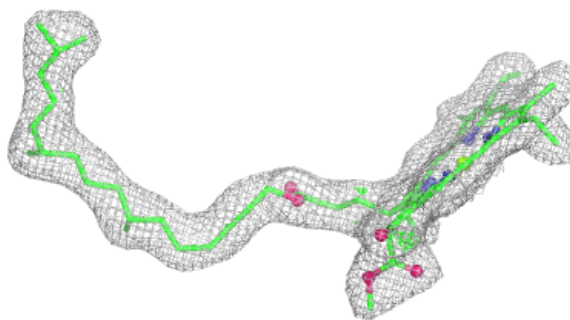
**Electron density around CLA B 611:**

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

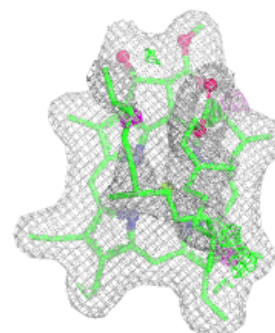
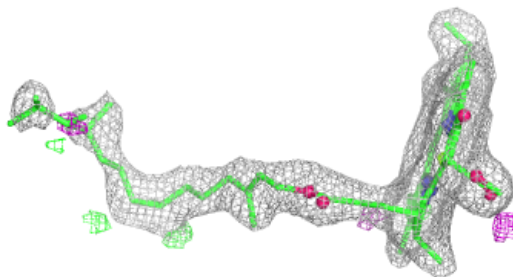
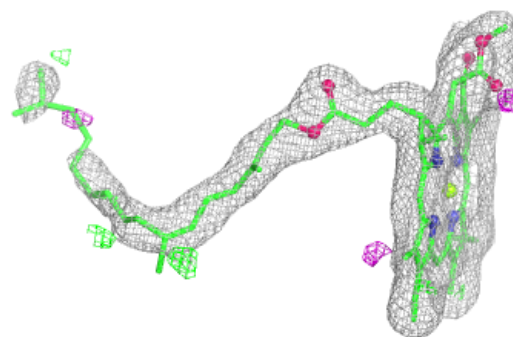


Electron density around CLA D 403:

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

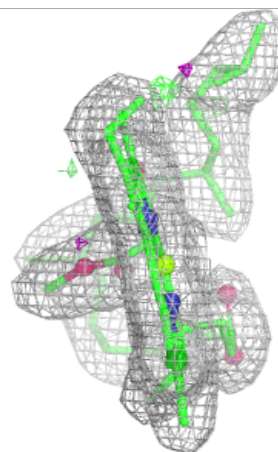
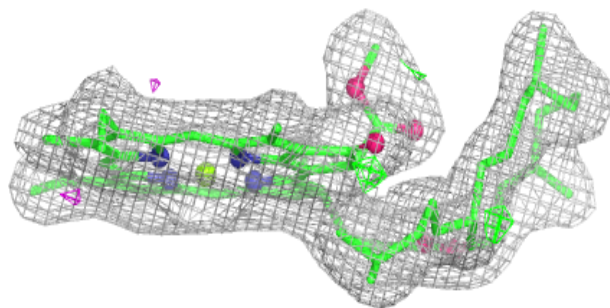
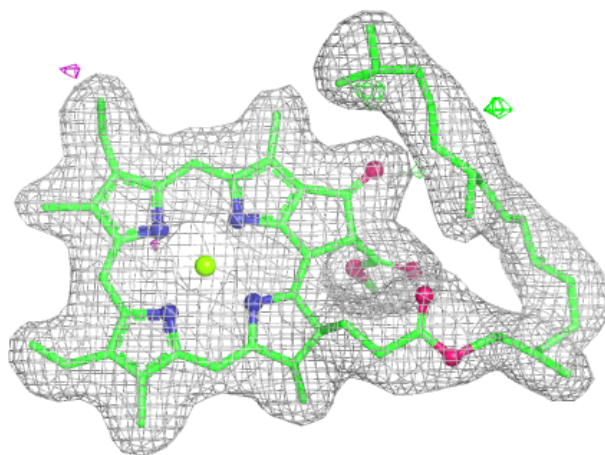
**Electron density around CLA D 404:**

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



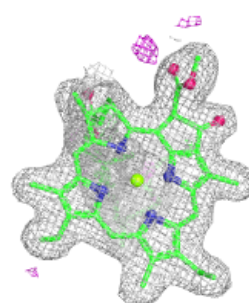
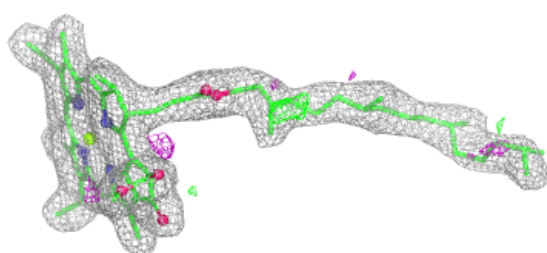
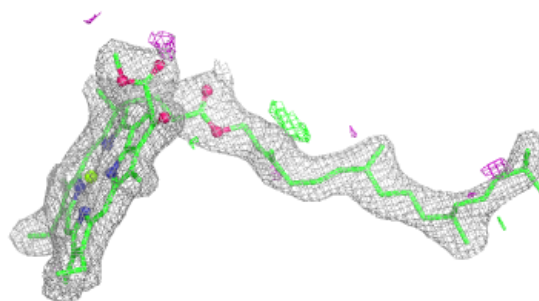
Electron density around CLA B 609:

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

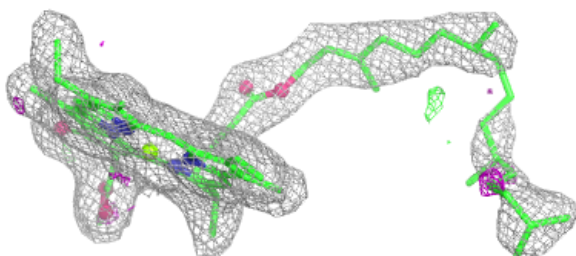
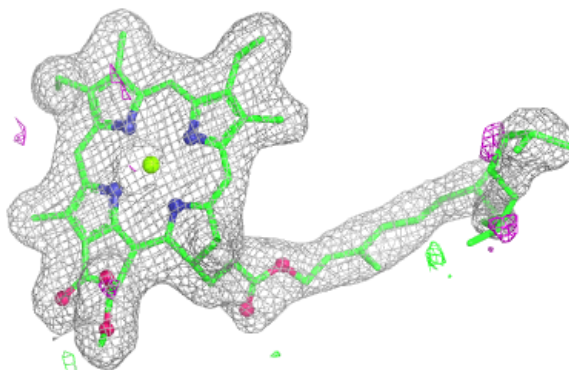


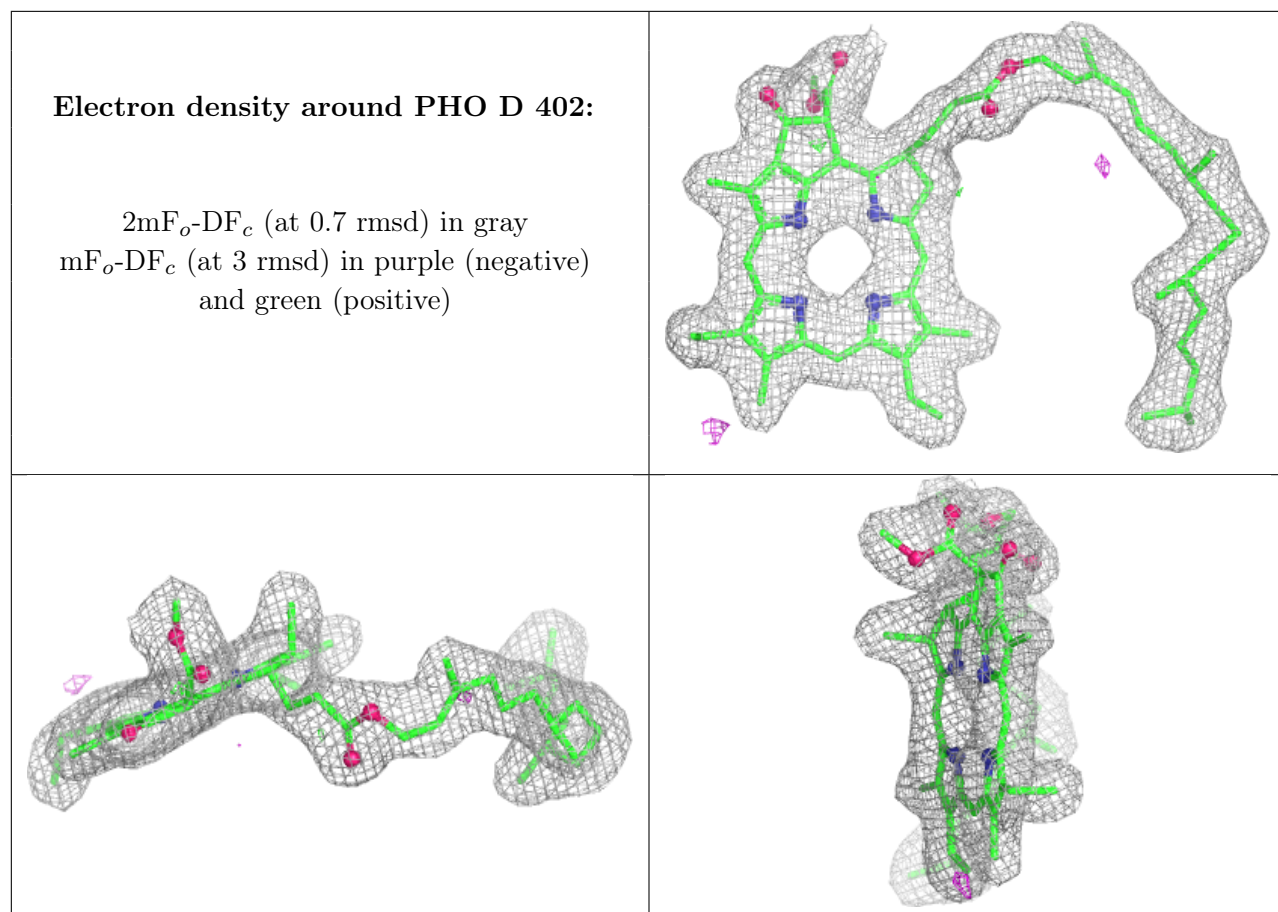
Electron density around CLA B 603:

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

**Electron density around CLA a 407:**

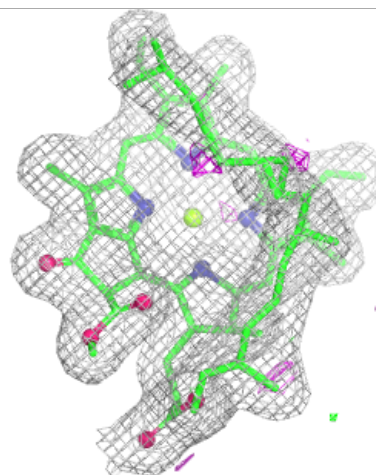
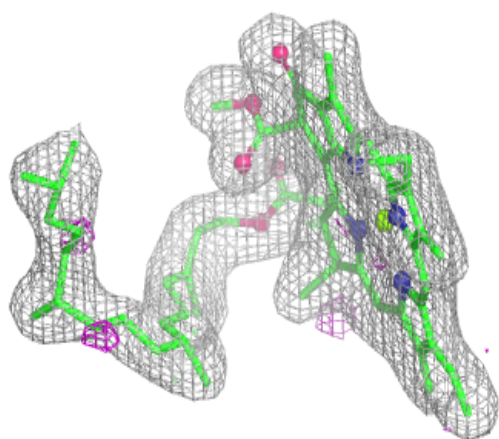
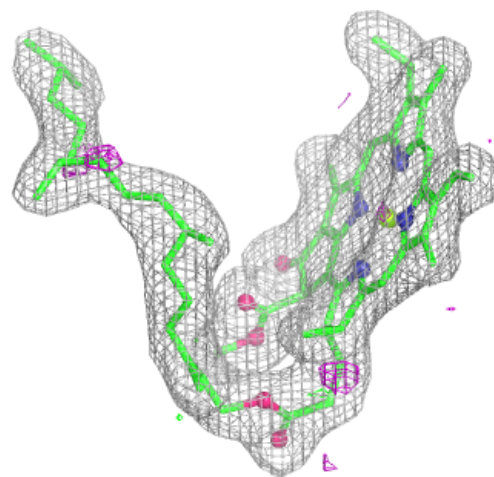
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





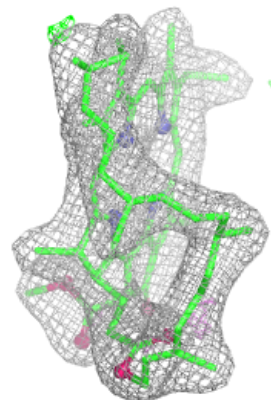
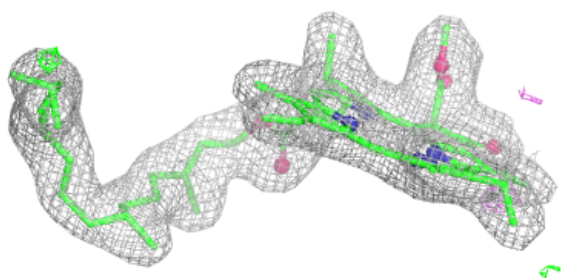
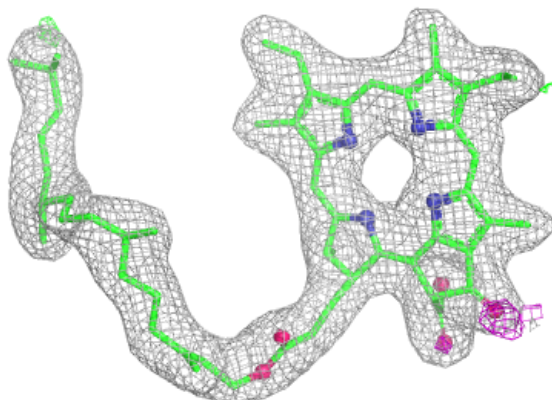
Electron density around CLA B 612:

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

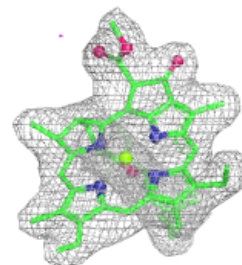
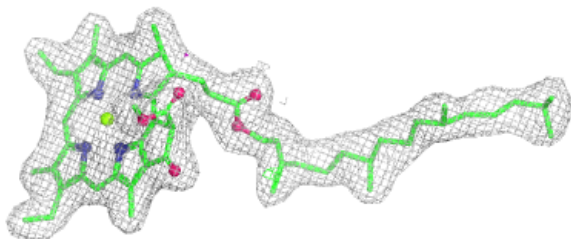
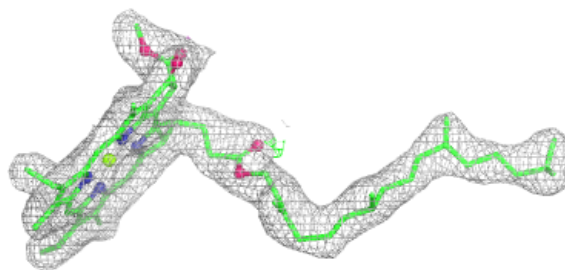


Electron density around PHO a 414:

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

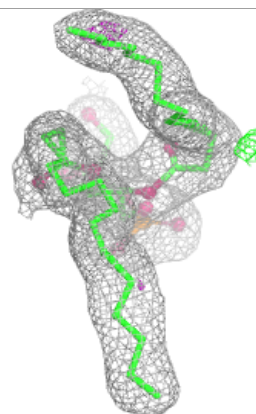
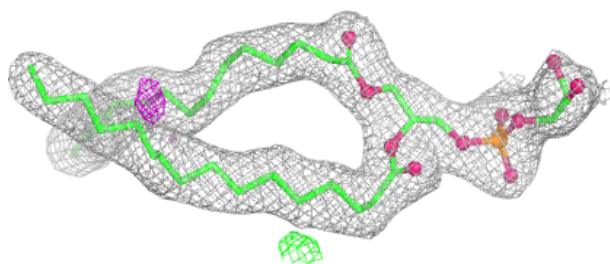
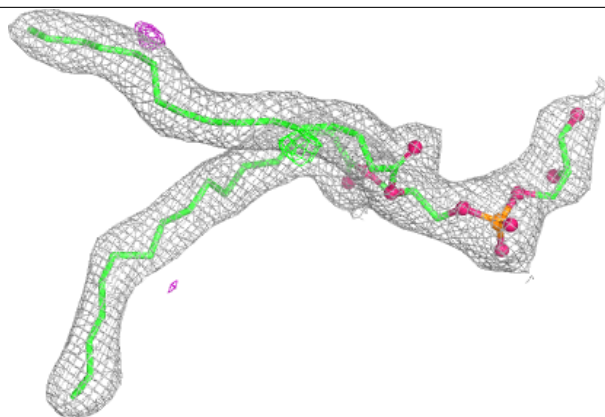
**Electron density around CLA c 503:**

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

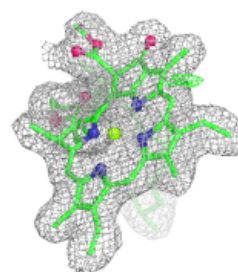
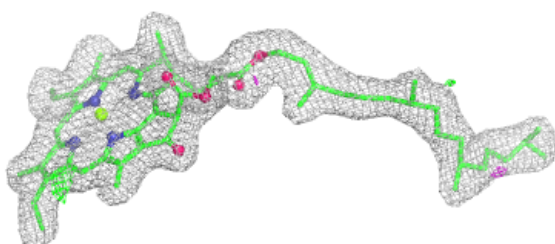
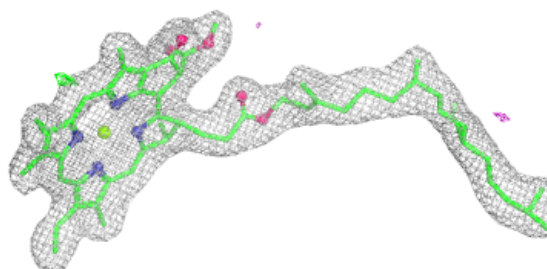


Electron density around LHG D 408:

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

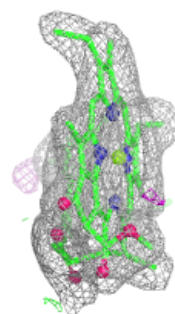
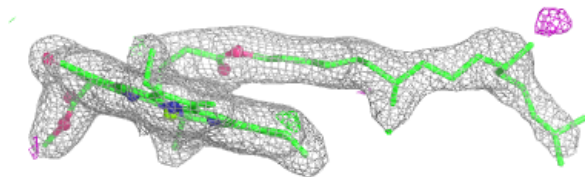
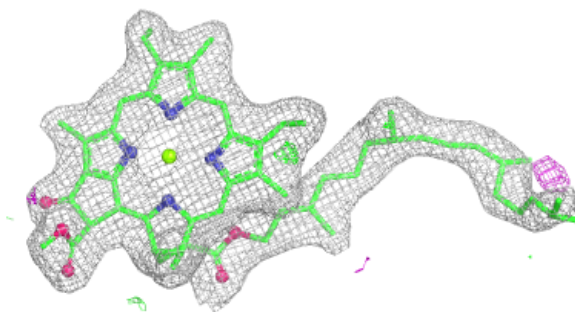
**Electron density around CLA A 403:**

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



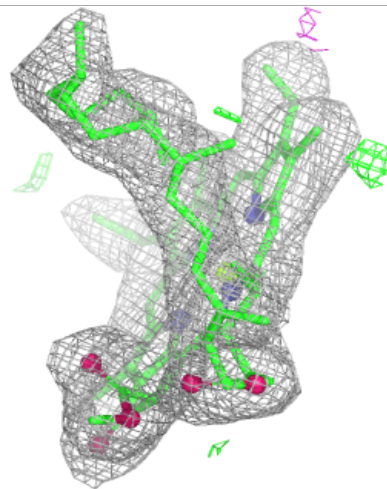
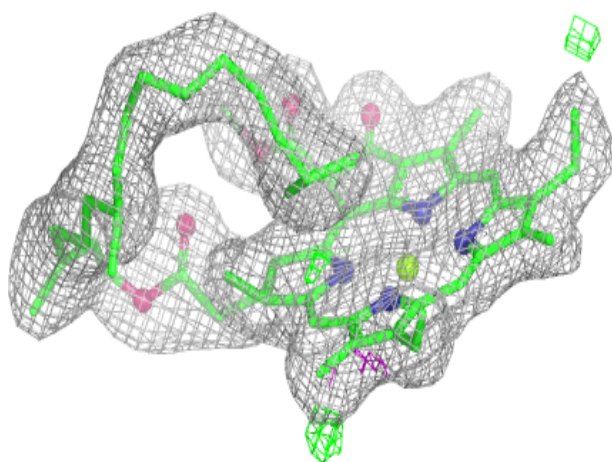
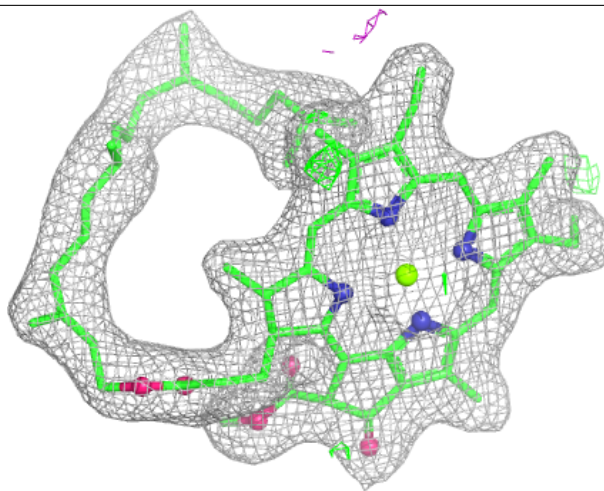
Electron density around CLA b 605:

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



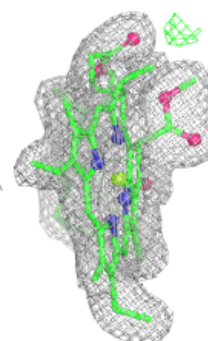
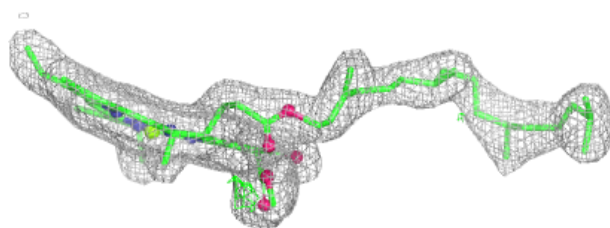
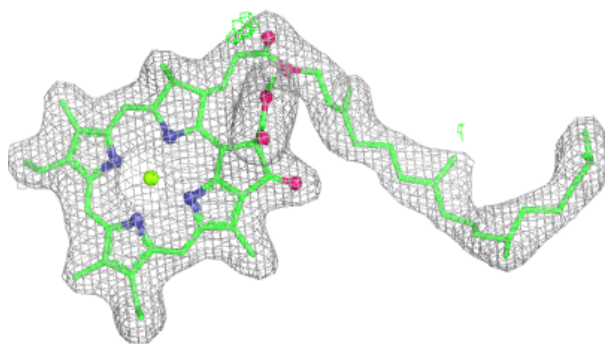
Electron density around CLA B 614:

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

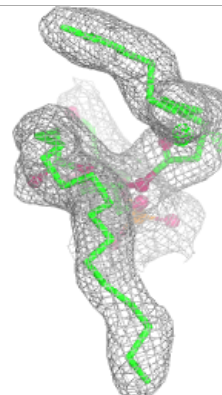
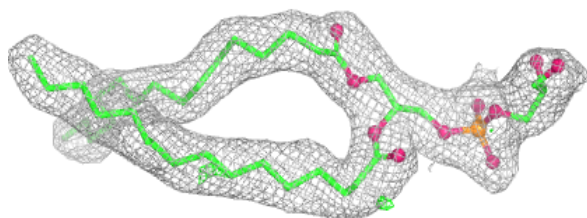
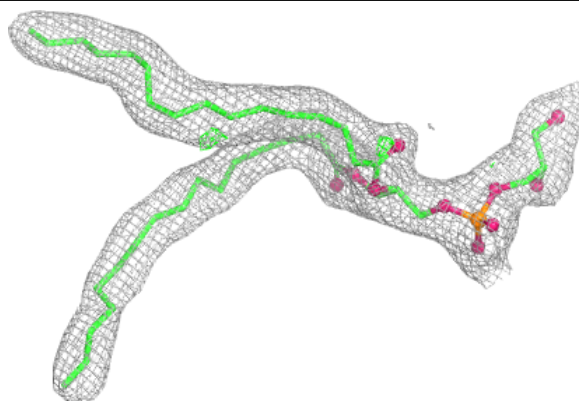


Electron density around CLA B 601:

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

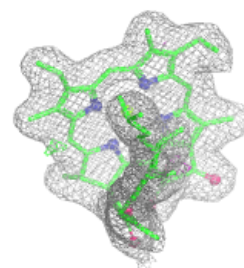
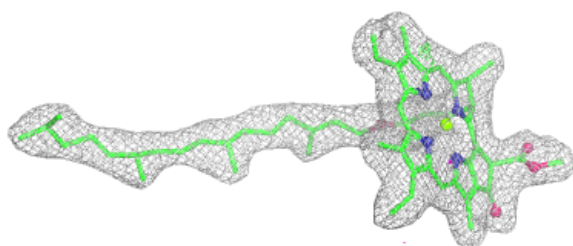
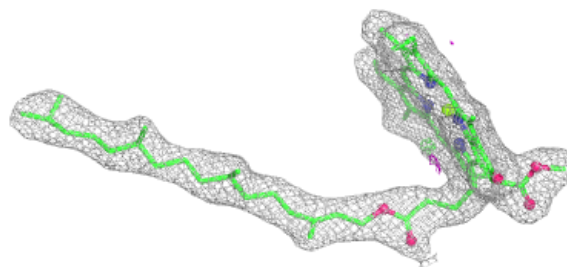
**Electron density around LHG d 406:**

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

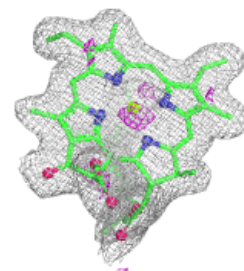
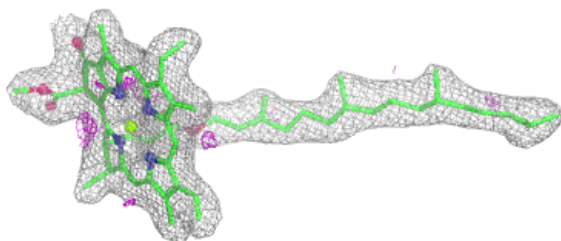
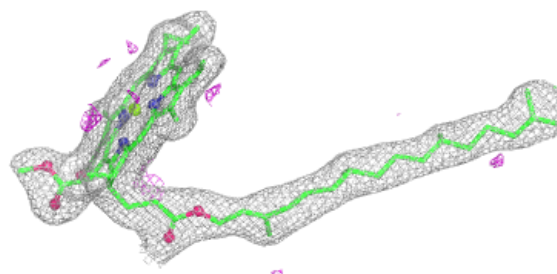


Electron density around CLA B 606:

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

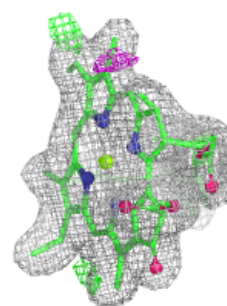
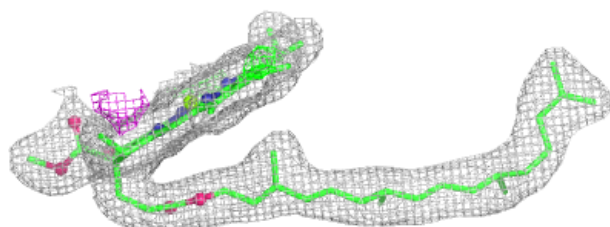
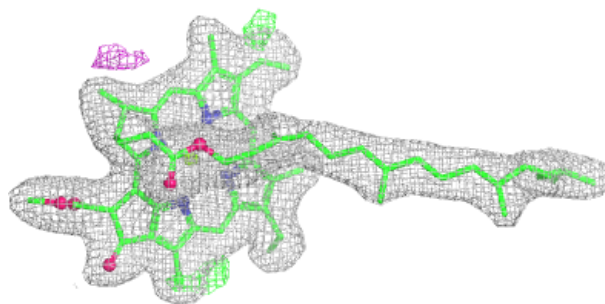
**Electron density around CLA b 609:**

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

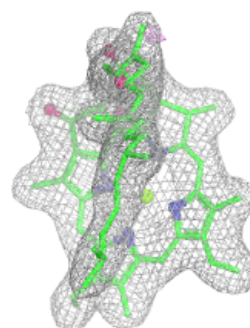
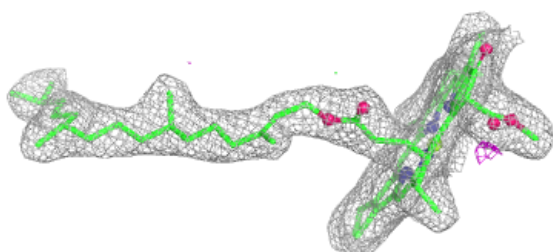
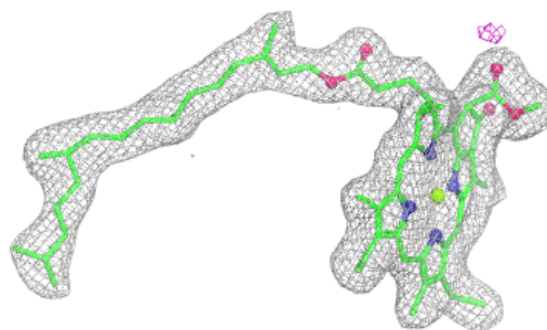


Electron density around CLA B 607:

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

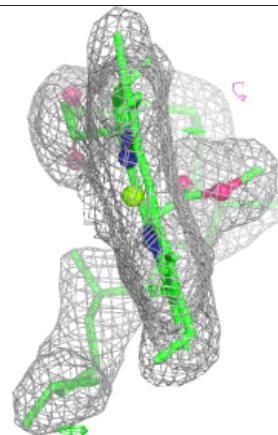
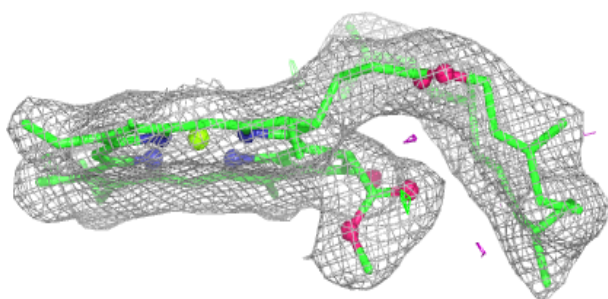
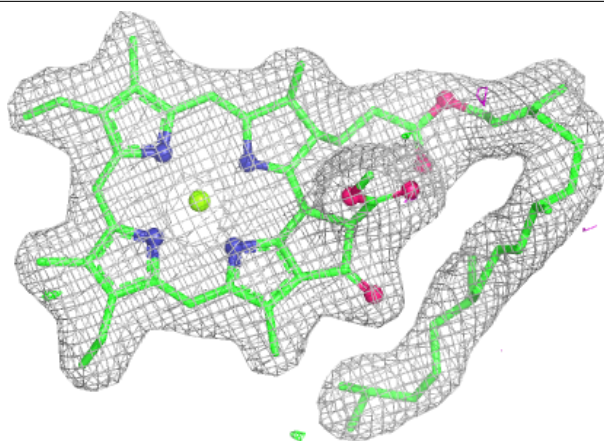
**Electron density around CLA B 608:**

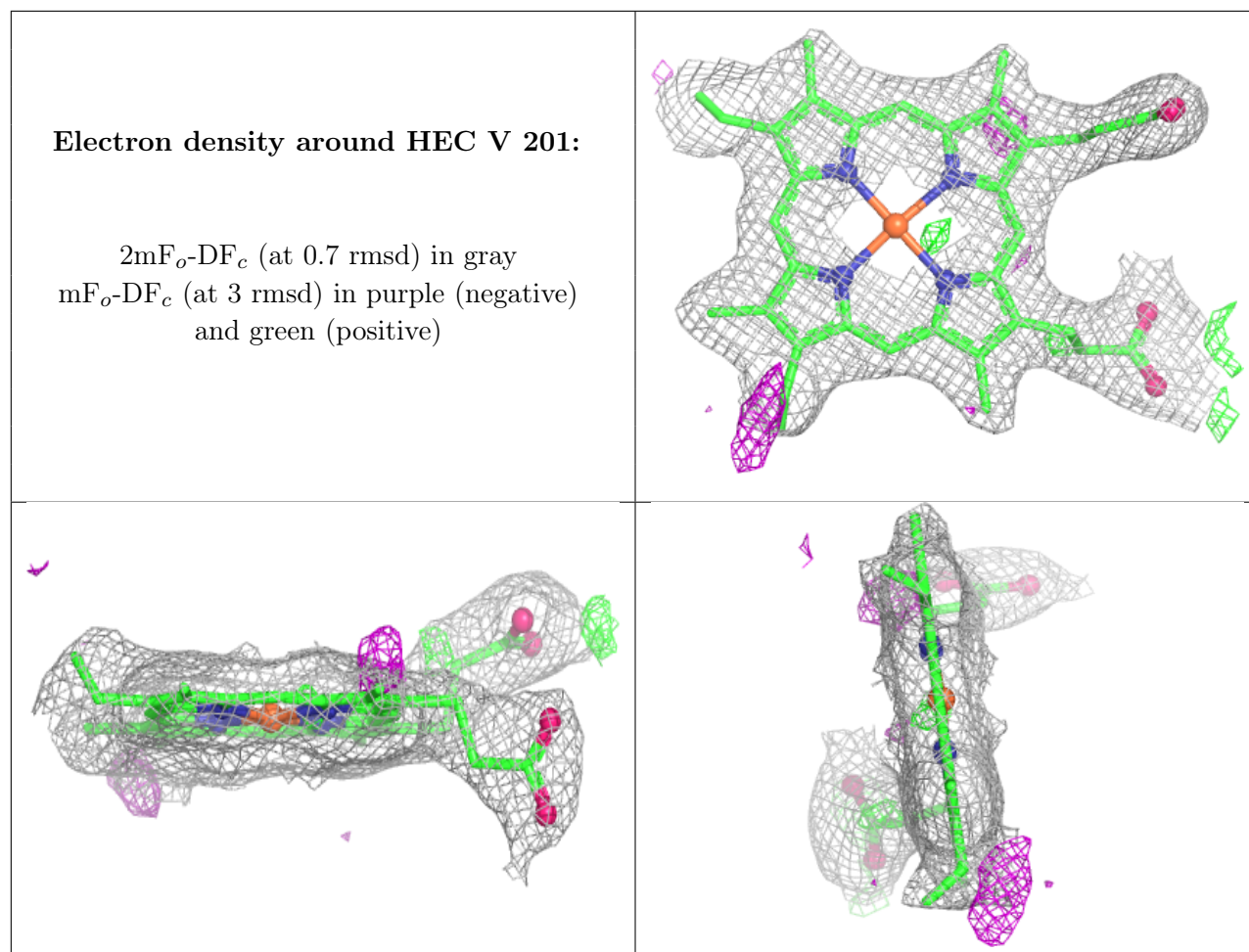
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

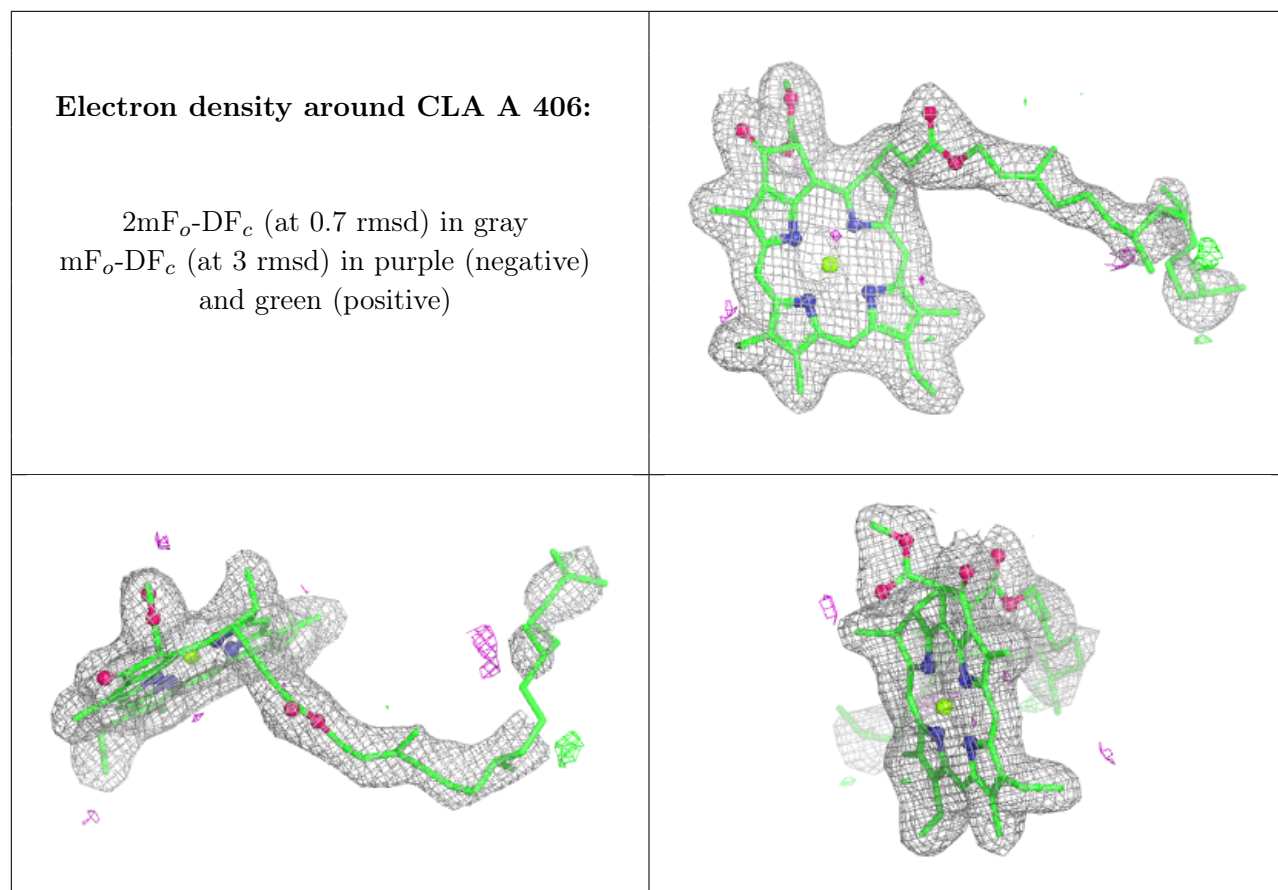


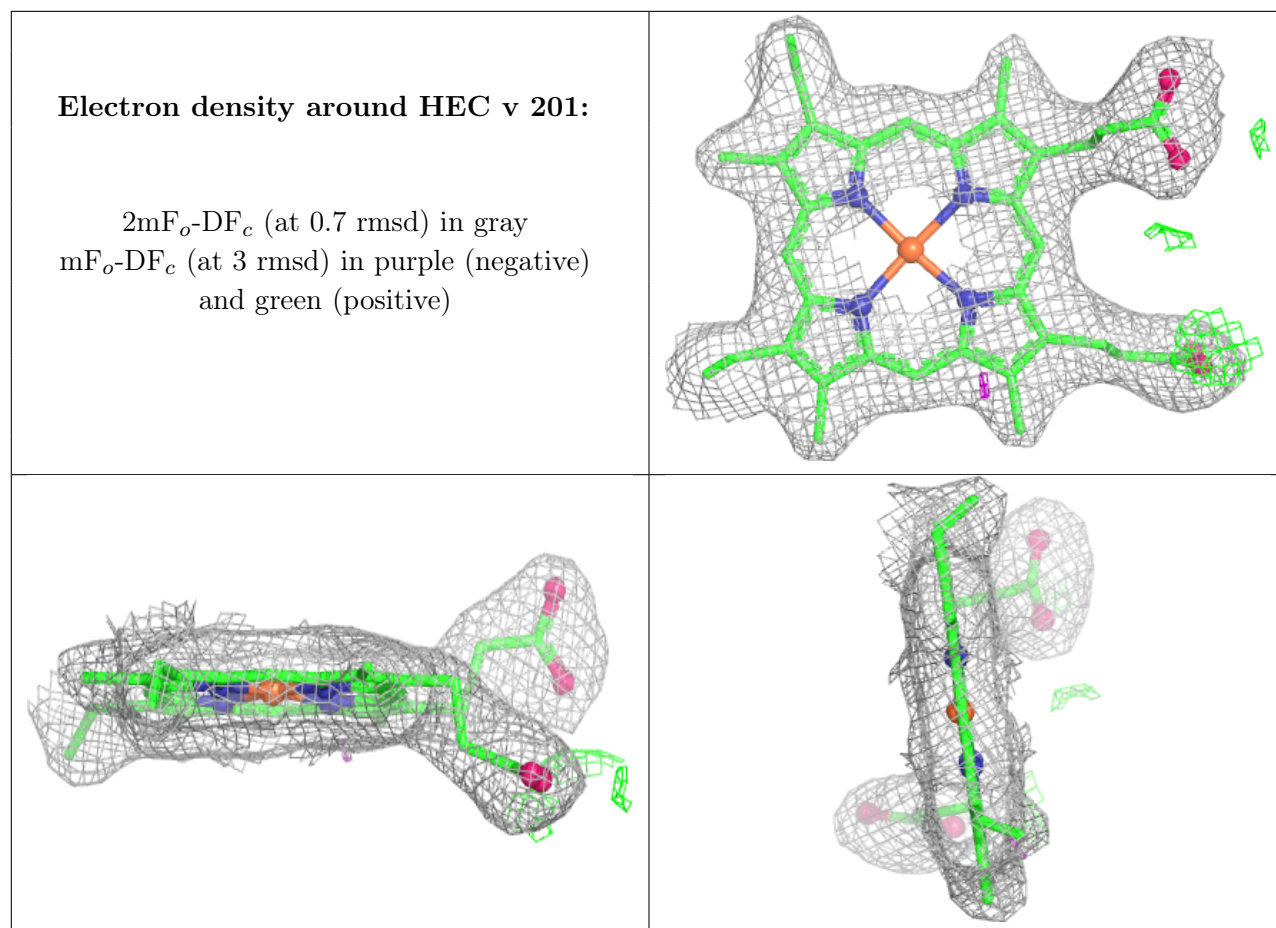
Electron density around CLA b 612:

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









6.5 Other polymers [i](#)

There are no such residues in this entry.