



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 01:06 PM UTC

PDB ID : 7RF2 / pdb_00007rf2
Title : RT XFEL structure of dark-stable state of Photosystem II (0F, S1 rich) at 2.08 Angstrom
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.08 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)
Xtrriage (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)

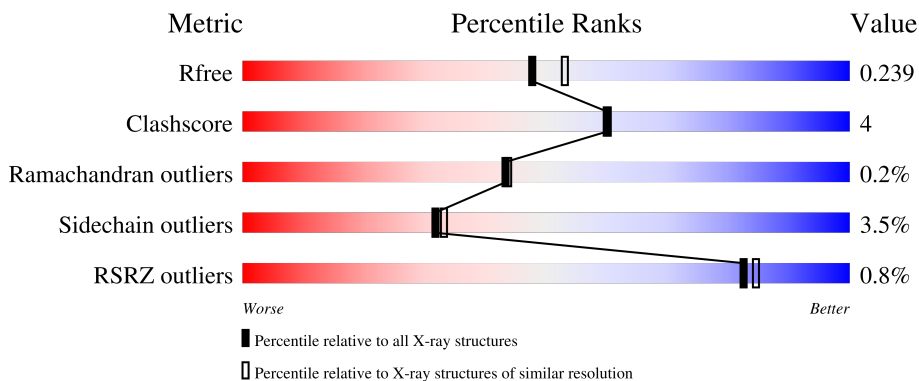
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


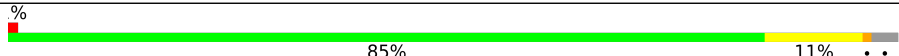
The reported resolution of this entry is 2.08 Å.

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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)







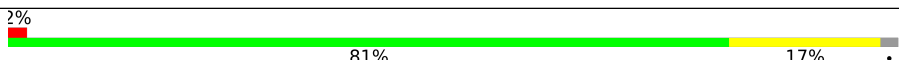
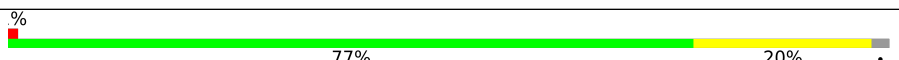


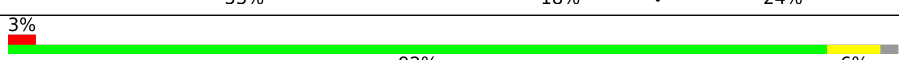
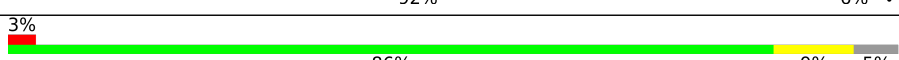
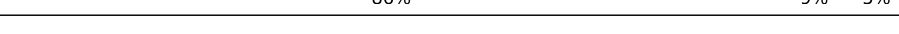


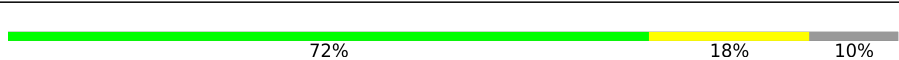




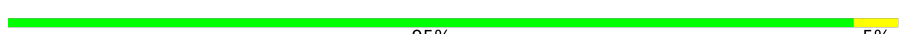
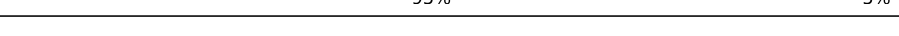


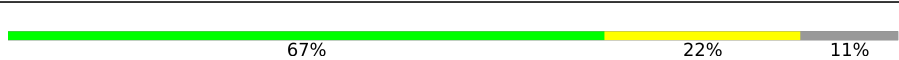
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	 85% 11% .
1	a	344	 85% 11% ..

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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

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Mol	Chain	Length	Quality of chain
2	B	510	 88% 11% ..
2	b	510	 89% 10% .
3	C	461	 89% 7% .
3	c	461	 86% 11% .
4	D	352	 87% 9% ..
4	d	352	 81% 16% .
5	E	84	 81% 17% .
5	e	84	 77% 20% .
6	F	45	 64% 9% . 24%
6	f	45	 53% 18% . 24%
7	H	66	 92% 6% .
7	h	66	 86% 9% 5%
8	I	38	 79% 16% 5%
8	i	38	 79% 13% . 5%
9	J	40	 72% 18% 10%
9	j	40	 58% 28% 5% 10%
10	K	46	 63% 17% 20%
10	k	46	 61% 17% . 20%
11	L	37	 95% 5%
11	l	37	 84% 11% ..
12	M	36	 86% 6% 8%
12	m	36	 67% 22% 11%
13	O	272	 79% 10% . 10%
13	o	272	 79% 11% 10%
14	R	41	 51% 17% 32%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	406	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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	507	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	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	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	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	c	501	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	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103670 atoms, of which 51532 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	H	N	O				S
1	A	334	5141	1717	2519	431	459	15	0	0	0
1	a	334	5128	1714	2509	431	459	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	H	N	O				S
2	B	505	7878	2631	3873	666	695	13	0	5	0
2	b	505	7814	2610	3836	665	690	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	H	N	O				S
3	C	442	6781	2249	3355	571	593	13	0	2	0
3	c	451	6926	2290	3426	587	610	13	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
4	D	341	5338	1800	2621	444	461	12	0	0	0
4	d	341	5350	1804	2627	444	463	12	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
6	F	34	Total	C	H	N	O	S	0	0	0
			557	187	282	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			557	187	282	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	H	65	Total	C	H	N	O	S	0	0	0
			1042	341	532	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
8	I	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
10	K	37	Total 598	C 204	H 305	N 43	O 46	0	0	0
10	k	37	Total 598	C 204	H 305	N 43	O 46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
11	L	37	Total 620	C 202	H 316	N 48	O 53	S 1	0	0	0
11	l	36	Total 600	C 197	H 304	N 47	O 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	H	N	O				S
12	M	33	Total 525	C 171	H 269	N 37	O 47	S 1	0	0	0
12	m	32	Total 518	C 168	H 267	N 36	O 46	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
13	O	244	Total 3700	C 1168	H 1830	N 313	O 385	S 4	0	1	0
13	o	244	Total 3720	C 1170	H 1846	N 317	O 383	S 4	0	0	0

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
14	R	28	Total 459	C 151	H 238	N 38	O 32	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
15	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
15	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
17	V	137	Total	C	H	N	O	S	0	0	0
			2137	675	1073	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2137	675	1073	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
19	Y	27	Total 413	C 128	H 217	N 35	O 30	S 3	0	0	0
19	y	30	Total 459	C 144	H 241	N 35	O 36	S 3	0	0	0

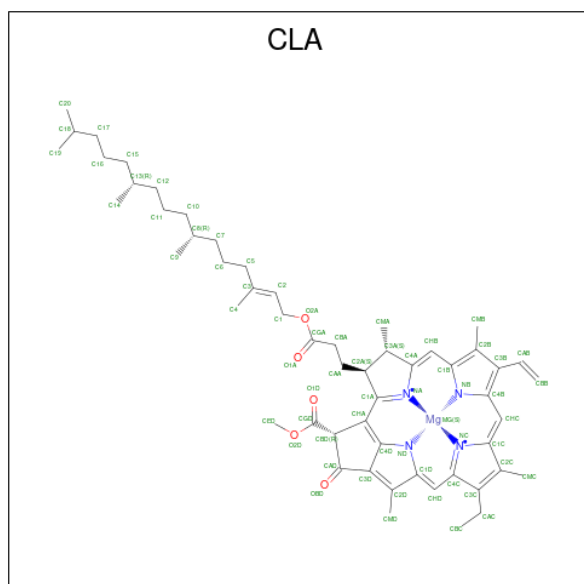
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
20	Z	62	Total 995	C 328	H 516	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

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

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

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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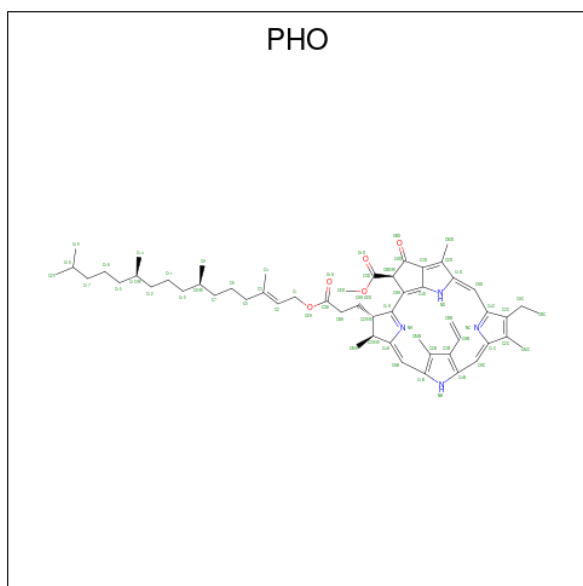
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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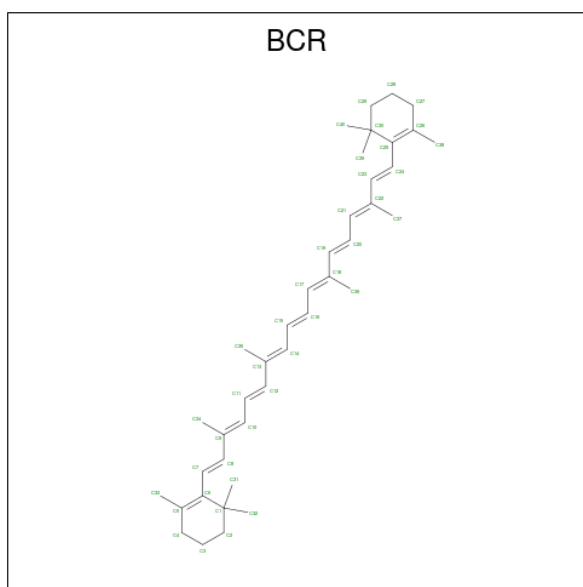
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	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	
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

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



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

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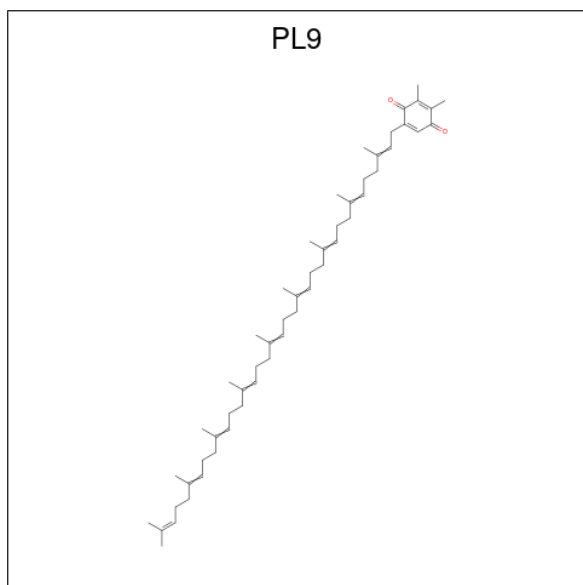
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

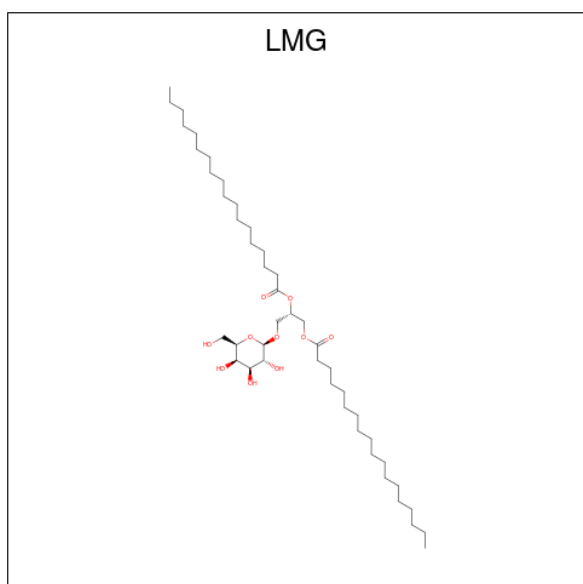
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



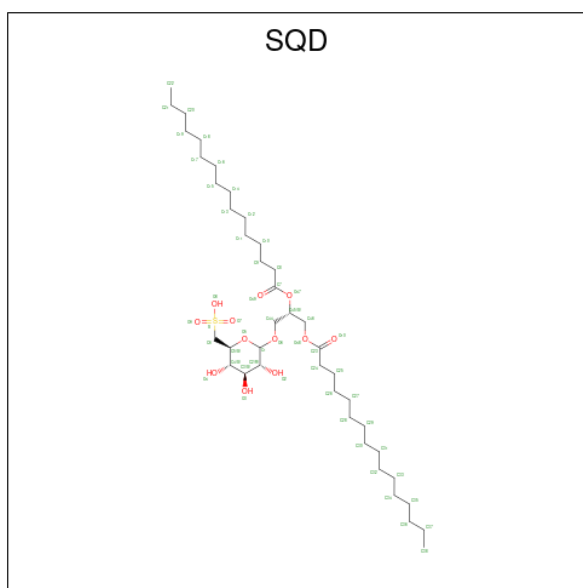
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
26	A	1	135	53	80	2	0	0
26	D	1	135	53	80	2	0	0
26	a	1	135	53	80	2	0	0
26	d	1	135	53	80	2	0	0

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



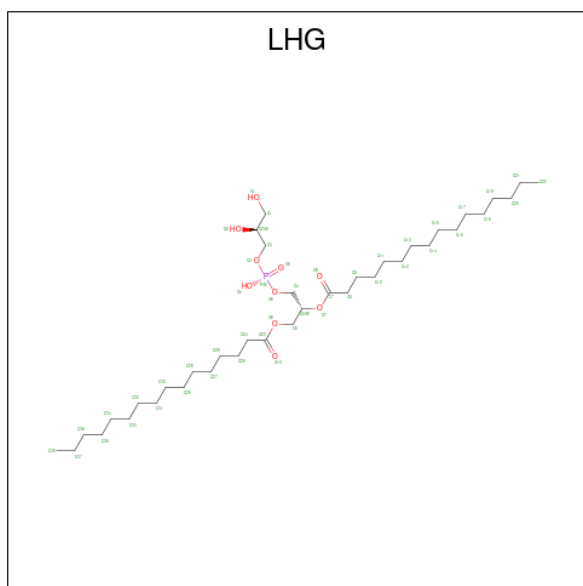
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			77	27	45	5		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	Y	1	Total	C	H	O	0	0
			114	38	66	10		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	h	1	Total	C	H	O	0	0
			57	21	34	2		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



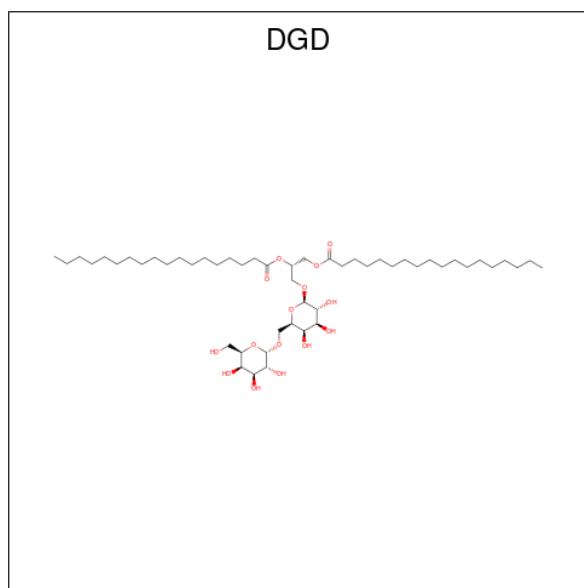
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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

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



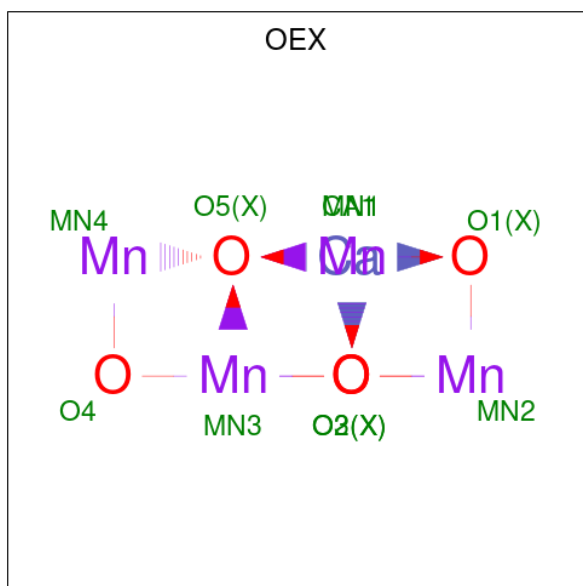
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
30	A	1	Total 162	C 51	H 96	O 15	0	0
30	C	1	Total 144	C 47	H 82	O 15	0	0
30	C	1	Total 144	C 47	H 82	O 15	0	0
30	C	1	Total 144	C 47	H 82	O 15	0	0

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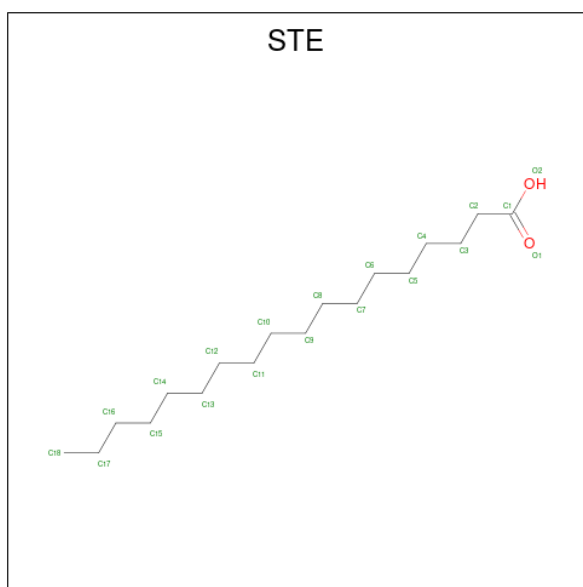
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			143	47	81	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		
30	o	1	Total	C	H	O	0	0
			119	39	75	5		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: $\text{C}_{18}\text{H}_{36}\text{O}_2$).



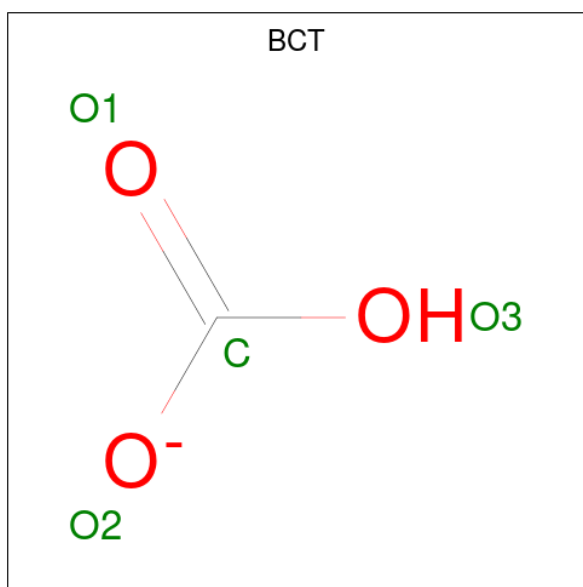
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			34	12	20	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	O		0	0
			16	14	2			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H		0	0
			47	16	31			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	D	1	Total	C	H	O	0	0
			55	18	35	2		
32	D	1	Total	C	O		0	0
			15	13	2			
32	E	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			

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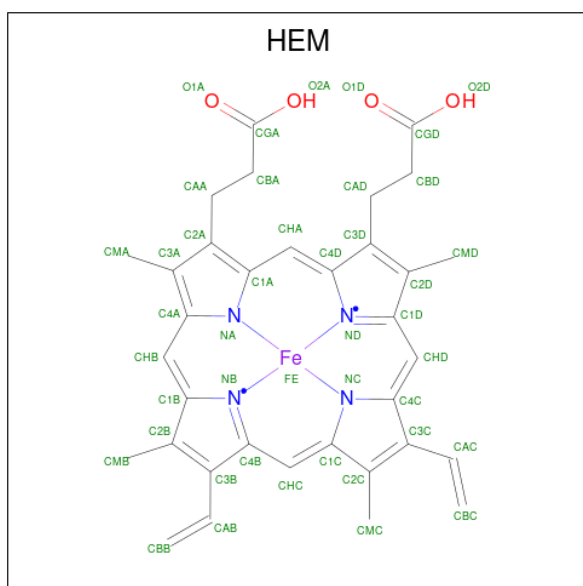
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	T	1	Total C H 44 15 29	0	0
32	a	1	Total C H 26 10 16	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 28 10 16 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	d	1	Total C H O 55 18 35 2	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	m	1	Total C H O 28 10 16 2	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	d	1	Total	C	H	O	0	0
			5	1	1	3		

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



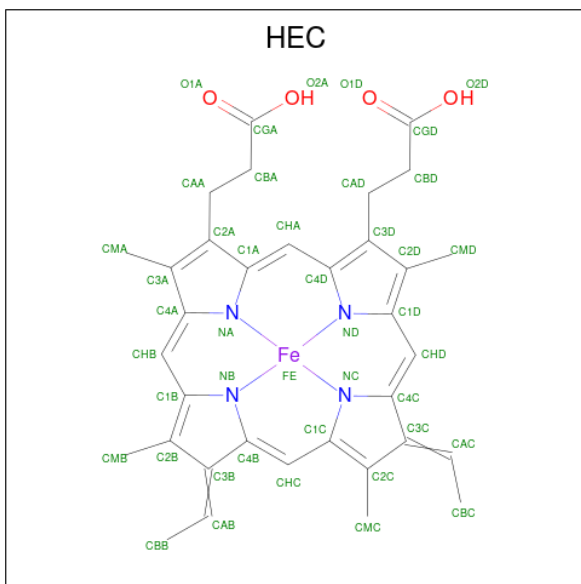
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
35	V	1	75	34	1	32	4	4	0	0
35	v	1	75	34	1	32	4	4	0	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	144	Total	O	0	0
			144	144		
36	B	204	Total	O	0	0
			204	204		
36	C	182	Total	O	0	0
			182	182		
36	D	136	Total	O	0	0
			136	136		
36	E	30	Total	O	0	0
			30	30		
36	F	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	H	37	Total O 37 37	0	0
36	I	10	Total O 10 10	0	0
36	J	16	Total O 16 16	0	0
36	K	8	Total O 8 8	0	0
36	L	8	Total O 8 8	0	0
36	M	7	Total O 7 7	0	0
36	O	90	Total O 90 90	0	0
36	T	10	Total O 10 10	0	0
36	U	52	Total O 52 52	0	0
36	V	65	Total O 65 65	0	0
36	X	12	Total O 12 12	0	0
36	Y	6	Total O 6 6	0	0
36	Z	2	Total O 2 2	0	0
36	a	126	Total O 126 126	0	0
36	b	206	Total O 206 206	0	0
36	c	181	Total O 181 181	0	0
36	d	111	Total O 111 111	0	0
36	e	21	Total O 21 21	0	0
36	f	8	Total O 8 8	0	0
36	h	36	Total O 36 36	0	0
36	i	13	Total O 13 13	0	0

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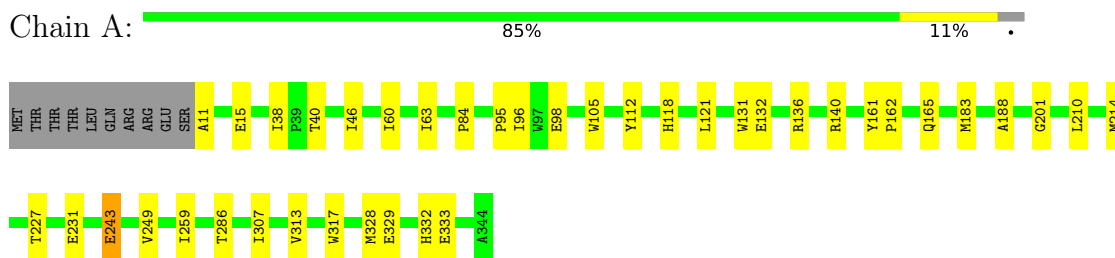
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	j	8	Total O 8 8	0	0
36	k	6	Total O 6 6	0	0
36	l	7	Total O 7 7	0	0
36	m	6	Total O 6 6	0	0
36	o	102	Total O 102 102	0	0
36	r	3	Total O 3 3	0	0
36	t	8	Total O 8 8	0	0
36	u	58	Total O 58 58	0	0
36	v	56	Total O 56 56	0	0
36	x	8	Total O 8 8	0	0
36	y	3	Total O 3 3	0	0
36	z	9	Total O 9 9	0	0

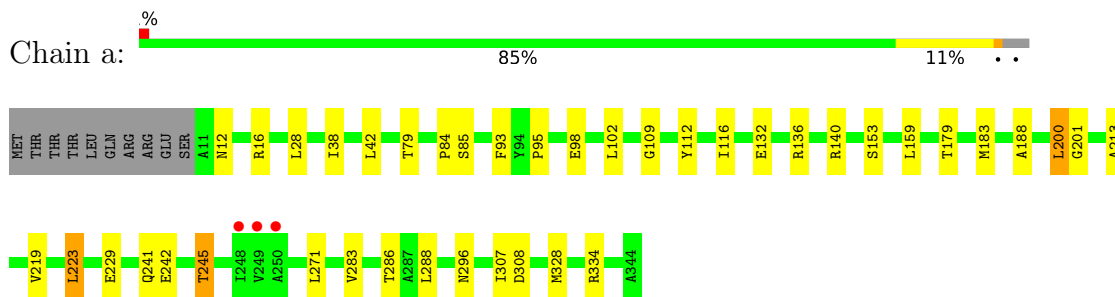
3 Residue-property plots [i](#)

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.

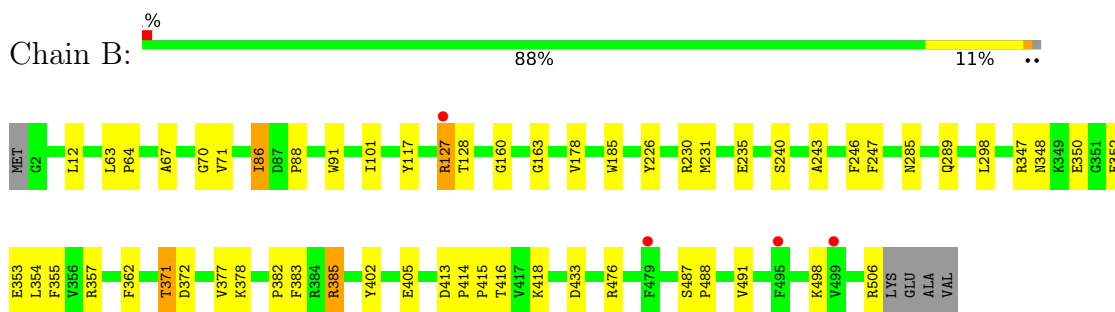
- Molecule 1: Photosystem II protein D1 1



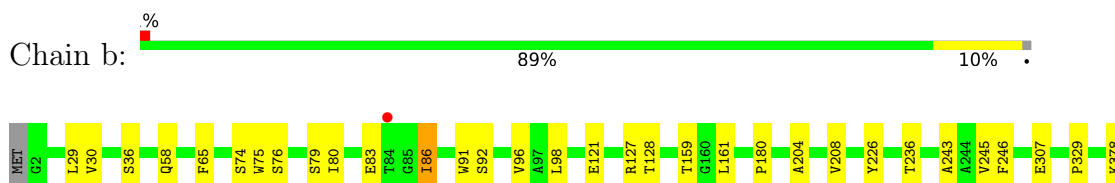
- Molecule 1: Photosystem II protein D1 1

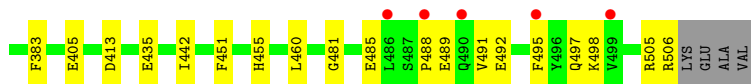


- Molecule 2: Photosystem II CP47 reaction center protein

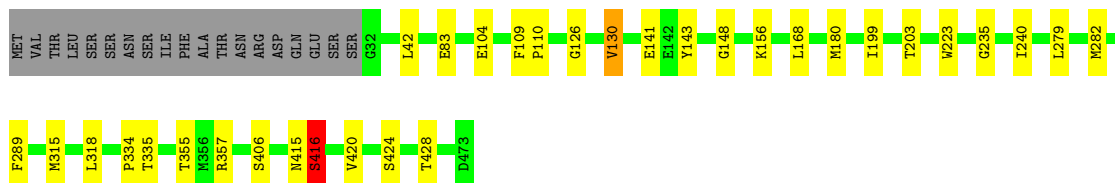
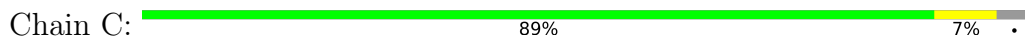


- Molecule 2: Photosystem II CP47 reaction center protein

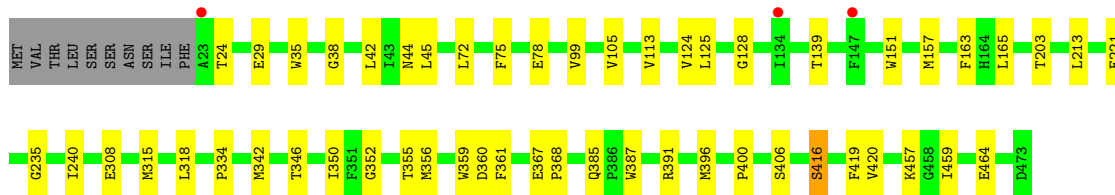
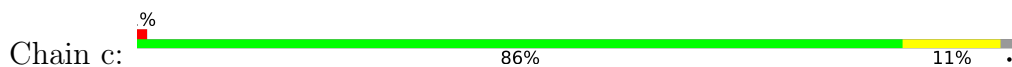




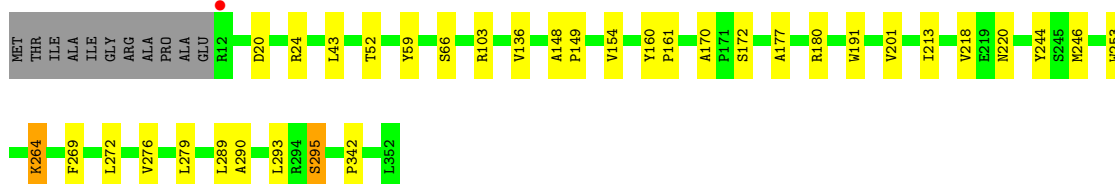
● Molecule 3: Photosystem II CP43 reaction center protein



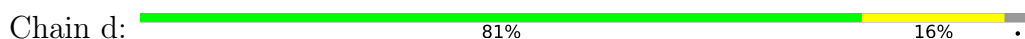
● Molecule 3: Photosystem II CP43 reaction center protein



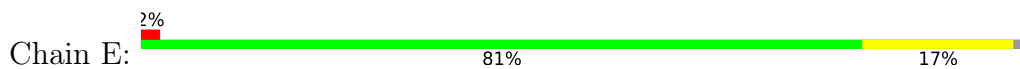
● Molecule 4: Photosystem II D2 protein



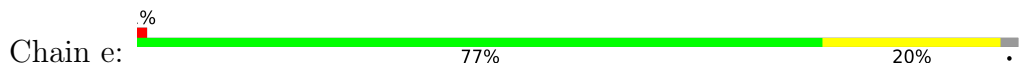
● Molecule 4: Photosystem II D2 protein



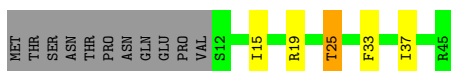
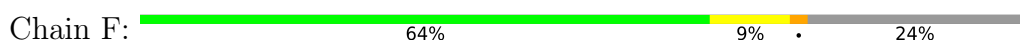
● Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



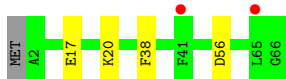
- Molecule 6: Cytochrome b559 subunit beta



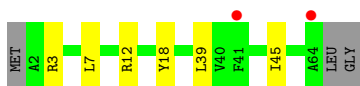
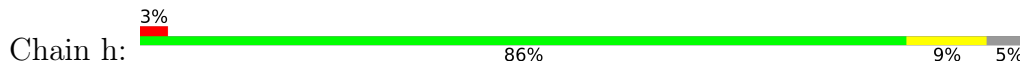
- Molecule 6: Cytochrome b559 subunit beta



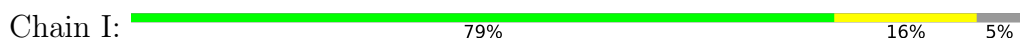
- Molecule 7: Photosystem II reaction center protein H




- Molecule 7: Photosystem II reaction center protein H

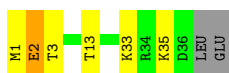


- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  79% 13% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  72% 18% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 58% 28% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  63% 17% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  61% 17% 20%




- Molecule 11: Photosystem II reaction center protein L

Chain L:  95% 5%




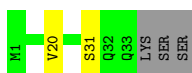
- Molecule 11: Photosystem II reaction center protein L

Chain l:  84% 11% 5% 2%



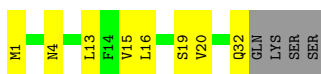
- Molecule 12: Photosystem II reaction center protein M

Chain M:  86% 6% 8%




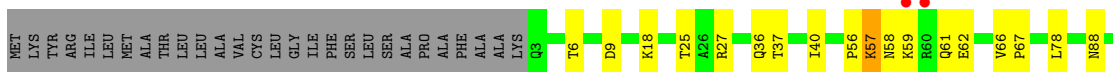
- Molecule 12: Photosystem II reaction center protein M

Chain m:  67% 22% 11%




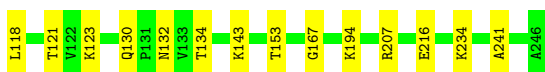
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  % 79% 10% 10%



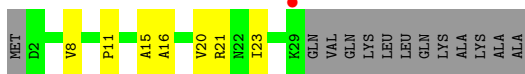
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  79% 11% 10%



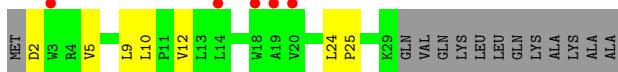
- Molecule 14: Photosystem II protein Y

Chain R:  2% 51% 17% 32%




- Molecule 14: Photosystem II protein Y

Chain r:  12% 51% 17% 32%




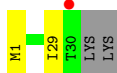
- Molecule 15: Photosystem II reaction center protein T

Chain T:  81% 9% 6%



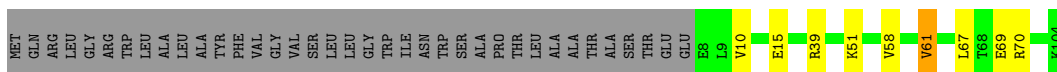
- Molecule 15: Photosystem II reaction center protein T

Chain t:  3% 88% 6% 6%



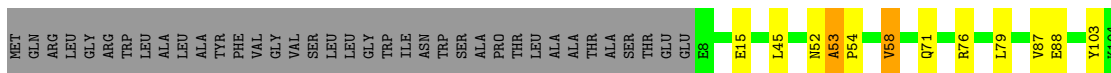
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:  66% 6% 28%



- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:  63% 7% 28%



- Molecule 17: Cytochrome c-550

Chain V:  74% 9% 16%




- Molecule 17: Cytochrome c-550

Chain v:  75% 7% 16%

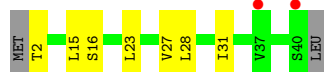
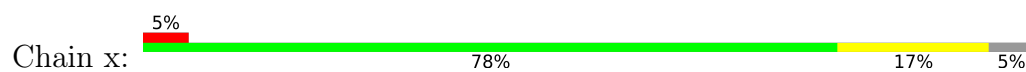


- Molecule 18: Photosystem II reaction center X protein

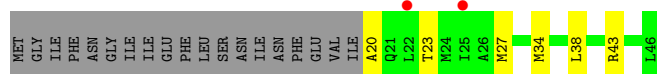
Chain X:  78% 15% 7%



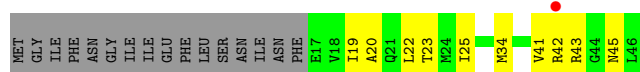
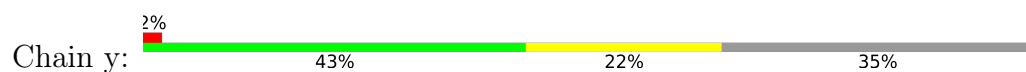
- Molecule 18: Photosystem II reaction center X protein



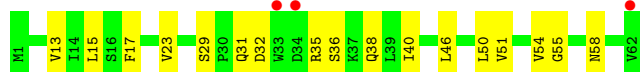
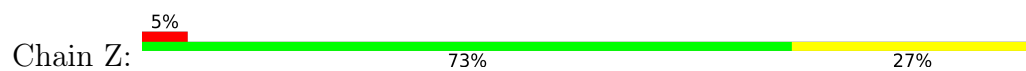
- Molecule 19: Photosystem II reaction center protein Ycf12



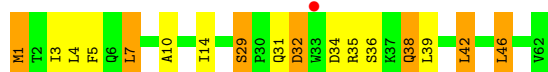
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 221.63Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.64 – 2.08 33.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.64-2.08) 85.0 (33.64-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.238 0.185 , 0.239	Depositor DCC
R_{free} test set	4226 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtrriage
Anisotropy	0.197	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103670	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	1/2707 (0.0%)	0.66	0/3692
1	a	0.58	1/2704 (0.0%)	0.65	0/3688
2	B	0.54	0/4161	0.60	0/5669
2	b	0.54	0/4118	0.60	0/5611
3	C	0.54	0/3547	0.61	0/4830
3	c	0.50	0/3619	0.58	0/4926
4	D	0.58	0/2812	0.64	0/3832
4	d	0.53	0/2821	0.62	0/3844
5	E	0.50	0/688	0.60	0/940
5	e	0.47	0/683	0.59	0/932
6	F	0.58	0/284	0.60	0/387
6	f	0.46	0/284	0.69	0/387
7	H	0.67	0/523	0.65	0/713
7	h	0.59	0/511	0.65	0/697
8	I	0.60	0/293	0.70	0/396
8	i	0.64	0/293	0.65	0/396
9	J	0.50	0/263	0.61	0/356
9	j	0.51	0/263	0.60	0/356
10	K	0.45	0/303	0.56	0/416
10	k	0.48	0/303	0.54	0/416
11	L	0.70	0/311	0.67	0/422
11	l	0.72	0/303	0.67	0/412
12	M	0.71	0/249	0.81	0/341
12	m	0.69	0/244	0.75	0/334
13	O	0.64	0/1904	0.71	0/2585
13	o	0.63	0/1905	0.68	0/2583
14	R	0.40	0/227	0.54	0/313
14	r	0.40	0/227	0.47	0/313
15	T	0.69	0/257	0.71	0/349
15	t	0.62	0/255	0.67	0/346
16	U	0.55	0/785	0.62	0/1064
16	u	0.75	1/785 (0.1%)	0.69	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.65	0/1085	0.69	0/1473
17	v	0.58	0/1085	0.63	0/1473
18	X	0.50	0/284	0.60	0/384
18	x	0.43	0/289	0.52	0/391
19	Y	0.48	0/197	0.57	0/264
19	y	0.44	0/219	0.56	0/294
20	Z	0.42	0/490	0.52	0/669
20	z	0.38	0/488	0.51	0/666
All	All	0.56	3/42769 (0.0%)	0.63	0/58224

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
17	V	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	u	103	TYR	CA-C	10.60	1.59	1.53
1	a	38	ILE	CA-CB	8.40	1.58	1.54
1	A	38	ILE	CA-CB	-7.59	1.50	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2519	2519	24	0
1	a	2619	2509	2509	26	0
2	B	4005	3873	3867	36	0
2	b	3978	3836	3836	28	0
3	C	3426	3355	3343	18	0
3	c	3500	3426	3426	30	0
4	D	2717	2621	2621	23	0
4	d	2723	2627	2627	36	0
5	E	666	651	651	11	0
5	e	664	648	648	15	0
6	F	275	282	282	4	0
6	f	275	282	282	9	0
7	H	510	532	532	3	0
7	h	498	518	518	3	0
8	I	296	311	311	2	0
8	i	296	311	311	3	0
9	J	257	268	268	5	0
9	j	257	268	268	12	0
10	K	293	305	305	4	0
10	k	293	305	305	7	0
11	L	304	316	316	2	0
11	l	296	304	304	2	0
12	M	256	269	269	2	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	17	0
13	o	1874	1846	1846	15	0
14	R	221	238	238	4	0
14	r	221	238	238	2	0
15	T	258	261	261	3	0
15	t	256	256	256	0	0
16	U	774	773	773	6	0
16	u	774	773	773	9	1
17	V	1064	1073	1073	10	1
17	v	1064	1073	1073	9	0
18	X	281	312	312	5	0
18	x	286	316	314	5	0
19	Y	196	217	217	3	0
19	y	218	241	241	4	0
20	Z	479	516	516	7	0
20	z	477	509	509	13	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	1035	1139	1139	13	0
22	C	839	922	922	10	0
22	D	195	216	216	3	0
22	a	195	216	216	2	0
22	b	1035	1139	1139	15	0
22	c	839	919	919	11	0
22	d	195	216	216	1	0
23	A	128	148	148	1	0
23	a	64	74	74	0	0
23	d	64	74	74	0	0
24	A	40	56	56	0	0
24	B	120	168	168	1	0
24	C	40	56	56	1	0
24	D	40	56	56	2	0
24	H	40	56	56	3	0
24	K	120	168	168	2	0
24	T	40	56	56	2	0
24	a	40	56	56	0	0
24	b	120	168	168	3	0
24	c	80	112	112	2	0
24	d	40	56	56	2	0
24	h	40	56	56	1	0
24	k	80	112	112	1	0
24	t	40	56	56	2	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	1	0
26	D	55	80	80	1	0
26	a	55	80	80	4	0
26	d	55	80	80	1	0
27	A	48	66	66	1	0
27	D	83	117	117	1	0
27	M	51	72	72	2	0
27	Y	48	66	66	0	0
27	a	49	68	68	0	0
27	b	55	86	86	0	0
27	c	85	113	112	0	0
27	d	44	58	58	0	0
27	h	23	34	34	0	0
27	m	51	72	72	1	0
28	A	91	135	135	2	0
28	B	54	78	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	F	36	46	45	0	0
28	a	90	134	133	0	0
28	b	49	65	65	1	0
28	f	41	48	48	2	0
29	A	49	74	74	3	0
29	D	145	215	215	4	0
29	L	49	74	74	1	0
29	a	49	74	74	1	0
29	d	88	125	125	1	0
29	e	42	57	57	2	0
29	l	49	74	74	1	0
30	A	66	96	96	5	0
30	C	186	246	245	1	0
30	H	62	82	80	0	0
30	c	186	245	241	2	0
30	h	62	82	80	0	0
30	o	44	75	75	3	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	B	105	137	161	4	0
32	C	40	63	63	0	0
32	D	35	35	57	1	0
32	E	12	16	16	0	0
32	H	18	35	35	1	0
32	I	15	26	26	2	0
32	J	12	16	16	0	0
32	M	43	73	73	1	0
32	T	15	29	29	0	0
32	a	22	32	32	0	0
32	b	82	141	141	1	0
32	c	32	51	51	2	0
32	d	37	61	61	1	0
32	j	12	16	16	0	0
32	m	12	16	16	0	0
33	D	4	1	1	0	0
33	d	4	1	1	0	0
34	F	43	30	30	1	0
34	f	43	30	30	6	0
35	V	43	32	30	2	0
35	v	43	32	30	2	0
36	A	144	0	0	5	0
36	B	204	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	C	182	0	0	0	0
36	D	136	0	0	1	0
36	E	30	0	0	2	0
36	F	7	0	0	0	0
36	H	37	0	0	0	0
36	I	10	0	0	0	0
36	J	16	0	0	2	0
36	K	8	0	0	0	0
36	L	8	0	0	0	0
36	M	7	0	0	0	0
36	O	90	0	0	3	0
36	T	10	0	0	1	0
36	U	52	0	0	2	0
36	V	65	0	0	1	0
36	X	12	0	0	1	0
36	Y	6	0	0	0	0
36	Z	2	0	0	0	0
36	a	126	0	0	2	0
36	b	206	0	0	6	0
36	c	181	0	0	5	0
36	d	111	0	0	0	0
36	e	21	0	0	1	0
36	f	8	0	0	0	0
36	h	36	0	0	0	0
36	i	13	0	0	0	0
36	j	8	0	0	2	0
36	k	6	0	0	1	0
36	l	7	0	0	2	0
36	m	6	0	0	0	0
36	o	102	0	0	5	0
36	r	3	0	0	0	0
36	t	8	0	0	0	0
36	u	58	0	0	5	0
36	v	56	0	0	2	0
36	x	8	0	0	0	0
36	y	3	0	0	0	0
36	z	9	0	0	1	0
All	All	52138	51532	51542	440	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 440 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)
16:u:53:ALA:O	36:u:201:HOH:O	1.77	1.02
16:u:15:GLU:OE1	36:u:202:HOH:O	1.89	0.90
2:B:235:GLU:HB3	36:B:701:HOH:O	1.71	0.89
3:c:44:ASN:O	36:c:601:HOH:O	1.99	0.81
16:u:88:GLU:OE1	36:u:203:HOH:O	1.98	0.80

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:70:GLU:OE2	16:u:76:ARG:HE[3_457]	1.57	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	36
1	a	332/344 (96%)	325 (98%)	7 (2%)	0	100	100
2	B	508/510 (100%)	503 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	494 (98%)	9 (2%)	0	100	100
3	C	442/461 (96%)	434 (98%)	7 (2%)	1 (0%)	43	44
3	c	451/461 (98%)	438 (97%)	12 (3%)	1 (0%)	43	44
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	226 (93%)	14 (6%)	3 (1%)	10	6
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	30	28
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	7
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	14
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	2	0
19	y	28/46 (61%)	24 (86%)	3 (11%)	1 (4%)	2	1
20	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
All	All	5231/5700 (92%)	5092 (97%)	128 (2%)	11 (0%)	43	44

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER

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Mol	Chain	Res	Type
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
3	c	416	SER

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%)	267 (99%)	3 (1%)	65	73
1	a	269/280 (96%)	259 (96%)	10 (4%)	30	31
2	B	408/407 (100%)	398 (98%)	10 (2%)	42	46
2	b	402/407 (99%)	386 (96%)	16 (4%)	28	28
3	C	346/362 (96%)	339 (98%)	7 (2%)	48	54
3	c	354/362 (98%)	341 (96%)	13 (4%)	30	31
4	D	276/283 (98%)	271 (98%)	5 (2%)	51	58
4	d	277/283 (98%)	269 (97%)	8 (3%)	37	40
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	42
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	26
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	32
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	16
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	13
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	38
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	7
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	11
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	10
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	34
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	29
14	R	22/33 (67%)	21 (96%)	1 (4%)	24	24
14	r	22/33 (67%)	19 (86%)	3 (14%)	3	2
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	30
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	28
16	U	84/112 (75%)	81 (96%)	3 (4%)	31	32
16	u	84/112 (75%)	83 (99%)	1 (1%)	63	70
17	V	117/138 (85%)	114 (97%)	3 (3%)	40	45
17	v	117/138 (85%)	113 (97%)	4 (3%)	32	34
18	X	31/34 (91%)	30 (97%)	1 (3%)	34	36
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	12
19	Y	19/37 (51%)	19 (100%)	0	100	100
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	44 (86%)	7 (14%)	3	2
All	All	4321/4654 (93%)	4170 (96%)	151 (4%)	32	33

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	k	35	LEU
19	y	45	ASN
11	l	30	LEU
14	r	9	LEU
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	322	GLN
13	o	147	ASN
4	d	186	GLN
7	h	59	ASN
20	z	58	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	i	1	8	8,9,10	1.30	1 (12%)	8,9,11	1.42	1 (12%)
12	FME	M	1	12	8,9,10	1.04	0	8,9,11	0.85	0
8	FME	I	1	8	8,9,10	0.98	0	8,9,11	1.15	1 (12%)
15	FME	t	1	15	8,9,10	1.22	1 (12%)	8,9,11	1.07	0
15	FME	T	1	15	8,9,10	1.14	1 (12%)	8,9,11	0.92	0
12	FME	m	1	12	8,9,10	1.16	1 (12%)	8,9,11	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	T	1	15	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-3.07	1.42	1.46
12	m	1	FME	CA-N	-2.53	1.42	1.46
15	t	1	FME	CA-N	-2.34	1.43	1.46
15	T	1	FME	CN-N	2.13	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CB-CA-N	3.03	116.04	110.52
8	I	1	FME	CB-CA-N	2.05	114.25	110.52

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	O-C-CA-CB
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	CB-CG-SD-CE
8	I	1	FME	C-CA-CB-CG
8	i	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 187 ligands modelled in this entry, 6 are monoatomic - leaving 181 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
23	PHO	A	404	-	58,69,69	1.88	14 (24%)	55,99,99	1.46	9 (16%)
28	SQD	A	412	-	50,52,54	1.08	5 (10%)	60,63,65	1.68	8 (13%)
32	STE	C	519	-	15,15,19	0.73	0	14,14,19	0.27	0
32	STE	C	520	-	11,11,19	0.55	0	11,11,19	1.52	1 (9%)
32	STE	c	520	-	19,19,19	0.71	1 (5%)	19,19,19	0.91	1 (5%)
22	CLA	B	605	-	69,73,73	1.23	10 (14%)	82,113,113	1.50	11 (13%)
28	SQD	B	621	-	52,54,54	1.01	3 (5%)	62,65,65	1.77	12 (19%)
27	LMG	D	410	-	31,31,55	1.20	3 (9%)	33,33,63	1.14	1 (3%)
27	LMG	M	101	-	51,51,55	1.13	2 (3%)	59,59,63	1.44	7 (11%)
30	DGD	C	516	-	63,63,67	1.28	8 (12%)	77,77,81	1.43	9 (11%)
32	STE	b	621	-	15,15,19	0.49	0	14,14,19	0.69	0
22	CLA	C	505	-	69,73,73	1.17	7 (10%)	82,113,113	1.44	10 (12%)
22	CLA	b	615	-	69,73,73	1.59	12 (17%)	82,113,113	1.42	7 (8%)
22	CLA	D	402	-	69,73,73	1.19	7 (10%)	82,113,113	1.39	11 (13%)
24	BCR	T	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.17	2 (3%)
22	CLA	c	502	-	69,73,73	1.16	7 (10%)	82,113,113	1.33	9 (10%)
22	CLA	c	506	-	69,73,73	1.24	9 (13%)	82,113,113	1.16	6 (7%)
32	STE	D	412	-	19,19,19	0.76	1 (5%)	19,19,19	0.98	0
24	BCR	t	101	-	41,41,41	1.06	3 (7%)	56,56,56	1.56	12 (21%)
33	BCT	D	401	21	3,3,3	1.11	0	2,3,3	2.76	2 (100%)
22	CLA	d	405	-	69,73,73	1.20	7 (10%)	82,113,113	1.18	10 (12%)
22	CLA	b	612	-	69,73,73	1.13	7 (10%)	82,113,113	1.26	9 (10%)
22	CLA	c	512	-	69,73,73	1.32	10 (14%)	82,113,113	1.23	7 (8%)
22	CLA	B	609	-	69,73,73	1.27	7 (10%)	82,113,113	1.37	8 (9%)
32	STE	B	627	-	15,15,19	0.85	1 (6%)	15,15,19	1.27	2 (13%)
24	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.26	7 (12%)
31	OEX	a	416	1,3,36	0,15,15	-	-	-	-	-
24	BCR	h	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	9 (16%)
23	PHO	A	405	-	58,69,69	1.96	8 (13%)	55,99,99	1.51	6 (10%)
28	SQD	f	102	-	39,41,54	1.14	4 (10%)	49,52,65	1.86	11 (22%)
27	LMG	D	407	-	51,51,55	1.01	1 (1%)	59,59,63	1.33	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	M	103	-	9,9,19	0.55	0	8,8,19	0.66	0
22	CLA	d	403	-	69,73,73	1.13	7 (10%)	82,113,113	1.14	8 (9%)
29	LHG	L	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.18	3 (5%)
22	CLA	b	604	-	69,73,73	1.44	10 (14%)	82,113,113	1.50	8 (9%)
32	STE	m	102	-	11,11,19	0.67	0	11,11,19	1.73	2 (18%)
22	CLA	C	503	-	69,73,73	1.42	10 (14%)	82,113,113	1.43	8 (9%)
22	CLA	D	404	-	69,73,73	1.48	11 (15%)	82,113,113	1.10	3 (3%)
32	STE	b	626	-	9,9,19	0.51	0	8,8,19	0.60	0
27	LMG	d	410	-	44,44,55	1.24	4 (9%)	52,52,63	1.42	6 (11%)
24	BCR	b	618	-	41,41,41	1.23	2 (4%)	56,56,56	1.20	8 (14%)
23	PHO	d	401	-	58,69,69	2.07	9 (15%)	55,99,99	1.69	11 (20%)
22	CLA	b	601	36	69,73,73	1.46	10 (14%)	82,113,113	1.38	7 (8%)
22	CLA	b	611	-	69,73,73	1.27	10 (14%)	82,113,113	1.60	9 (10%)
27	LMG	A	411	-	48,48,55	1.05	1 (2%)	56,56,63	1.45	8 (14%)
30	DGD	c	517	-	63,63,67	1.15	8 (12%)	77,77,81	1.38	10 (12%)
32	STE	D	413	-	14,14,19	0.88	1 (7%)	14,14,19	1.09	1 (7%)
30	DGD	c	516	-	63,63,67	1.38	7 (11%)	77,77,81	1.29	6 (7%)
22	CLA	C	511	3	69,73,73	1.24	7 (10%)	82,113,113	1.27	3 (3%)
29	LHG	d	408	-	48,48,48	0.94	1 (2%)	51,54,54	1.15	2 (3%)
22	CLA	c	505	-	69,73,73	1.10	8 (11%)	82,113,113	1.28	8 (9%)
32	STE	M	102	-	14,14,19	1.03	1 (7%)	14,14,19	0.77	1 (7%)
22	CLA	C	512	-	69,73,73	1.50	8 (11%)	82,113,113	1.25	8 (9%)
29	LHG	D	408	-	48,48,48	1.01	2 (4%)	51,54,54	1.27	7 (13%)
22	CLA	A	406	-	58,62,73	1.36	9 (15%)	68,99,113	1.51	9 (13%)
27	LMG	Y	101	-	48,48,55	0.97	2 (4%)	56,56,63	1.47	10 (17%)
29	LHG	d	409	-	38,38,48	1.02	2 (5%)	41,44,54	1.07	4 (9%)
24	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.12	5 (8%)
22	CLA	b	602	-	69,73,73	1.33	9 (13%)	82,113,113	1.34	8 (9%)
22	CLA	c	513	-	69,73,73	1.43	10 (14%)	82,113,113	1.19	11 (13%)
24	BCR	k	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.20	4 (7%)
22	CLA	C	509	-	69,73,73	1.31	11 (15%)	82,113,113	1.29	7 (8%)
22	CLA	c	504	36	64,68,73	1.30	10 (15%)	76,107,113	1.34	10 (13%)
32	STE	b	625	-	19,19,19	0.67	0	19,19,19	1.26	3 (15%)
22	CLA	C	507	36	69,73,73	1.46	10 (14%)	82,113,113	1.58	9 (10%)
32	STE	M	104	-	17,17,19	0.37	0	16,16,19	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	618	-	41,41,41	1.12	3 (7%)	56,56,56	1.38	6 (10%)
22	CLA	B	603	-	69,73,73	1.34	9 (13%)	82,113,113	1.37	14 (17%)
32	STE	B	626	-	11,11,19	0.75	0	11,11,19	0.92	0
22	CLA	C	510	-	69,73,73	1.19	7 (10%)	82,113,113	1.20	7 (8%)
32	STE	T	102	-	14,14,19	0.43	0	13,13,19	0.83	0
32	STE	c	522	-	11,11,19	0.86	0	11,11,19	1.17	1 (9%)
29	LHG	l	101	-	48,48,48	0.63	0	51,54,54	1.26	6 (11%)
22	CLA	B	604	-	69,73,73	1.29	7 (10%)	82,113,113	1.57	12 (14%)
32	STE	B	623	-	11,11,19	0.93	1 (9%)	11,11,19	1.07	1 (9%)
24	BCR	B	619	-	41,41,41	1.23	2 (4%)	56,56,56	1.43	8 (14%)
32	STE	d	412	-	19,19,19	0.73	0	19,19,19	0.77	1 (5%)
22	CLA	b	608	-	69,73,73	1.31	9 (13%)	82,113,113	1.40	10 (12%)
24	BCR	K	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.36	6 (10%)
32	STE	J	101	-	11,11,19	0.70	0	11,11,19	1.58	2 (18%)
29	LHG	a	410	-	48,48,48	1.03	3 (6%)	51,54,54	1.45	6 (11%)
32	STE	B	622	-	13,13,19	0.57	0	13,13,19	1.32	3 (23%)
34	HEM	F	101	5,6	50,50,50	1.37	7 (14%)	67,82,82	1.20	6 (8%)
22	CLA	B	611	-	69,73,73	1.26	8 (11%)	82,113,113	1.38	12 (14%)
24	BCR	K	103	-	41,41,41	1.14	4 (9%)	56,56,56	1.30	9 (16%)
32	STE	B	625	-	15,15,19	0.49	0	14,14,19	0.71	0
29	LHG	D	411	-	48,48,48	0.88	3 (6%)	51,54,54	1.38	8 (15%)
24	BCR	C	514	-	41,41,41	1.27	3 (7%)	56,56,56	1.28	7 (12%)
26	PL9	D	406	-	55,55,55	1.39	7 (12%)	68,69,69	1.68	17 (25%)
30	DGD	o	301	-	43,43,67	1.15	2 (4%)	45,45,81	1.49	5 (11%)
27	LMG	a	414	-	49,49,55	1.01	5 (10%)	57,57,63	1.33	6 (10%)
24	BCR	k	101	-	41,41,41	1.05	4 (9%)	56,56,56	1.08	3 (5%)
22	CLA	C	504	36	63,67,73	1.18	8 (12%)	74,105,113	1.33	9 (12%)
28	SQD	a	411	-	52,54,54	0.98	3 (5%)	62,65,65	2.16	14 (22%)
32	STE	C	518	-	11,11,19	0.68	0	11,11,19	1.11	1 (9%)
22	CLA	C	508	-	69,73,73	1.39	7 (10%)	82,113,113	1.38	7 (8%)
22	CLA	b	616	-	64,68,73	1.13	6 (9%)	76,107,113	1.56	13 (17%)
35	HEC	V	201	17	46,50,50	1.73	5 (10%)	58,82,82	1.89	11 (18%)
22	CLA	B	608	-	69,73,73	1.45	11 (15%)	82,113,113	1.28	9 (10%)
24	BCR	b	617	-	41,41,41	1.26	3 (7%)	56,56,56	1.36	7 (12%)
26	PL9	d	407	-	55,55,55	1.58	7 (12%)	68,69,69	1.79	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	a	415	-	11,11,19	0.75	0	11,11,19	1.20	1 (9%)
22	CLA	b	605	-	69,73,73	1.17	7 (10%)	82,113,113	1.49	13 (15%)
29	LHG	D	409	-	46,46,48	0.98	3 (6%)	49,52,54	1.25	5 (10%)
22	CLA	B	607	36	69,73,73	1.17	7 (10%)	82,113,113	1.45	10 (12%)
23	PHO	a	404	-	58,69,69	2.00	10 (17%)	55,99,99	1.54	9 (16%)
28	SQD	F	102	-	34,36,54	0.99	2 (5%)	42,45,65	1.86	10 (23%)
22	CLA	b	607	36	69,73,73	1.39	12 (17%)	82,113,113	1.24	10 (12%)
22	CLA	B	615	-	69,73,73	1.46	9 (13%)	82,113,113	1.33	7 (8%)
30	DGD	h	103	-	63,63,67	1.22	8 (12%)	77,77,81	1.38	11 (14%)
26	PL9	A	410	-	55,55,55	0.89	2 (3%)	68,69,69	1.48	13 (19%)
28	SQD	A	414	-	38,38,54	1.08	3 (7%)	40,40,65	1.30	3 (7%)
32	STE	a	413	-	9,9,19	0.65	0	8,8,19	0.38	0
22	CLA	b	613	-	69,73,73	1.28	9 (13%)	82,113,113	1.43	12 (14%)
31	OEX	A	416	1,3,36	0,15,15	-	-	-	-	-
24	BCR	D	405	-	41,41,41	1.26	2 (4%)	56,56,56	1.20	7 (12%)
22	CLA	b	614	-	69,73,73	1.25	10 (14%)	82,113,113	1.15	7 (8%)
22	CLA	c	501	-	69,73,73	1.14	7 (10%)	82,113,113	1.47	8 (9%)
22	CLA	D	403	36	69,73,73	1.31	5 (7%)	82,113,113	1.31	5 (6%)
24	BCR	d	406	-	41,41,41	1.30	2 (4%)	56,56,56	1.24	6 (10%)
29	LHG	e	101	-	41,41,48	1.01	3 (7%)	44,47,54	1.24	4 (9%)
32	STE	E	101	-	11,11,19	1.04	1 (9%)	11,11,19	0.89	0
22	CLA	c	509	-	69,73,73	1.17	7 (10%)	82,113,113	1.56	11 (13%)
24	BCR	b	619	-	41,41,41	1.20	2 (4%)	56,56,56	1.34	9 (16%)
27	LMG	b	623	-	55,55,55	1.03	4 (7%)	63,63,63	1.76	11 (17%)
30	DGD	c	518	-	63,63,67	1.20	7 (11%)	77,77,81	1.47	12 (15%)
22	CLA	B	602	-	69,73,73	1.28	9 (13%)	82,113,113	1.35	9 (10%)
22	CLA	a	403	36	69,73,73	1.20	9 (13%)	82,113,113	1.36	9 (10%)
22	CLA	C	513	-	69,73,73	1.20	10 (14%)	82,113,113	1.37	8 (9%)
22	CLA	B	601	36	69,73,73	1.52	10 (14%)	82,113,113	1.41	8 (9%)
22	CLA	b	610	36	69,73,73	1.18	4 (5%)	82,113,113	1.40	12 (14%)
24	BCR	A	407	-	41,41,41	1.21	3 (7%)	56,56,56	1.41	8 (14%)
32	STE	I	101	-	14,14,19	0.62	0	13,13,19	0.36	0
22	CLA	b	606	-	69,73,73	1.48	8 (11%)	82,113,113	1.37	7 (8%)
22	CLA	B	612	-	69,73,73	1.11	5 (7%)	82,113,113	1.39	10 (12%)
22	CLA	C	506	-	69,73,73	1.68	9 (13%)	82,113,113	1.19	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	503	-	69,73,73	1.20	10 (14%)	82,113,113	1.39	9 (10%)
32	STE	H	103	-	17,17,19	0.41	0	16,16,19	0.84	0
27	LMG	c	519	-	37,37,55	1.22	5 (13%)	45,45,63	1.38	6 (13%)
32	STE	d	411	-	16,16,19	0.67	0	16,16,19	1.03	1 (6%)
22	CLA	C	501	-	69,73,73	1.47	12 (17%)	82,113,113	1.39	9 (10%)
29	LHG	A	413	-	48,48,48	1.00	3 (6%)	51,54,54	1.20	2 (3%)
32	STE	B	620	-	16,16,19	0.87	0	16,16,19	0.76	0
28	SQD	a	412	-	35,35,54	1.25	2 (5%)	37,37,65	1.67	6 (16%)
22	CLA	B	614	-	69,73,73	1.32	7 (10%)	82,113,113	1.28	10 (12%)
28	SQD	b	620	-	47,49,54	0.93	2 (4%)	57,60,65	2.34	14 (24%)
22	CLA	B	610	36	69,73,73	1.39	9 (13%)	82,113,113	1.44	12 (14%)
24	BCR	c	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.30	5 (8%)
32	STE	j	101	-	11,11,19	0.97	1 (9%)	11,11,19	1.44	2 (18%)
32	STE	b	622	-	19,19,19	0.73	0	19,19,19	0.95	0
22	CLA	c	511	3	69,73,73	1.55	8 (11%)	82,113,113	1.34	5 (6%)
22	CLA	B	606	-	69,73,73	1.42	10 (14%)	82,113,113	1.45	9 (10%)
22	CLA	c	507	36	69,73,73	1.23	7 (10%)	82,113,113	1.31	9 (10%)
32	STE	b	624	-	15,15,19	0.85	1 (6%)	15,15,19	0.96	1 (6%)
27	LMG	h	102	-	21,21,55	0.96	1 (4%)	20,20,63	1.08	1 (5%)
22	CLA	C	502	-	69,73,73	1.22	8 (11%)	82,113,113	1.15	8 (9%)
30	DGD	H	102	-	63,63,67	1.31	8 (12%)	77,77,81	1.57	13 (16%)
22	CLA	b	603	-	69,73,73	1.32	10 (14%)	82,113,113	1.46	13 (15%)
22	CLA	d	404	36	69,73,73	1.44	7 (10%)	82,113,113	1.51	9 (10%)
22	CLA	B	616	-	64,68,73	1.57	11 (17%)	76,107,113	1.54	9 (11%)
24	BCR	a	406	-	41,41,41	1.24	4 (9%)	56,56,56	1.20	5 (8%)
22	CLA	a	405	-	69,73,73	1.25	10 (14%)	82,113,113	1.26	5 (6%)
30	DGD	A	415	-	67,67,67	1.43	10 (14%)	81,81,81	1.50	13 (16%)
30	DGD	C	517	-	63,63,67	1.28	7 (11%)	77,77,81	1.40	10 (12%)
24	BCR	B	617	-	41,41,41	1.18	3 (7%)	56,56,56	1.24	5 (8%)
22	CLA	A	402	-	69,73,73	1.41	8 (11%)	82,113,113	1.31	5 (6%)
22	CLA	c	510	-	69,73,73	1.25	7 (10%)	82,113,113	1.45	9 (10%)
24	BCR	K	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	3 (5%)
30	DGD	C	515	-	63,63,67	1.65	13 (20%)	77,77,81	1.45	12 (15%)
32	STE	B	624	-	17,17,19	0.66	0	17,17,19	1.18	1 (5%)
22	CLA	A	403	36	69,73,73	1.23	7 (10%)	82,113,113	1.32	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	402	-	69,73,73	1.37	9 (13%)	82,113,113	1.31	7 (8%)
35	HEC	v	201	17	46,50,50	1.88	6 (13%)	58,82,82	1.95	13 (22%)
26	PL9	a	409	-	55,55,55	1.31	3 (5%)	68,69,69	1.84	12 (17%)
22	CLA	B	613	-	69,73,73	1.64	13 (18%)	82,113,113	1.42	10 (12%)
22	CLA	b	609	-	69,73,73	1.34	11 (15%)	82,113,113	1.24	8 (9%)
27	LMG	m	101	-	51,51,55	1.15	6 (11%)	59,59,63	1.49	11 (18%)
22	CLA	c	508	-	68,72,73	1.41	9 (13%)	80,111,113	1.35	12 (15%)
34	HEM	f	101	5,6	50,50,50	1.45	8 (16%)	67,82,82	1.29	7 (10%)
27	LMG	c	521	-	48,48,55	1.25	7 (14%)	56,56,63	1.20	4 (7%)
33	BCT	d	402	21	3,3,3	1.22	0	2,3,3	3.07	2 (100%)

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
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
28	SQD	A	412	-	-	15/47/67/69	0/1/1/1
32	STE	C	519	-	-	5/13/13/17	-
32	STE	C	520	-	-	5/9/9/17	-
32	STE	c	520	-	-	13/17/17/17	-
22	CLA	B	605	-	1/1/20/20	7/39/115/115	-
28	SQD	B	621	-	-	19/49/69/69	0/1/1/1
27	LMG	D	410	-	-	13/33/33/70	-
27	LMG	M	101	-	-	25/46/66/70	0/1/1/1
30	DGD	C	516	-	-	20/51/91/95	0/2/2/2
32	STE	b	621	-	-	8/13/13/17	-
22	CLA	C	505	-	1/1/20/20	12/39/115/115	-
22	CLA	b	615	-	1/1/20/20	9/39/115/115	-
22	CLA	D	402	-	-	6/39/115/115	-
24	BCR	T	101	-	-	14/29/63/63	0/2/2/2
22	CLA	c	502	-	-	6/39/115/115	-
22	CLA	c	506	-	1/1/20/20	13/39/115/115	-
32	STE	D	412	-	-	7/17/17/17	-
24	BCR	t	101	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	405	-	1/1/20/20	4/39/115/115	-
22	CLA	b	612	-	1/1/20/20	5/39/115/115	-
22	CLA	c	512	-	1/1/20/20	18/39/115/115	-
22	CLA	B	609	-	-	3/39/115/115	-
32	STE	B	627	-	-	8/13/13/17	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
24	BCR	h	101	-	-	3/29/63/63	0/2/2/2
23	PHO	A	405	-	-	1/37/103/103	0/5/6/6
28	SQD	f	102	-	-	17/36/56/69	0/1/1/1
27	LMG	D	407	-	-	14/46/66/70	0/1/1/1
32	STE	M	103	-	-	4/7/7/17	-
22	CLA	d	403	-	-	12/39/115/115	-
29	LHG	L	101	-	-	17/53/53/53	-
22	CLA	b	604	-	1/1/20/20	9/39/115/115	-
32	STE	m	102	-	-	1/9/9/17	-
22	CLA	C	503	-	1/1/20/20	4/39/115/115	-
22	CLA	D	404	-	1/1/20/20	12/39/115/115	-
32	STE	b	626	-	-	4/7/7/17	-
27	LMG	d	410	-	-	12/39/59/70	0/1/1/1
24	BCR	b	618	-	-	5/29/63/63	0/2/2/2
23	PHO	d	401	-	-	5/37/103/103	0/5/6/6
22	CLA	b	601	36	1/1/20/20	18/39/115/115	-
22	CLA	b	611	-	1/1/20/20	7/39/115/115	-
27	LMG	A	411	-	-	16/43/63/70	0/1/1/1
30	DGD	c	517	-	-	20/51/91/95	0/2/2/2
32	STE	D	413	-	-	7/12/12/17	-
30	DGD	c	516	-	-	27/51/91/95	0/2/2/2
22	CLA	C	511	3	1/1/20/20	8/39/115/115	-
29	LHG	d	408	-	-	20/53/53/53	-
22	CLA	c	505	-	1/1/20/20	8/39/115/115	-
32	STE	M	102	-	-	5/12/12/17	-
22	CLA	C	512	-	1/1/20/20	14/39/115/115	-
29	LHG	D	408	-	-	23/53/53/53	-
22	CLA	A	406	-	1/1/17/20	3/26/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	Y	101	-	-	23/43/63/70	0/1/1/1
29	LHG	d	409	-	-	13/43/43/53	-
24	BCR	c	514	-	-	7/29/63/63	0/2/2/2
22	CLA	c	513	-	1/1/20/20	11/39/115/115	-
22	CLA	b	602	-	-	9/39/115/115	-
24	BCR	k	102	-	-	0/29/63/63	0/2/2/2
22	CLA	C	509	-	1/1/20/20	14/39/115/115	-
22	CLA	c	504	36	1/1/19/20	7/33/109/115	-
32	STE	b	625	-	-	10/17/17/17	-
22	CLA	C	507	36	1/1/20/20	5/39/115/115	-
32	STE	M	104	-	-	7/15/15/17	-
24	BCR	B	618	-	-	10/29/63/63	0/2/2/2
22	CLA	B	603	-	1/1/20/20	10/39/115/115	-
32	STE	B	626	-	-	3/9/9/17	-
22	CLA	C	510	-	1/1/20/20	9/39/115/115	-
32	STE	T	102	-	-	7/12/12/17	-
32	STE	c	522	-	-	4/9/9/17	-
29	LHG	l	101	-	-	21/53/53/53	-
22	CLA	B	604	-	1/1/20/20	11/39/115/115	-
32	STE	B	623	-	-	5/9/9/17	-
24	BCR	B	619	-	-	3/29/63/63	0/2/2/2
32	STE	d	412	-	-	11/17/17/17	-
22	CLA	b	608	-	-	6/39/115/115	-
24	BCR	K	101	-	-	8/29/63/63	0/2/2/2
32	STE	J	101	-	-	5/9/9/17	-
29	LHG	a	410	-	-	17/53/53/53	-
32	STE	B	622	-	-	2/11/11/17	-
34	HEM	F	101	5,6	-	3/14/54/54	-
22	CLA	B	611	-	1/1/20/20	6/39/115/115	-
24	BCR	K	103	-	-	4/29/63/63	0/2/2/2
32	STE	B	625	-	-	7/13/13/17	-
29	LHG	D	411	-	-	19/53/53/53	-
24	BCR	C	514	-	-	7/29/63/63	0/2/2/2
26	PL9	D	406	-	-	10/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	o	301	-	-	20/45/45/95	-
27	LMG	a	414	-	-	23/44/64/70	0/1/1/1
24	BCR	k	101	-	-	12/29/63/63	0/2/2/2
22	CLA	C	504	36	1/1/18/20	4/32/108/115	-
28	SQD	a	411	-	-	23/49/69/69	0/1/1/1
32	STE	C	518	-	-	4/9/9/17	-
22	CLA	C	508	-	-	6/39/115/115	-
22	CLA	b	616	-	1/1/19/20	13/33/109/115	-
22	CLA	B	608	-	-	3/39/115/115	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
32	STE	a	415	-	-	4/9/9/17	-
22	CLA	b	605	-	1/1/20/20	7/39/115/115	-
29	LHG	D	409	-	-	21/51/51/53	-
22	CLA	B	607	36	1/1/20/20	4/39/115/115	-
23	PHO	a	404	-	-	5/37/103/103	0/5/6/6
28	SQD	F	102	-	-	12/28/48/69	0/1/1/1
22	CLA	b	607	36	1/1/20/20	13/39/115/115	-
22	CLA	B	615	-	1/1/20/20	7/39/115/115	-
30	DGD	h	103	-	-	19/51/91/95	0/2/2/2
26	PL9	A	410	-	-	23/53/73/73	0/1/1/1
28	SQD	A	414	-	-	17/39/39/69	-
32	STE	a	413	-	-	5/7/7/17	-
22	CLA	b	613	-	1/1/20/20	7/39/115/115	-
24	BCR	D	405	-	-	5/29/63/63	0/2/2/2
22	CLA	b	614	-	1/1/20/20	15/39/115/115	-
22	CLA	c	501	-	1/1/20/20	2/39/115/115	-
22	CLA	D	403	36	-	6/39/115/115	-
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
29	LHG	e	101	-	-	21/46/46/53	-
32	STE	E	101	-	-	3/9/9/17	-
22	CLA	c	509	-	1/1/20/20	15/39/115/115	-
24	BCR	b	619	-	-	4/29/63/63	0/2/2/2
27	LMG	b	623	-	-	25/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	c	518	-	-	16/51/91/95	0/2/2/2
22	CLA	B	602	-	1/1/20/20	6/39/115/115	-
22	CLA	a	403	36	1/1/20/20	13/39/115/115	-
22	CLA	C	513	-	1/1/20/20	15/39/115/115	-
22	CLA	B	601	36	1/1/20/20	21/39/115/115	-
22	CLA	b	610	36	1/1/20/20	3/39/115/115	-
24	BCR	A	407	-	-	7/29/63/63	0/2/2/2
32	STE	I	101	-	-	5/12/12/17	-
22	CLA	b	606	-	1/1/20/20	5/39/115/115	-
22	CLA	B	612	-	1/1/20/20	11/39/115/115	-
22	CLA	C	506	-	-	9/39/115/115	-
22	CLA	c	503	-	1/1/20/20	10/39/115/115	-
32	STE	H	103	-	-	9/15/15/17	-
27	LMG	c	519	-	-	11/31/51/70	0/1/1/1
32	STE	d	411	-	-	8/14/14/17	-
22	CLA	C	501	-	1/1/20/20	3/39/115/115	-
29	LHG	A	413	-	-	27/53/53/53	-
32	STE	B	620	-	-	8/14/14/17	-
28	SQD	a	412	-	-	16/37/37/69	-
22	CLA	B	614	-	1/1/20/20	8/39/115/115	-
28	SQD	b	620	-	-	24/44/64/69	0/1/1/1
22	CLA	B	610	36	1/1/20/20	4/39/115/115	-
24	BCR	c	515	-	-	2/29/63/63	0/2/2/2
32	STE	j	101	-	-	3/9/9/17	-
32	STE	b	622	-	-	12/17/17/17	-
22	CLA	c	511	3	1/1/20/20	9/39/115/115	-
22	CLA	B	606	-	1/1/20/20	15/39/115/115	-
22	CLA	c	507	36	1/1/20/20	12/39/115/115	-
32	STE	b	624	-	-	5/13/13/17	-
27	LMG	h	102	-	-	11/17/17/70	-
22	CLA	C	502	-	1/1/20/20	8/39/115/115	-
30	DGD	H	102	-	-	19/51/91/95	0/2/2/2
22	CLA	b	603	-	1/1/20/20	8/39/115/115	-
22	CLA	d	404	36	1/1/20/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	616	-	1/1/19/20	8/33/109/115	-
24	BCR	a	406	-	-	0/29/63/63	0/2/2/2
22	CLA	a	405	-	1/1/20/20	5/39/115/115	-
30	DGD	A	415	-	-	33/55/95/95	0/2/2/2
30	DGD	C	517	-	-	14/51/91/95	0/2/2/2
24	BCR	B	617	-	-	6/29/63/63	0/2/2/2
22	CLA	A	402	-	1/1/20/20	3/39/115/115	-
22	CLA	c	510	-	1/1/20/20	6/39/115/115	-
24	BCR	K	102	-	-	5/29/63/63	0/2/2/2
30	DGD	C	515	-	-	19/51/91/95	0/2/2/2
32	STE	B	624	-	-	14/15/15/17	-
22	CLA	A	403	36	-	14/39/115/115	-
22	CLA	a	402	-	1/1/20/20	4/39/115/115	-
35	HEC	v	201	17	-	6/14/54/54	-
26	PL9	a	409	-	-	19/53/73/73	0/1/1/1
22	CLA	B	613	-	1/1/20/20	14/39/115/115	-
22	CLA	b	609	-	-	8/39/115/115	-
27	LMG	m	101	-	-	16/46/66/70	0/1/1/1
22	CLA	c	508	-	-	6/38/114/115	-
34	HEM	f	101	5,6	-	5/14/54/54	-
27	LMG	c	521	-	-	25/43/63/70	0/1/1/1
35	HEC	V	201	17	-	6/14/54/54	-

The worst 5 of 924 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C1B-C2B	9.07	1.49	1.39
23	d	401	PHO	C3B-C4B	9.04	1.50	1.41
23	a	404	PHO	C1B-C2B	8.87	1.49	1.39
23	A	405	PHO	C1B-C2B	8.36	1.48	1.39
23	A	405	PHO	C3B-C4B	7.87	1.49	1.41

The worst 5 of 1224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	620	SQD	O6-C1-C2	10.28	123.88	108.27
28	a	411	SQD	O6-C1-C2	9.94	123.37	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C4A-NA-C1A	8.90	110.74	106.68
22	C	507	CLA	C4A-NA-C1A	8.48	110.55	106.68
22	b	611	CLA	C4A-NA-C1A	8.26	110.45	106.68

5 of 57 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	406	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND

5 of 1793 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	403	CLA	C2B-C3B-CAB-CBB
22	A	403	CLA	C4B-C3B-CAB-CBB
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

100 monomers are involved in 130 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	c	520	STE	2	0
22	B	605	CLA	1	0
28	B	621	SQD	1	0
27	D	410	LMG	1	0
27	M	101	LMG	2	0
30	C	516	DGD	1	0
22	b	615	CLA	3	0
22	D	402	CLA	1	0
24	T	101	BCR	2	0
22	c	506	CLA	1	0
24	t	101	BCR	2	0
22	b	612	CLA	1	0
22	c	512	CLA	1	0
32	B	627	STE	2	0
24	H	101	BCR	3	0
24	h	101	BCR	1	0

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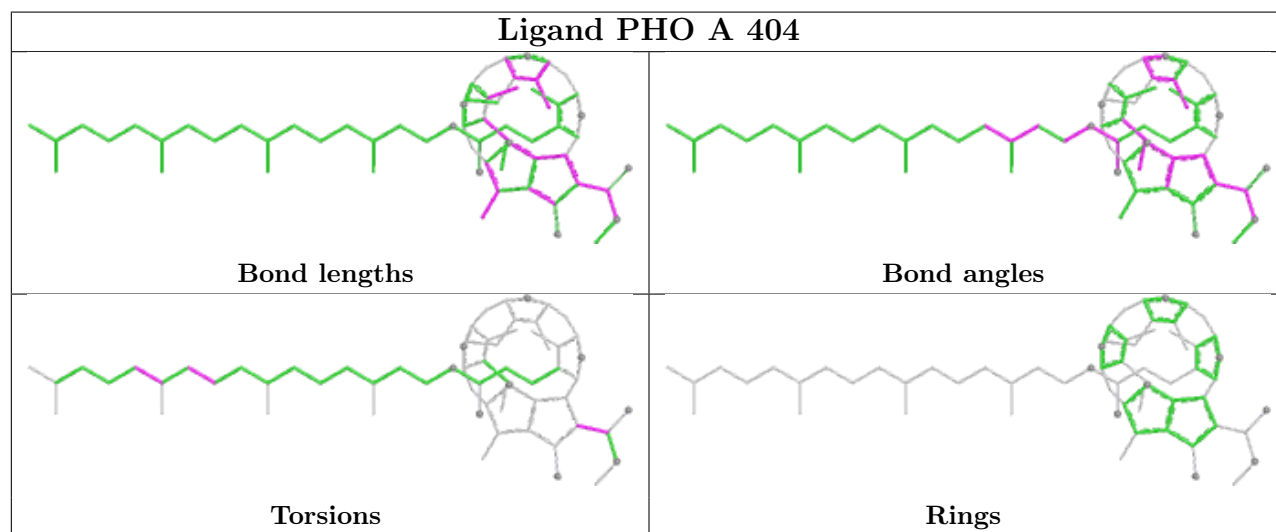
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	405	PHO	1	0
28	f	102	SQD	2	0
29	L	101	LHG	1	0
22	b	604	CLA	2	0
22	D	404	CLA	1	0
24	b	618	BCR	2	0
22	b	601	CLA	2	0
27	A	411	LMG	1	0
30	c	517	DGD	1	0
32	D	413	STE	1	0
22	C	511	CLA	1	0
29	d	408	LHG	1	0
22	C	512	CLA	2	0
29	D	408	LHG	1	0
22	A	406	CLA	1	0
24	c	514	BCR	1	0
22	b	602	CLA	2	0
22	c	513	CLA	1	0
24	k	102	BCR	1	0
22	C	509	CLA	1	0
22	C	507	CLA	1	0
32	M	104	STE	1	0
22	C	510	CLA	1	0
29	l	101	LHG	1	0
22	B	604	CLA	1	0
24	B	619	BCR	1	0
32	d	412	STE	1	0
29	a	410	LHG	1	0
34	F	101	HEM	1	0
22	B	611	CLA	1	0
29	D	411	LHG	3	0
24	C	514	BCR	1	0
26	D	406	PL9	1	0
30	o	301	DGD	3	0
22	C	508	CLA	1	0
22	b	616	CLA	2	0
35	V	201	HEC	2	0
26	d	407	PL9	1	0
22	b	605	CLA	1	0
22	B	607	CLA	1	0
26	A	410	PL9	1	0
28	A	414	SQD	2	0

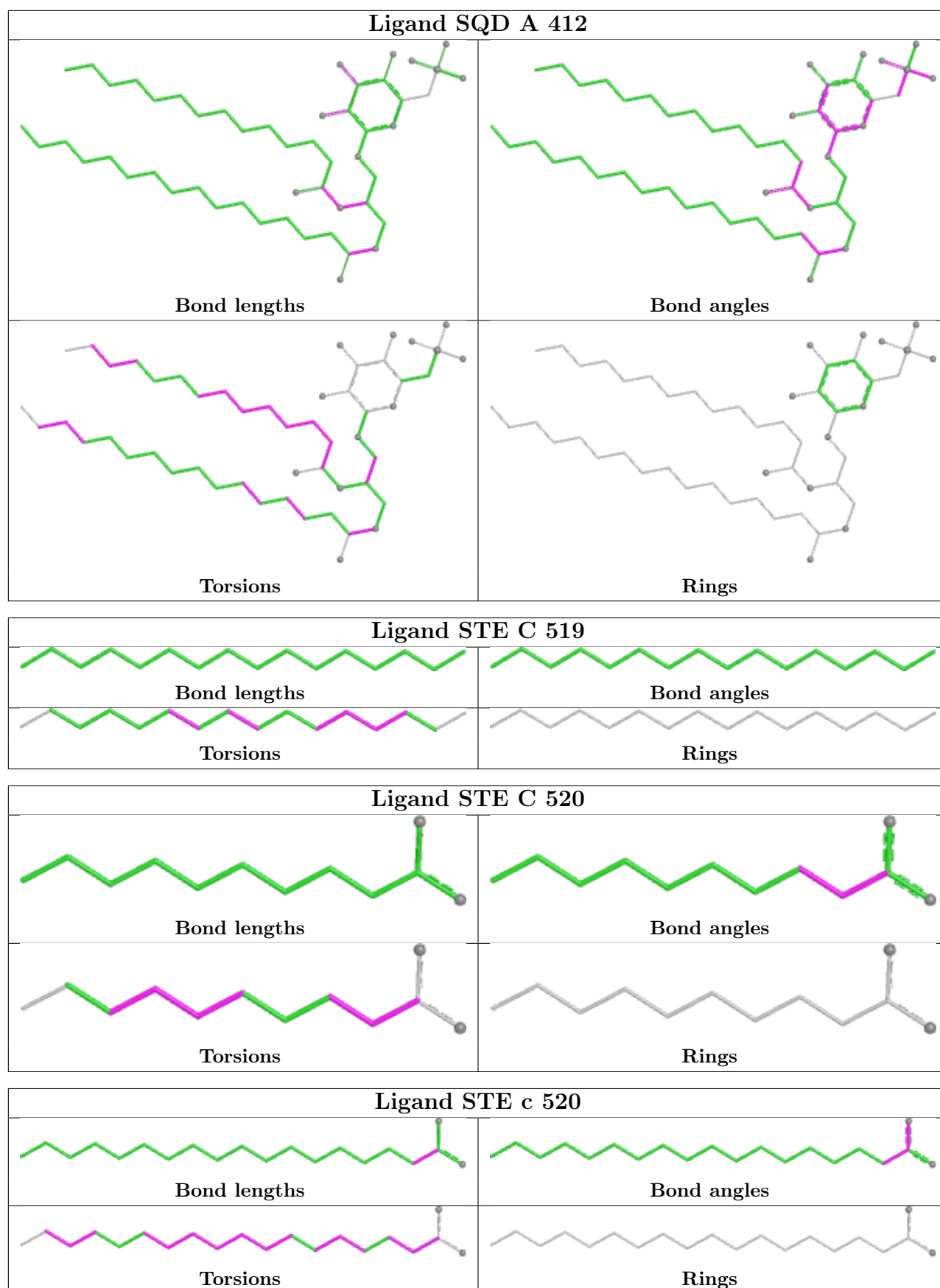
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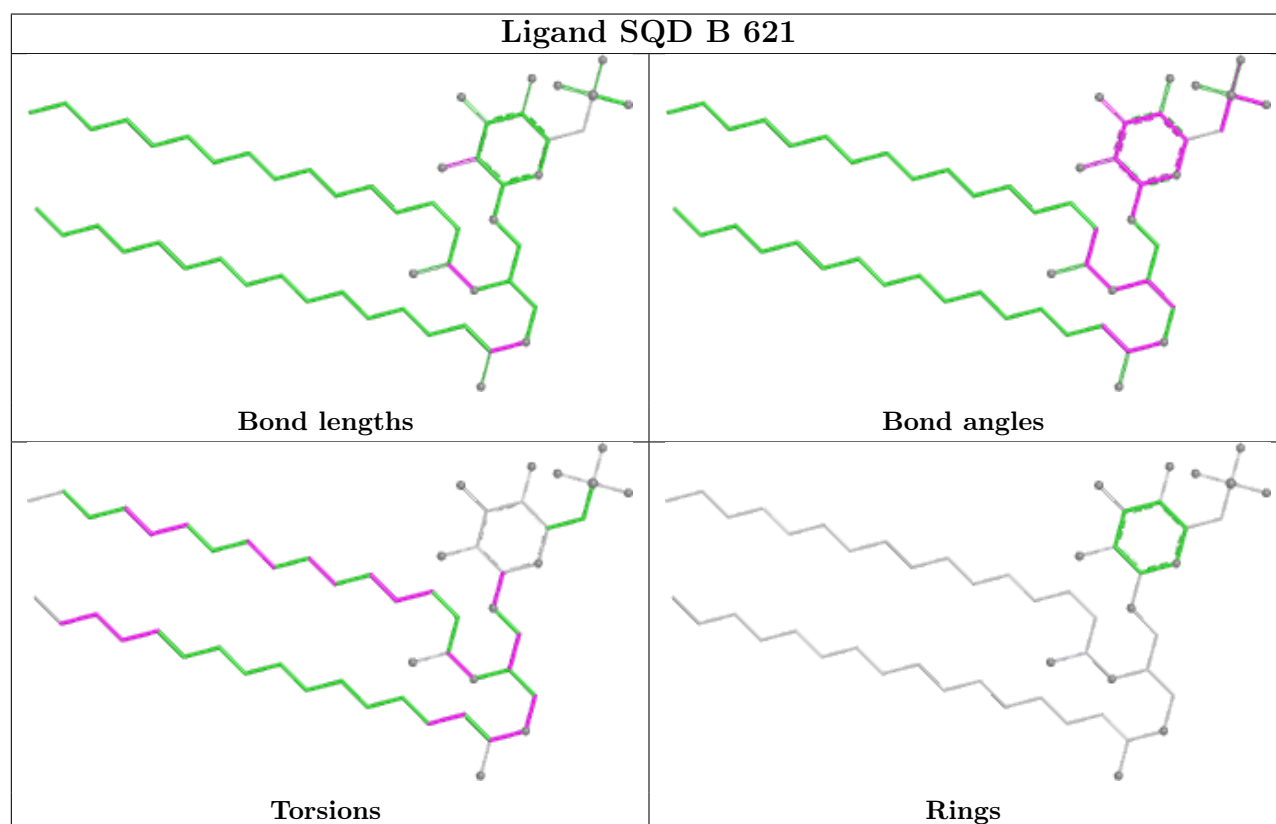
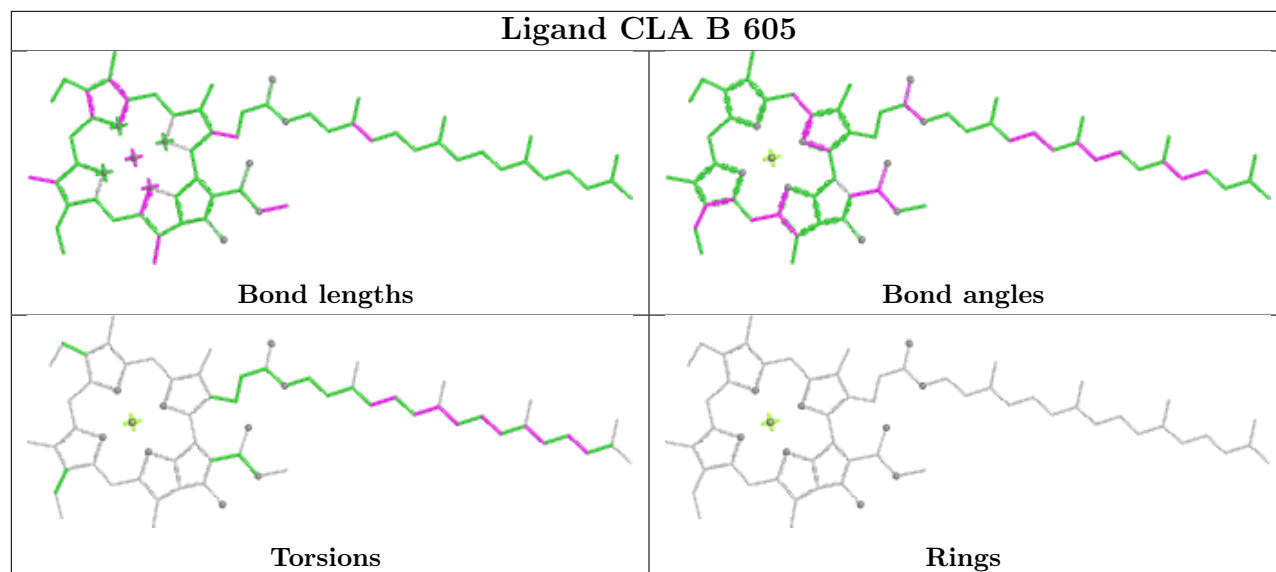
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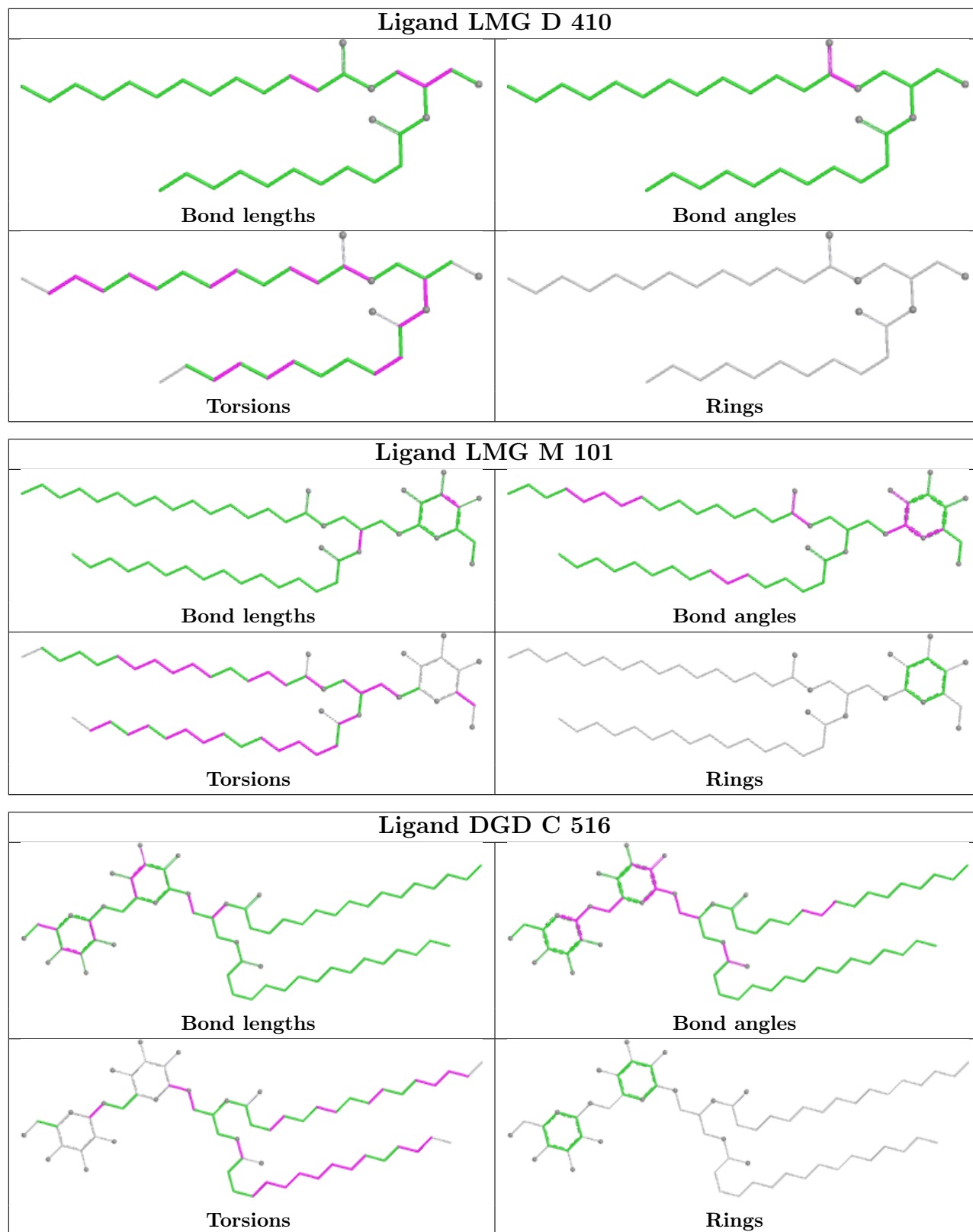
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	405	BCR	2	0
22	b	614	CLA	1	0
22	c	501	CLA	2	0
22	D	403	CLA	1	0
24	d	406	BCR	2	0
29	e	101	LHG	2	0
22	c	509	CLA	2	0
24	b	619	BCR	1	0
30	c	518	DGD	1	0
22	B	602	CLA	1	0
22	C	513	CLA	1	0
22	B	601	CLA	4	0
22	b	610	CLA	1	0
32	I	101	STE	2	0
22	b	606	CLA	2	0
22	B	612	CLA	1	0
22	C	506	CLA	1	0
22	c	503	CLA	2	0
32	H	103	STE	1	0
22	C	501	CLA	2	0
29	A	413	LHG	3	0
32	B	620	STE	1	0
22	B	614	CLA	1	0
28	b	620	SQD	1	0
24	c	515	BCR	1	0
32	b	622	STE	1	0
22	c	511	CLA	2	0
22	B	606	CLA	2	0
22	c	507	CLA	1	0
22	C	502	CLA	1	0
22	d	404	CLA	1	0
22	B	616	CLA	1	0
22	a	405	CLA	1	0
30	A	415	DGD	5	0
22	c	510	CLA	2	0
24	K	102	BCR	2	0
32	B	624	STE	1	0
22	a	402	CLA	1	0
35	v	201	HEC	2	0
26	a	409	PL9	4	0
27	m	101	LMG	1	0
34	f	101	HEM	6	0

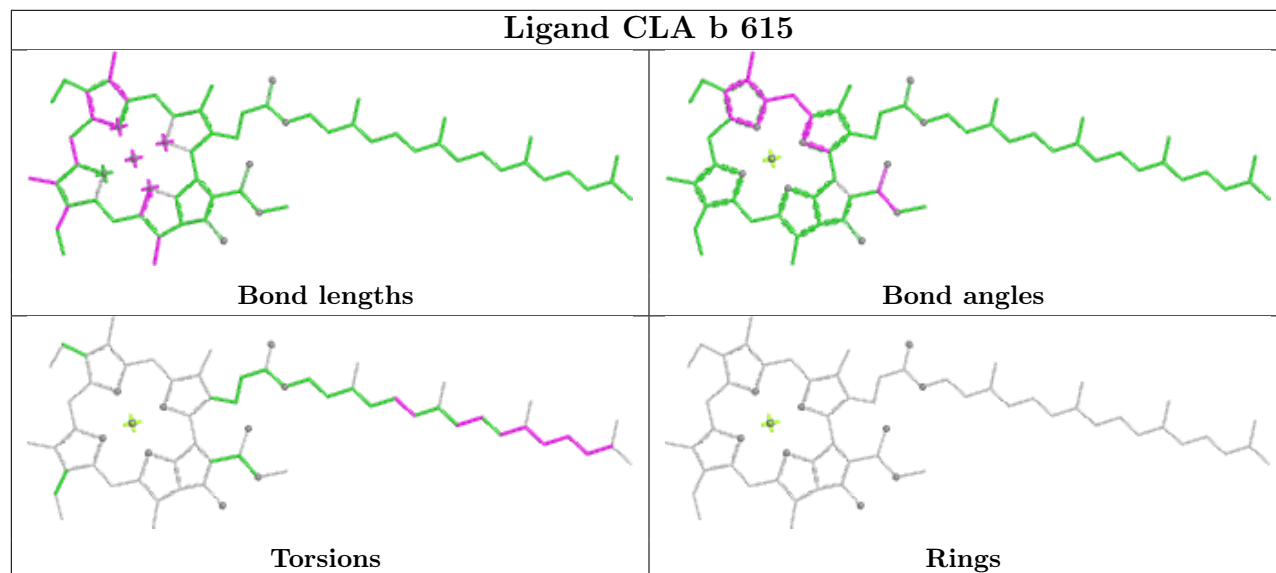
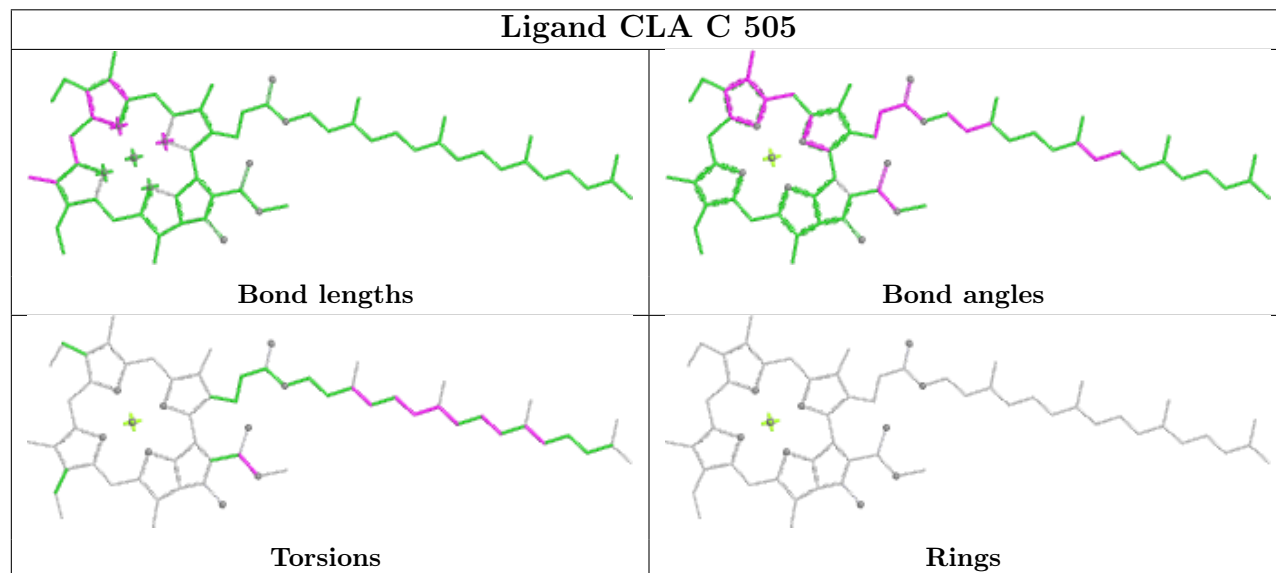
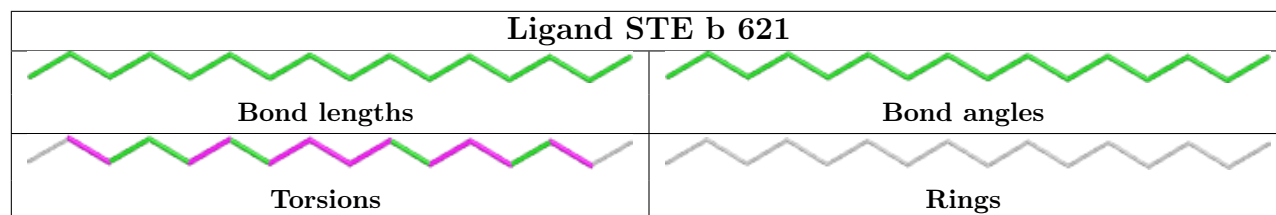
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

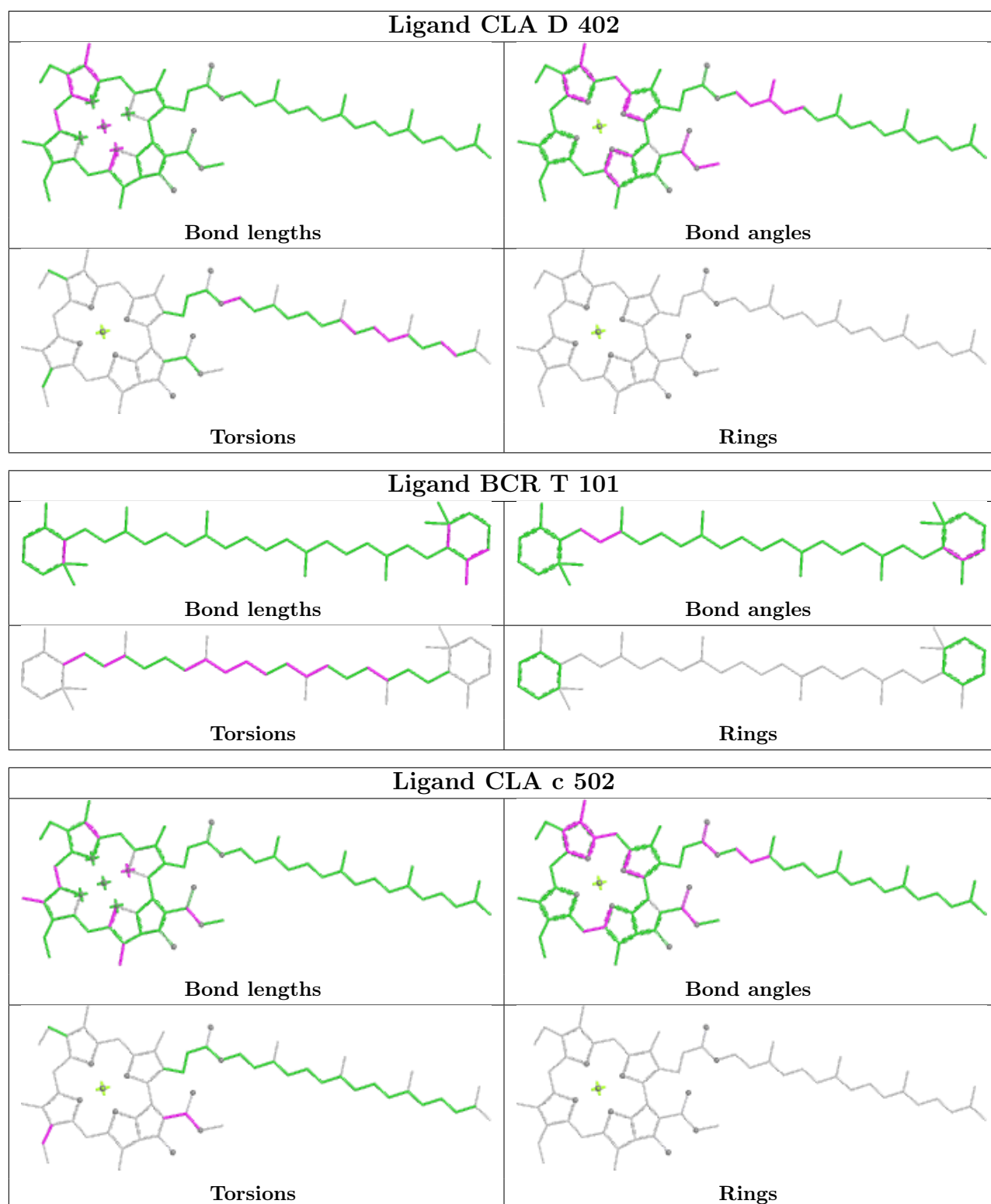


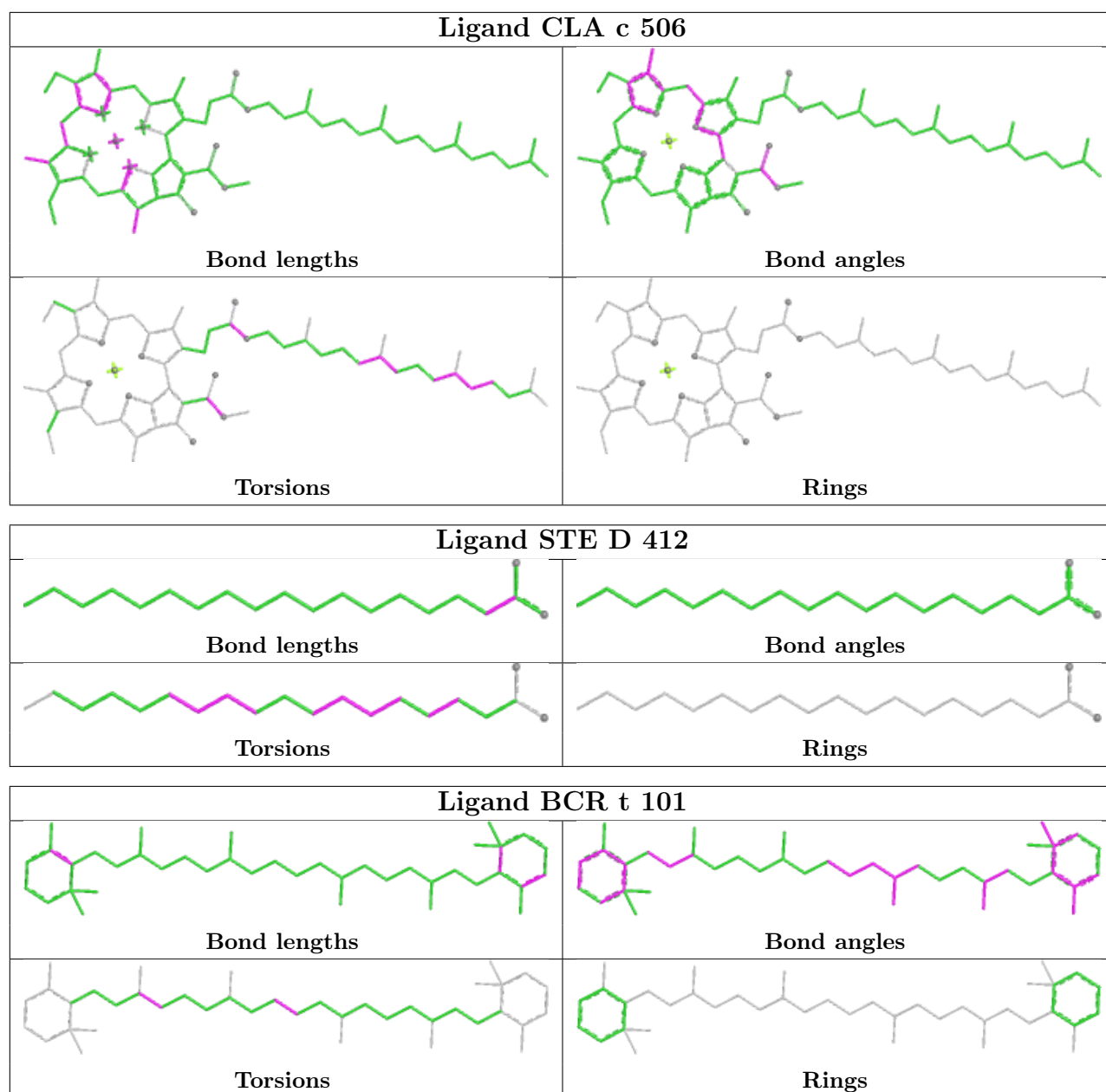


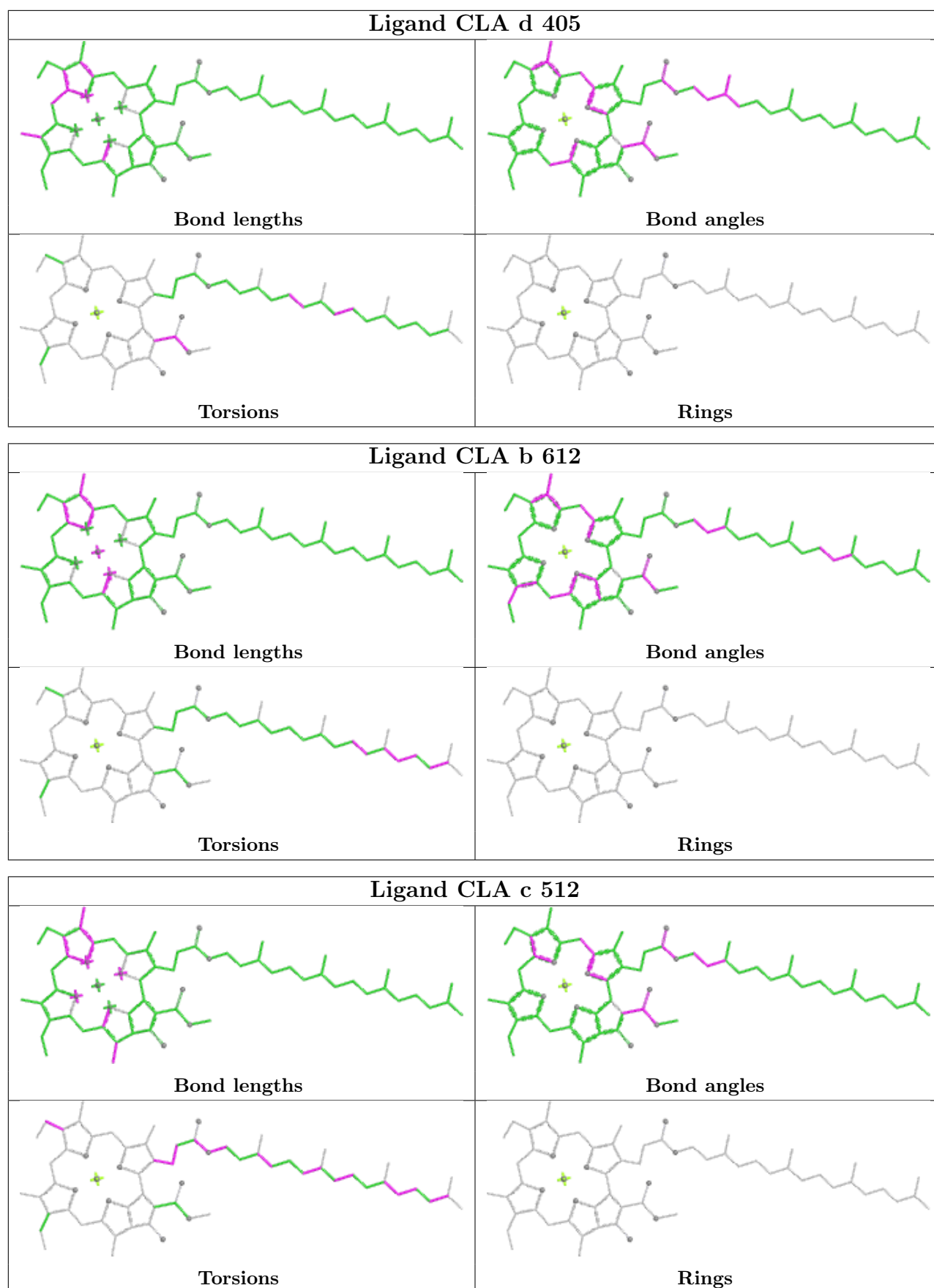


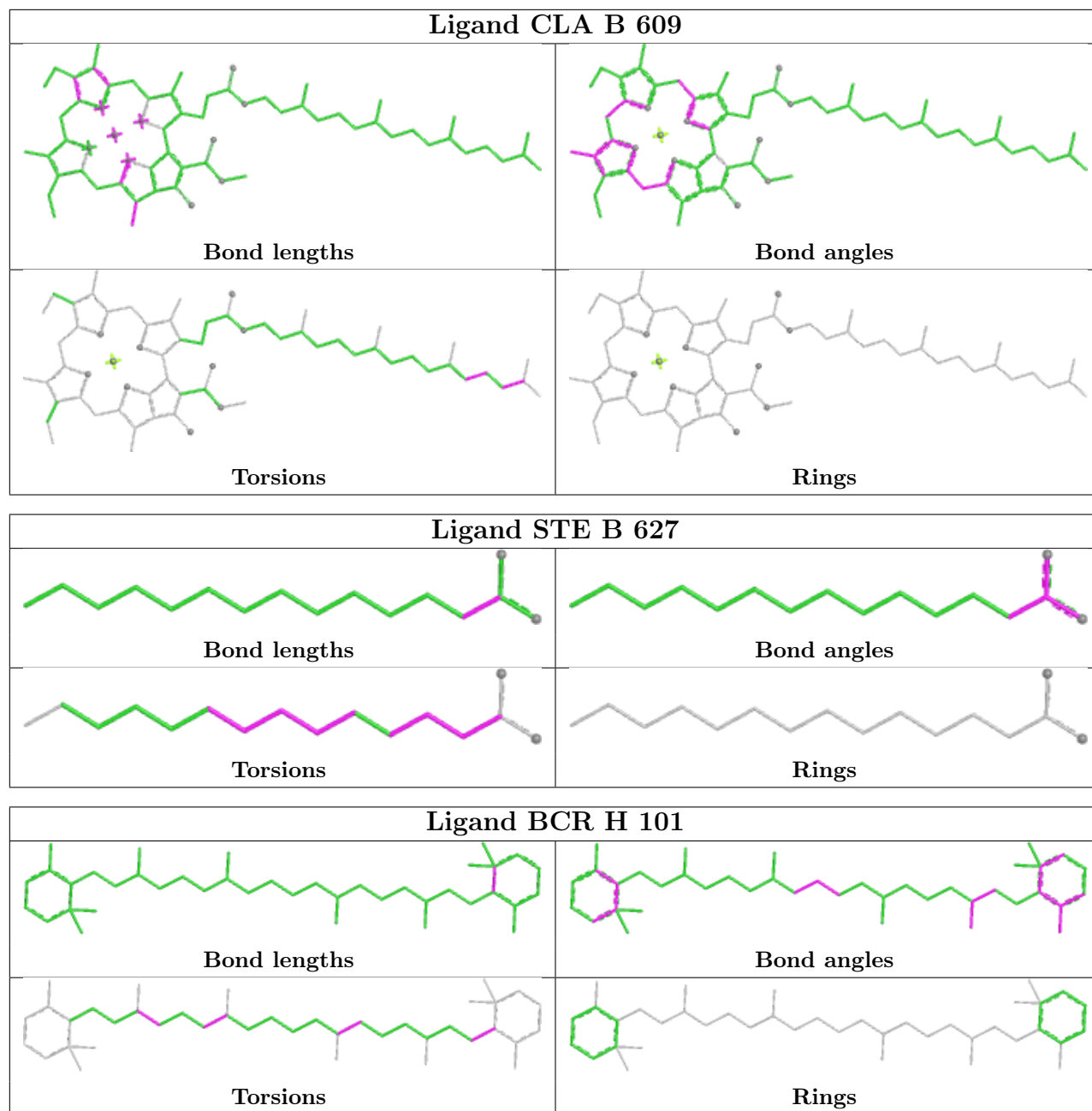


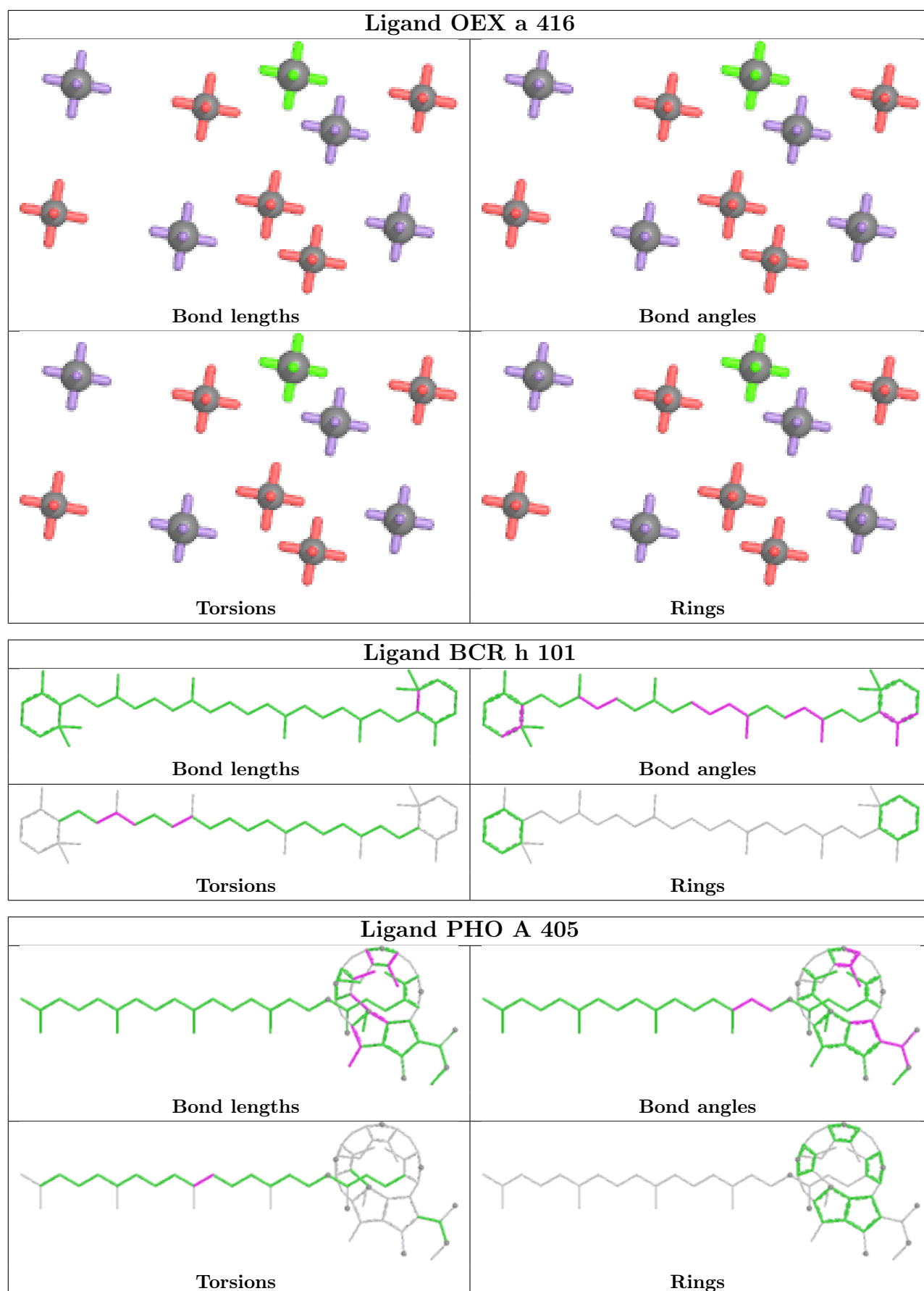


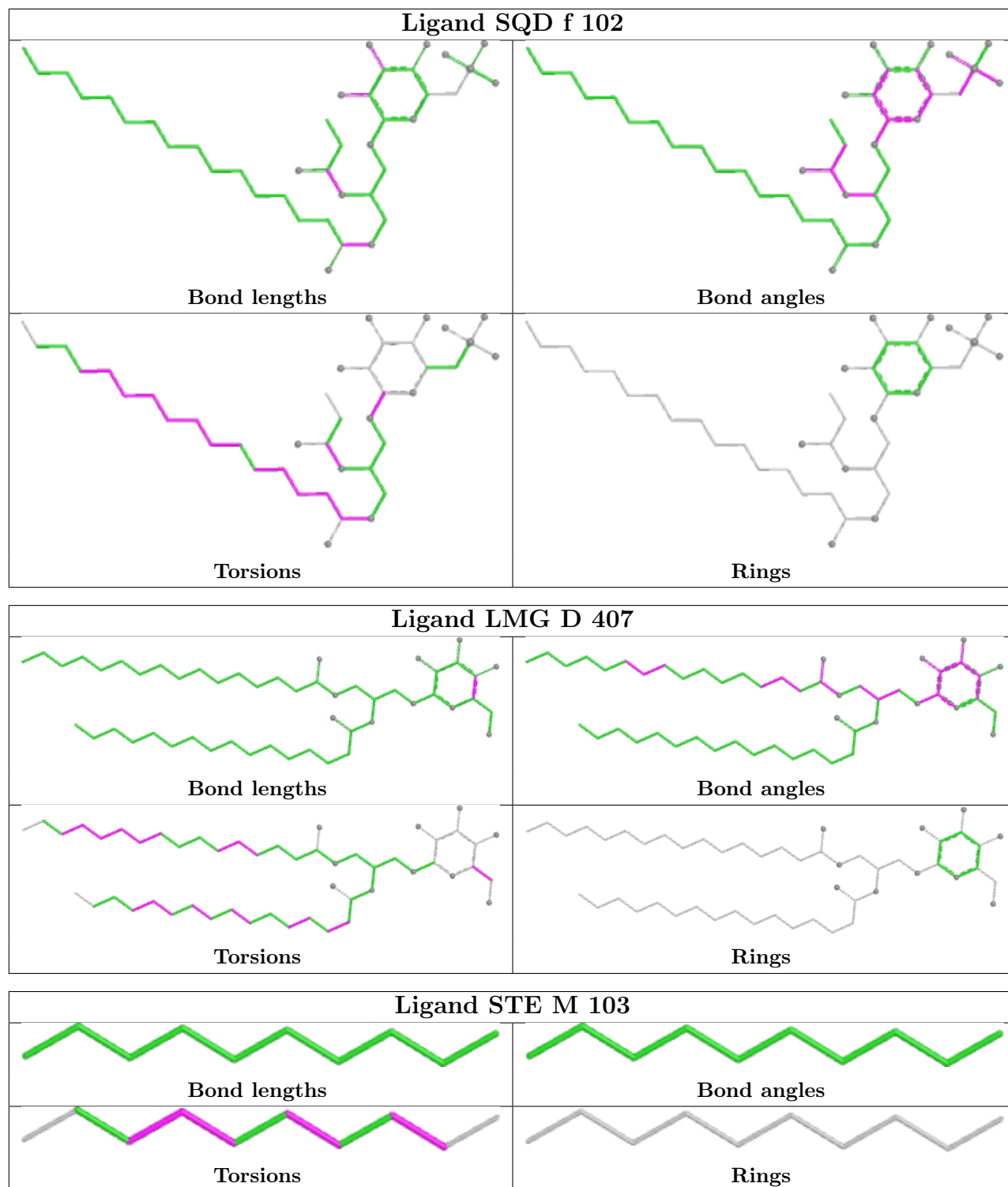


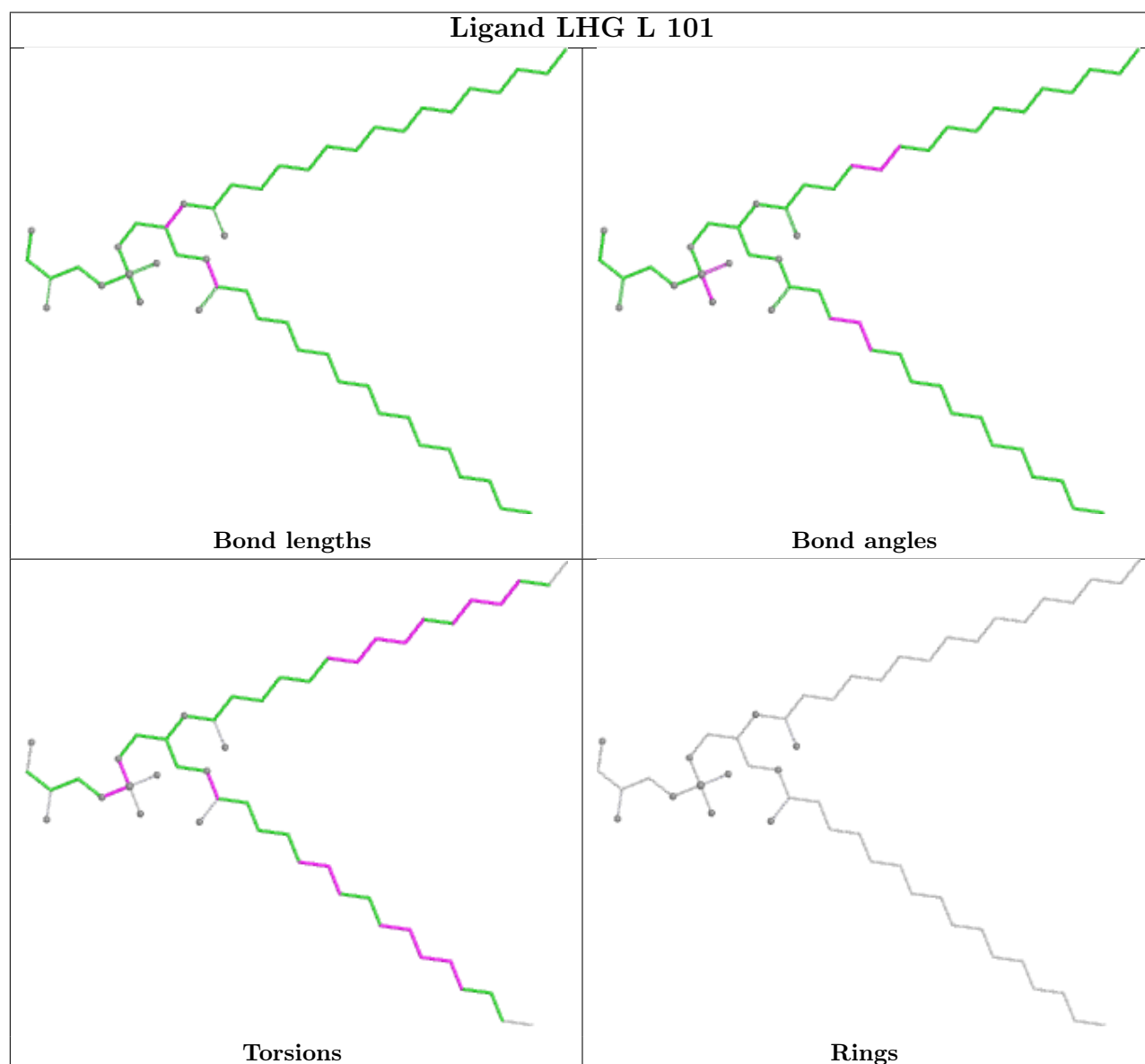
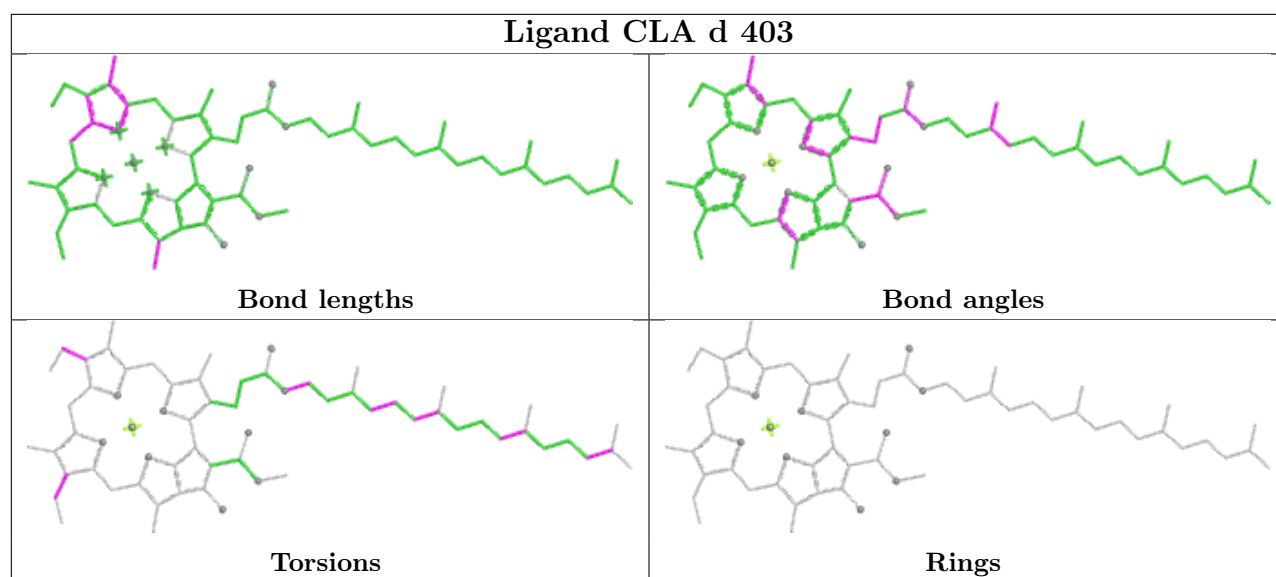


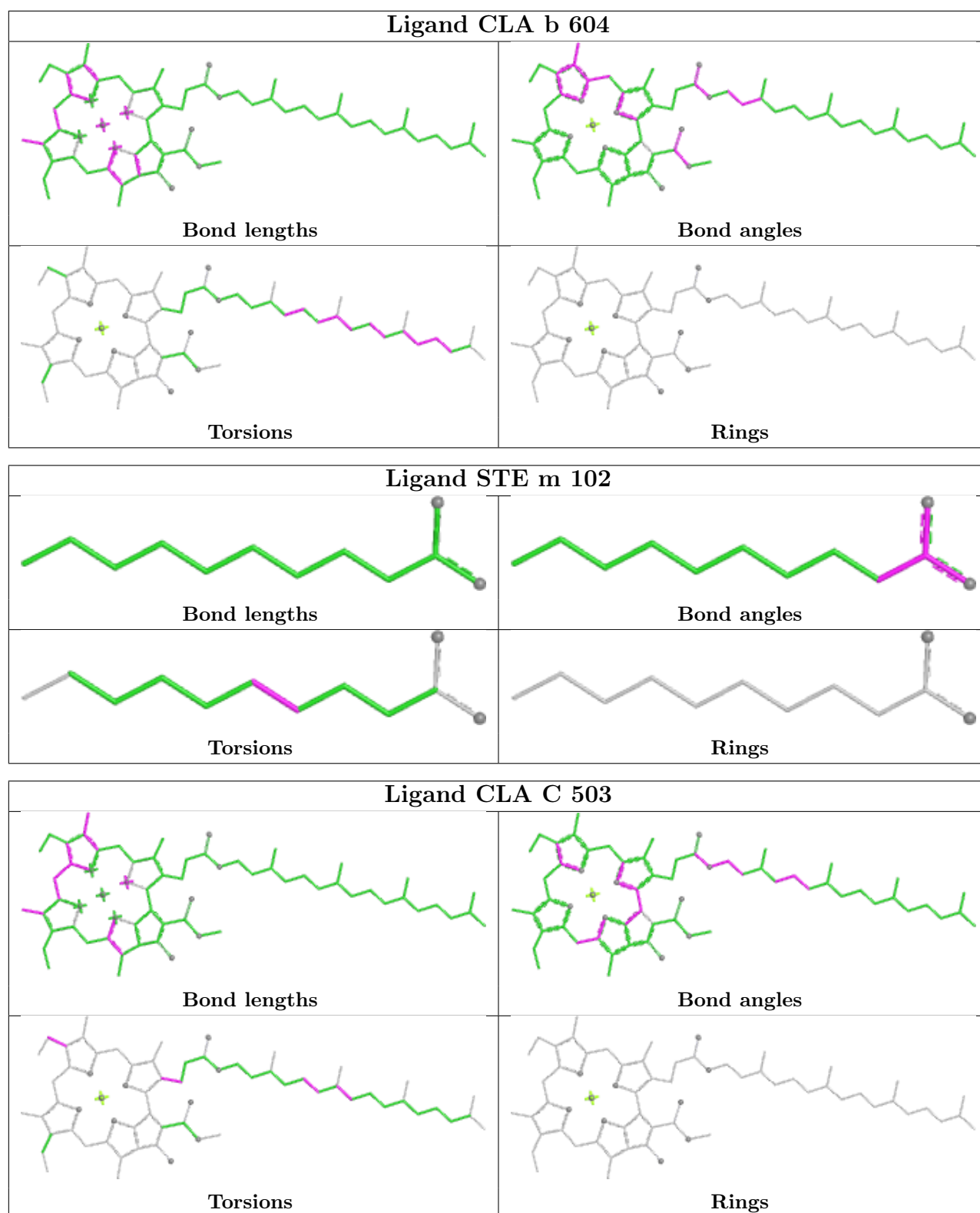


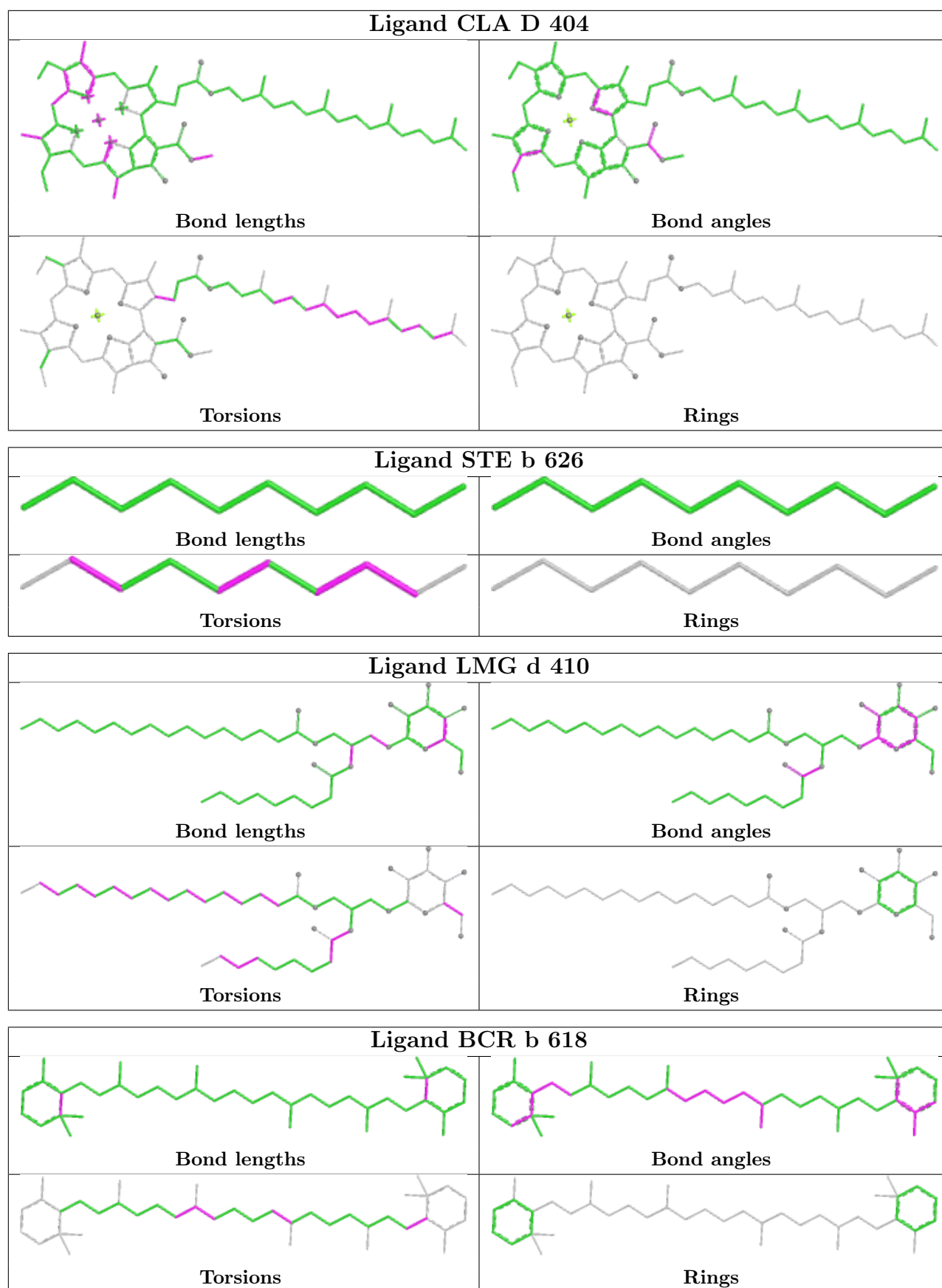


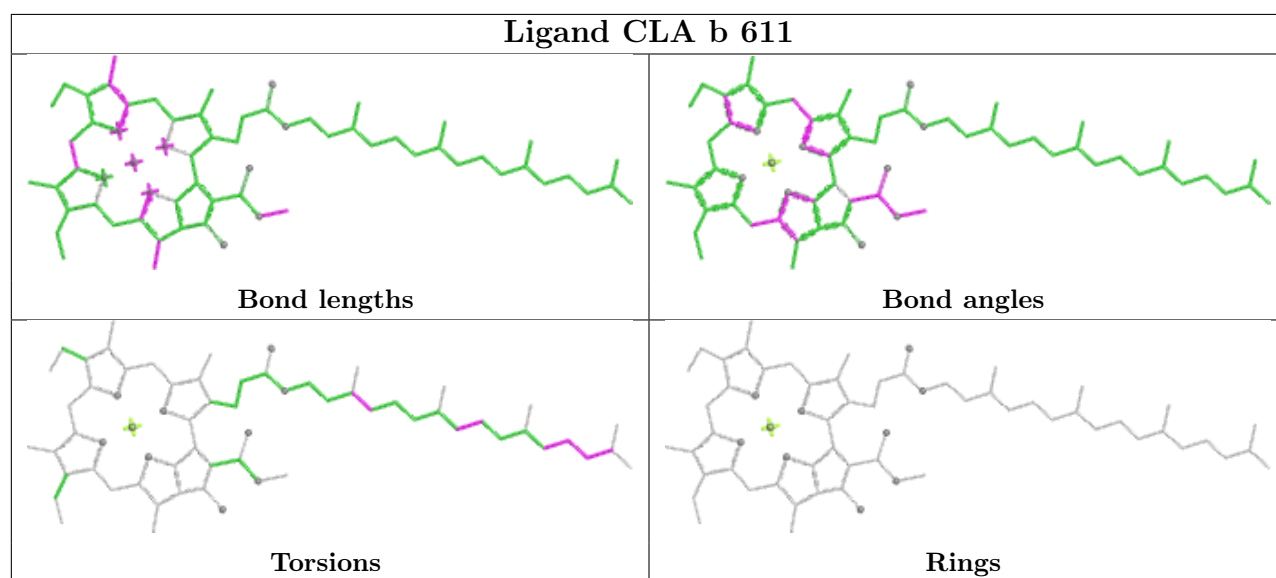
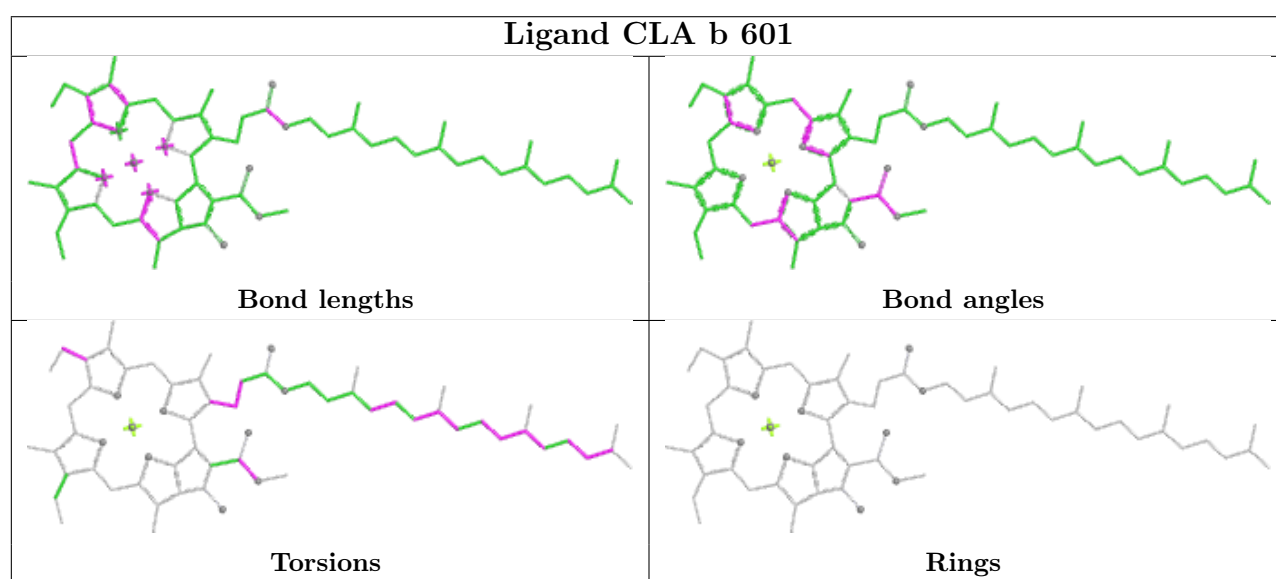
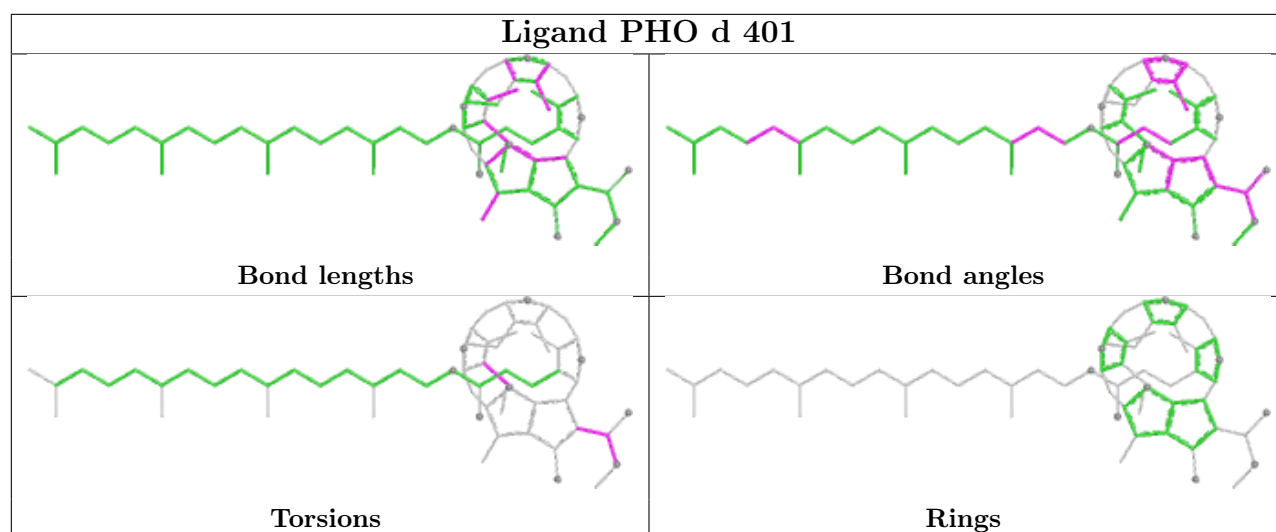


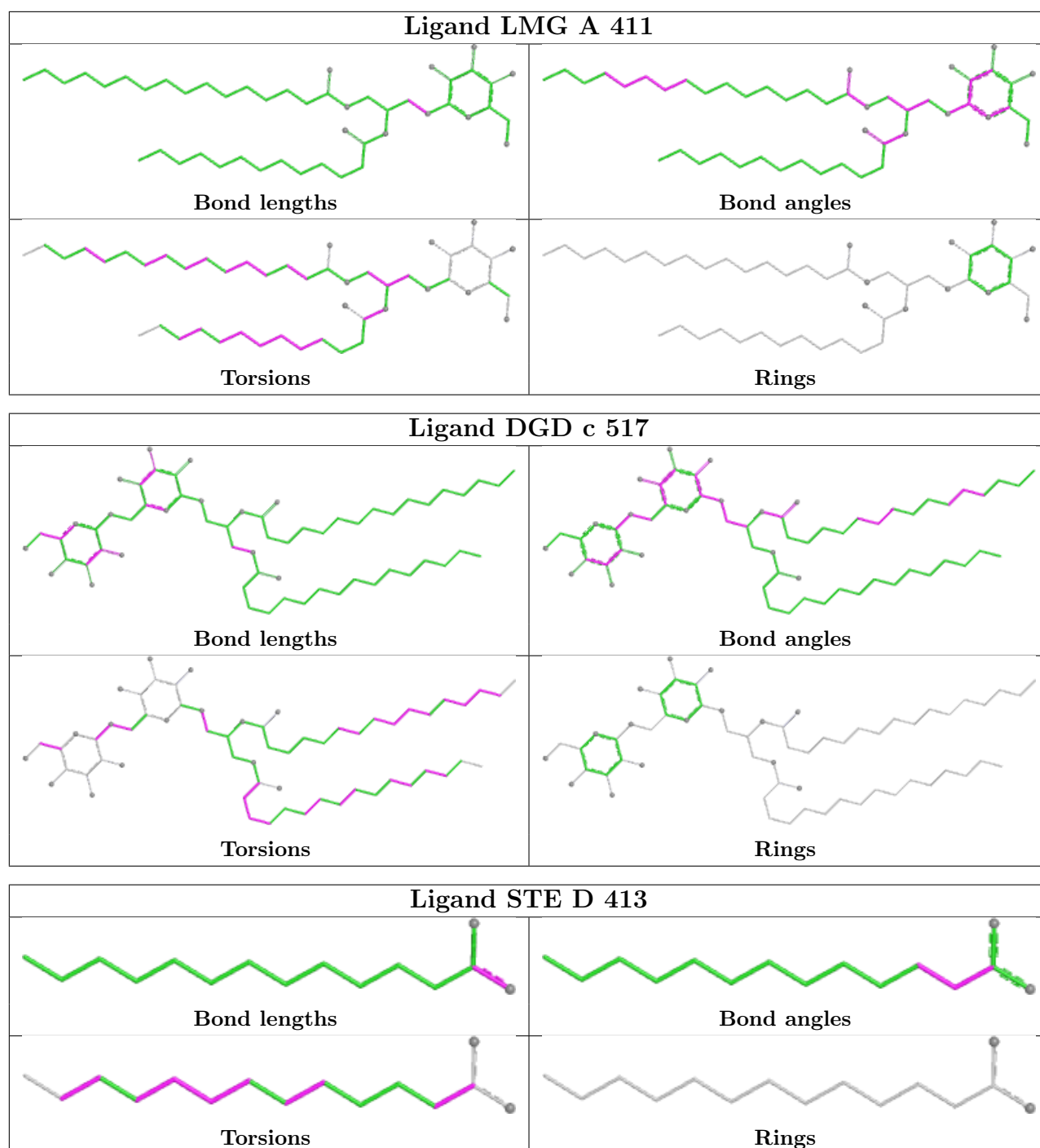


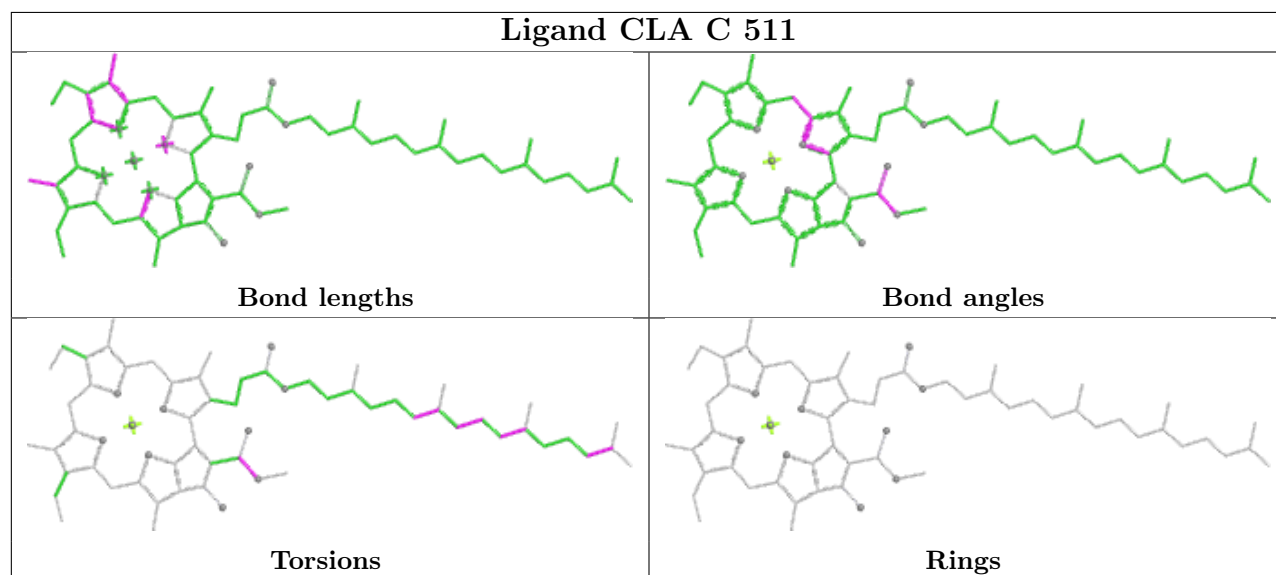
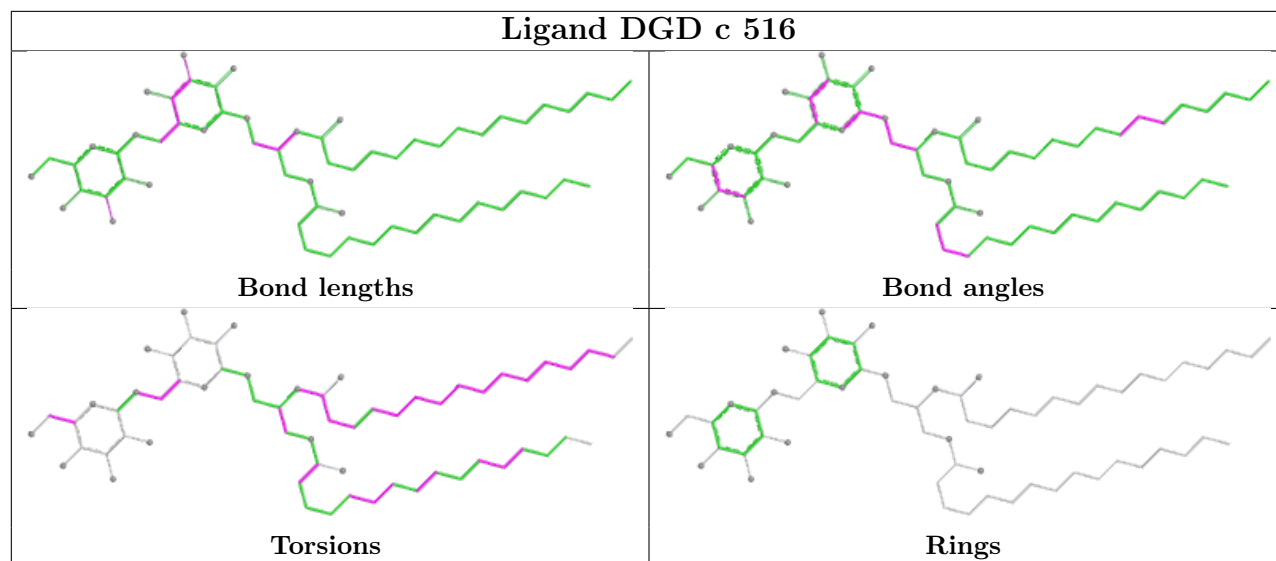


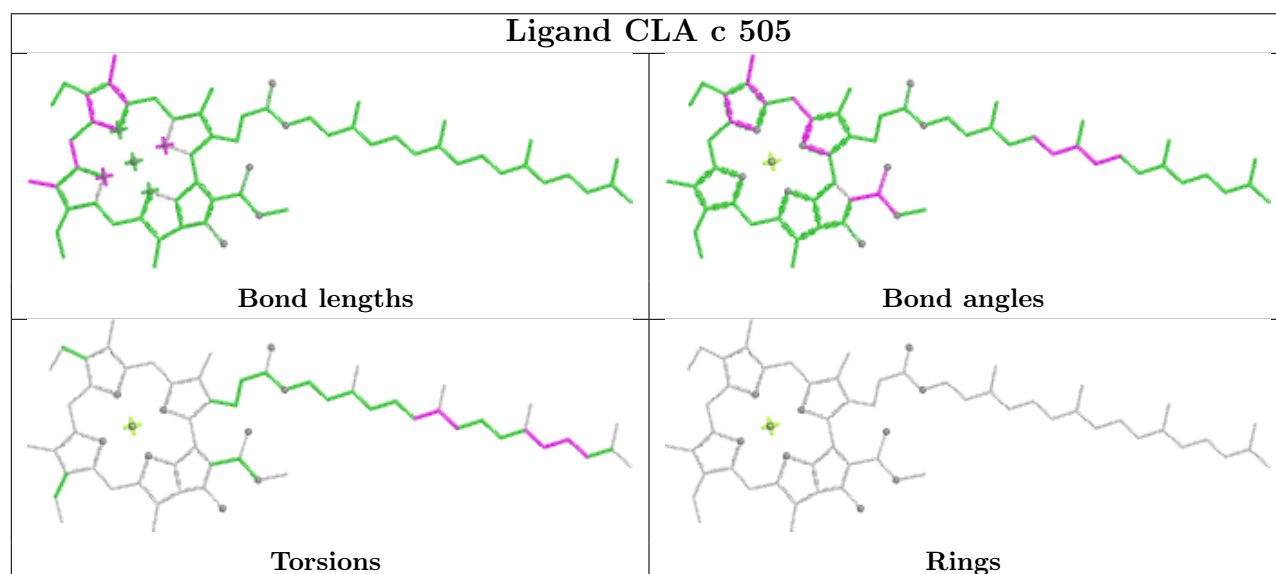
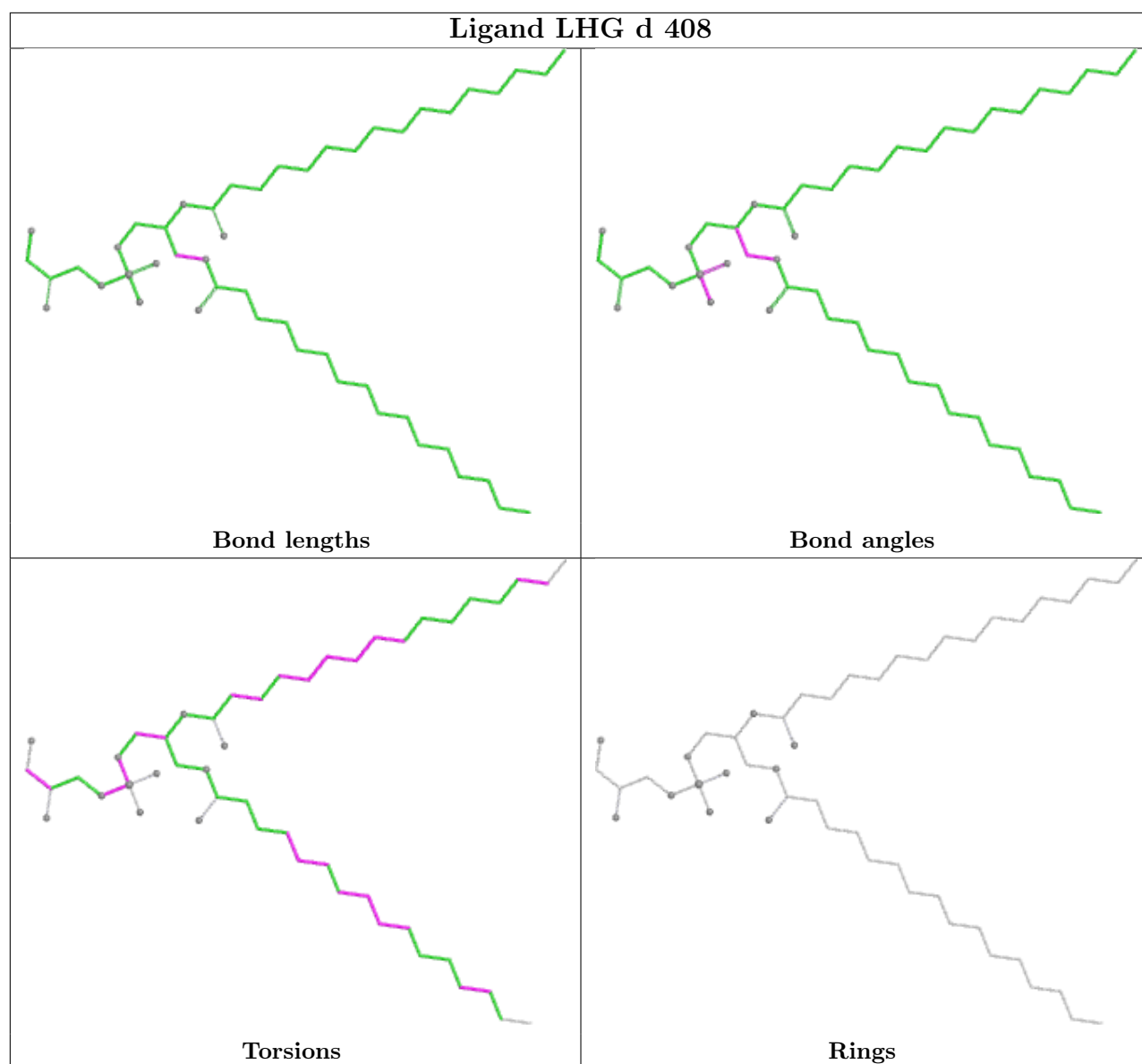


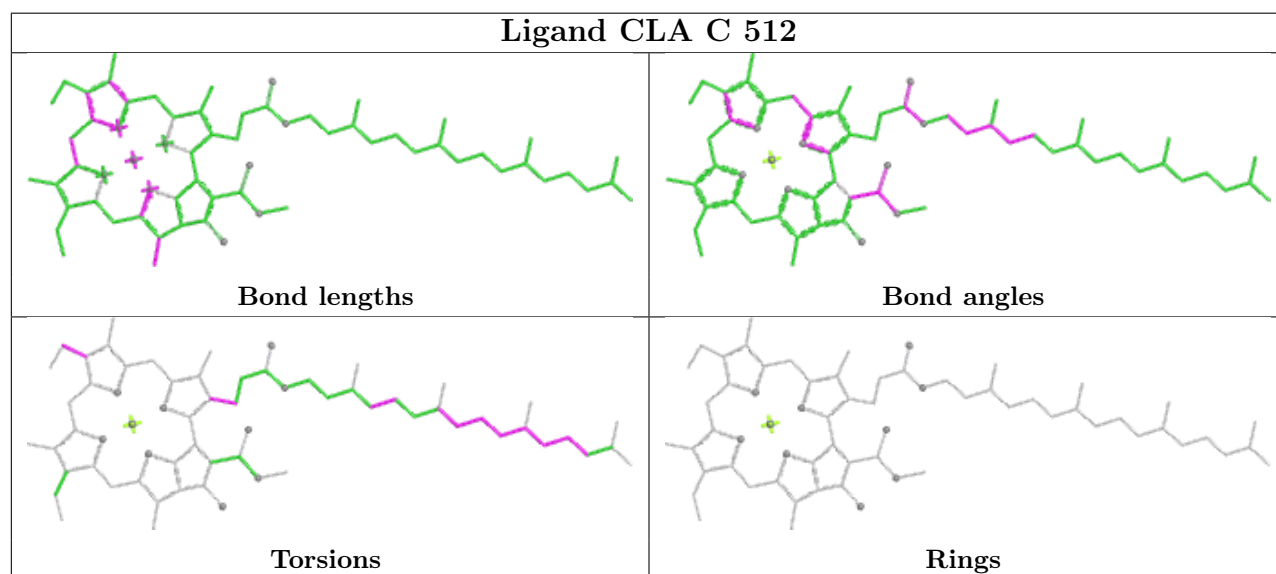
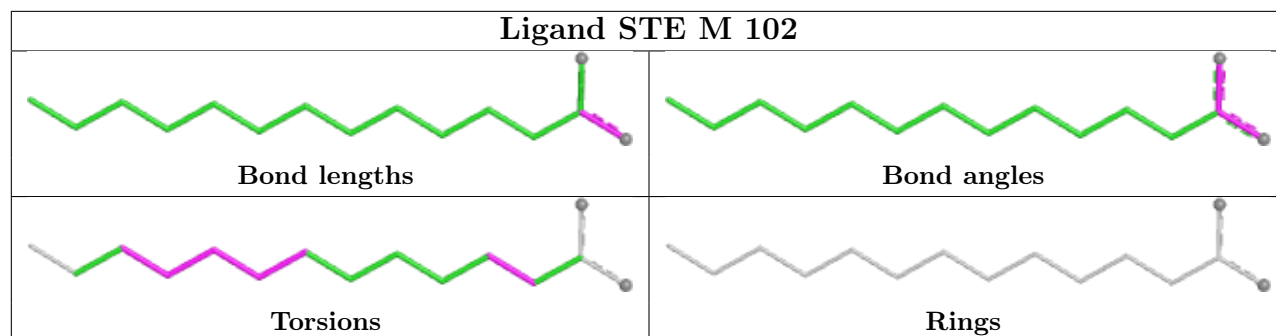


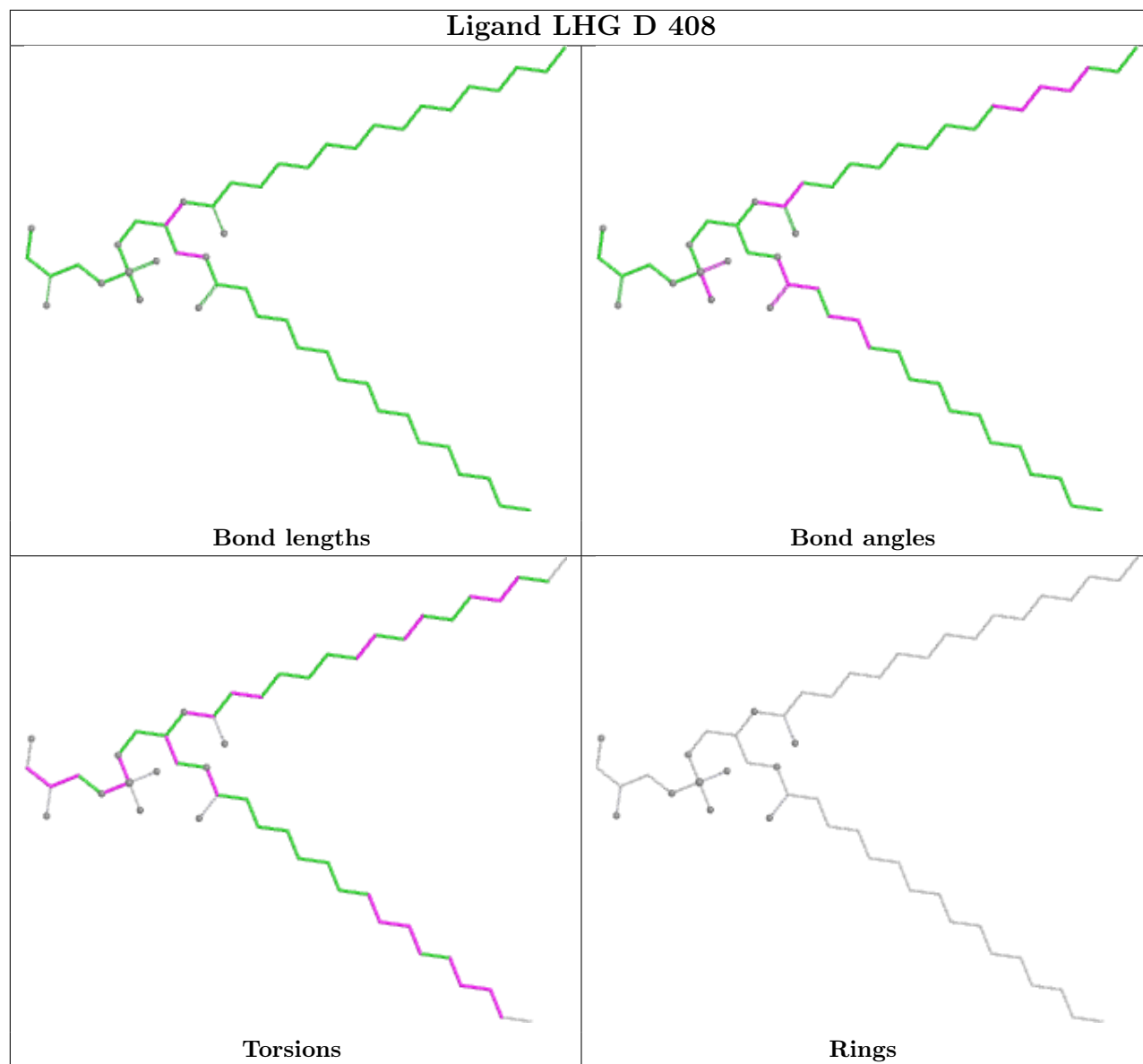


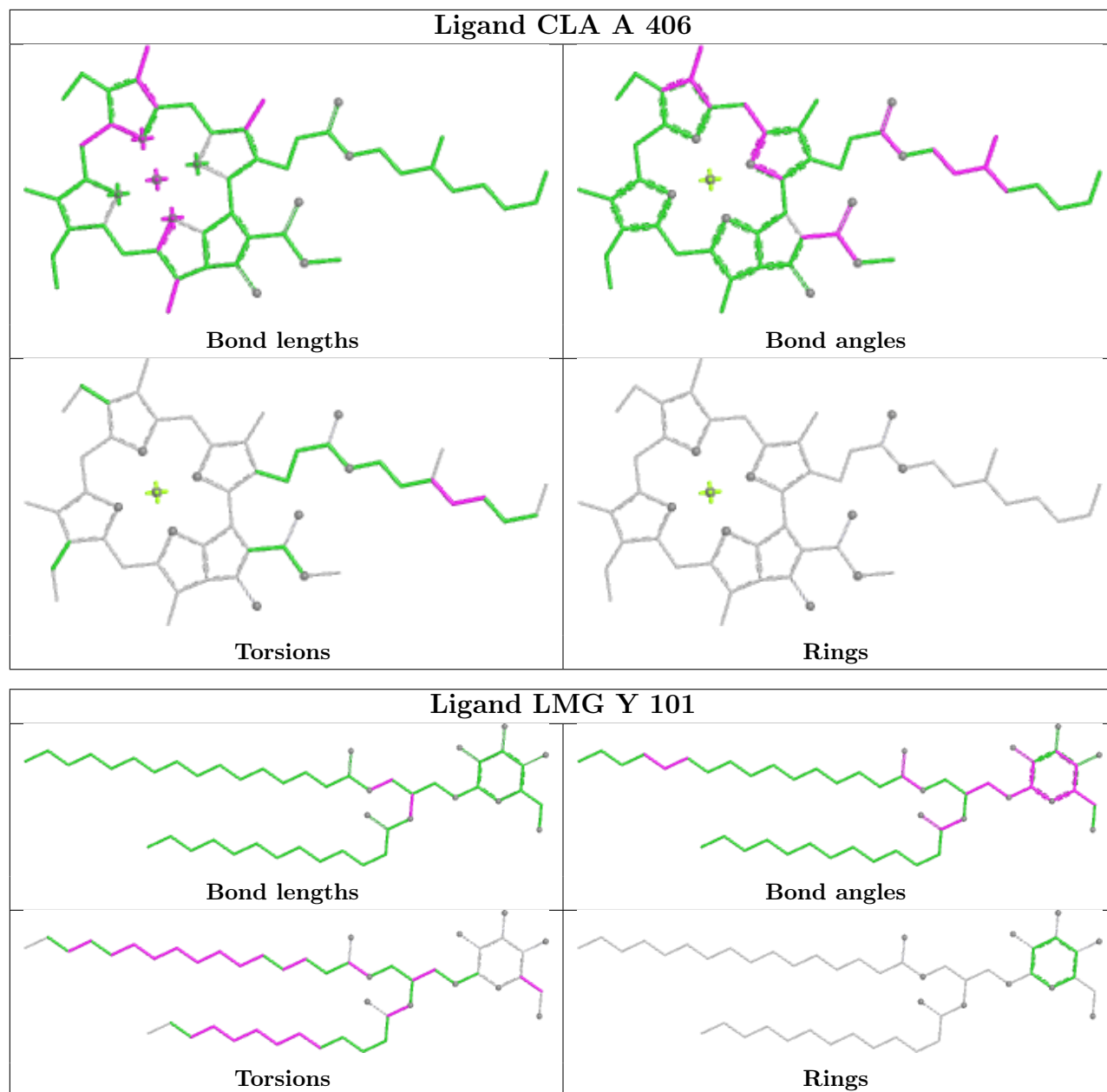


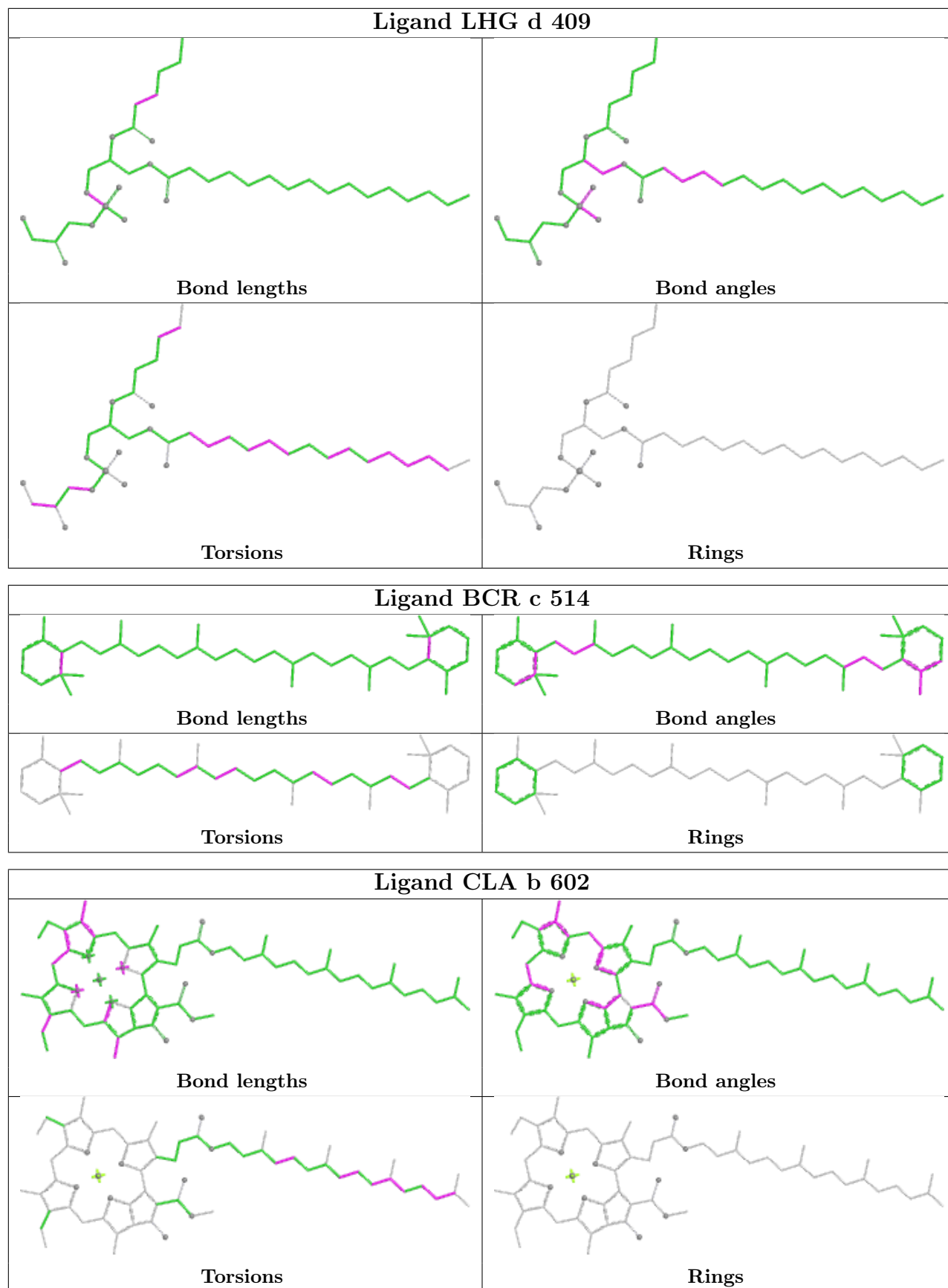


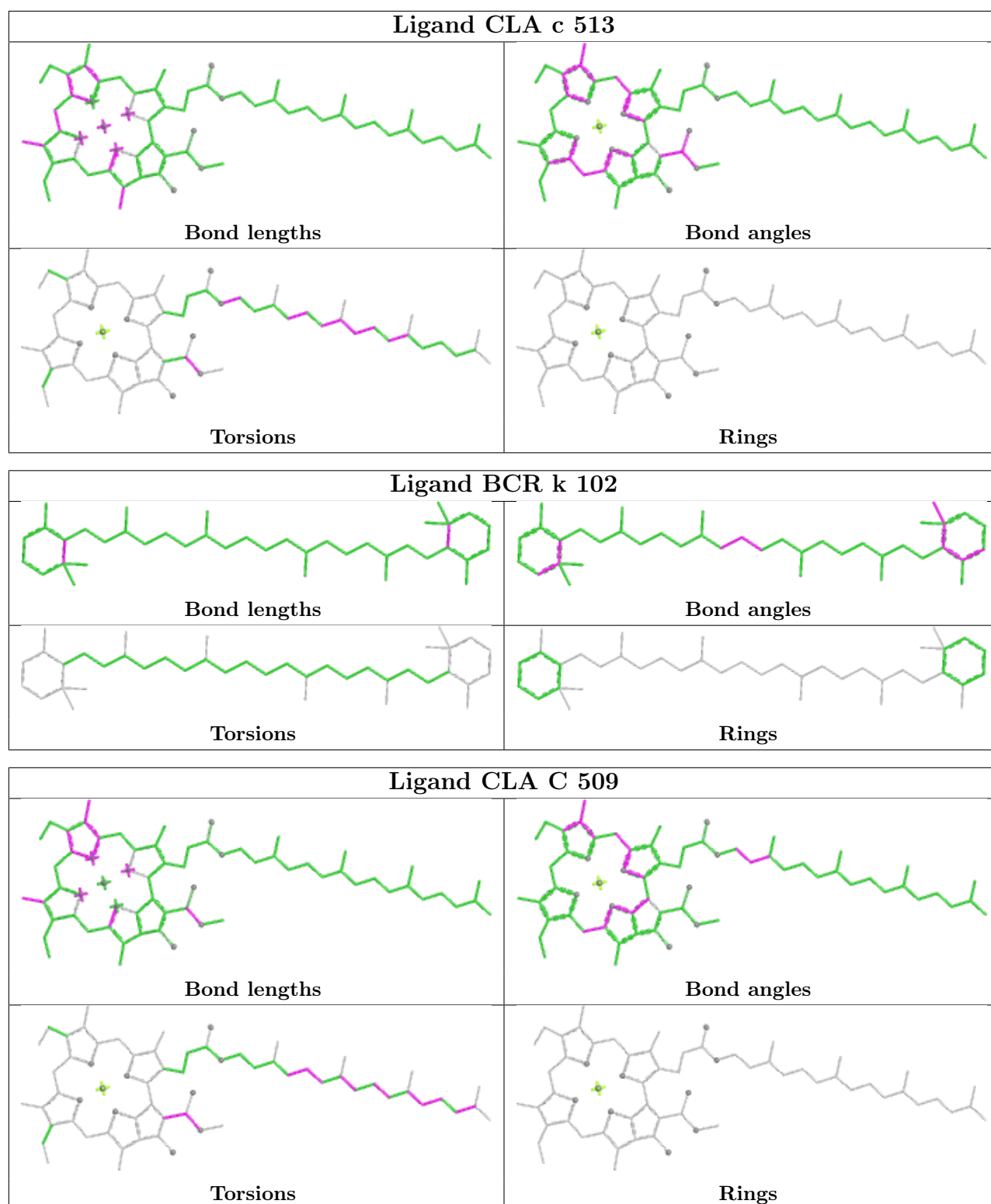


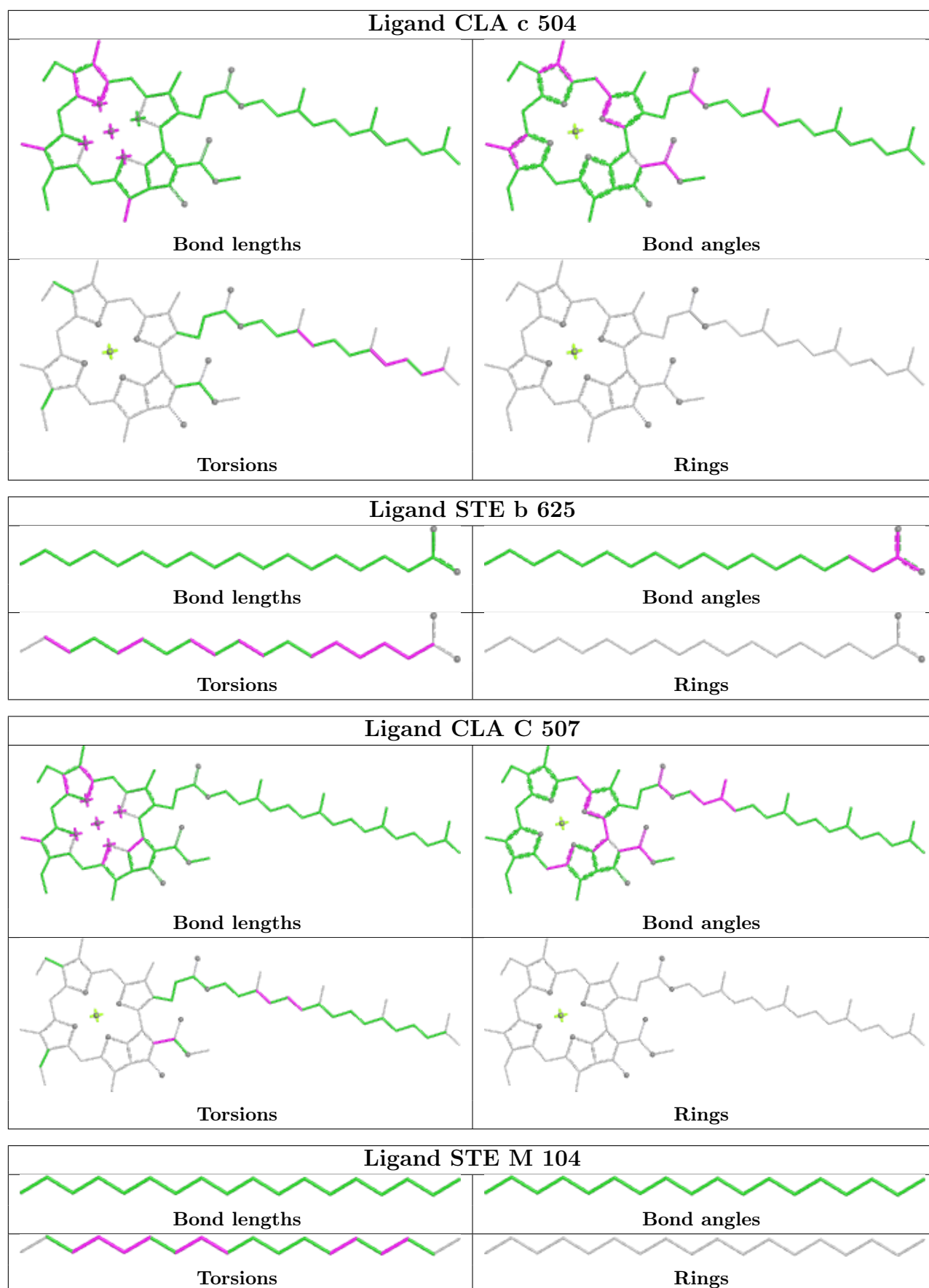


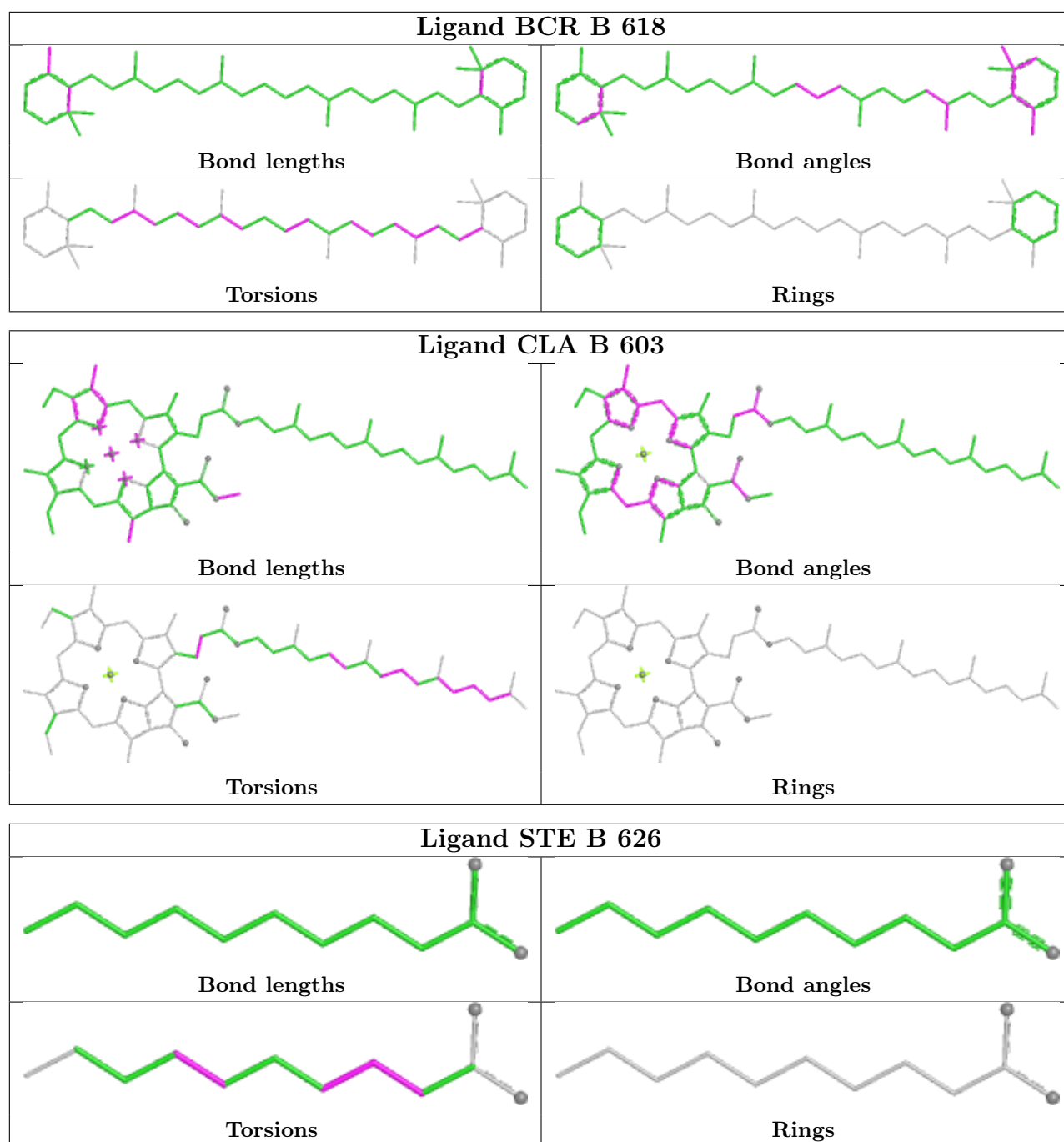


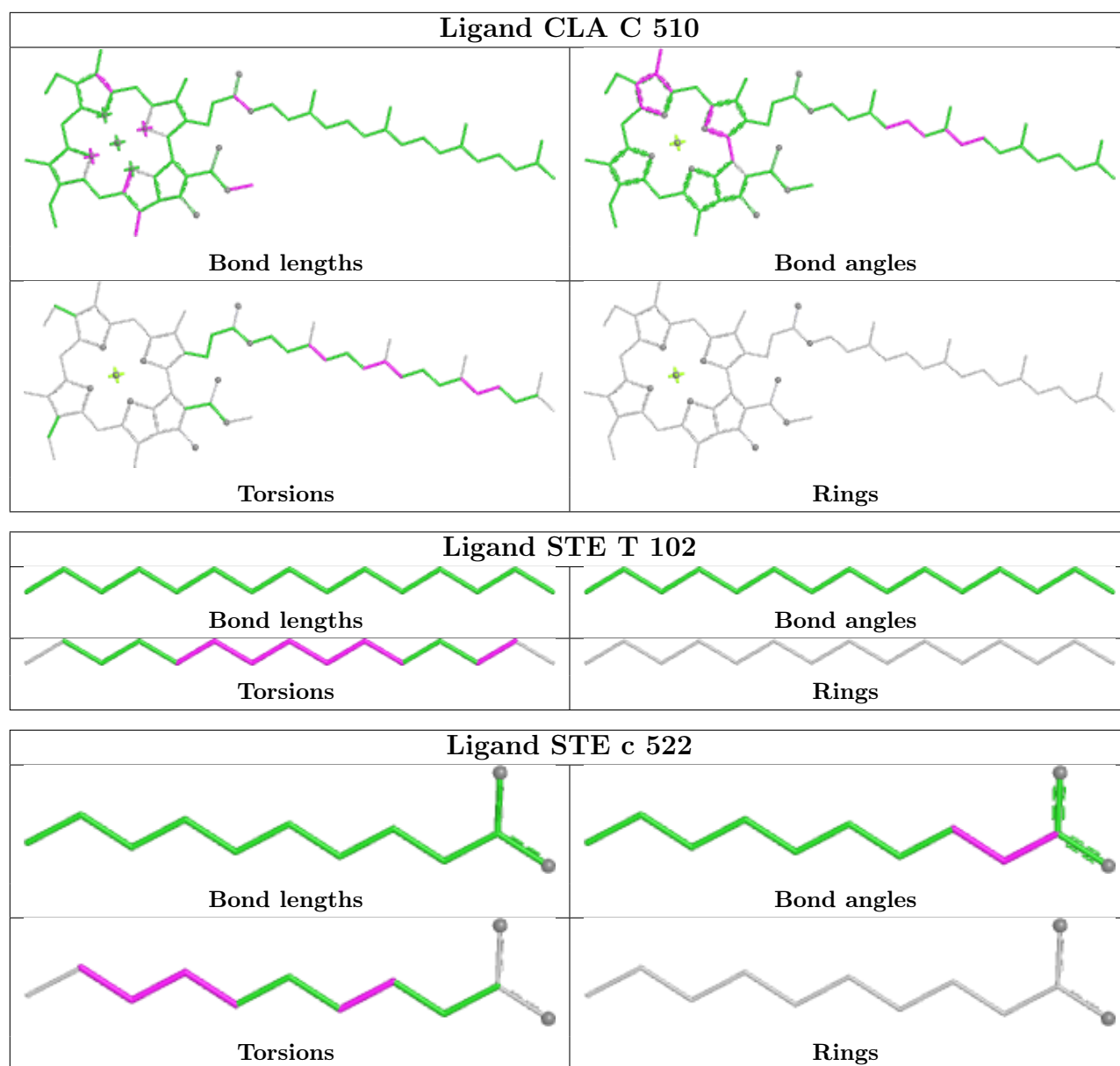


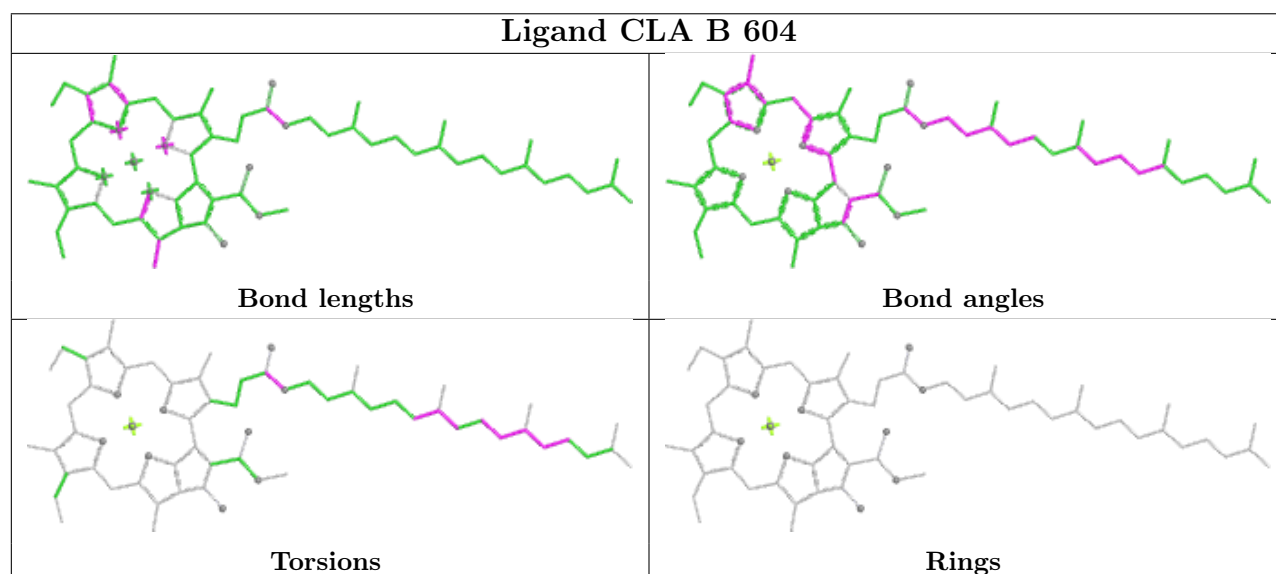
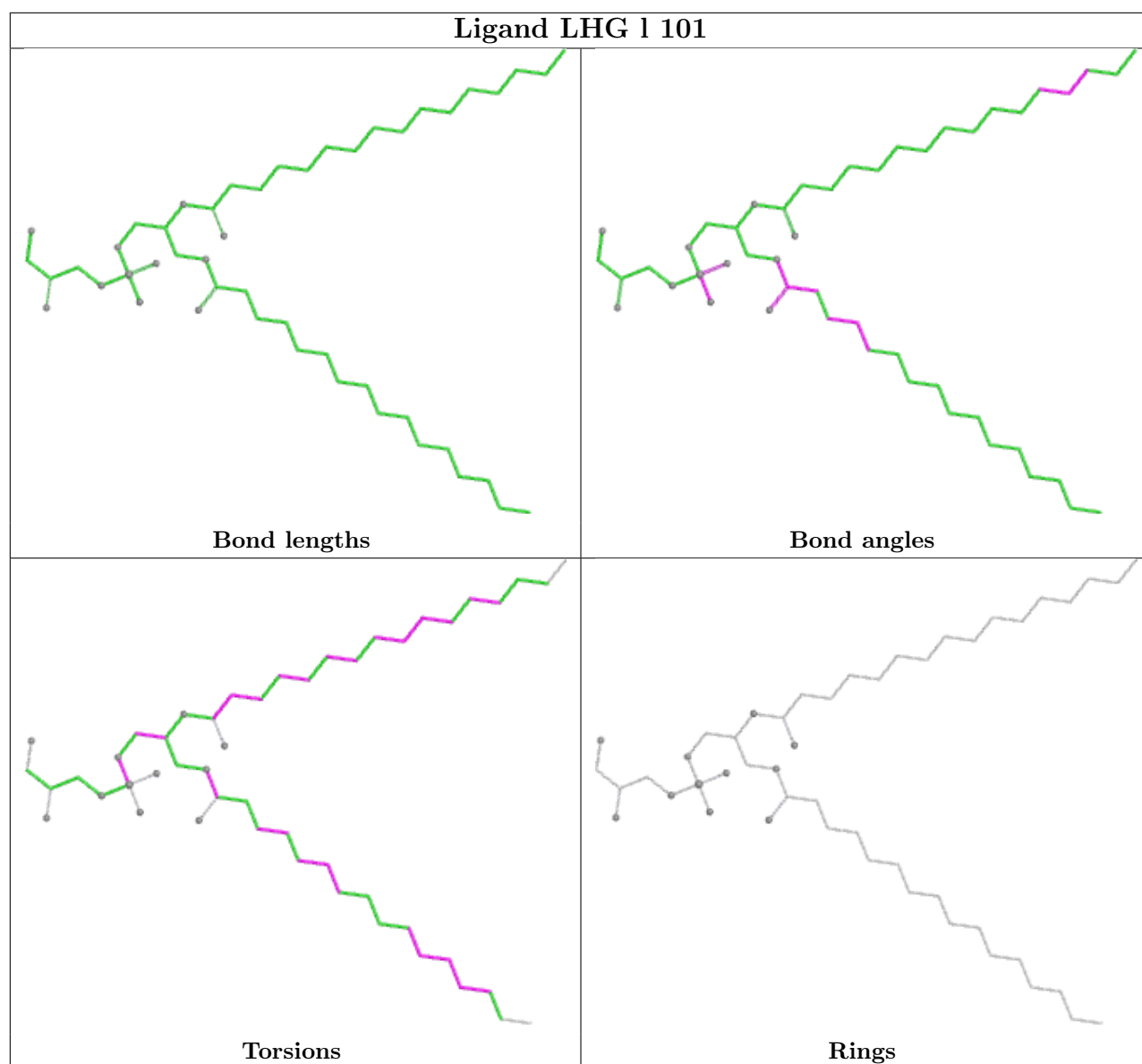


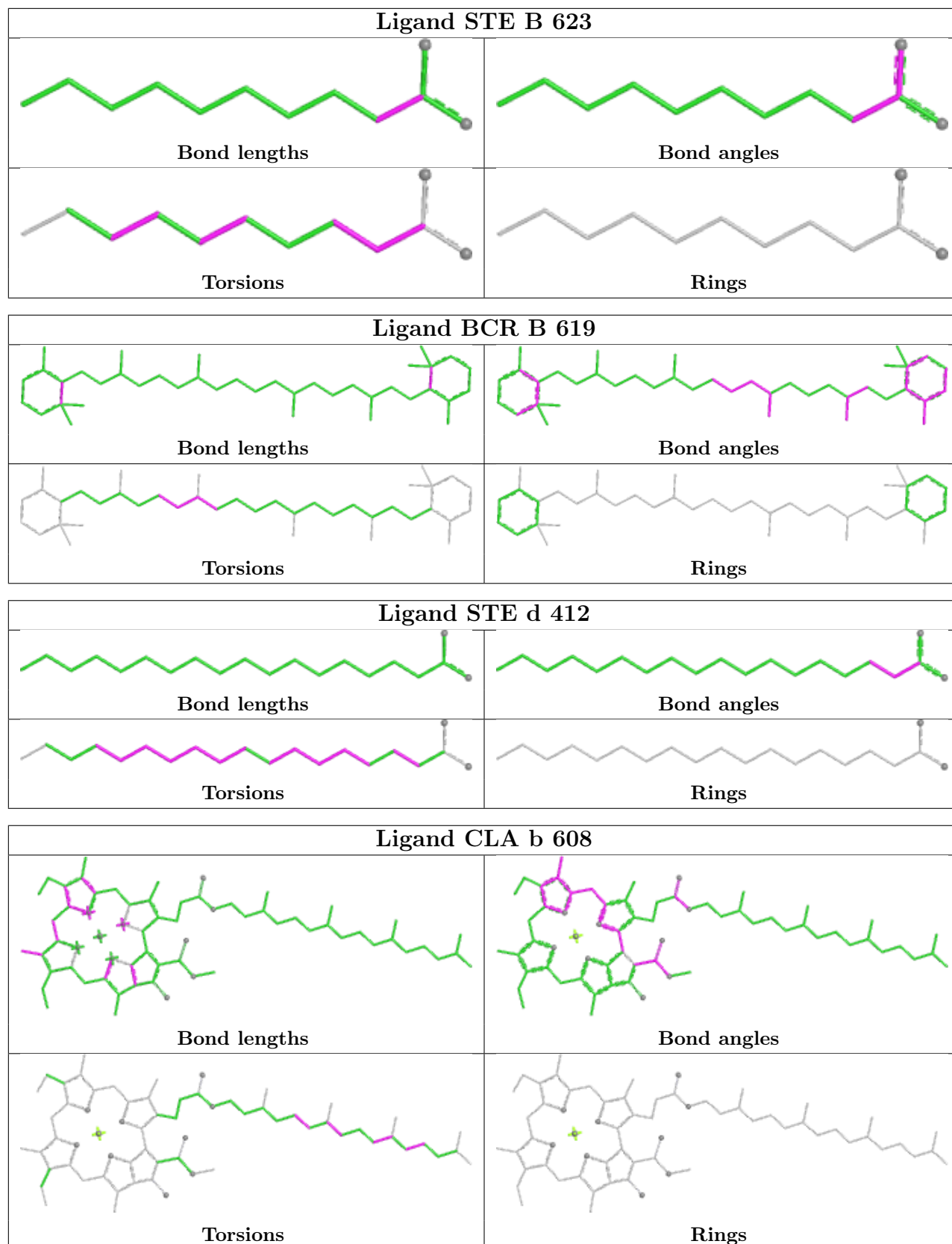


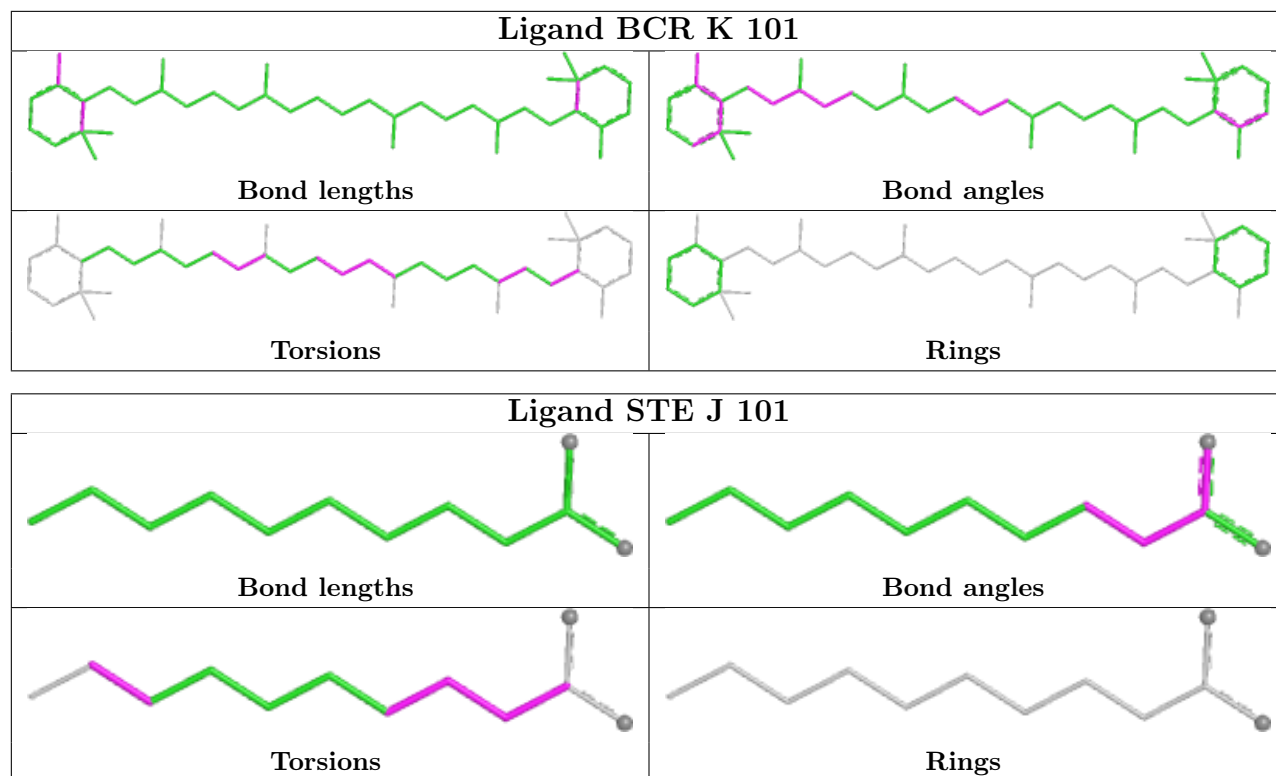


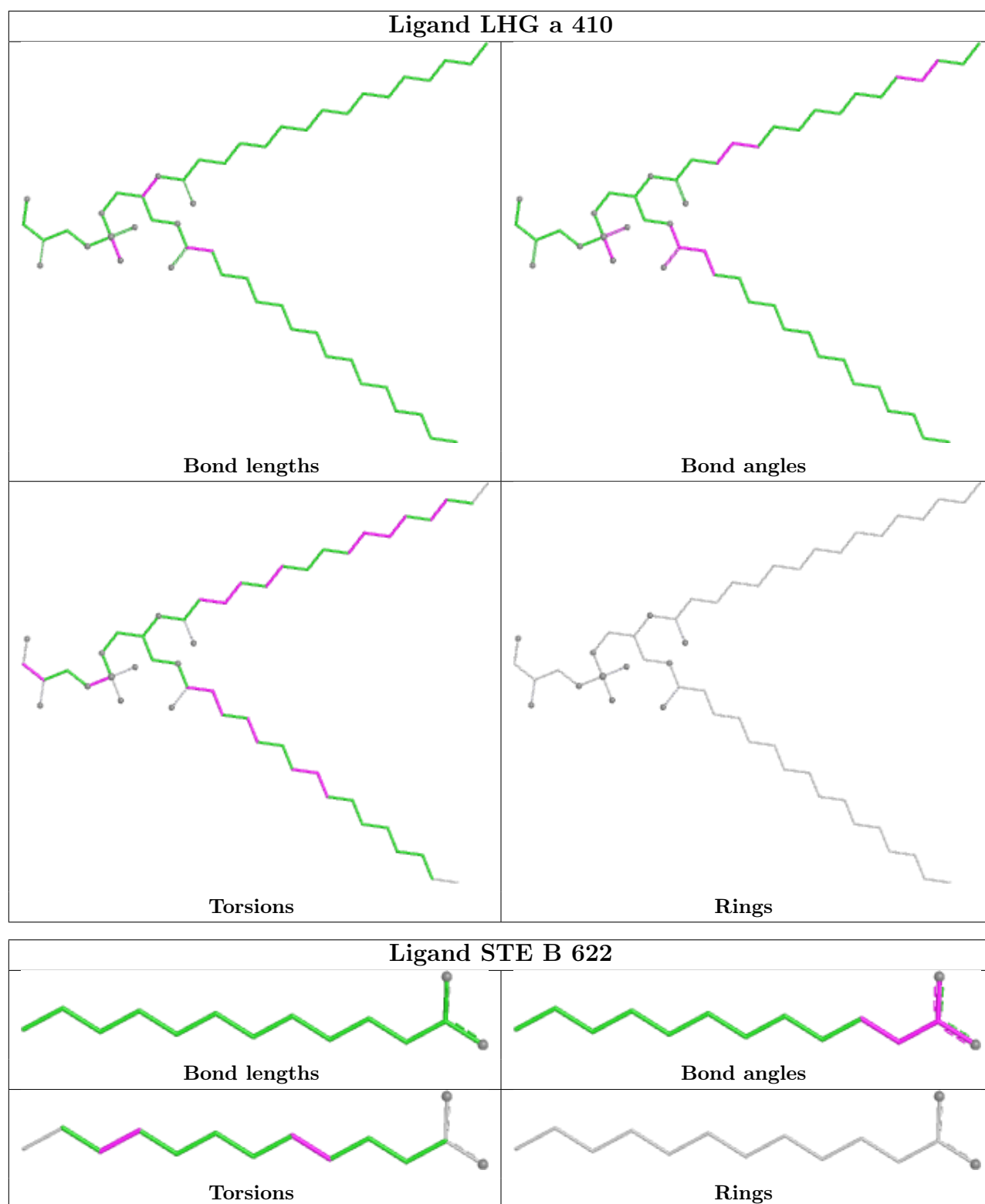


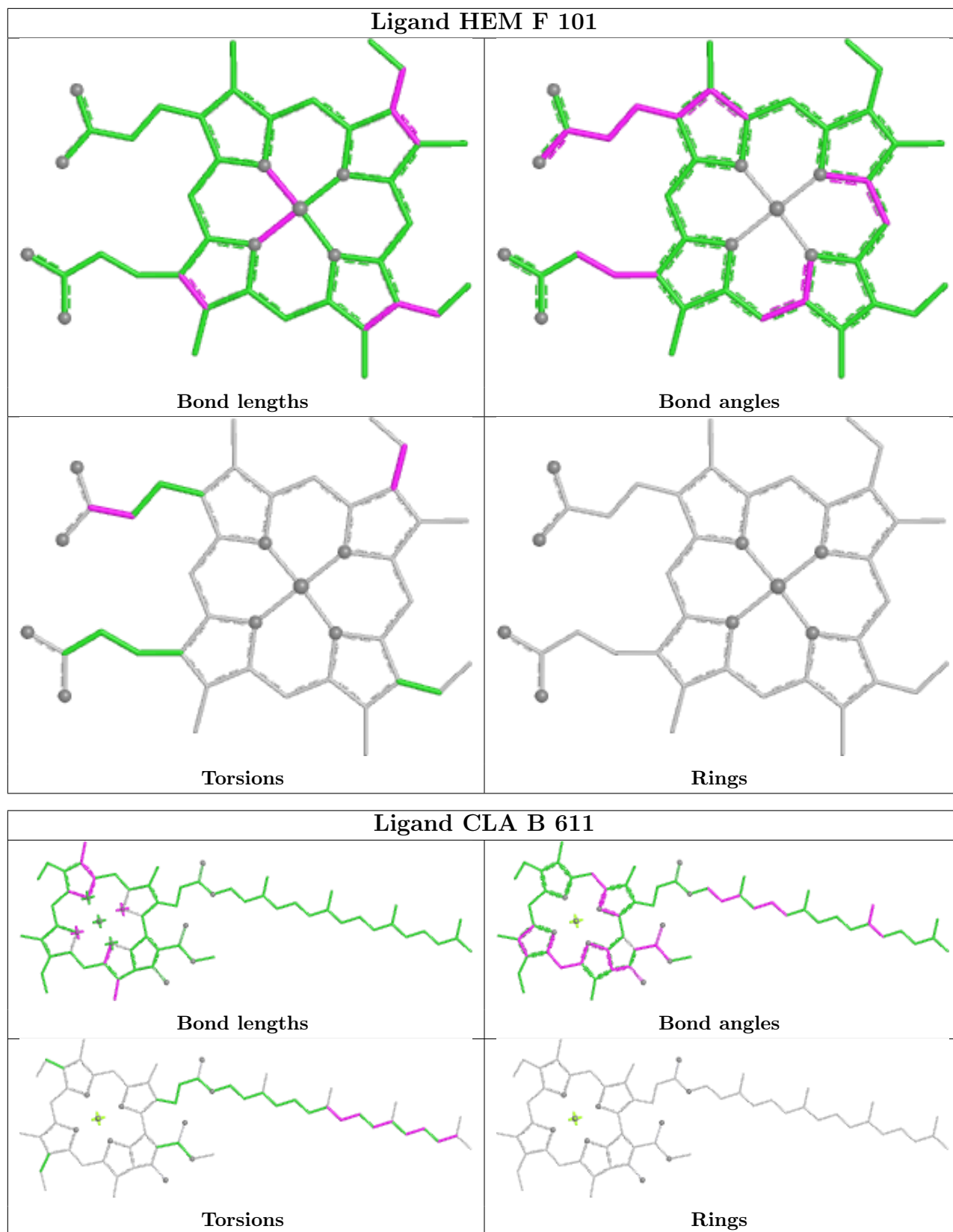


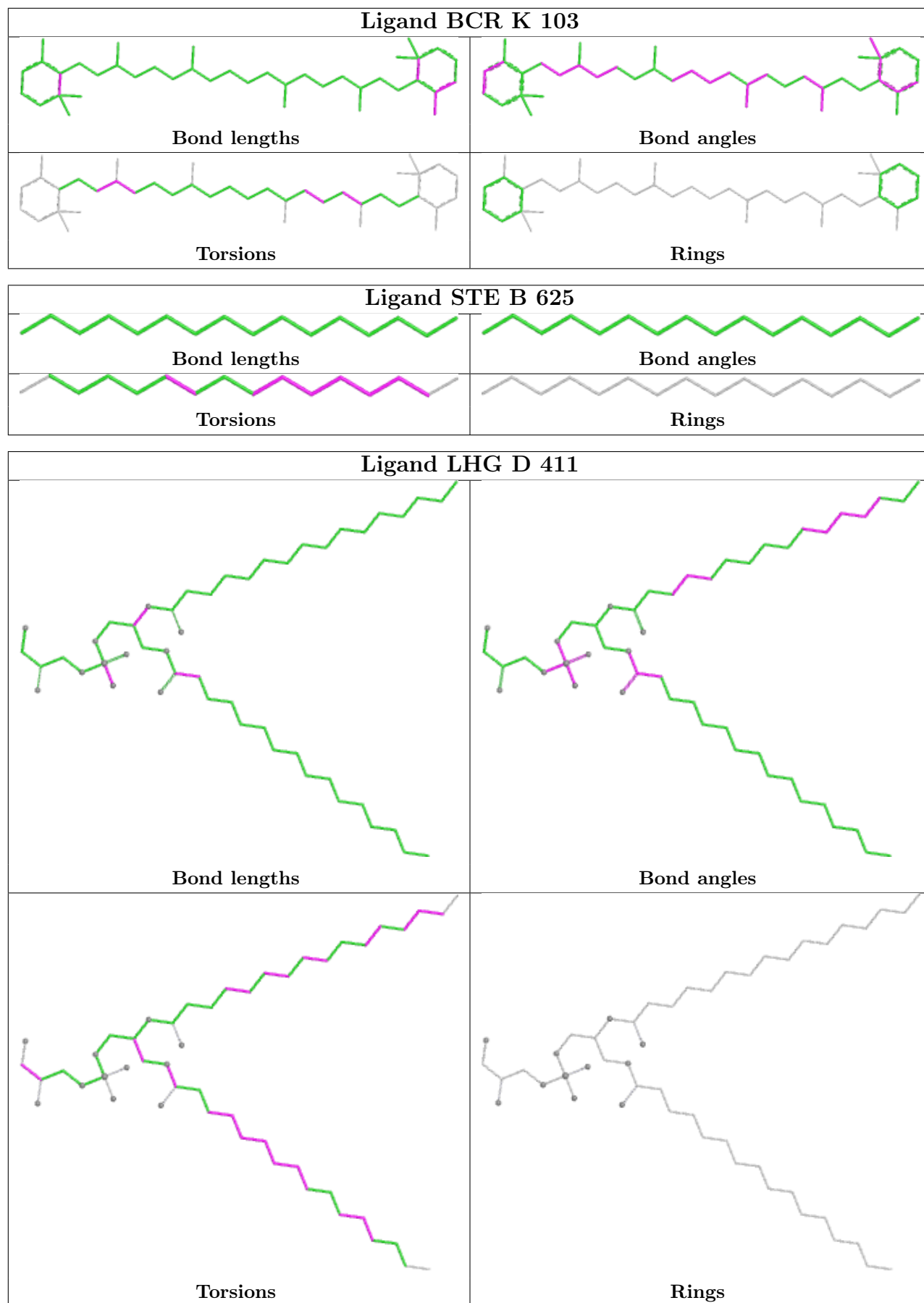


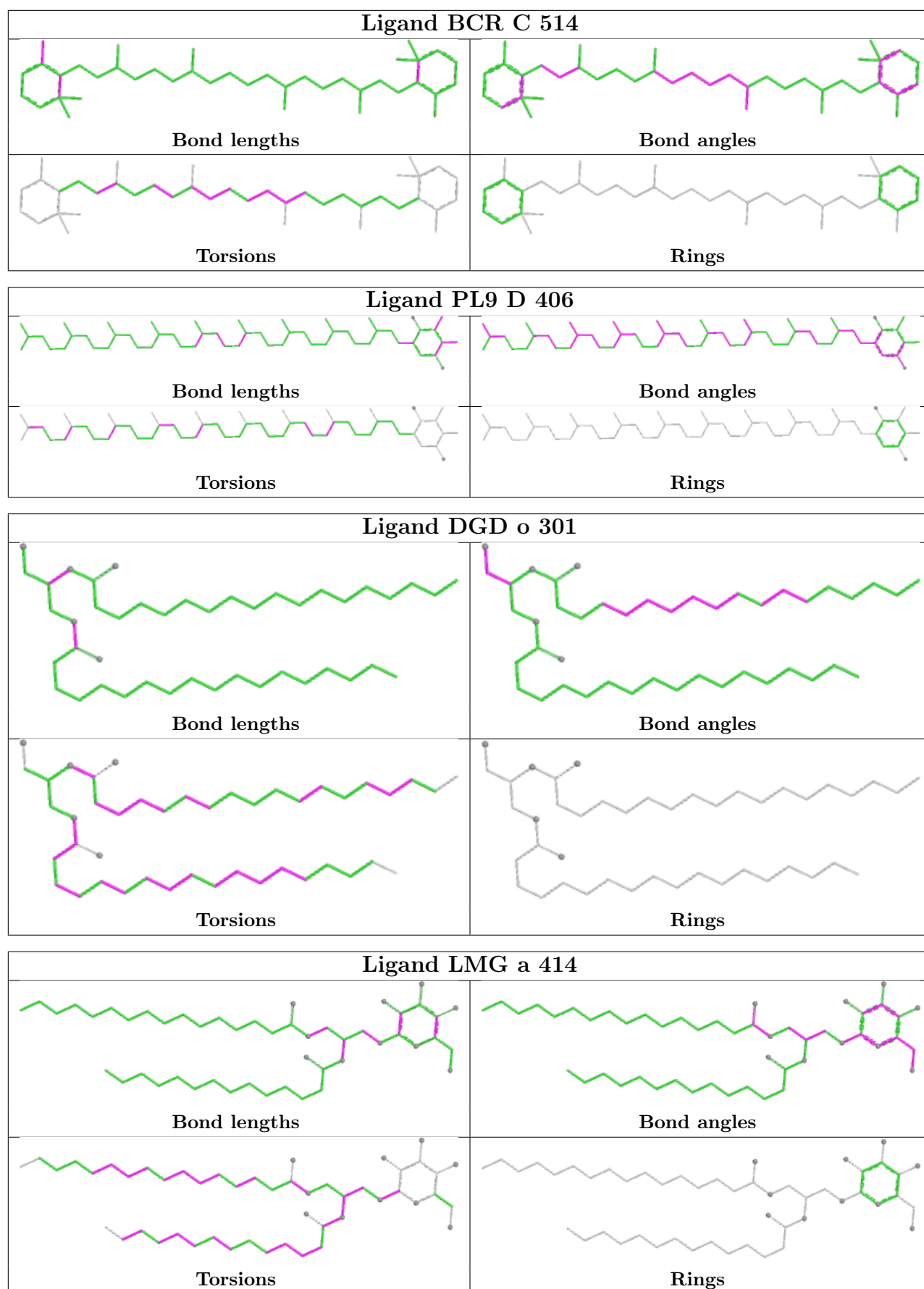


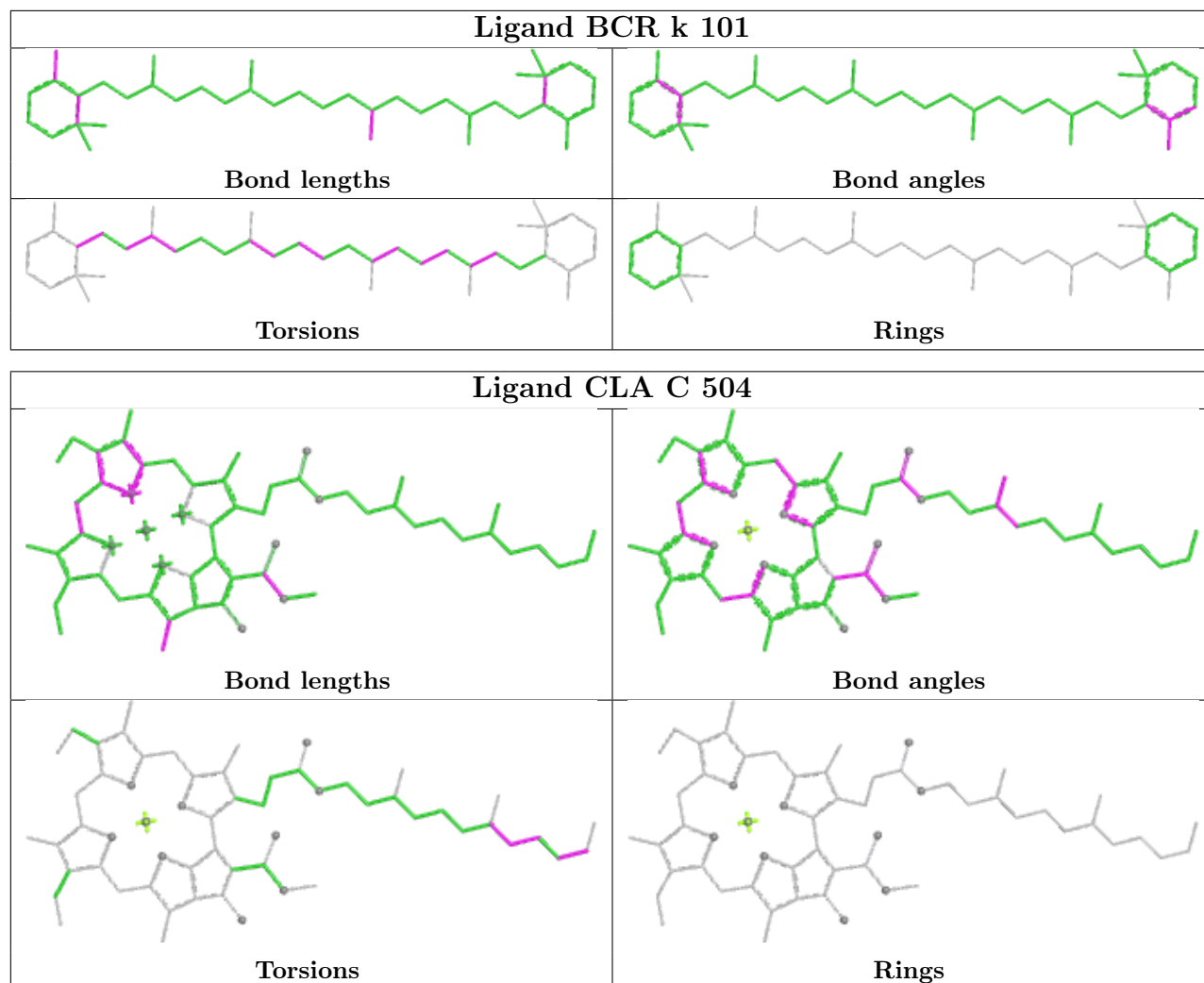


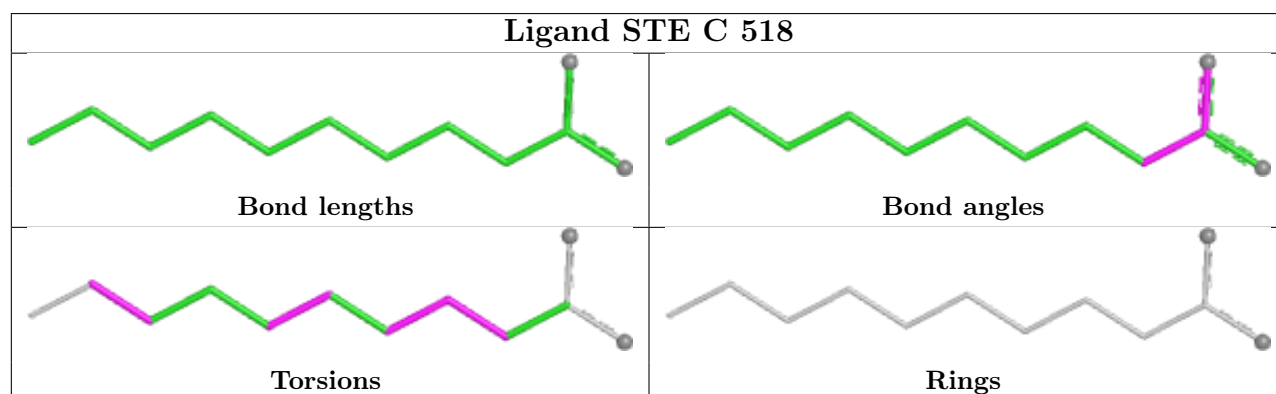
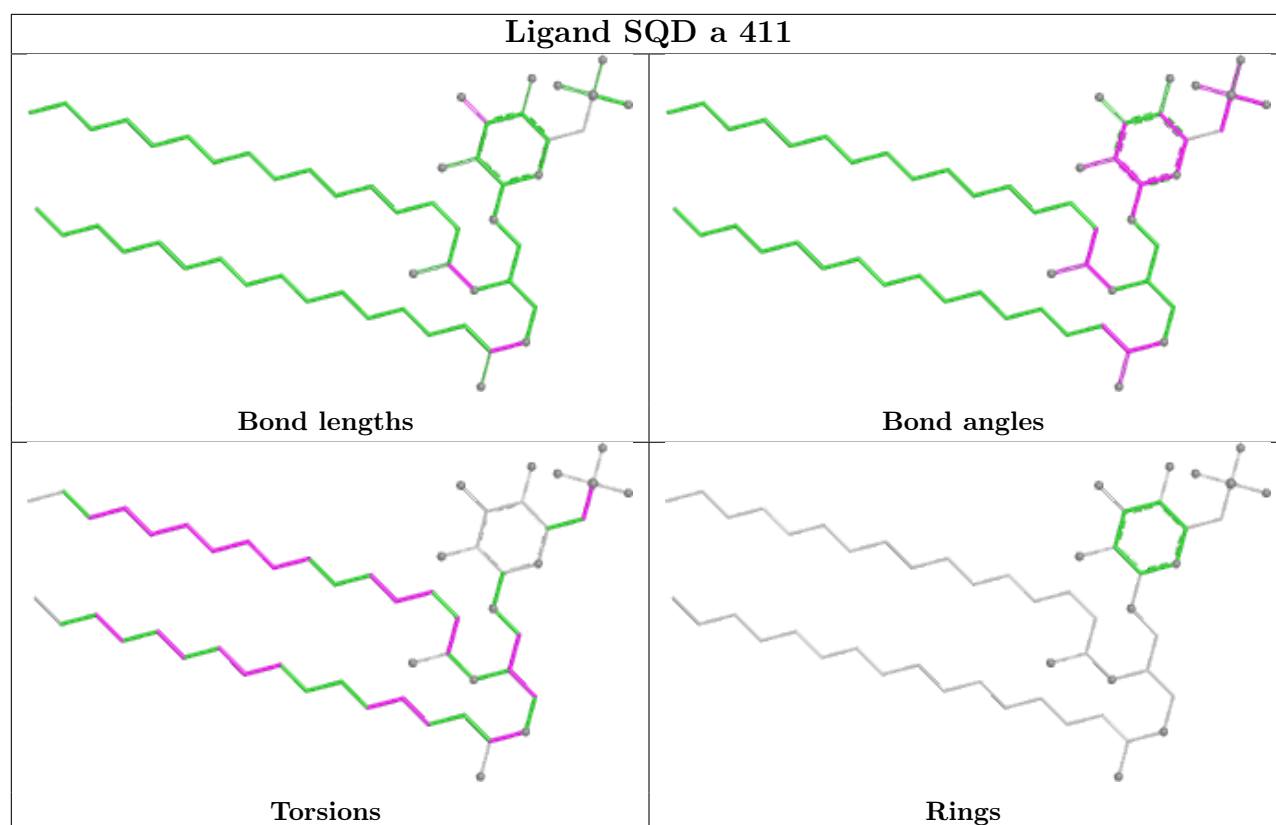


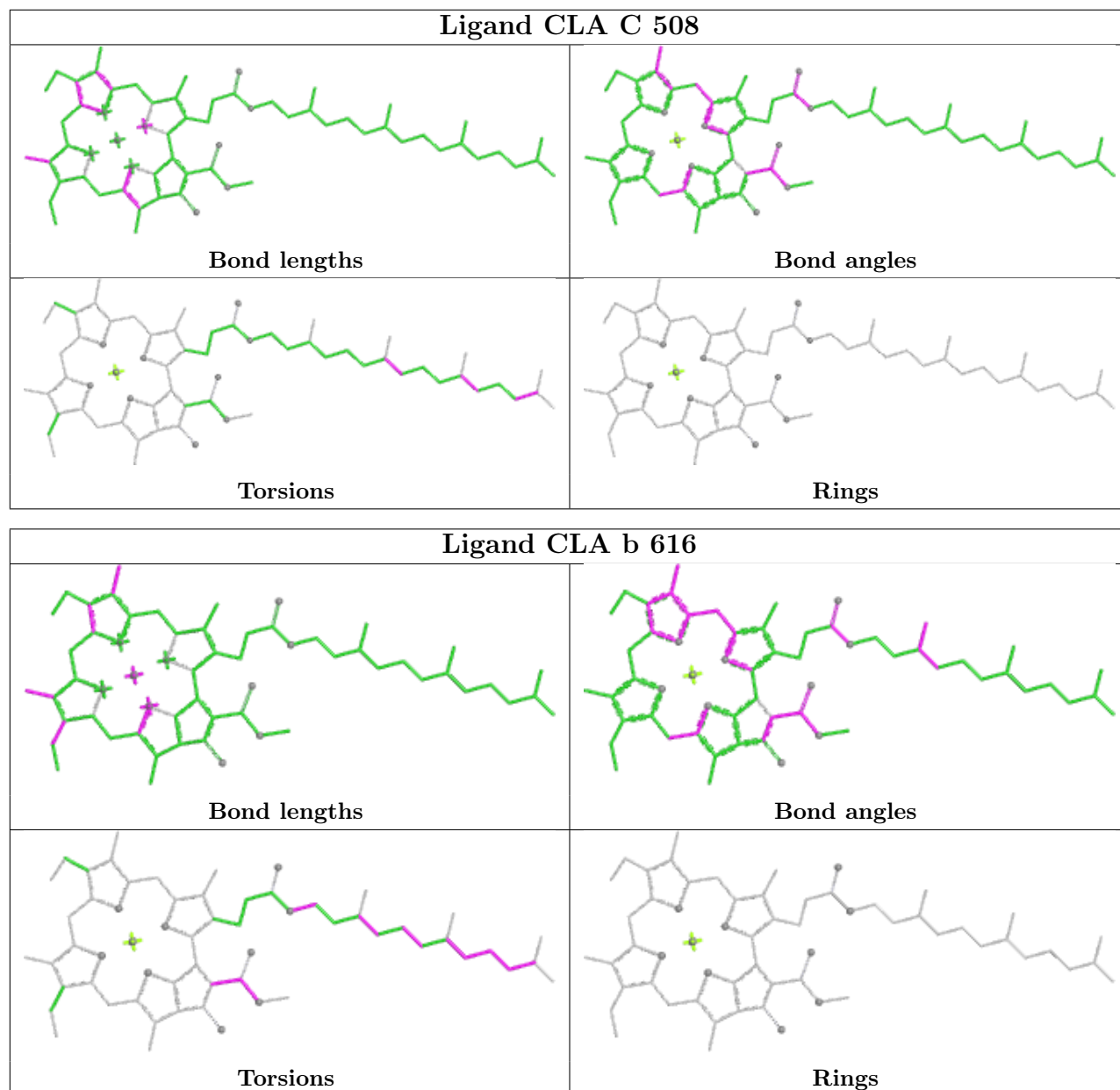


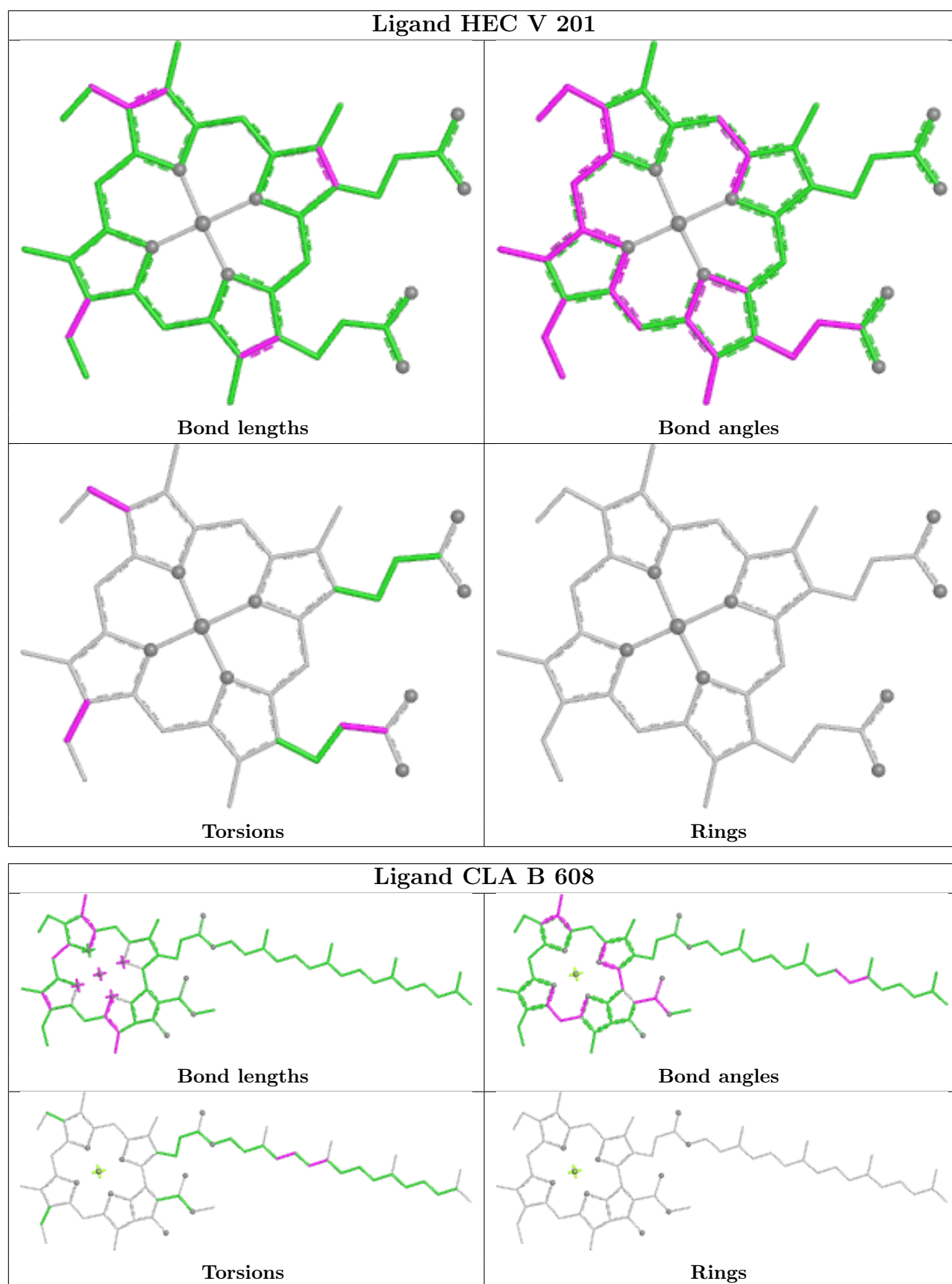


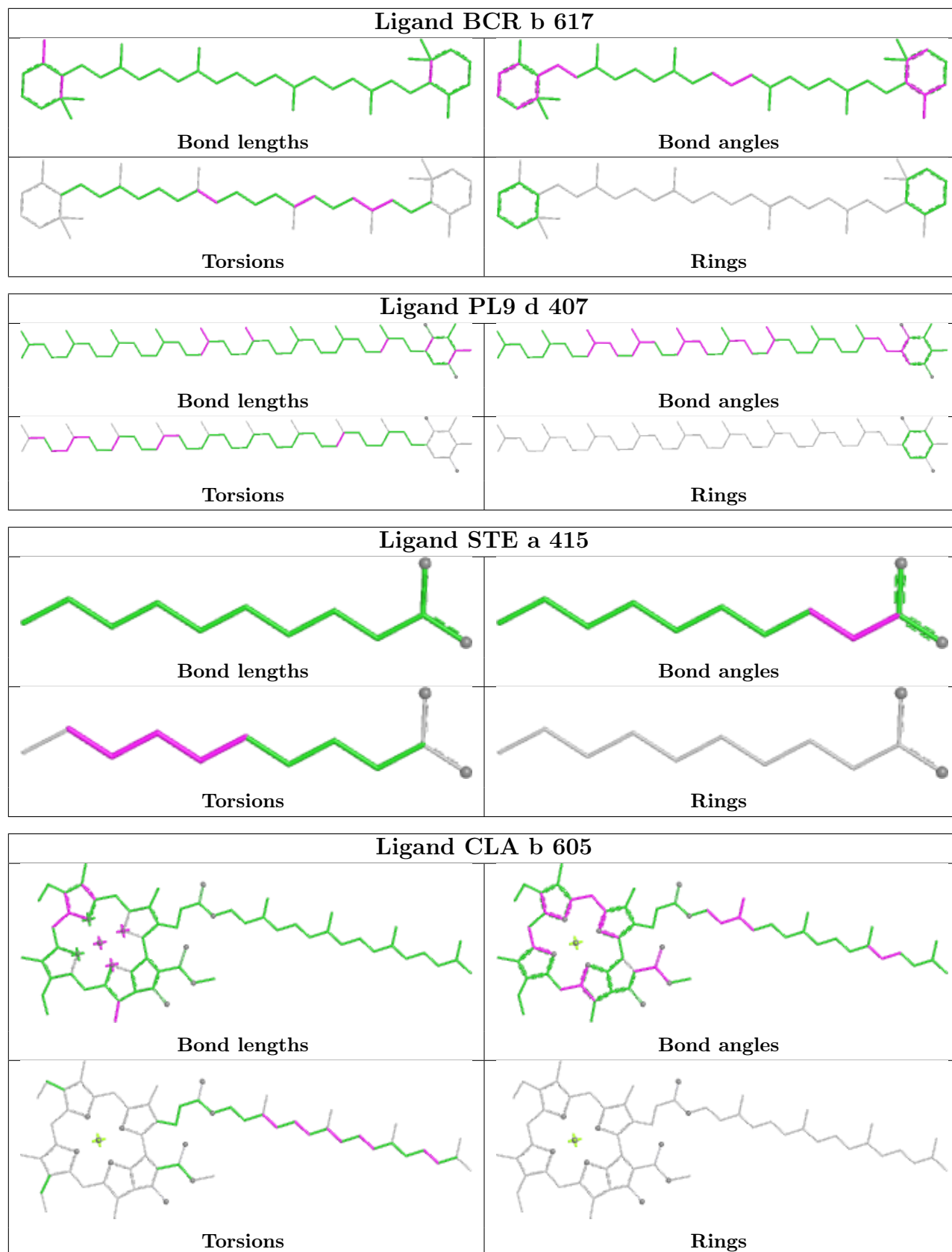


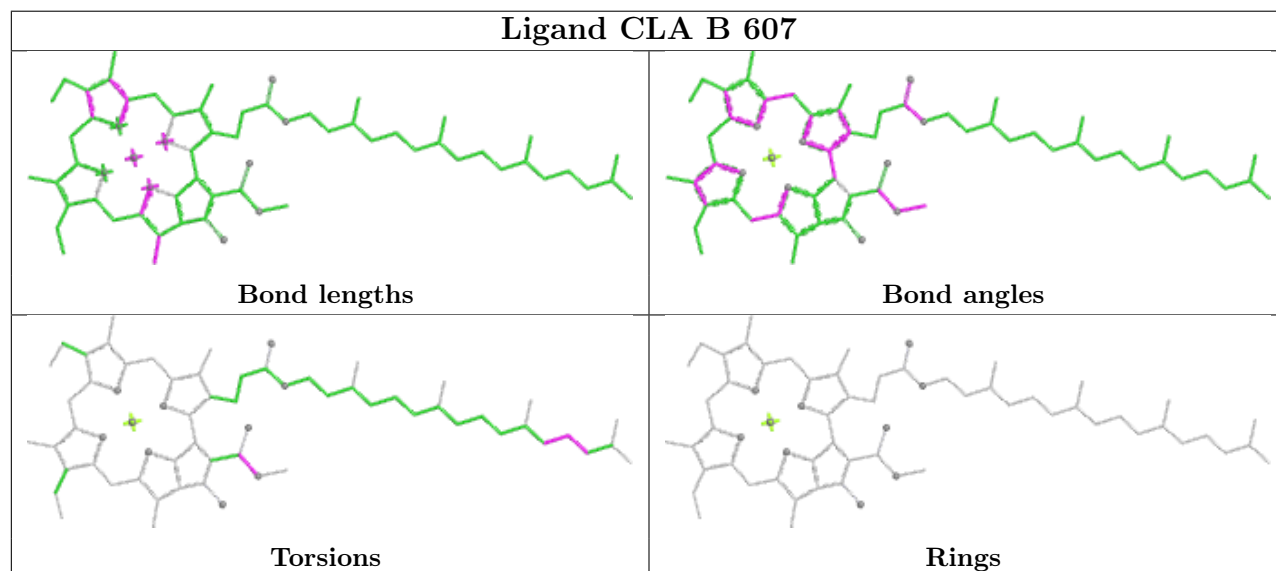
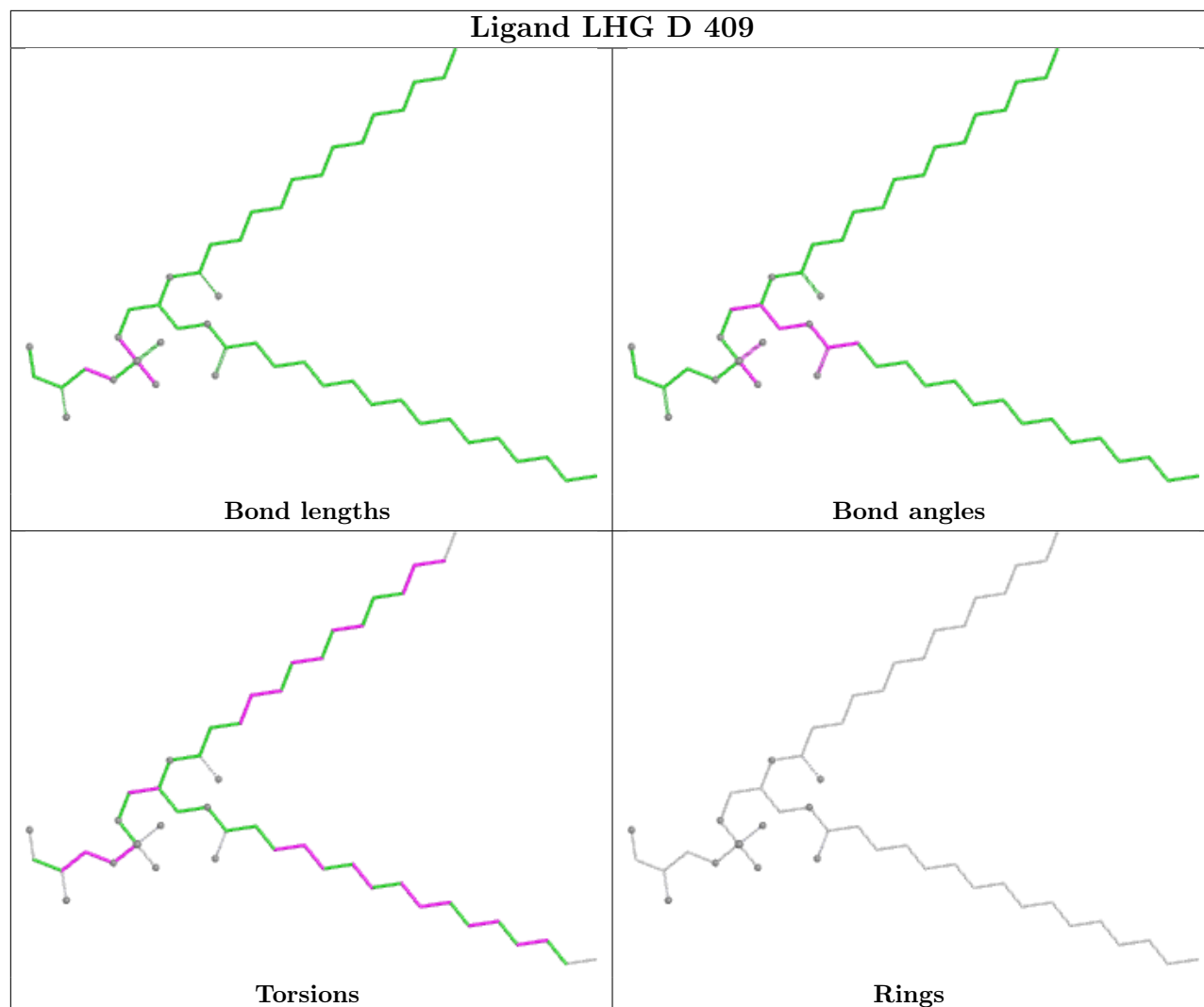


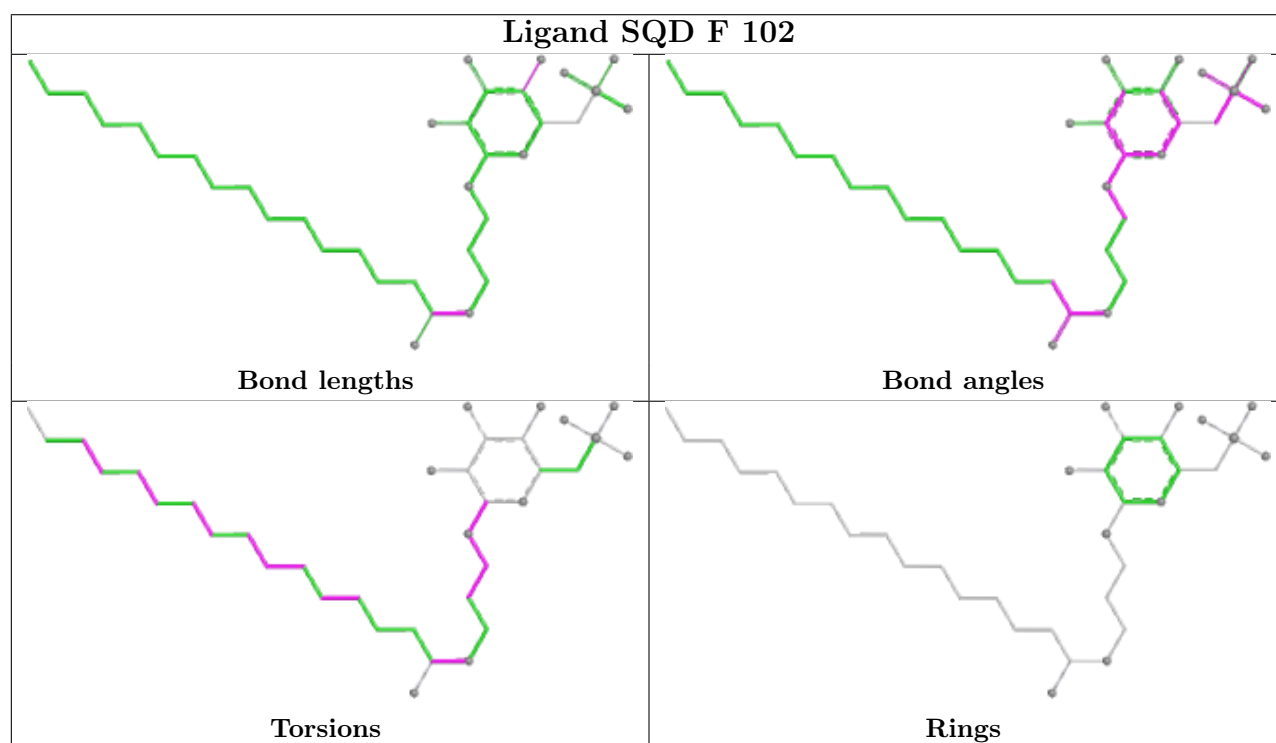
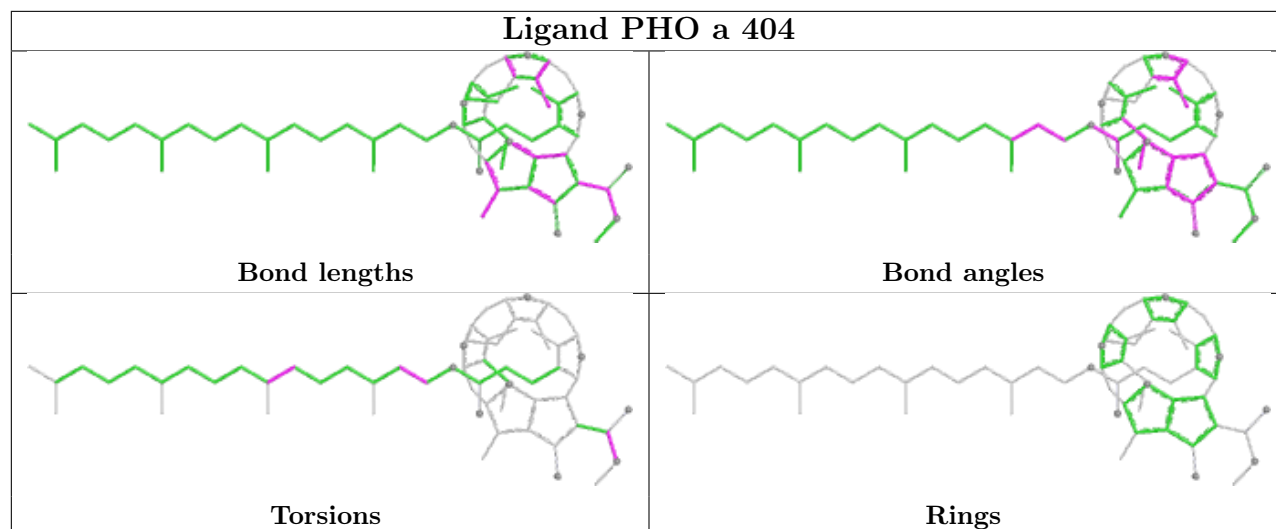


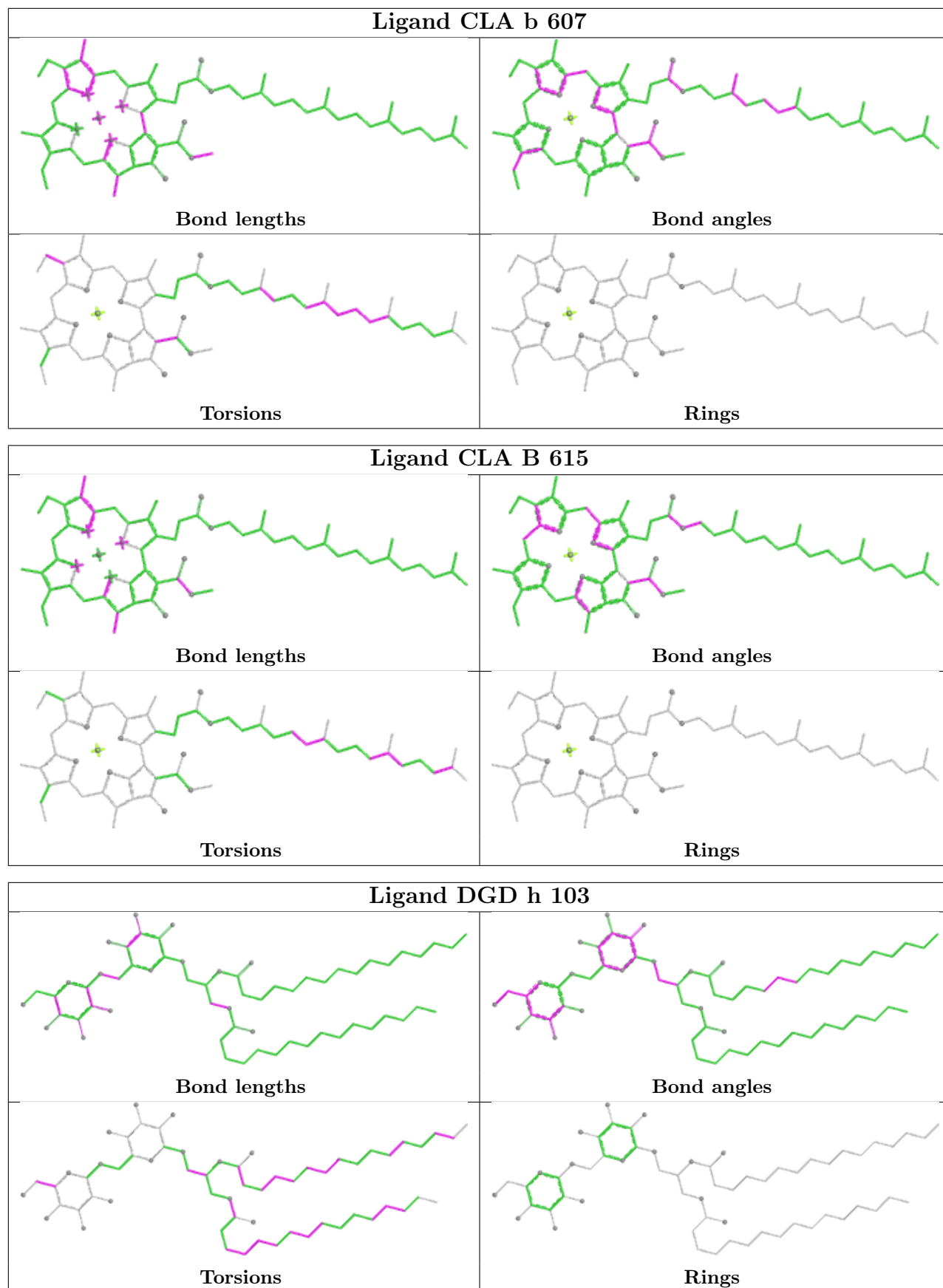


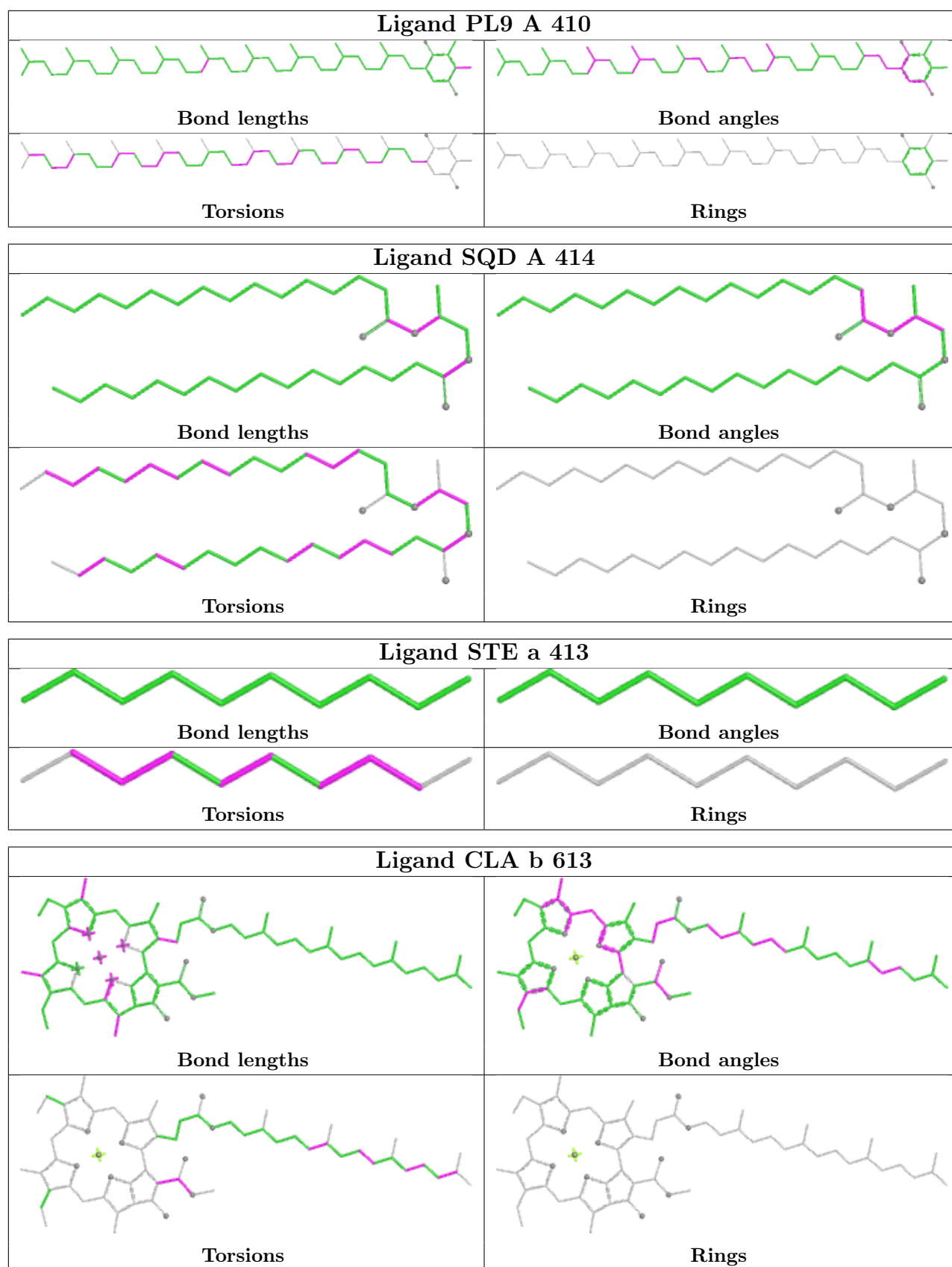


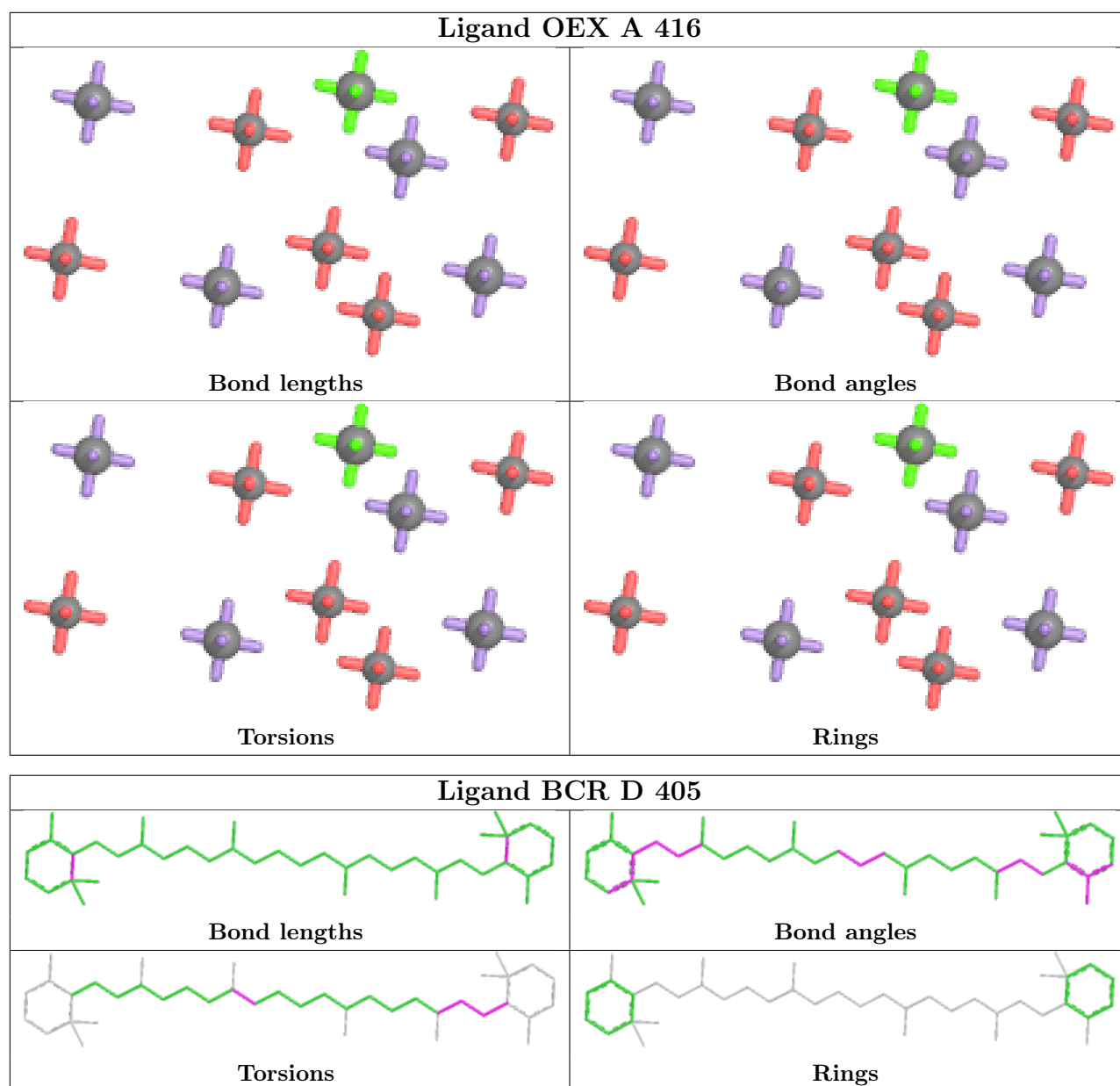


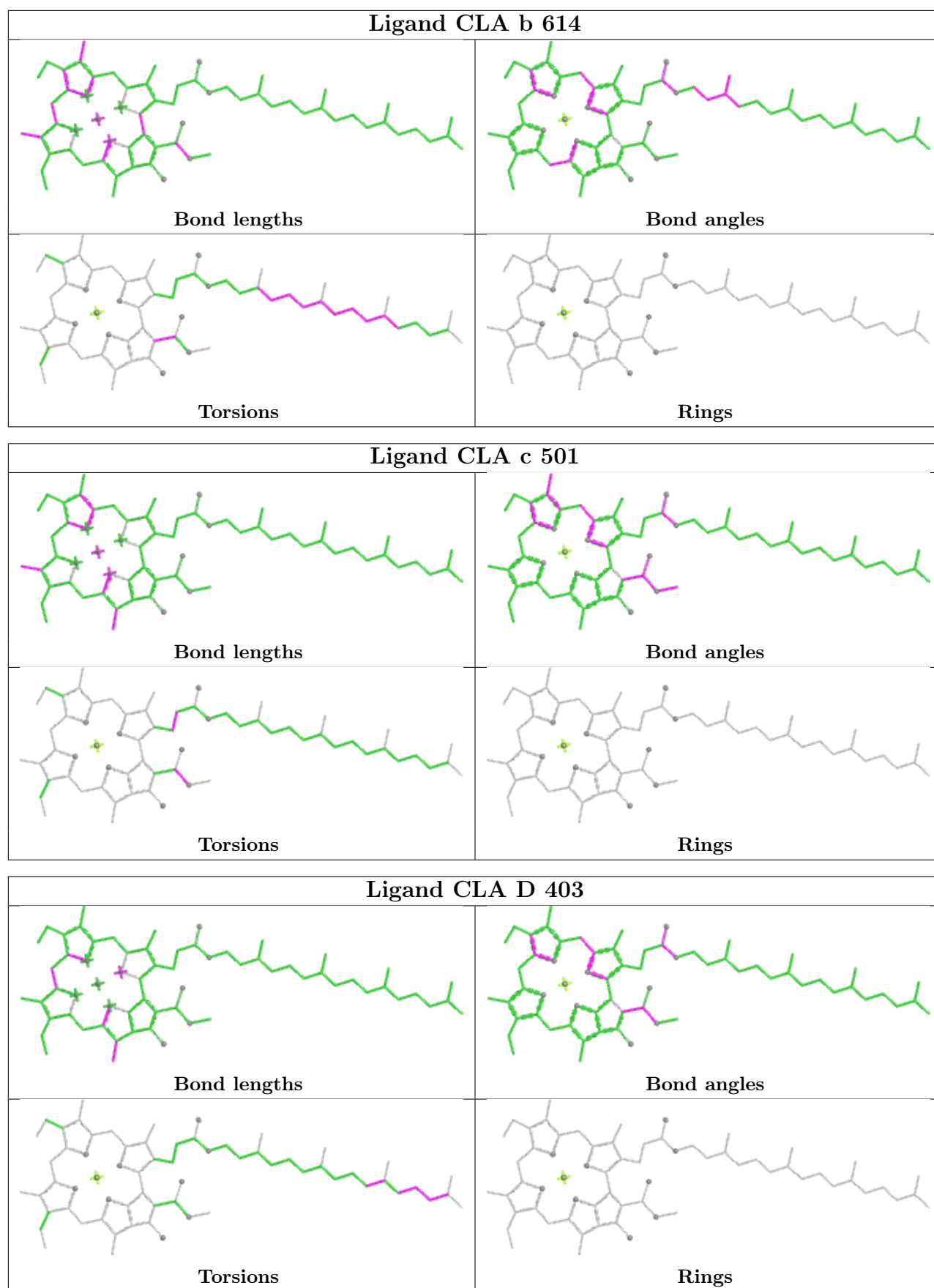


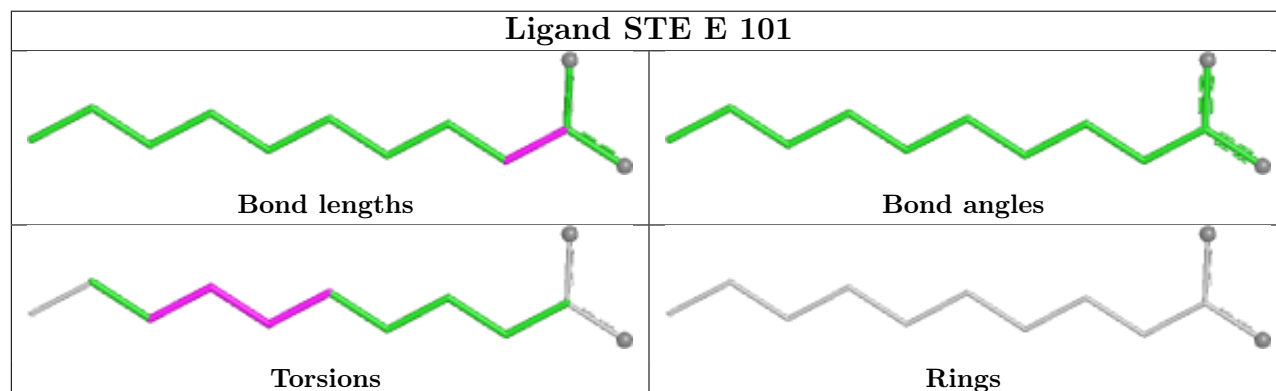
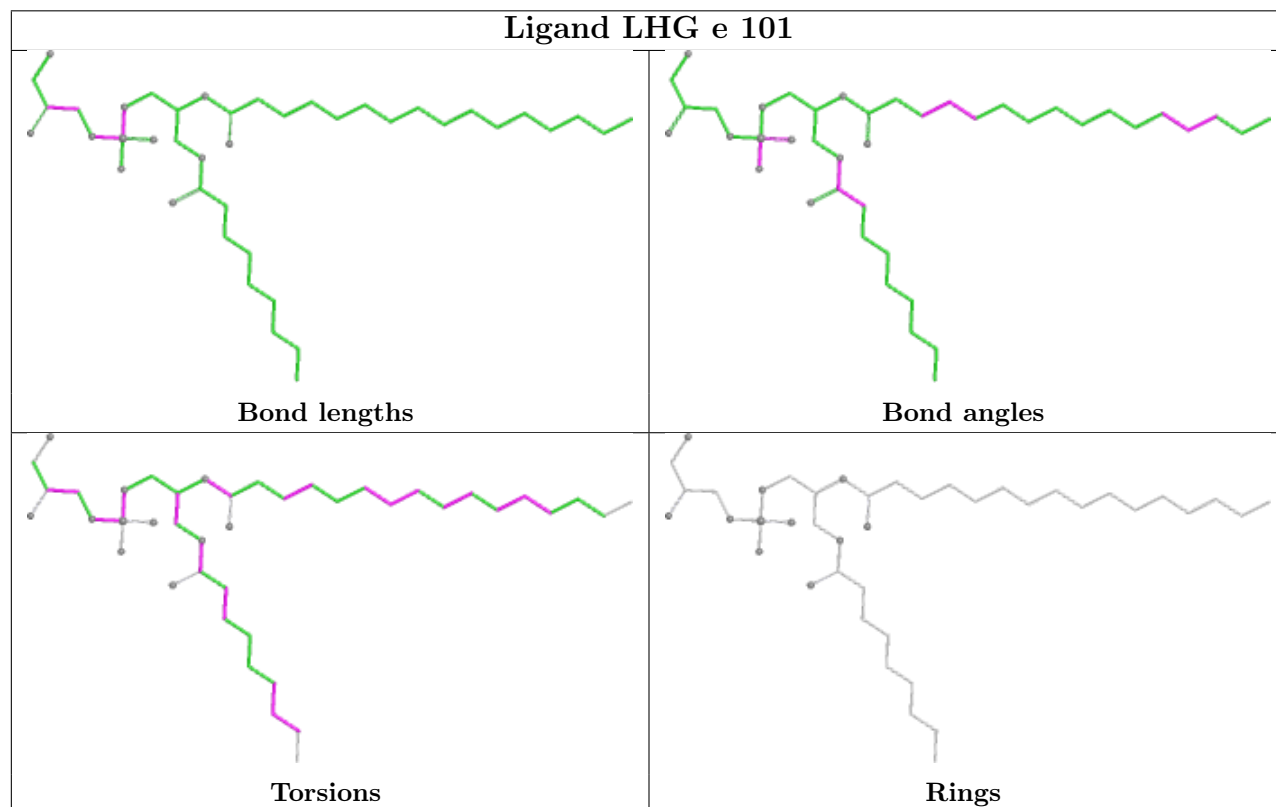
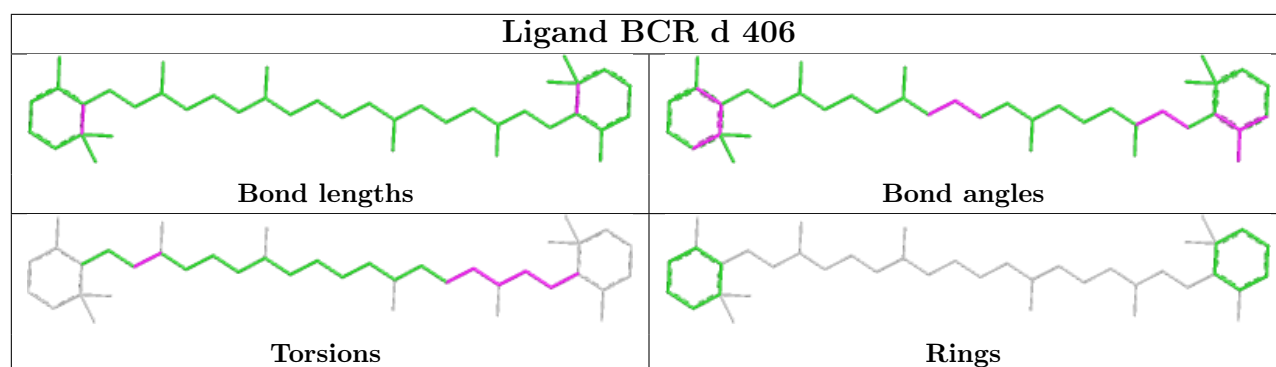


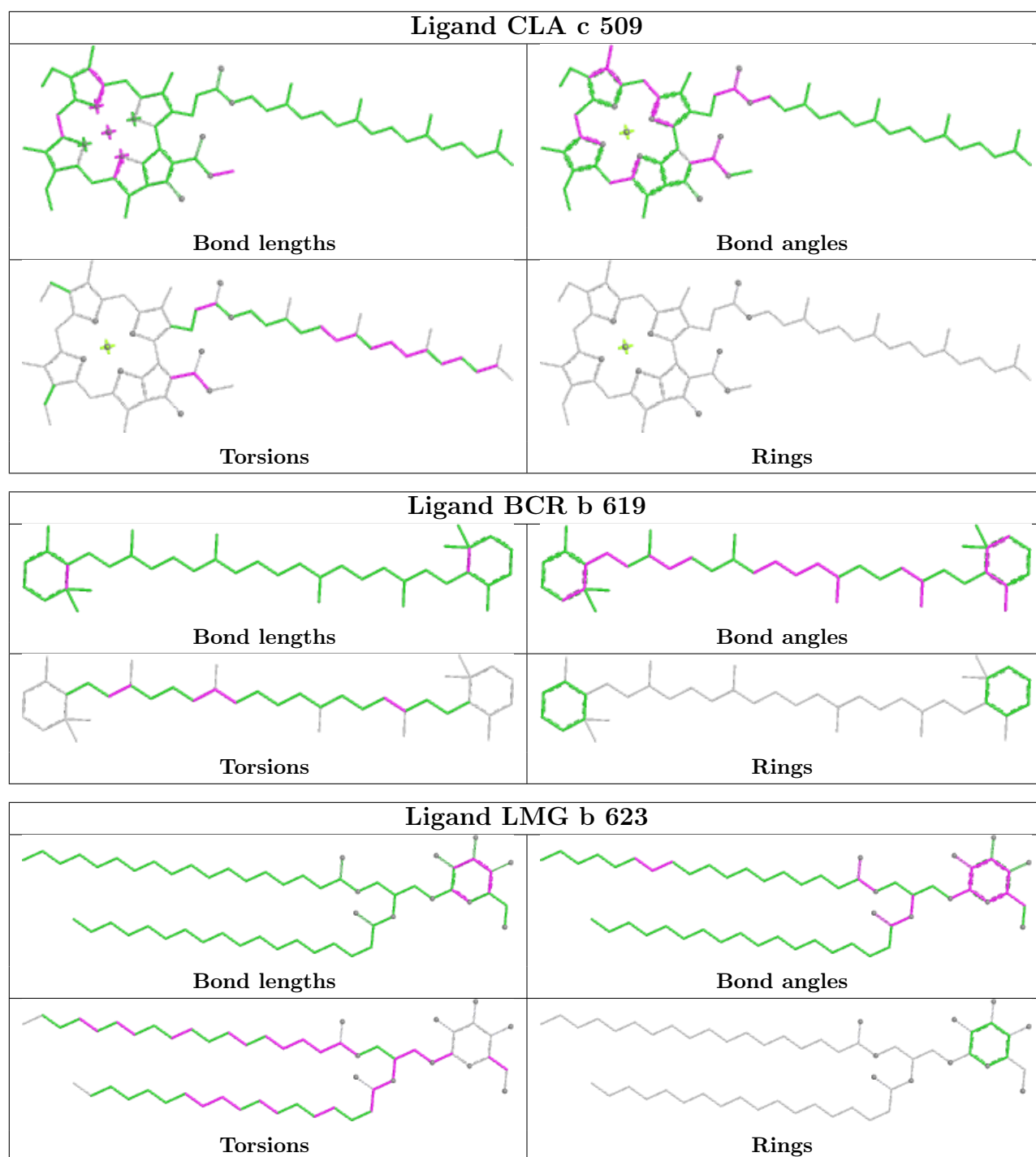


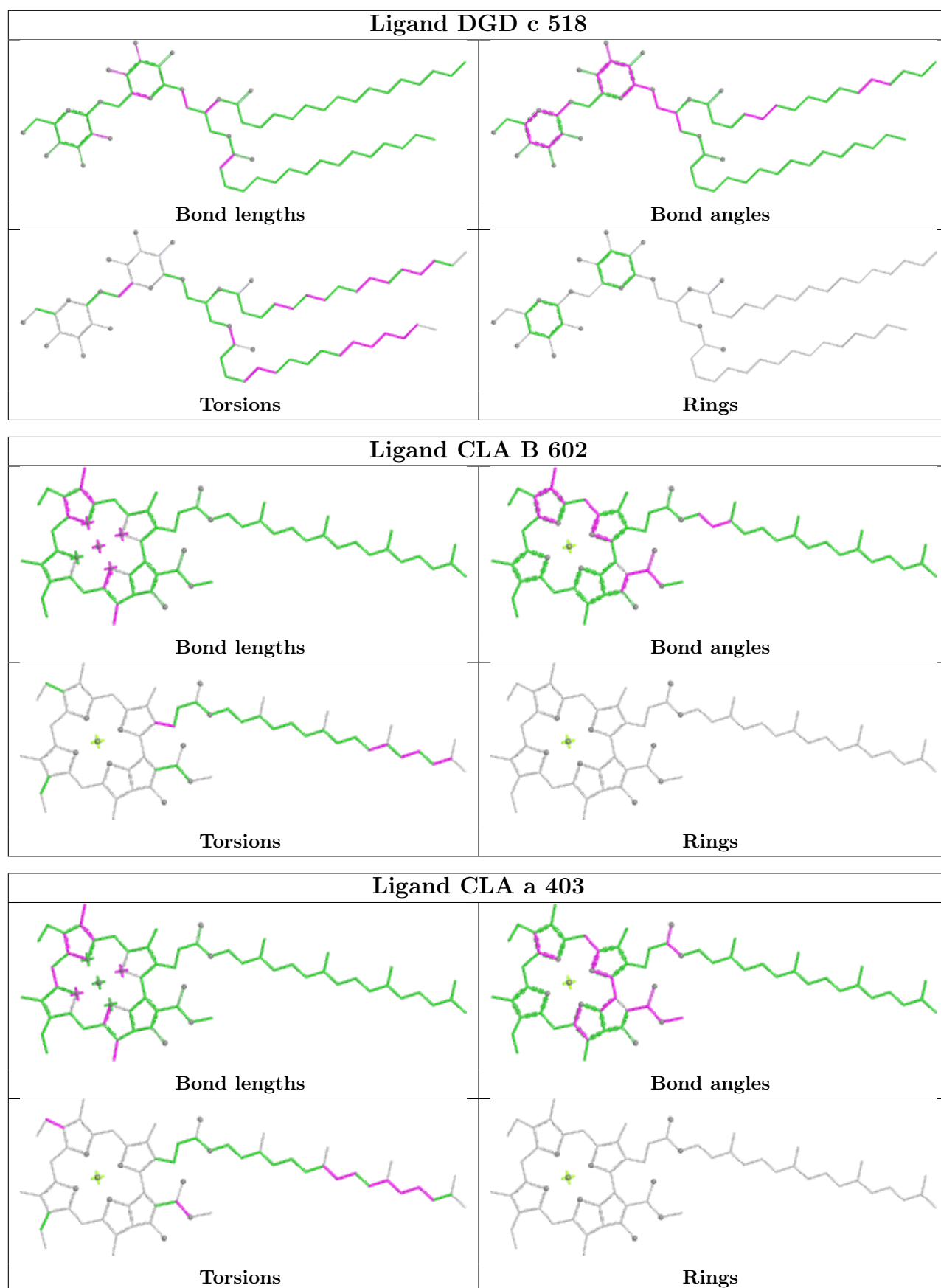


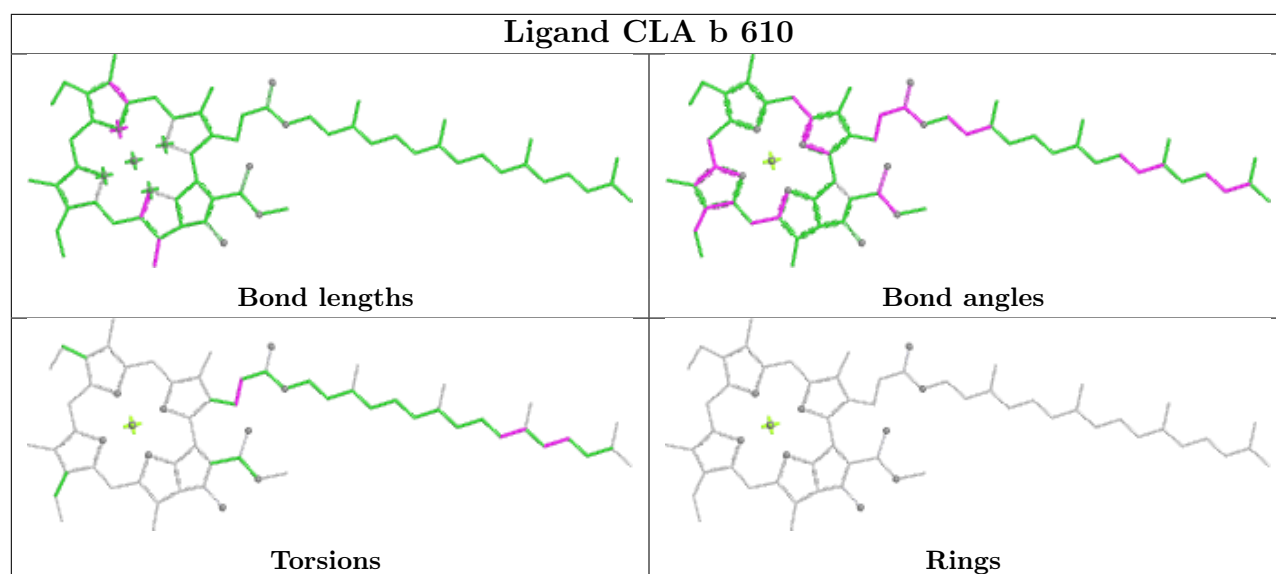
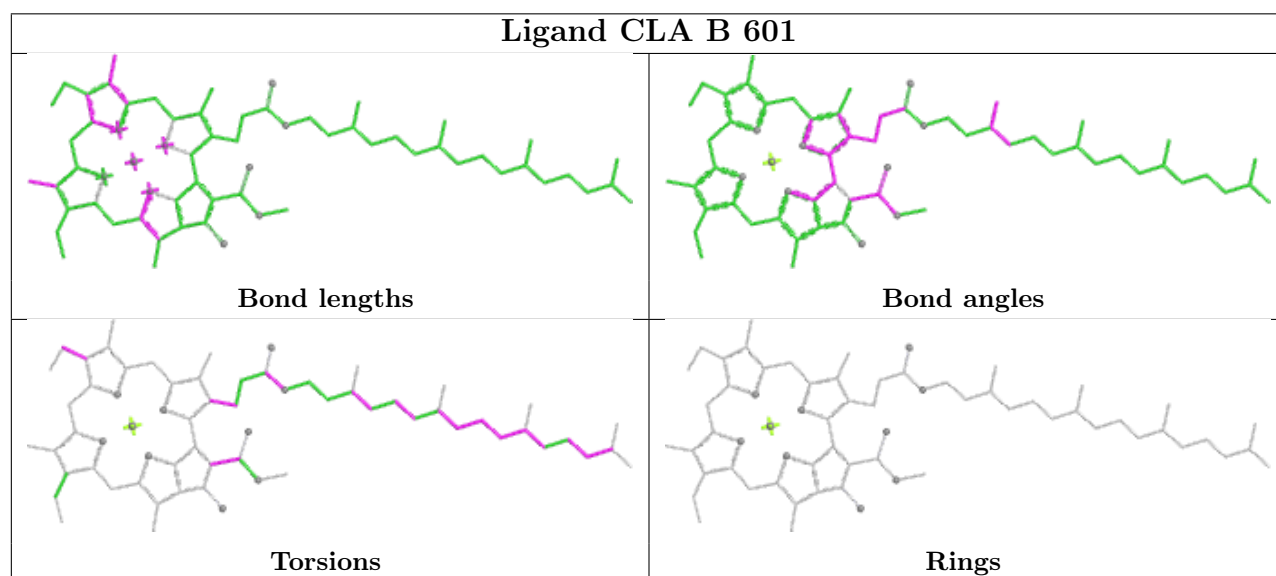
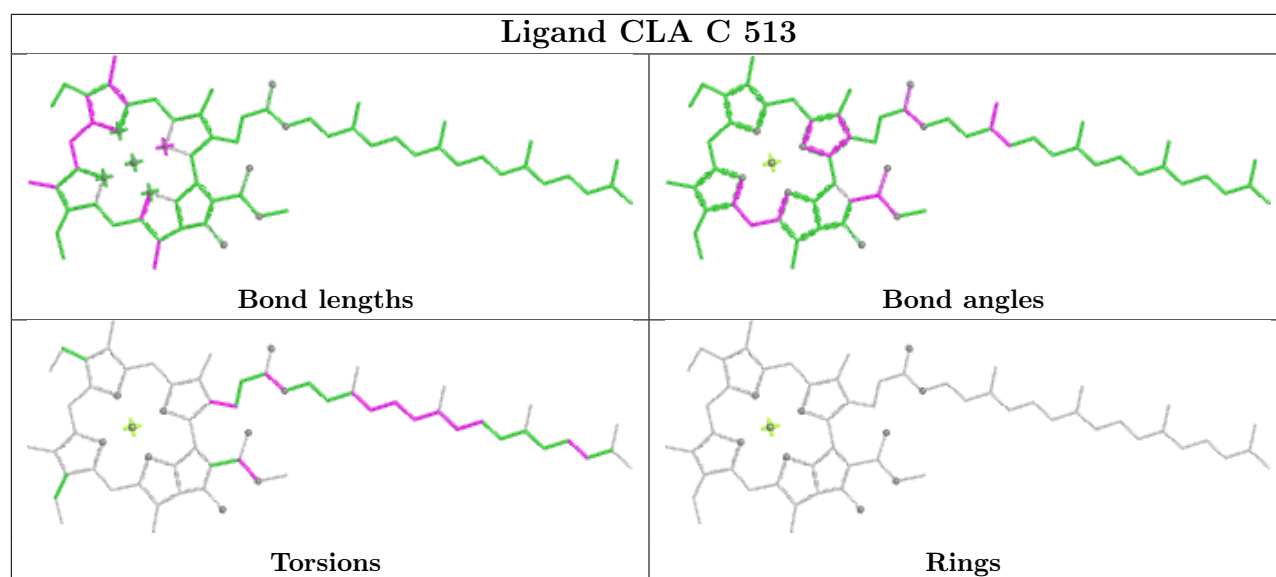


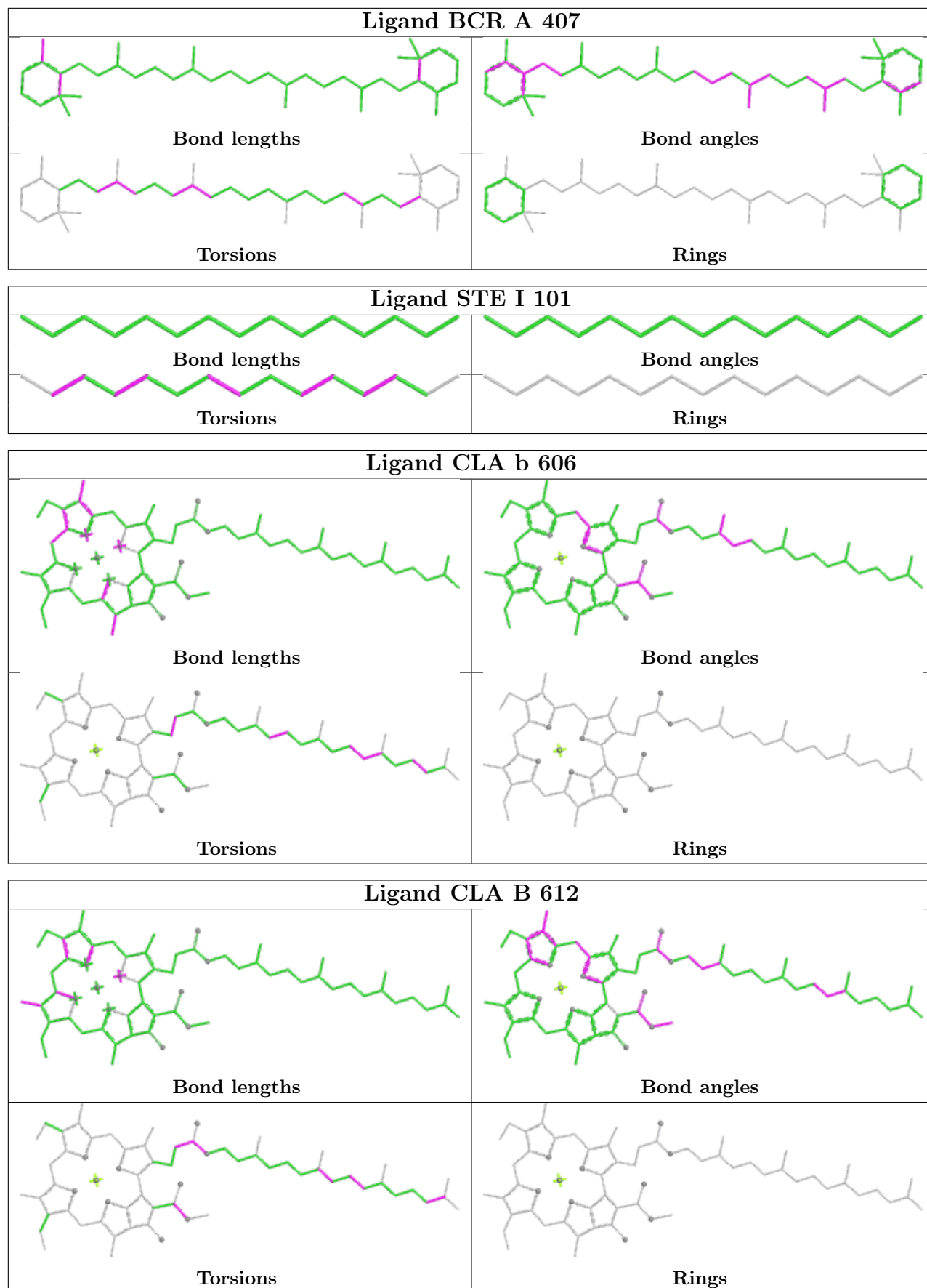


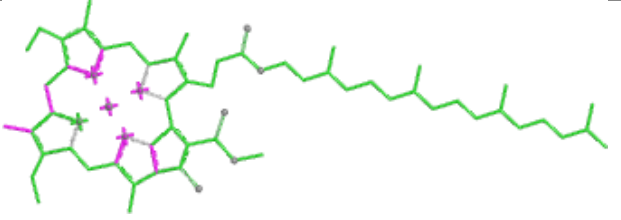
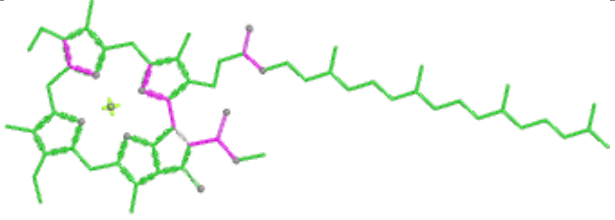
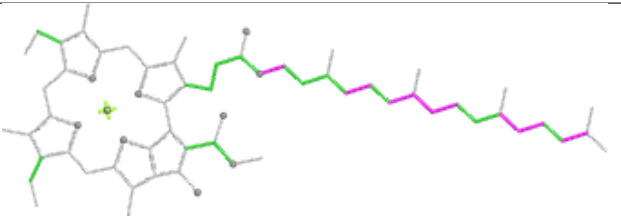
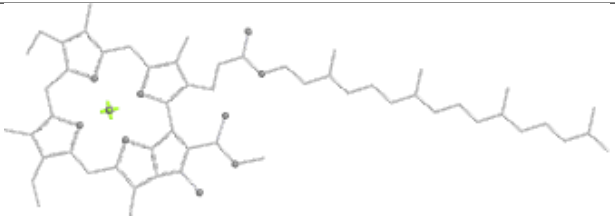
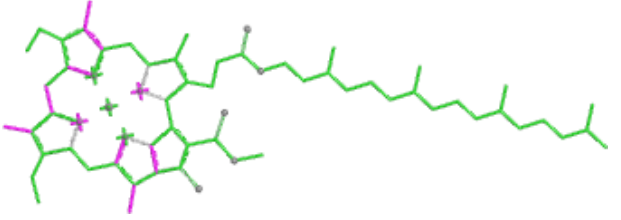
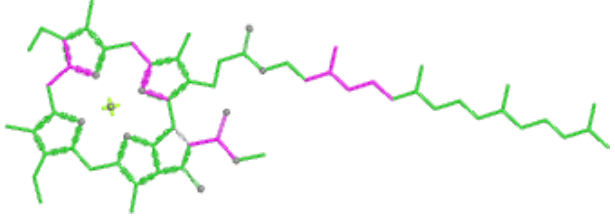
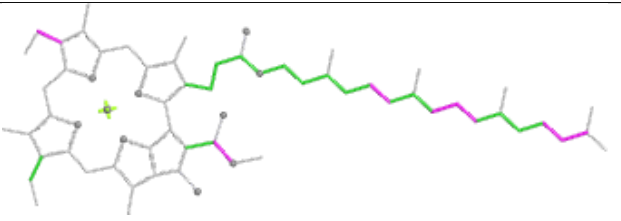
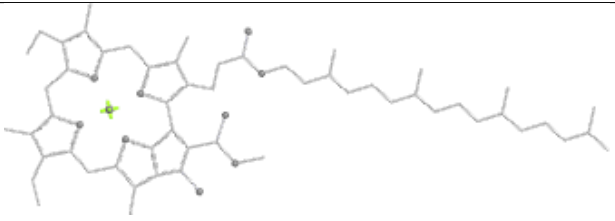






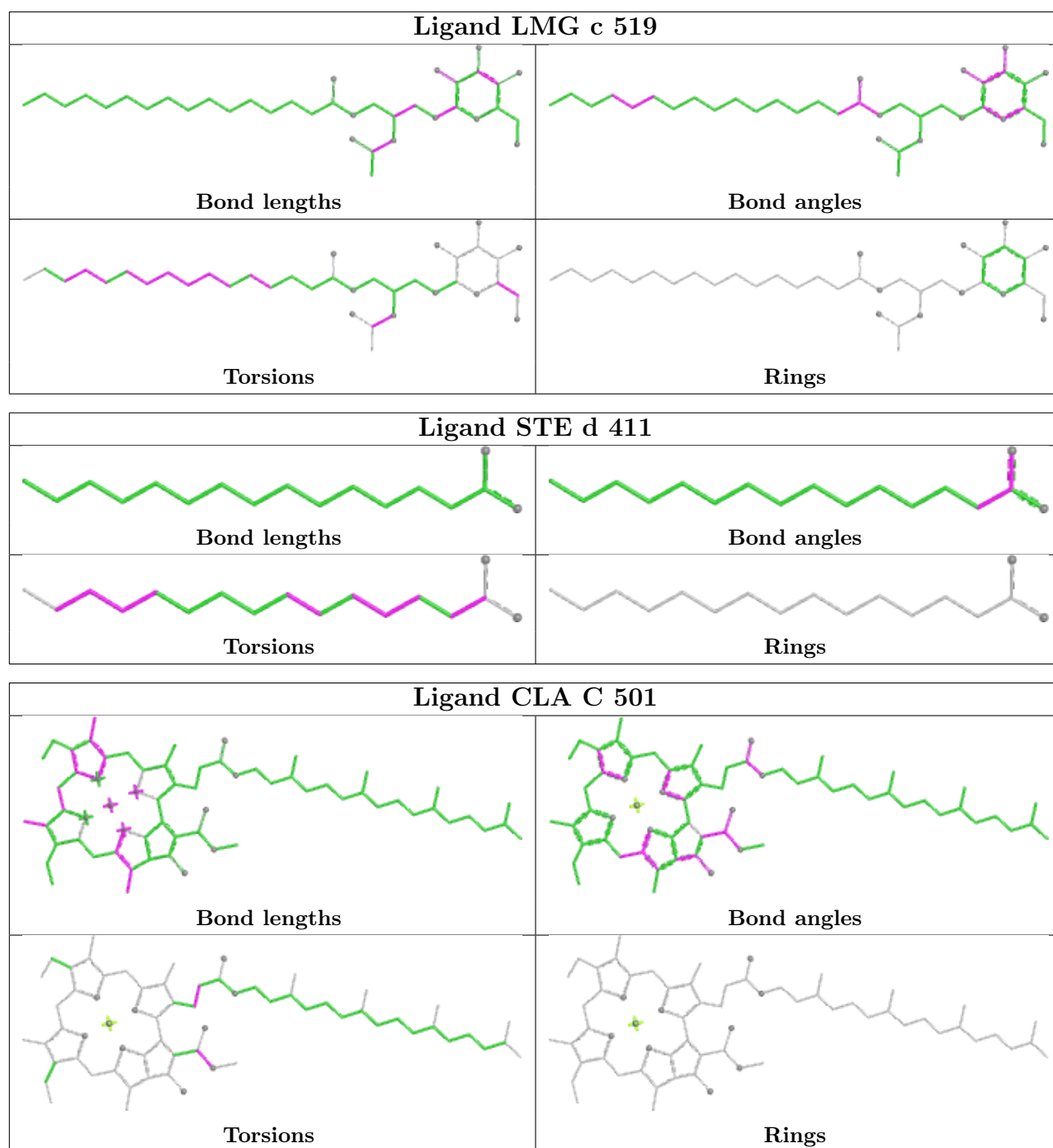


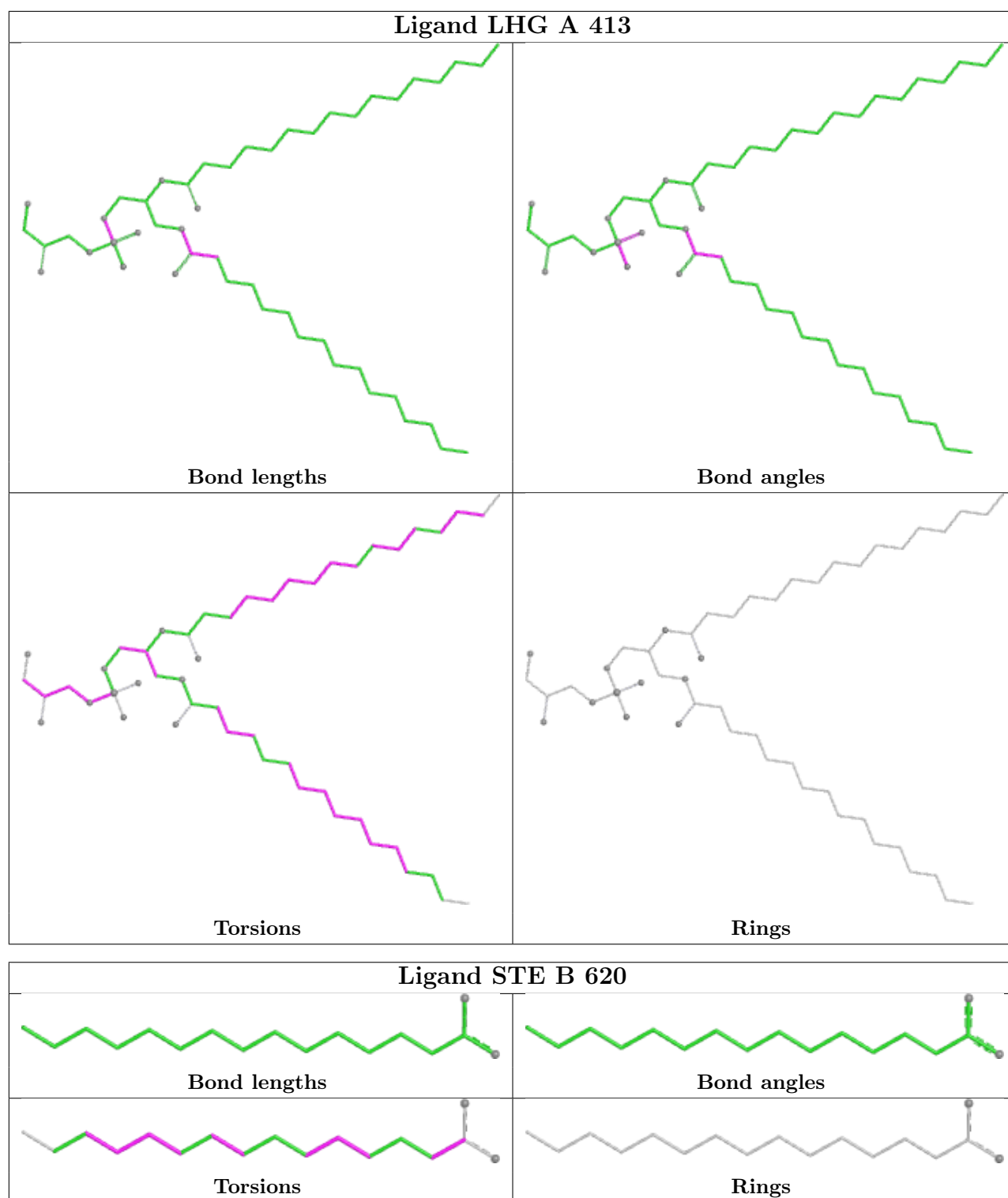


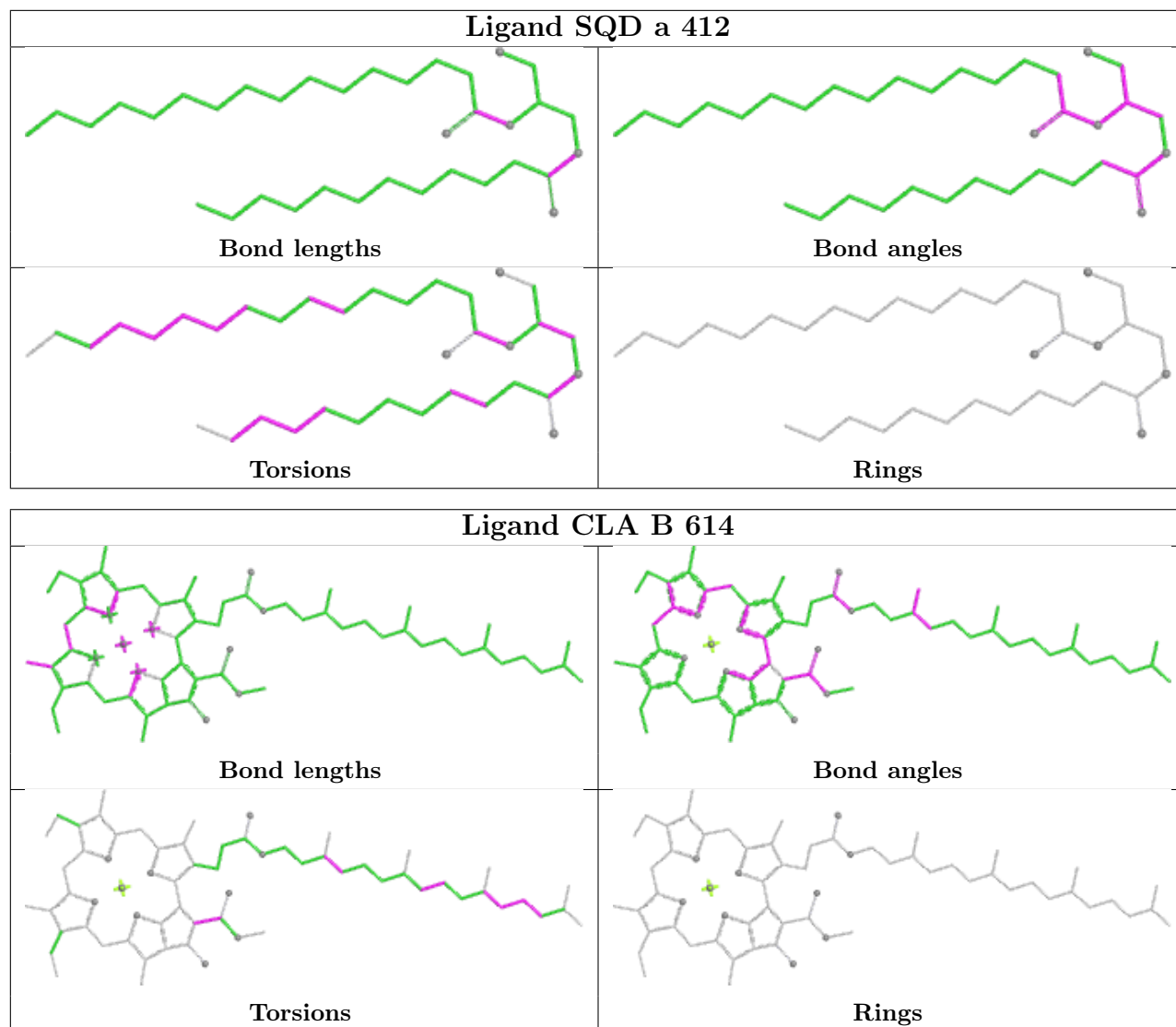


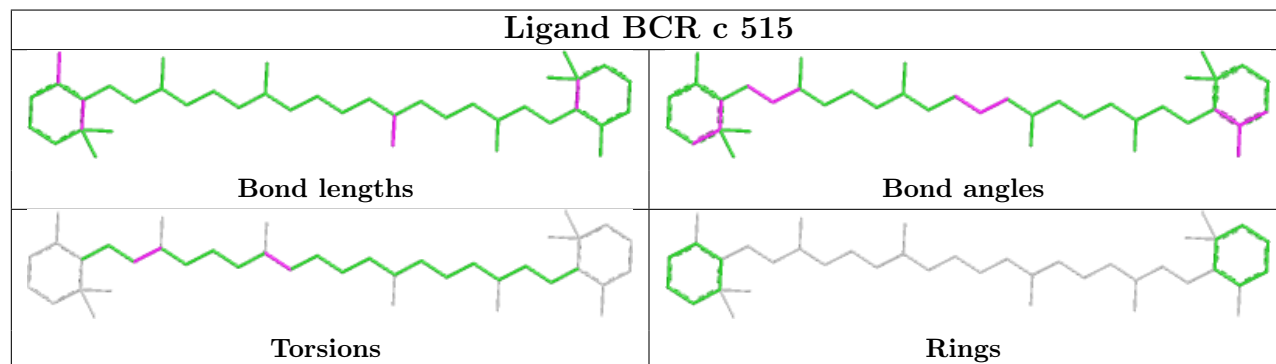
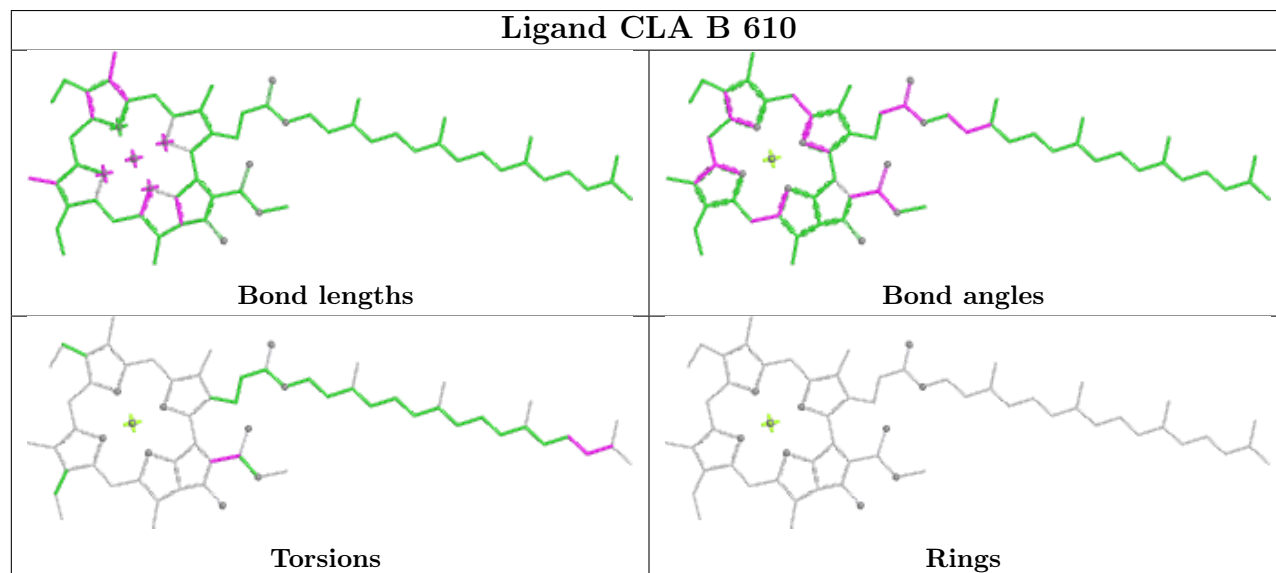
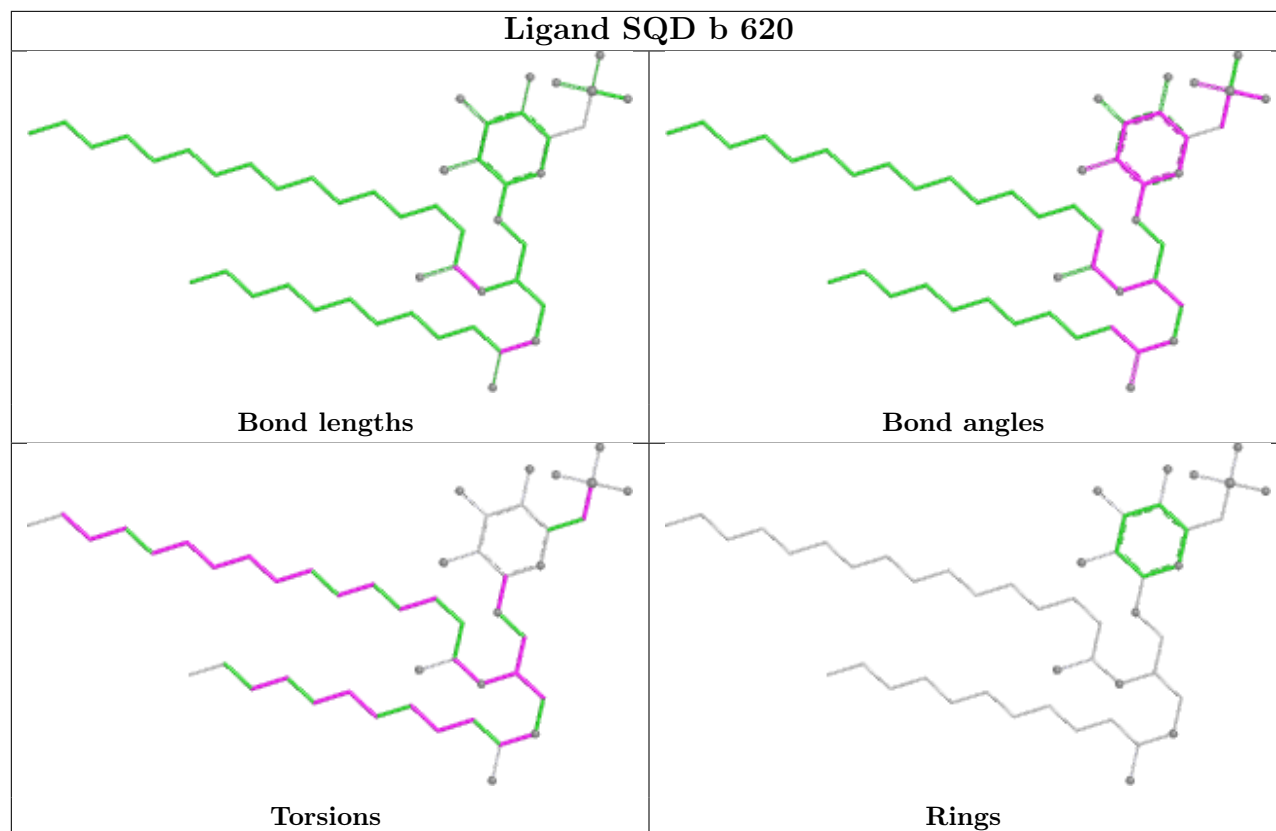


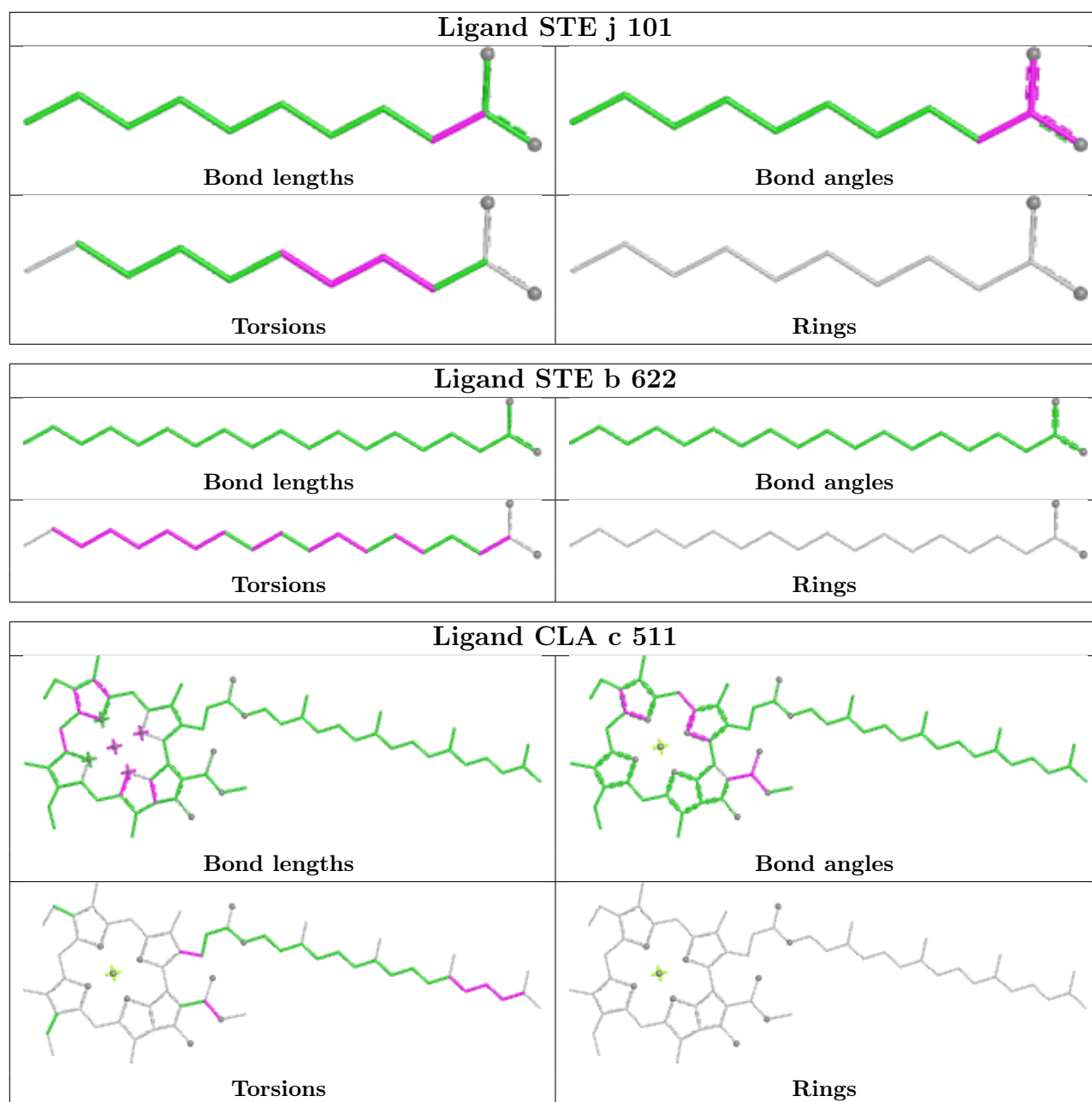
Ligand CLA C 506	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA c 503	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand STE H 103	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

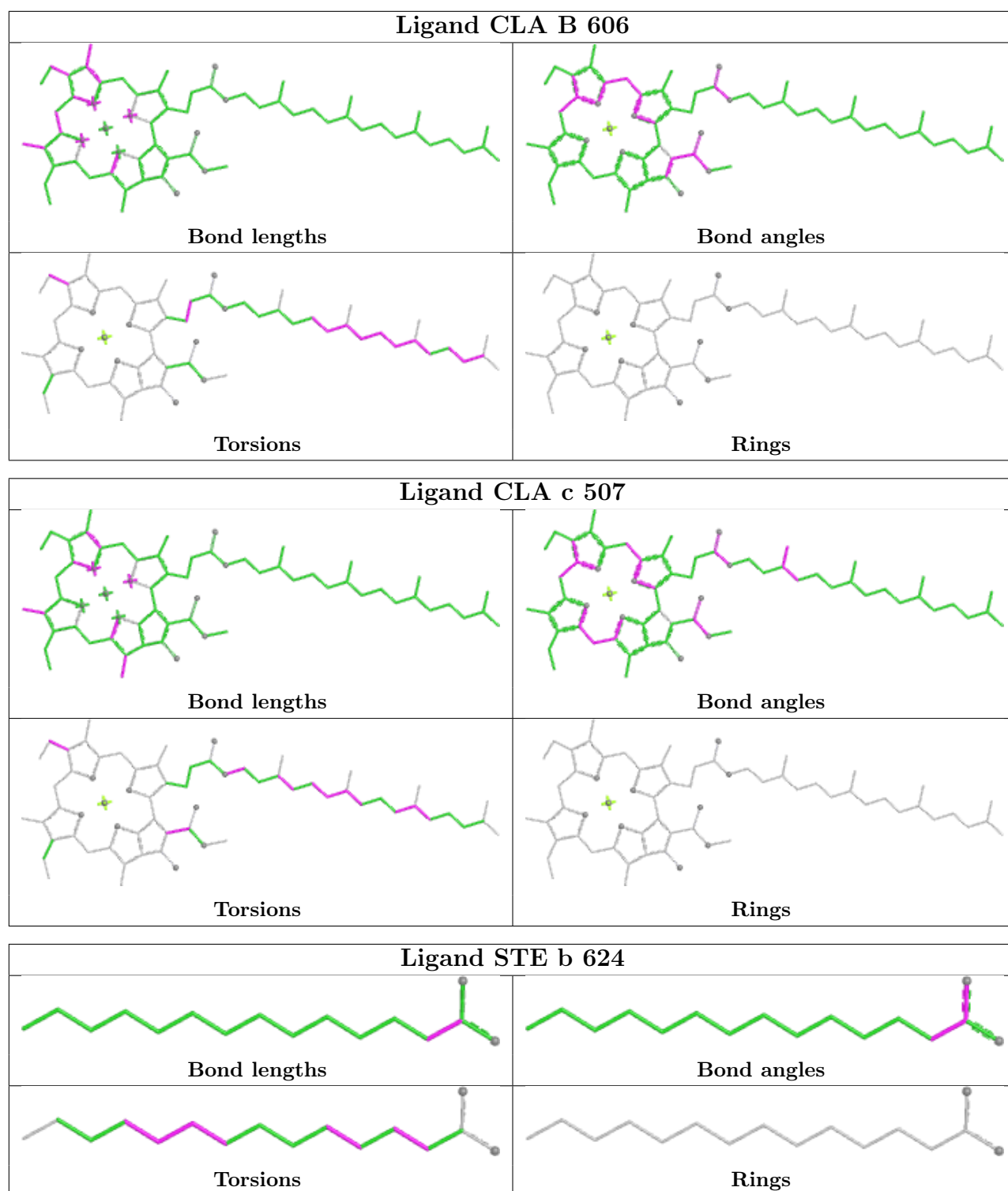


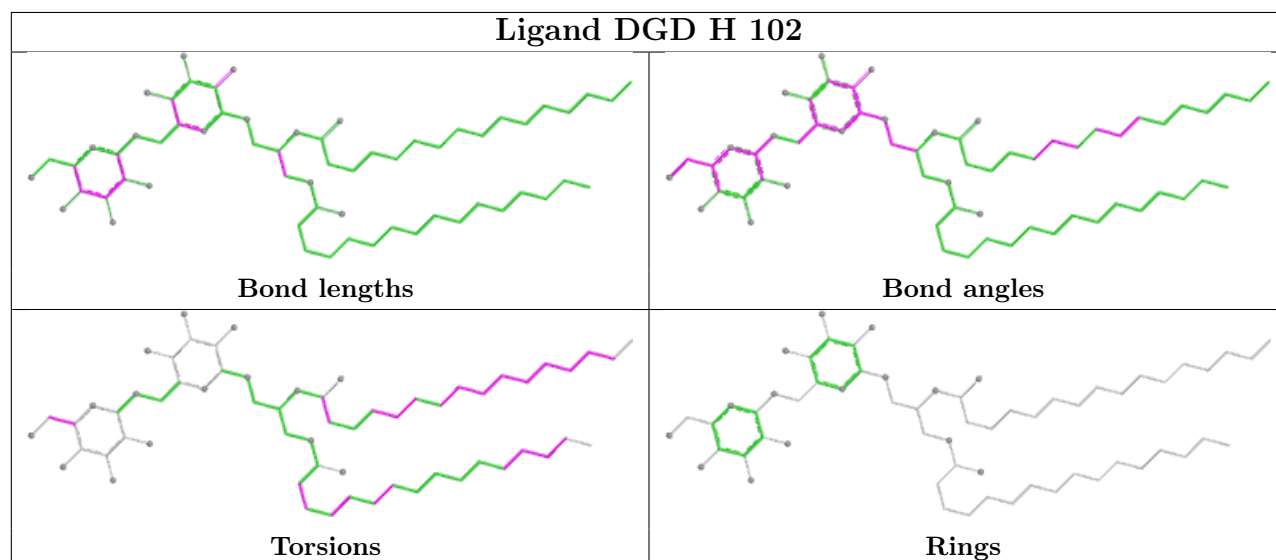
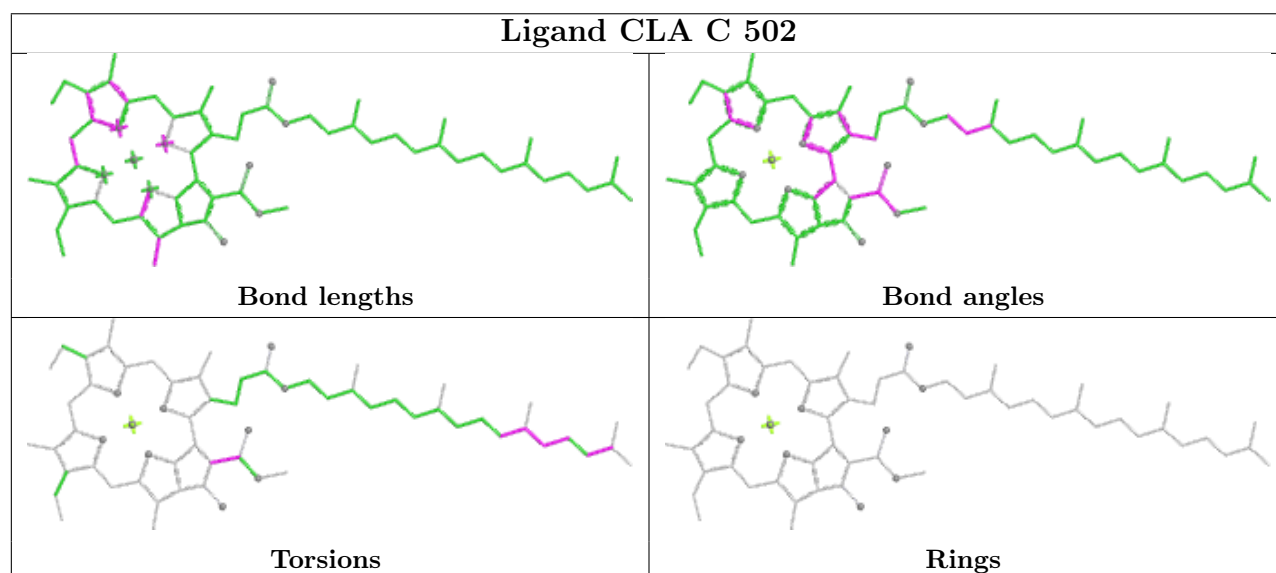
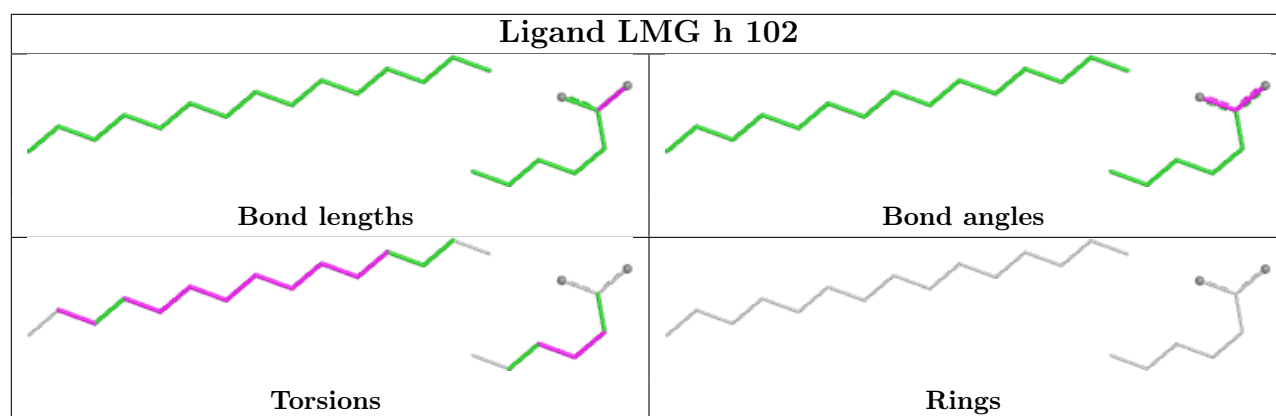


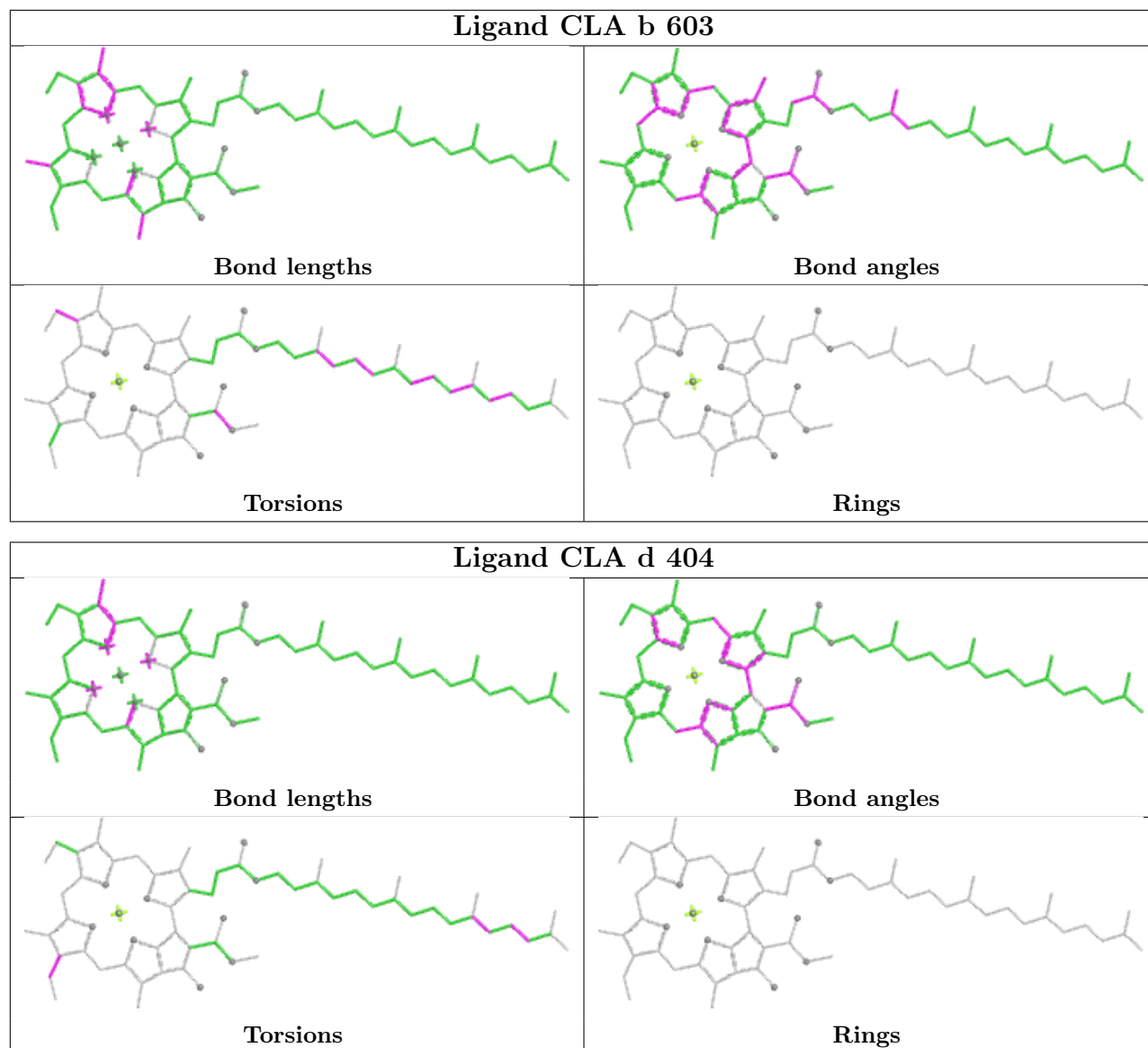


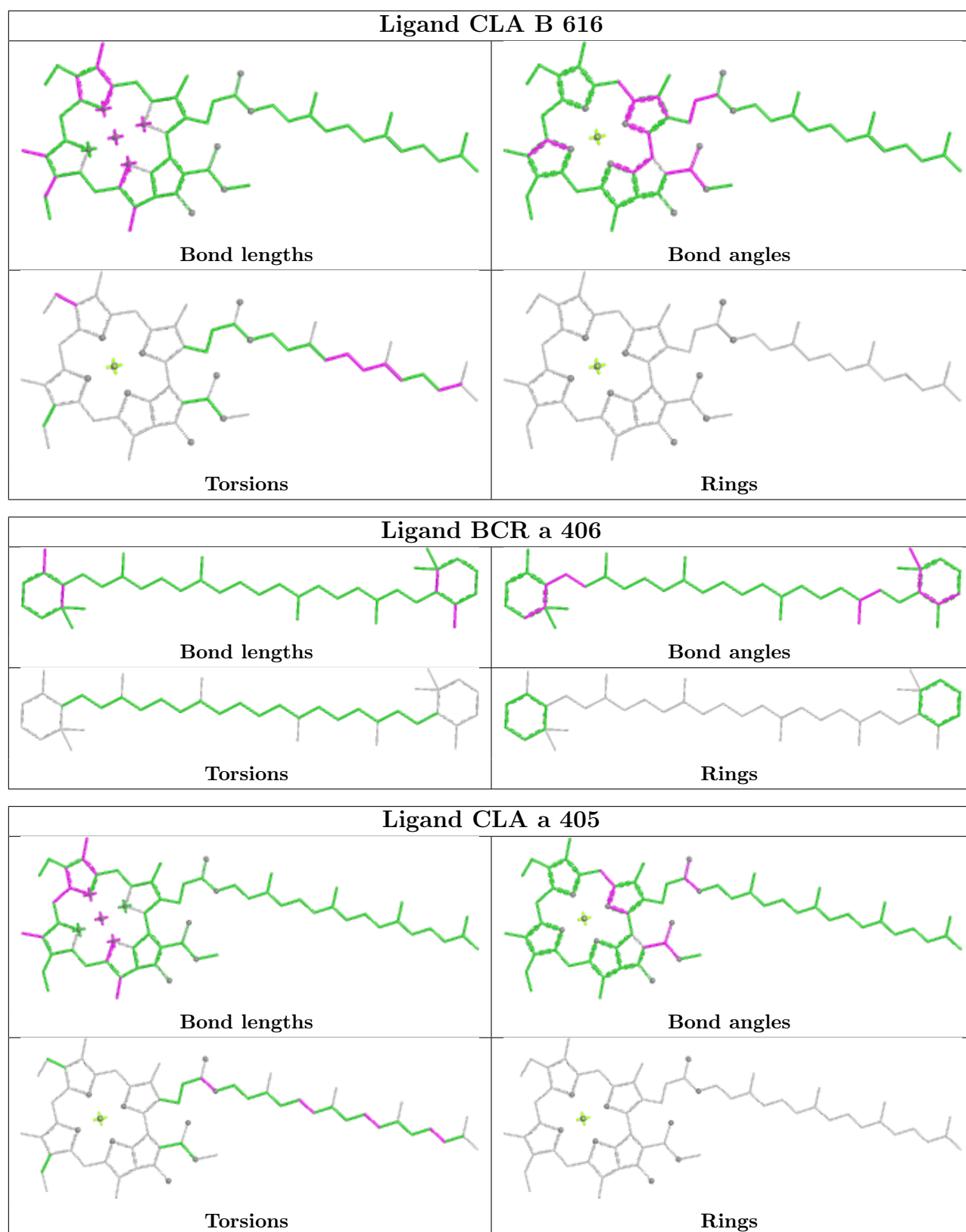


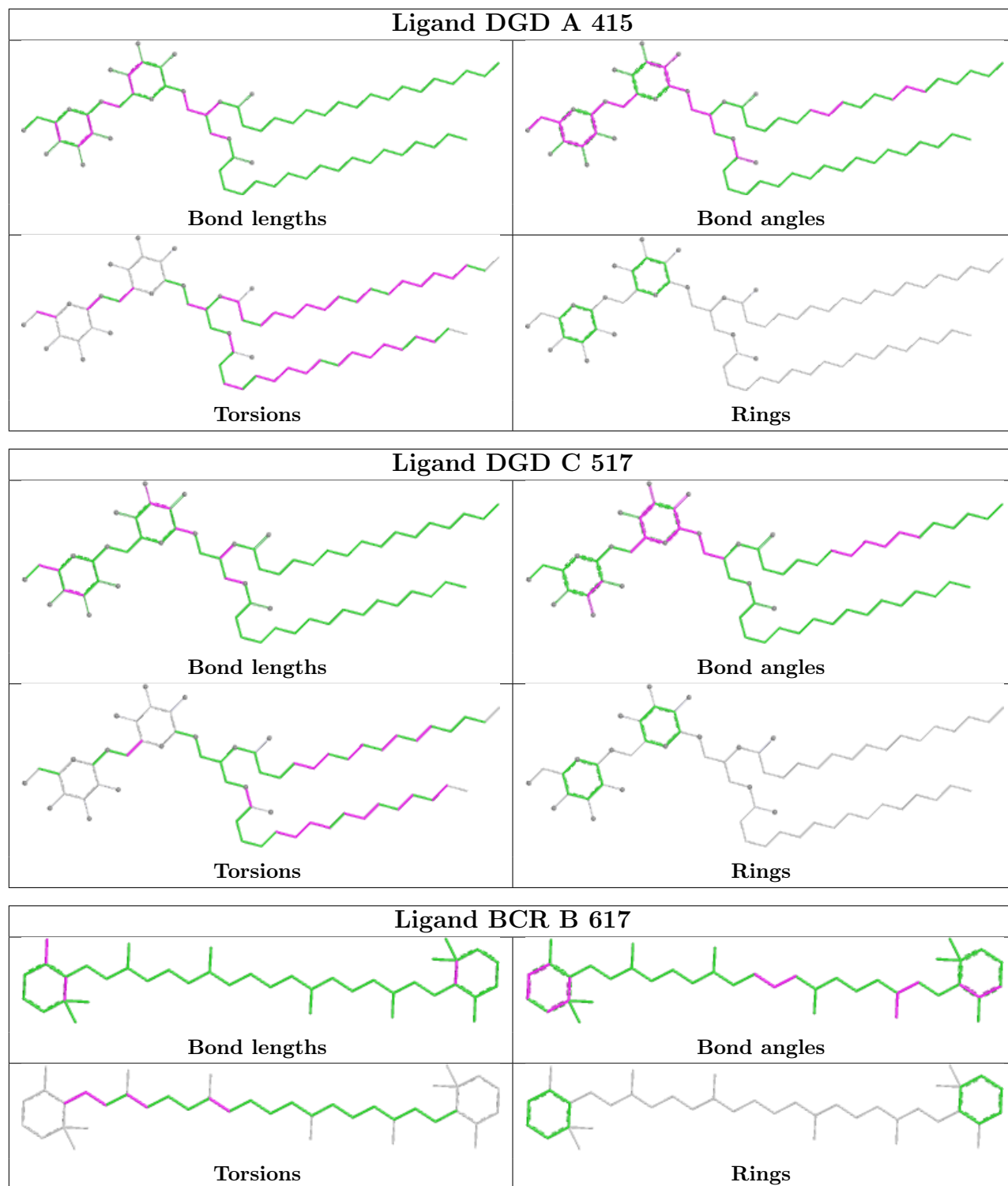


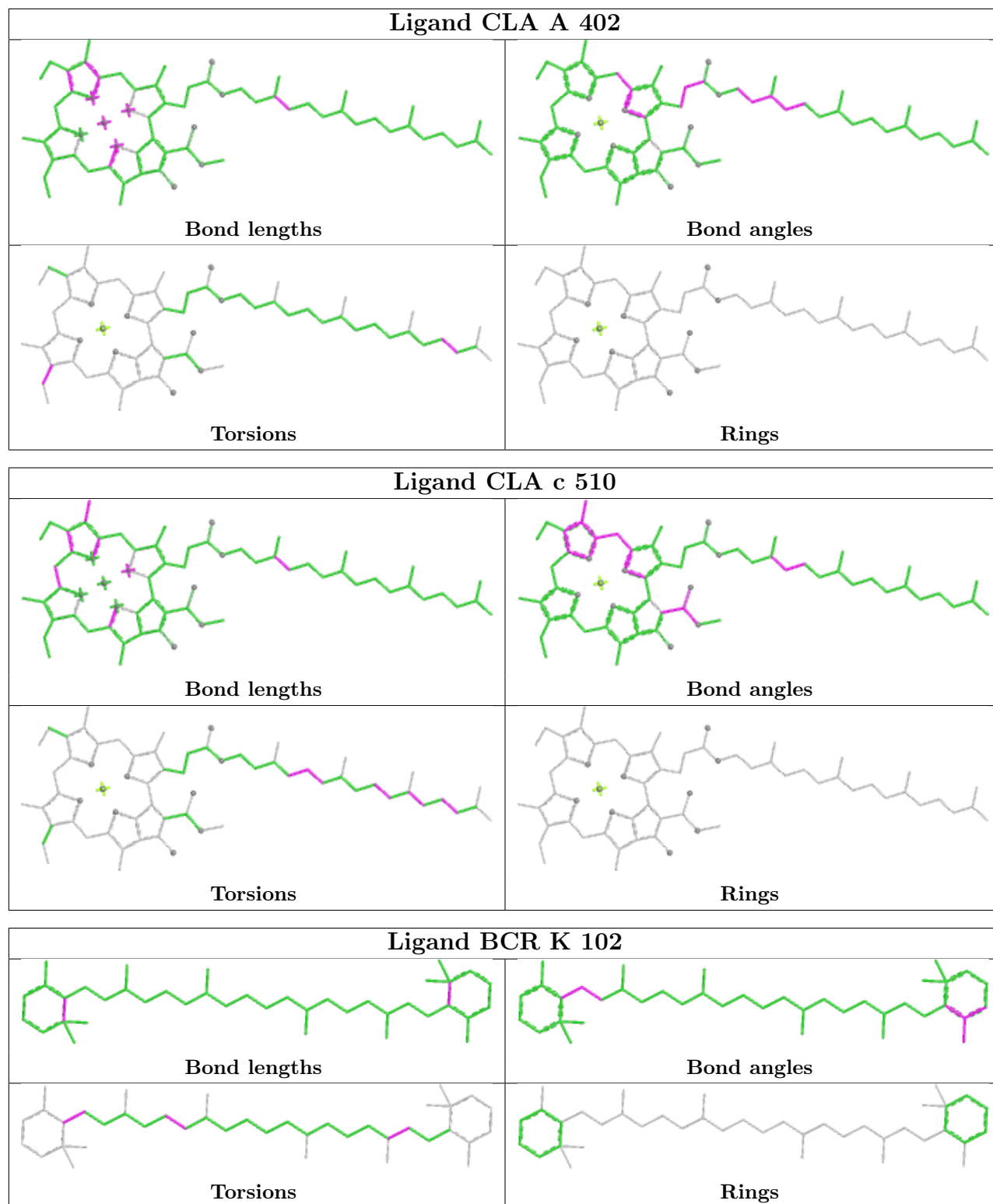


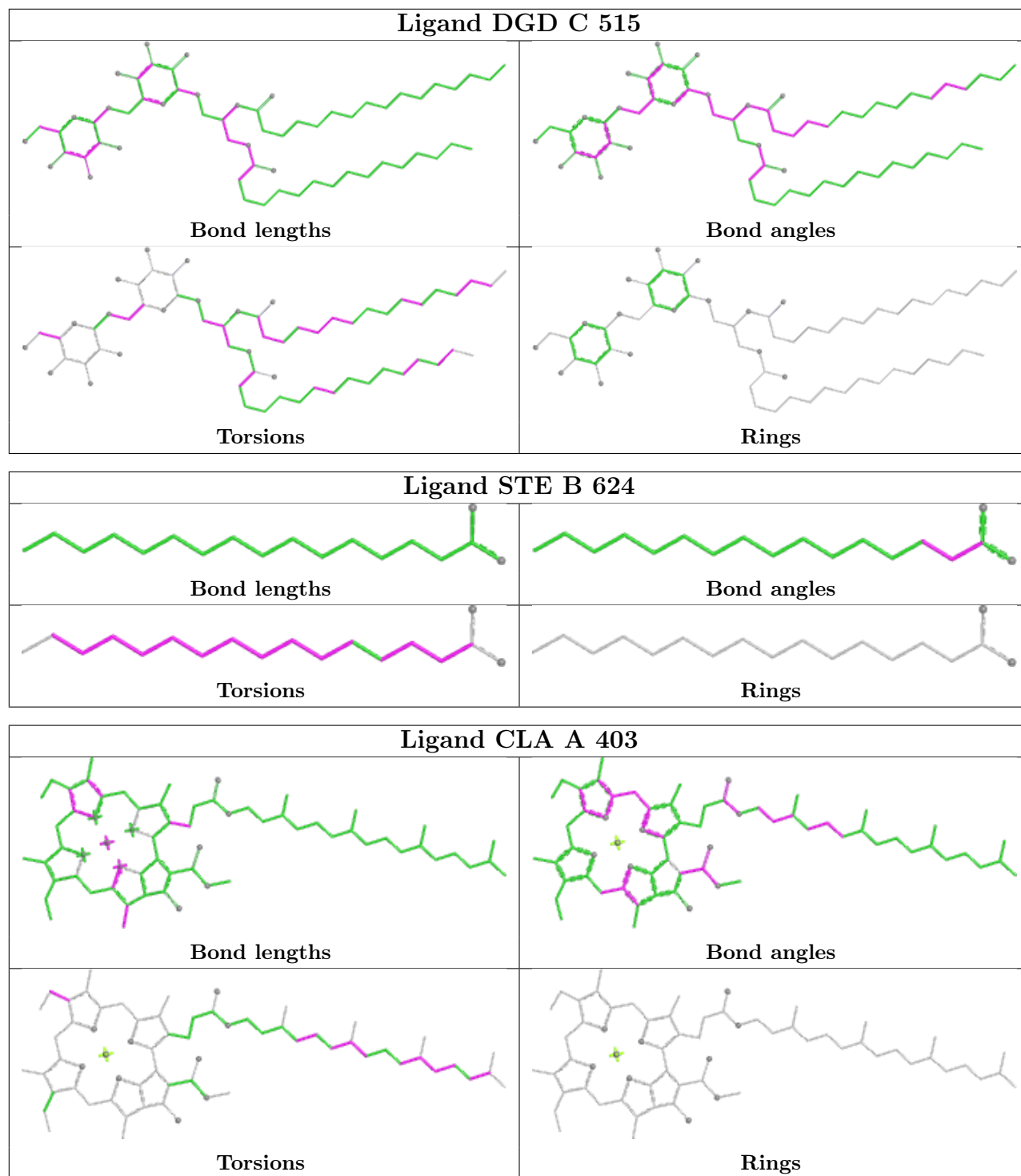


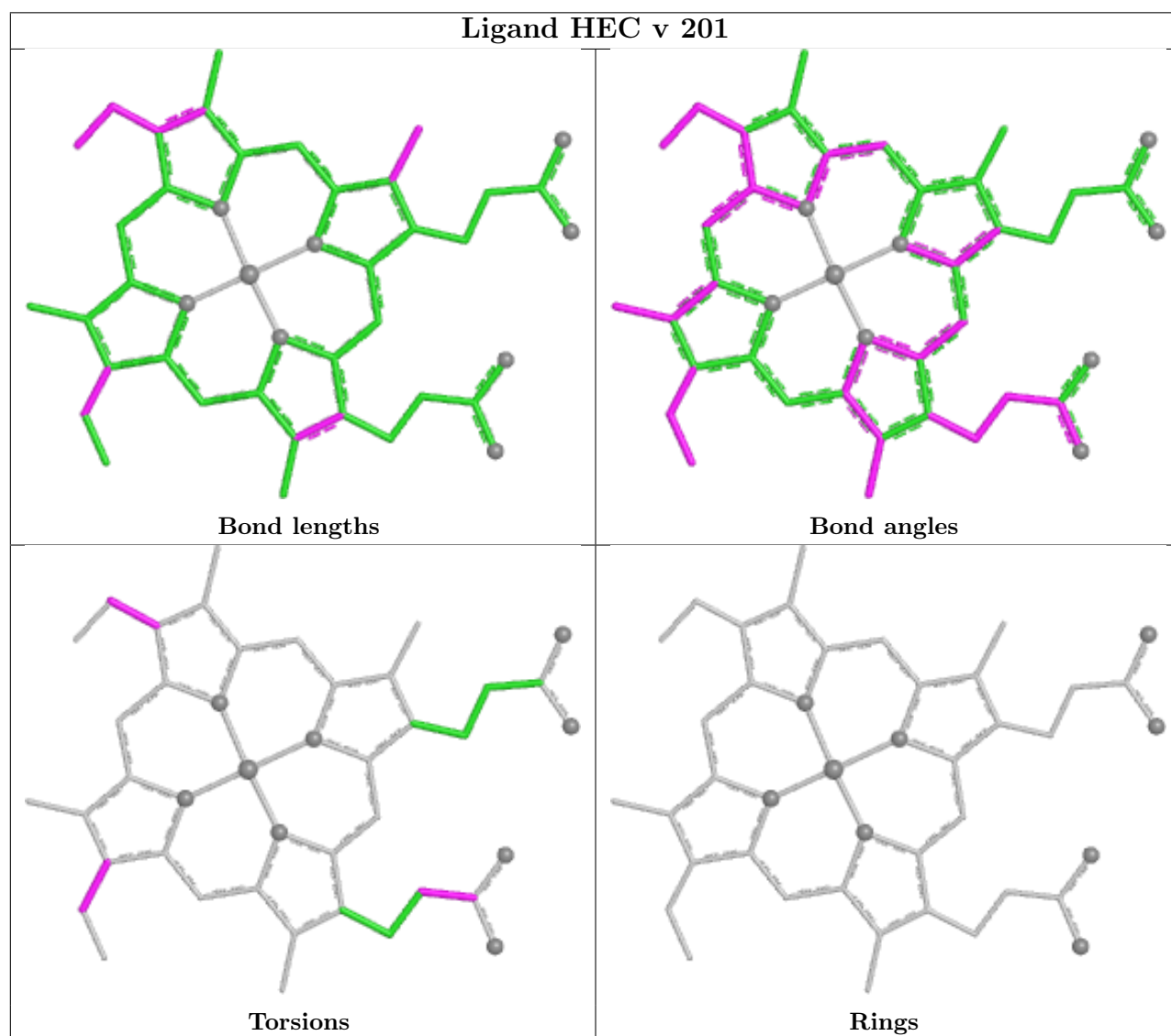
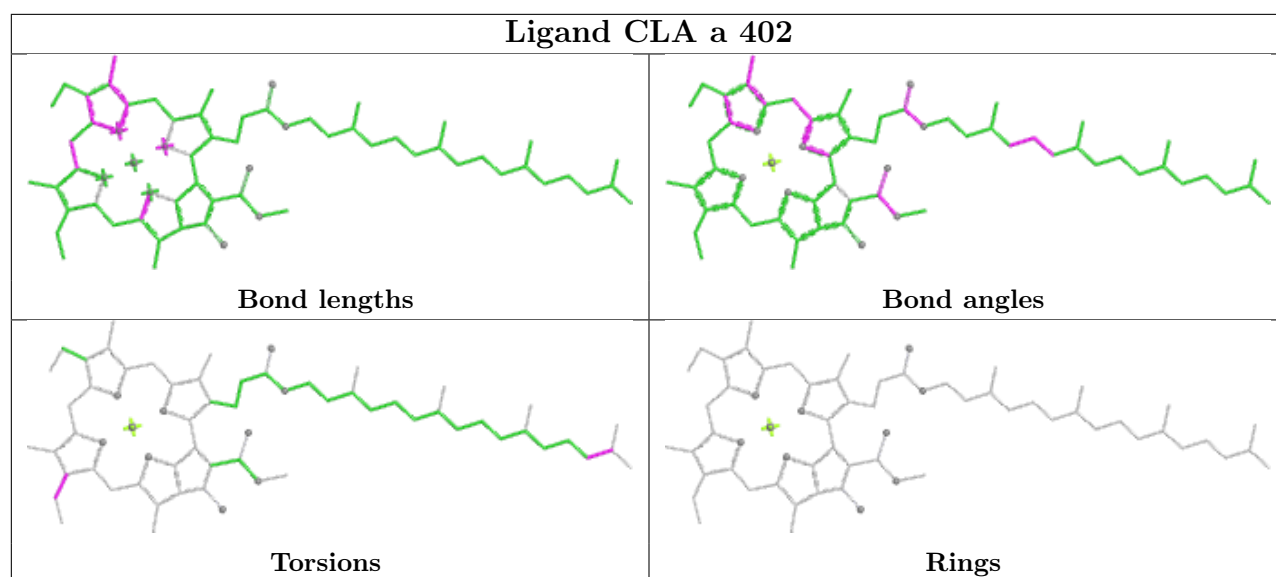


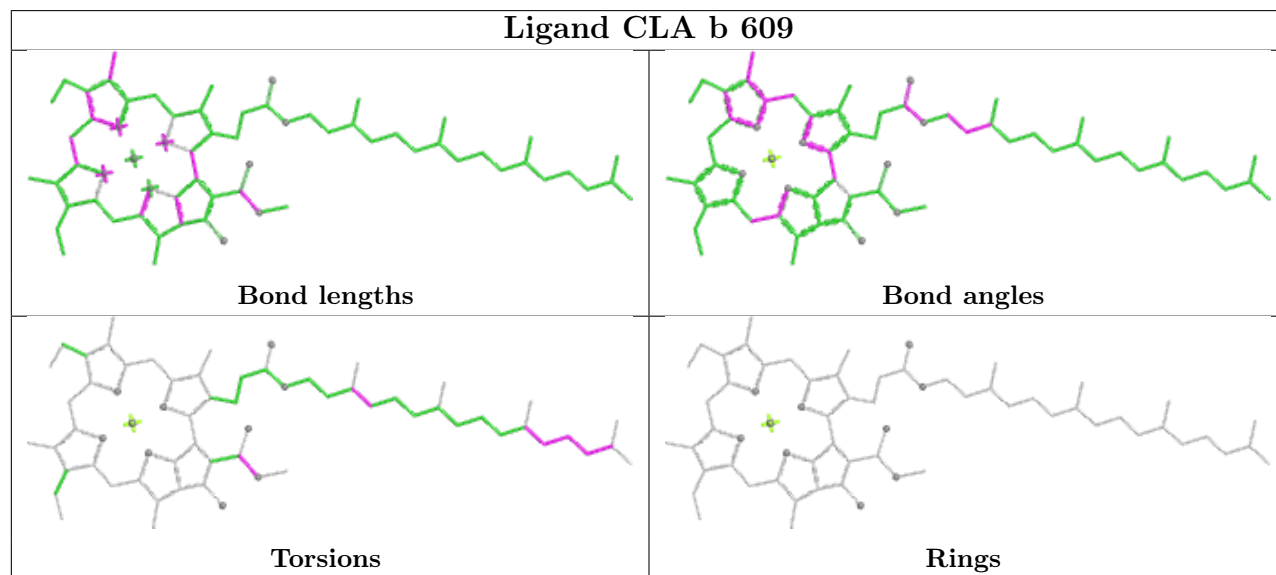
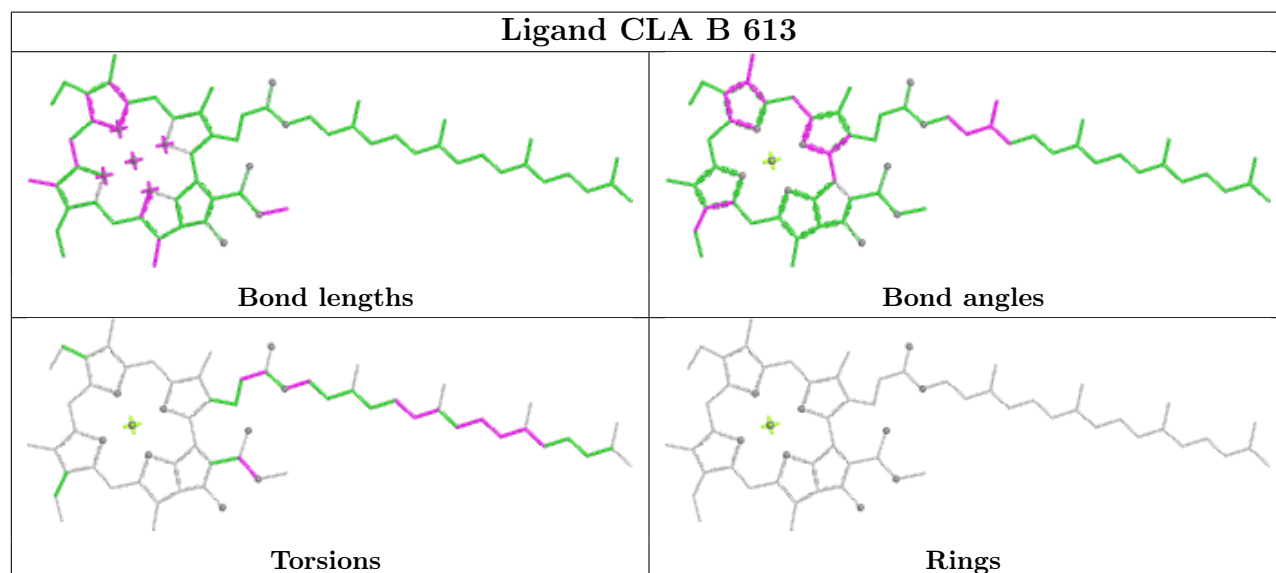
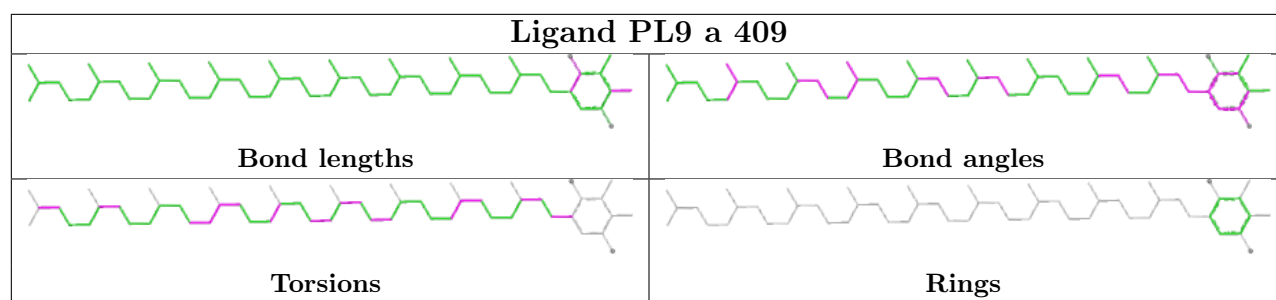


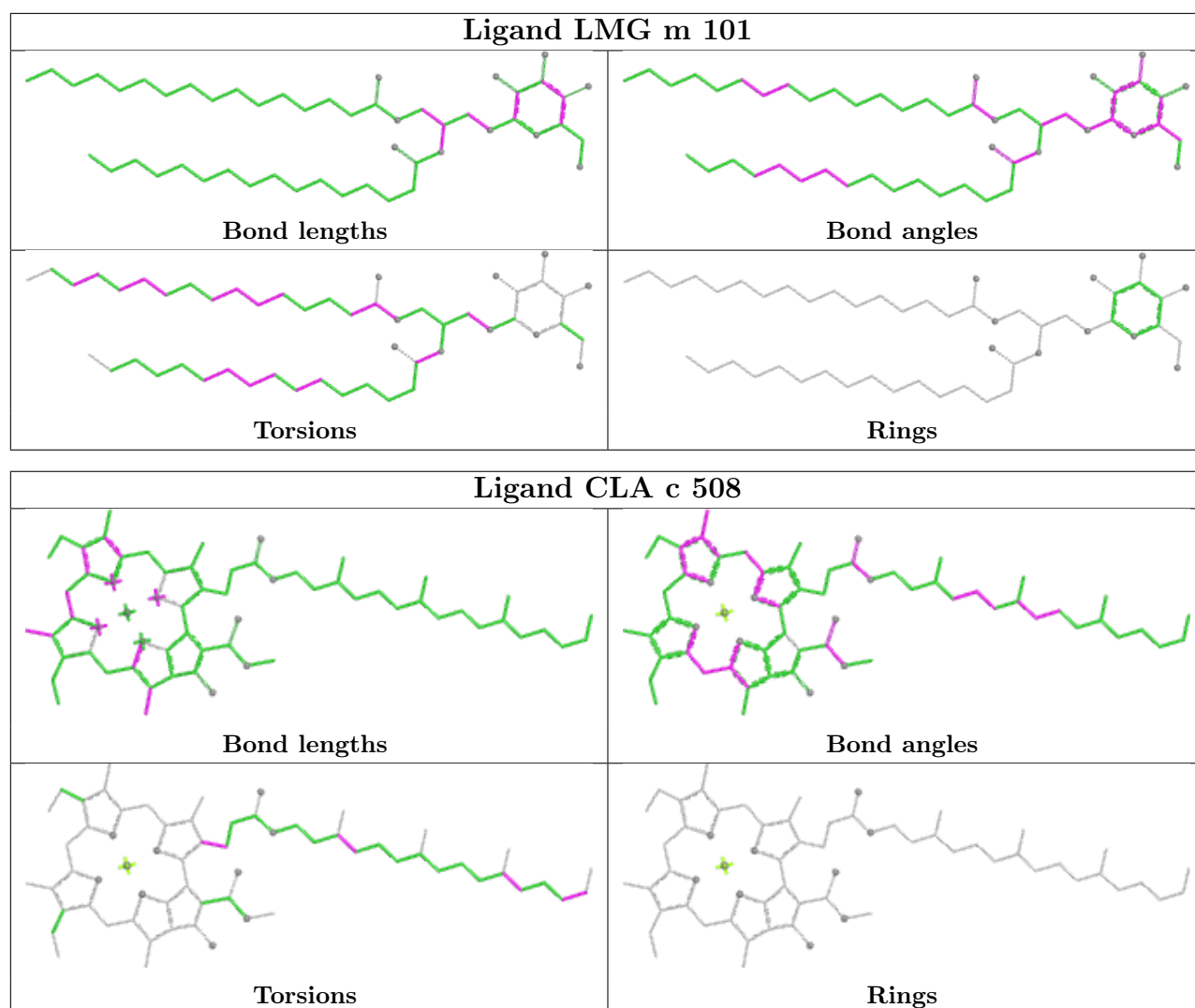


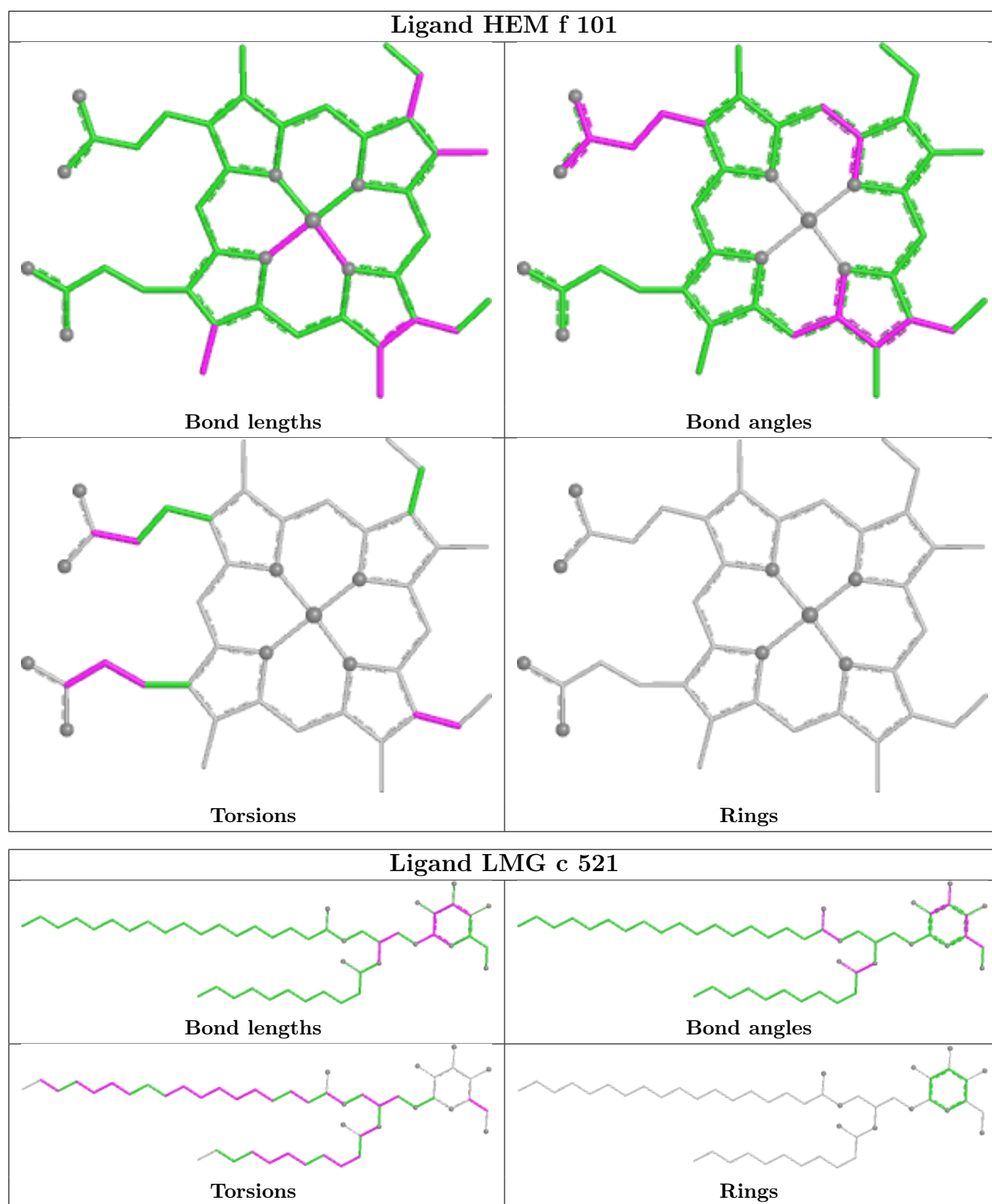












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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	334/344 (97%)	-0.58	0 100 100	23, 31, 52, 80	0
1	a	334/344 (97%)	-0.49	3 (0%) 81 83	22, 33, 60, 76	0
2	B	505/510 (99%)	-0.42	4 (0%) 82 84	18, 35, 63, 92	4 (0%)
2	b	505/510 (99%)	-0.27	6 (1%) 76 78	24, 39, 72, 109	0
3	C	442/461 (95%)	-0.39	0 100 100	16, 38, 54, 83	1 (0%)
3	c	451/461 (97%)	-0.26	3 (0%) 84 86	20, 42, 62, 92	2 (0%)
4	D	341/352 (96%)	-0.57	1 (0%) 90 91	22, 32, 51, 84	0
4	d	341/352 (96%)	-0.41	0 100 100	23, 36, 58, 86	1 (0%)
5	E	82/84 (97%)	0.15	2 (2%) 59 62	31, 55, 72, 78	1 (1%)
5	e	82/84 (97%)	0.25	1 (1%) 76 78	42, 63, 79, 91	0
6	F	34/45 (75%)	-0.07	0 100 100	37, 45, 70, 93	0
6	f	34/45 (75%)	0.08	0 100 100	45, 53, 84, 96	0
7	H	65/66 (98%)	-0.25	2 (3%) 51 53	32, 43, 61, 73	0
7	h	63/66 (95%)	0.02	2 (3%) 50 52	43, 52, 62, 76	0
8	I	35/38 (92%)	-0.38	0 100 100	31, 40, 68, 84	0
8	i	35/38 (92%)	-0.21	0 100 100	33, 42, 78, 84	0
9	J	36/40 (90%)	-0.00	0 100 100	36, 52, 82, 96	0
9	j	36/40 (90%)	0.18	1 (2%) 55 57	41, 55, 89, 101	0
10	K	37/46 (80%)	-0.01	0 100 100	44, 55, 74, 77	0
10	k	37/46 (80%)	0.18	0 100 100	48, 59, 72, 78	0
11	L	37/37 (100%)	-0.64	0 100 100	25, 32, 65, 71	0
11	l	36/37 (97%)	-0.56	0 100 100	26, 32, 72, 86	0
12	M	32/36 (88%)	-0.55	0 100 100	27, 36, 56, 69	0
12	m	31/36 (86%)	-0.54	0 100 100	28, 36, 50, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.27	2 (0%) 82 84	25, 42, 79, 134	1 (0%)
13	o	244/272 (89%)	-0.24	1 (0%) 88 90	23, 42, 81, 114	0
14	R	28/41 (68%)	0.81	1 (3%) 46 48	60, 76, 85, 102	0
14	r	28/41 (68%)	1.45	5 (17%) 3 4	68, 98, 119, 133	0
15	T	29/32 (90%)	-0.60	0 100 100	27, 33, 60, 76	0
15	t	29/32 (90%)	-0.45	1 (3%) 48 50	27, 34, 75, 94	0
16	U	97/134 (72%)	-0.26	0 100 100	31, 44, 68, 89	0
16	u	97/134 (72%)	-0.32	0 100 100	31, 42, 58, 81	0
17	V	137/163 (84%)	-0.38	0 100 100	31, 42, 58, 73	0
17	v	137/163 (84%)	-0.12	0 100 100	33, 49, 69, 87	0
18	X	38/41 (92%)	-0.10	0 100 100	41, 53, 72, 82	0
18	x	39/41 (95%)	0.22	2 (5%) 33 35	48, 62, 91, 107	0
19	Y	27/46 (58%)	0.96	2 (7%) 20 22	54, 75, 91, 101	0
19	y	30/46 (65%)	0.74	1 (3%) 49 51	62, 75, 90, 101	0
20	Z	62/62 (100%)	0.71	3 (4%) 35 37	55, 72, 119, 128	0
20	z	62/62 (100%)	0.65	1 (1%) 70 73	61, 75, 108, 125	0
All	All	5293/5700 (92%)	-0.28	44 (0%) 82 84	16, 40, 75, 134	10 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.7
15	t	30	THR	3.9
18	x	40	SER	3.5
20	Z	62	VAL	3.4
20	z	33	TRP	3.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.95	0.07	40,48,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	FME	T	1	10/11	0.95	0.08	27,46,62,62	0
15	FME	t	1	10/11	0.95	0.07	29,43,65,65	0
12	FME	m	1	10/11	0.96	0.07	35,43,58,66	0
8	FME	i	1	10/11	0.96	0.10	39,48,60,60	0
12	FME	M	1	10/11	0.96	0.08	39,53,66,71	0

6.3 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	STE	b	626	10/20	0.74	0.20	45,57,66,79	0
32	STE	b	625	20/20	0.76	0.17	45,67,80,91	0
32	STE	I	101	15/20	0.76	0.19	43,60,76,80	0
26	PL9	a	409	55/55	0.77	0.18	44,72,88,94	0
29	LHG	A	413	49/49	0.77	0.15	48,83,110,124	0
32	STE	E	101	12/20	0.77	0.18	52,76,90,92	0
32	STE	m	102	12/20	0.78	0.19	49,64,81,90	0
32	STE	j	101	12/20	0.79	0.14	42,57,69,72	0
27	LMG	h	102	23/55	0.79	0.19	47,65,83,88	0
32	STE	c	522	12/20	0.80	0.13	58,71,85,89	0
26	PL9	A	410	55/55	0.80	0.16	46,66,88,93	0
29	LHG	e	101	42/49	0.80	0.15	64,84,110,118	0
32	STE	a	415	12/20	0.81	0.14	45,68,76,82	0
32	STE	C	519	16/20	0.81	0.14	45,58,76,76	0
32	STE	a	413	10/20	0.81	0.15	40,65,68,69	0
32	STE	H	103	18/20	0.82	0.18	54,82,92,98	0
32	STE	B	625	16/20	0.82	0.14	37,64,85,88	0
32	STE	B	627	16/20	0.82	0.19	39,47,69,72	0
27	LMG	c	521	48/55	0.83	0.15	50,77,103,106	0
27	LMG	b	623	55/55	0.84	0.15	46,71,92,102	0
32	STE	d	412	20/20	0.84	0.13	47,65,79,80	0
30	DGD	o	301	44/66	0.84	0.14	38,58,81,95	0
22	CLA	b	601	65/65	0.84	0.12	46,66,84,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	STE	b	621	16/20	0.85	0.14	41,52,70,71	0
32	STE	b	622	20/20	0.85	0.12	37,59,81,84	0
32	STE	D	413	15/20	0.85	0.17	33,40,65,65	0
28	SQD	a	412	36/54	0.85	0.14	32,66,92,99	0
27	LMG	D	410	32/55	0.86	0.13	36,58,75,85	0
28	SQD	f	102	41/54	0.86	0.14	57,92,112,114	0
32	STE	T	102	15/20	0.86	0.14	52,65,79,81	0
32	STE	b	624	16/20	0.86	0.14	44,61,82,89	0
30	DGD	A	415	66/66	0.86	0.11	47,63,79,89	0
27	LMG	A	411	48/55	0.87	0.11	43,58,72,79	0
32	STE	c	520	20/20	0.87	0.12	43,58,91,99	0
28	SQD	A	414	39/54	0.87	0.13	44,62,91,95	0
32	STE	d	411	17/20	0.87	0.13	44,57,65,77	0
32	STE	J	101	12/20	0.87	0.12	46,58,69,77	0
32	STE	B	620	17/20	0.87	0.11	35,52,71,82	0
27	LMG	Y	101	48/55	0.87	0.12	32,67,84,92	0
32	STE	M	103	10/20	0.88	0.13	36,47,60,69	0
32	STE	B	626	12/20	0.88	0.14	57,69,80,85	0
28	SQD	b	620	49/54	0.88	0.10	43,59,84,98	0
32	STE	B	623	12/20	0.88	0.11	37,49,69,82	0
24	BCR	K	101	40/40	0.88	0.12	44,58,74,78	0
28	SQD	B	621	54/54	0.89	0.10	42,65,90,100	0
32	STE	M	104	18/20	0.89	0.11	35,52,79,82	0
27	LMG	c	519	37/55	0.89	0.11	40,63,78,78	0
32	STE	B	624	18/20	0.89	0.10	38,60,76,78	0
24	BCR	k	101	40/40	0.90	0.10	43,60,72,77	0
32	STE	C	520	12/20	0.90	0.10	35,49,59,59	0
27	LMG	m	101	51/55	0.90	0.10	35,54,76,95	0
22	CLA	B	601	65/65	0.90	0.10	32,62,87,99	0
27	LMG	a	414	49/55	0.90	0.10	30,59,83,100	0
32	STE	B	622	14/20	0.90	0.10	39,49,62,66	0
32	STE	C	518	12/20	0.90	0.11	45,56,65,67	0
32	STE	M	102	15/20	0.90	0.12	33,50,71,73	0
30	DGD	C	516	62/66	0.91	0.10	31,52,95,110	0
28	SQD	F	102	36/54	0.91	0.11	45,74,95,99	0
24	BCR	c	514	40/40	0.91	0.10	41,60,71,72	0
24	BCR	h	101	40/40	0.91	0.09	34,52,73,80	0
32	STE	D	412	20/20	0.91	0.10	36,52,75,78	0
27	LMG	M	101	51/55	0.91	0.09	32,49,73,81	0
22	CLA	c	512	65/65	0.91	0.10	38,54,82,93	0
22	CLA	C	513	65/65	0.91	0.10	39,61,91,95	0
24	BCR	K	102	40/40	0.91	0.09	36,54,68,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	DGD	H	102	62/66	0.92	0.09	30,47,59,66	0
30	DGD	h	103	62/66	0.92	0.09	27,47,63,72	0
22	CLA	c	513	65/65	0.92	0.10	39,65,104,105	0
24	BCR	B	618	40/40	0.92	0.07	23,39,49,53	0
24	BCR	D	405	40/40	0.92	0.10	23,46,83,85	0
24	BCR	d	406	40/40	0.92	0.11	30,52,86,93	0
24	BCR	H	101	40/40	0.93	0.08	33,48,66,72	0
24	BCR	K	103	40/40	0.93	0.10	37,51,65,66	0
29	LHG	d	409	39/49	0.93	0.09	28,41,68,74	0
24	BCR	T	101	40/40	0.93	0.07	25,37,49,51	0
28	SQD	a	411	54/54	0.93	0.10	40,62,96,97	0
24	BCR	C	514	40/40	0.93	0.09	25,39,50,58	0
24	BCR	c	515	40/40	0.93	0.09	25,44,55,64	0
22	CLA	C	503	65/65	0.94	0.07	31,41,50,62	0
24	BCR	A	407	40/40	0.94	0.07	25,35,44,44	0
22	CLA	C	510	65/65	0.94	0.07	25,43,59,61	0
24	BCR	b	617	40/40	0.94	0.07	24,41,52,54	0
24	BCR	b	618	40/40	0.94	0.07	23,39,52,56	0
24	BCR	b	619	40/40	0.94	0.07	31,46,61,65	0
24	BCR	B	619	40/40	0.94	0.07	27,43,59,67	0
22	CLA	c	505	65/65	0.94	0.08	24,40,64,67	0
29	LHG	D	409	47/49	0.94	0.10	24,51,77,89	0
29	LHG	a	410	49/49	0.94	0.10	32,52,70,77	0
22	CLA	c	509	65/65	0.94	0.08	31,47,67,72	0
22	CLA	c	511	65/65	0.94	0.09	37,52,68,71	0
27	LMG	d	410	44/55	0.94	0.09	32,54,88,100	0
22	CLA	C	512	65/65	0.94	0.09	35,53,82,90	0
24	BCR	k	102	40/40	0.94	0.09	42,53,69,69	0
30	DGD	c	517	62/66	0.94	0.08	30,50,87,88	0
28	SQD	A	412	52/54	0.94	0.09	35,58,85,88	0
22	CLA	C	509	65/65	0.95	0.08	25,46,61,69	0
27	LMG	D	407	51/55	0.95	0.09	23,55,83,89	0
22	CLA	d	405	65/65	0.95	0.09	29,48,81,89	0
23	PHO	d	401	64/64	0.95	0.07	23,38,47,59	0
22	CLA	B	615	65/65	0.95	0.07	20,37,57,63	0
24	BCR	B	617	40/40	0.95	0.06	26,38,56,56	0
22	CLA	C	511	65/65	0.95	0.08	28,48,63,72	0
22	CLA	B	616	60/65	0.95	0.10	25,38,88,95	0
22	CLA	C	502	65/65	0.95	0.07	27,40,52,54	0
22	CLA	a	403	65/65	0.95	0.09	24,41,88,95	0
22	CLA	B	606	65/65	0.95	0.07	23,36,64,71	0
22	CLA	b	606	65/65	0.95	0.08	23,39,67,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	b	609	65/65	0.95	0.08	29,44,61,69	0
22	CLA	b	614	65/65	0.95	0.07	23,39,71,79	0
22	CLA	b	615	65/65	0.95	0.07	25,39,59,59	0
24	BCR	a	406	40/40	0.95	0.06	19,33,49,50	0
22	CLA	b	616	60/65	0.95	0.08	26,43,84,91	0
22	CLA	c	503	65/65	0.95	0.07	32,42,53,59	0
22	CLA	c	504	60/65	0.95	0.07	29,44,74,85	0
22	CLA	C	504	59/65	0.95	0.07	30,42,77,79	0
22	CLA	c	506	65/65	0.95	0.09	31,49,95,99	0
22	CLA	c	507	65/65	0.95	0.08	29,44,58,67	0
29	LHG	D	411	49/49	0.95	0.08	30,45,61,73	0
22	CLA	c	508	64/65	0.95	0.08	29,44,87,101	0
22	CLA	C	505	65/65	0.95	0.08	20,40,69,72	0
22	CLA	c	510	65/65	0.95	0.07	30,47,62,65	0
24	BCR	t	101	40/40	0.95	0.06	26,37,50,54	0
30	DGD	C	515	62/66	0.95	0.10	18,39,69,77	0
22	CLA	C	506	65/65	0.95	0.09	28,45,78,89	0
30	DGD	C	517	62/66	0.95	0.08	26,47,73,79	0
26	PL9	D	406	55/55	0.95	0.06	21,33,47,53	0
22	CLA	C	508	65/65	0.95	0.07	26,42,91,97	0
30	DGD	c	518	62/66	0.95	0.08	26,52,78,83	0
26	PL9	d	407	55/55	0.95	0.06	22,34,41,47	0
22	CLA	b	608	65/65	0.96	0.07	23,42,61,66	0
22	CLA	B	609	65/65	0.96	0.07	26,38,59,66	0
22	CLA	b	610	65/65	0.96	0.08	24,37,50,55	0
22	CLA	b	611	65/65	0.96	0.06	19,35,52,60	0
22	CLA	b	612	65/65	0.96	0.07	17,34,48,58	0
22	CLA	b	613	65/65	0.96	0.07	19,35,66,78	0
22	CLA	B	610	65/65	0.96	0.07	19,33,44,50	0
22	CLA	C	507	65/65	0.96	0.07	21,39,57,60	0
22	CLA	B	611	65/65	0.96	0.06	20,31,51,54	0
22	CLA	c	501	65/65	0.96	0.06	28,40,52,55	0
22	CLA	c	502	65/65	0.96	0.07	30,42,59,62	0
22	CLA	B	612	65/65	0.96	0.07	21,32,45,58	0
22	CLA	B	614	65/65	0.96	0.08	20,37,67,77	0
22	CLA	A	402	65/65	0.96	0.06	17,27,45,49	0
22	CLA	B	604	65/65	0.96	0.07	19,32,70,84	0
22	CLA	C	501	65/65	0.96	0.06	19,35,46,56	0
22	CLA	a	402	65/65	0.96	0.06	20,30,42,55	0
22	CLA	B	605	65/65	0.96	0.07	18,31,47,49	0
29	LHG	L	101	49/49	0.96	0.07	26,43,57,64	0
22	CLA	a	405	65/65	0.96	0.08	18,37,74,82	0

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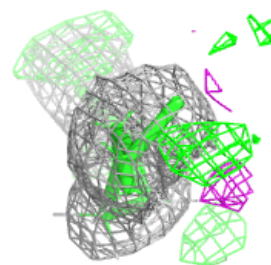
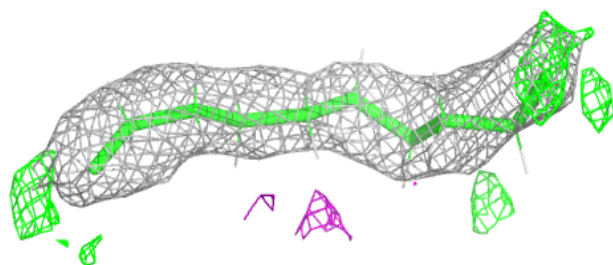
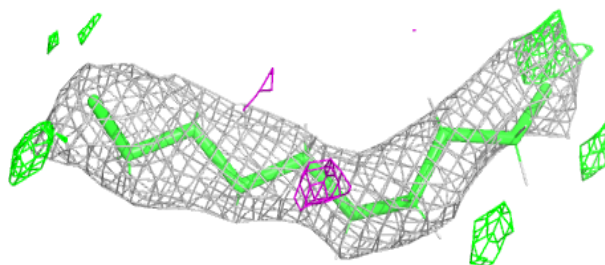
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CLA	A	403	65/65	0.96	0.08	22,34,95,103	0
22	CLA	b	602	65/65	0.96	0.08	26,43,62,65	0
29	LHG	l	101	49/49	0.96	0.07	25,46,58,60	0
22	CLA	b	603	65/65	0.96	0.07	19,36,61,68	0
22	CLA	d	403	65/65	0.96	0.07	18,35,54,59	0
22	CLA	d	404	65/65	0.96	0.06	18,30,45,53	0
22	CLA	b	604	65/65	0.96	0.07	21,34,68,80	0
23	PHO	A	404	64/64	0.96	0.06	17,28,42,48	0
30	DGD	c	516	62/66	0.96	0.08	22,43,76,81	0
23	PHO	A	405	64/64	0.96	0.06	22,32,42,46	0
23	PHO	a	404	64/64	0.96	0.06	20,31,38,44	0
22	CLA	b	605	65/65	0.96	0.06	21,34,48,52	0
22	CLA	B	608	65/65	0.96	0.06	20,34,55,59	0
33	BCT	d	402	4/4	0.96	0.07	32,38,45,52	0
22	CLA	B	603	65/65	0.97	0.07	17,32,65,67	0
22	CLA	b	607	65/65	0.97	0.07	17,36,64,75	0
29	LHG	d	408	49/49	0.97	0.07	22,42,57,67	0
22	CLA	B	602	65/65	0.97	0.06	23,35,53,66	0
22	CLA	B	613	65/65	0.97	0.07	18,31,66,75	0
22	CLA	D	402	65/65	0.97	0.06	17,27,53,64	0
22	CLA	D	403	65/65	0.97	0.06	19,28,49,59	0
29	LHG	D	408	49/49	0.97	0.07	23,42,56,61	0
22	CLA	D	404	65/65	0.97	0.07	24,41,96,106	0
33	BCT	D	401	4/4	0.97	0.07	22,26,32,35	0
22	CLA	B	607	65/65	0.97	0.07	15,35,60,62	0
34	HEM	F	101	43/43	0.97	0.08	37,48,61,62	0
34	HEM	f	101	43/43	0.97	0.09	45,58,77,83	0
25	CL	a	408	1/1	0.98	0.09	28,28,28,28	0
22	CLA	A	406	54/65	0.98	0.05	19,31,64,72	0
35	HEC	V	201	43/43	0.98	0.06	20,34,42,43	0
35	HEC	v	201	43/43	0.98	0.06	28,36,49,53	0
31	OEX	a	416	10/10	0.99	0.03	25,26,31,31	0
21	FE2	a	401	1/1	0.99	0.03	35,35,35,35	0
25	CL	A	408	1/1	0.99	0.03	28,28,28,28	0
25	CL	a	407	1/1	0.99	0.03	28,28,28,28	0
21	FE2	A	401	1/1	0.99	0.02	26,26,26,26	0
25	CL	A	409	1/1	1.00	0.02	31,31,31,31	0
31	OEX	A	416	10/10	1.00	0.02	22,26,29,31	0

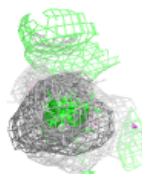
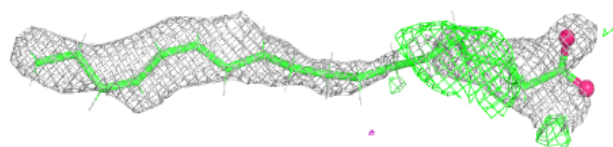
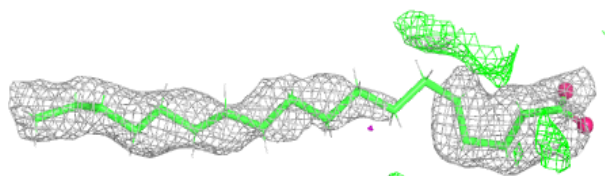
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE 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)

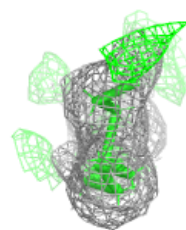
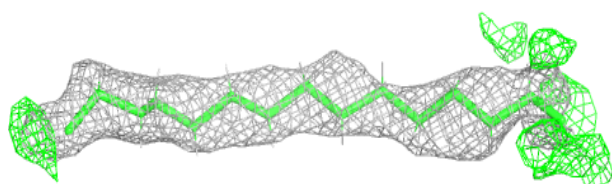
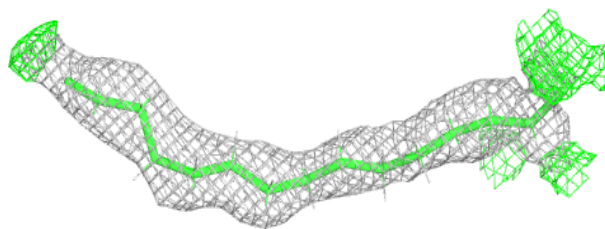
**Electron density around STE b 625:**

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

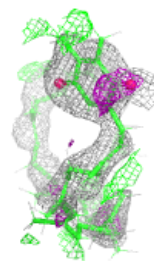
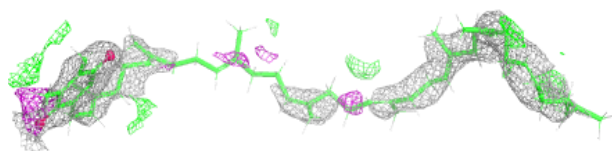
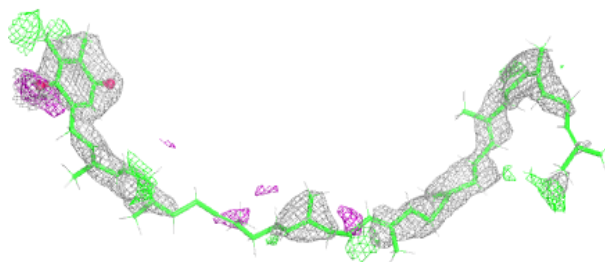


Electron density around STE I 101:

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

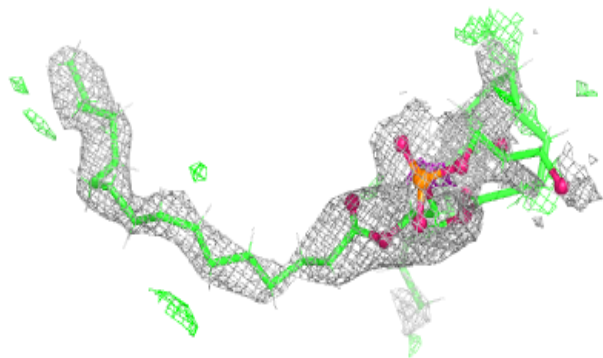
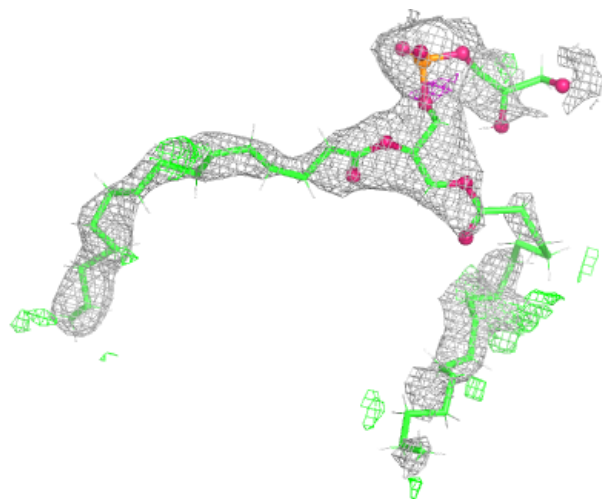
**Electron density around PL9 a 409:**

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



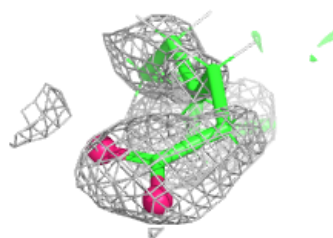
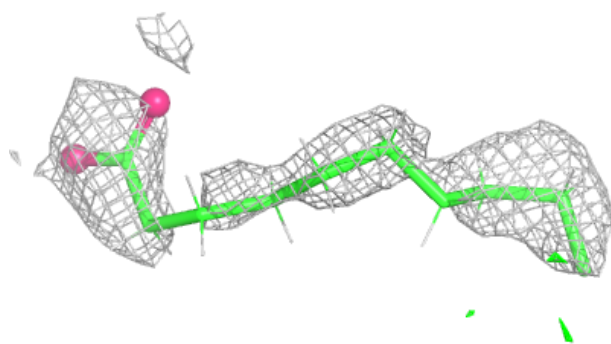
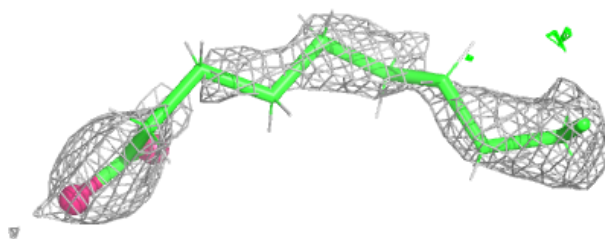
Electron density around LHG A 413:

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

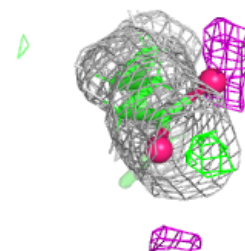
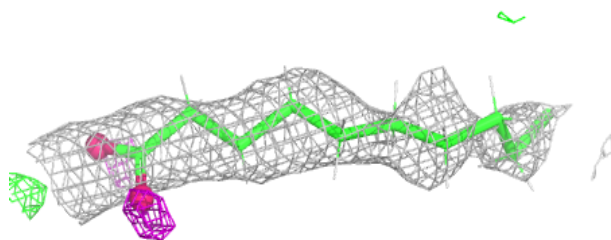
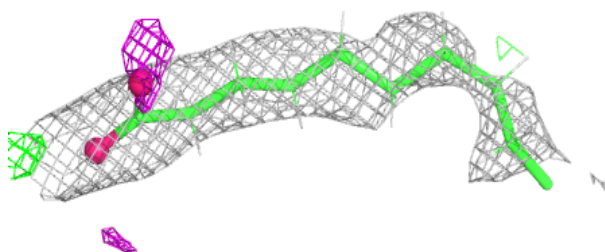


Electron density around STE E 101:

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

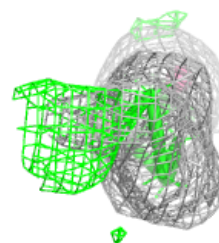
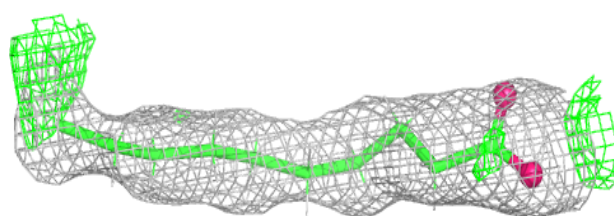
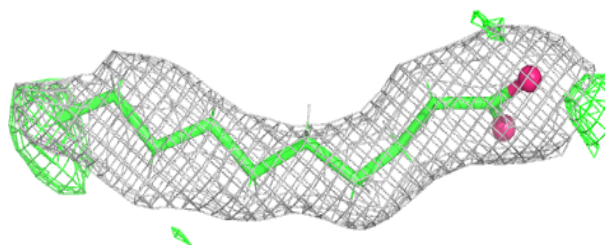
**Electron density around STE m 102:**

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

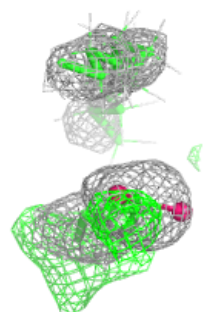
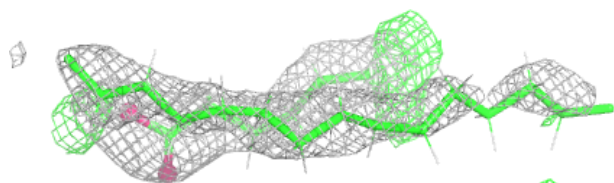
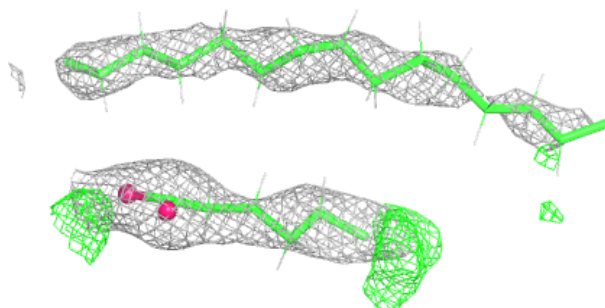


Electron density around STE j 101:

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

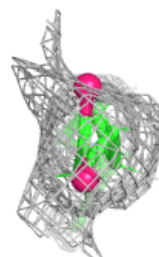
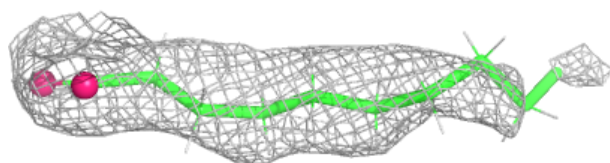
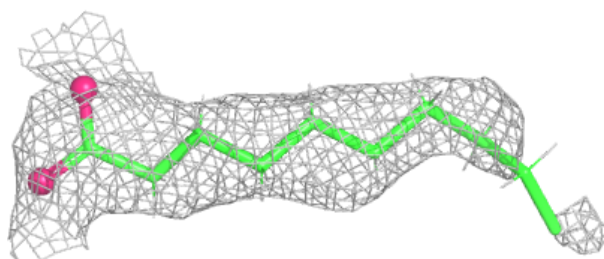
**Electron density around LMG h 102:**

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

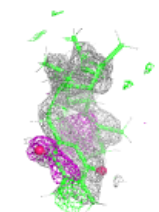
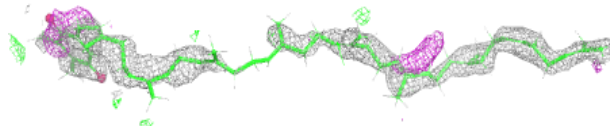
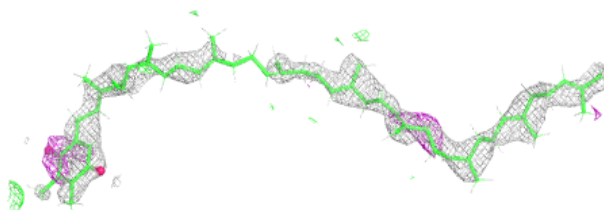


Electron density around STE c 522:

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

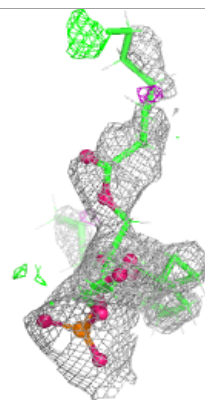
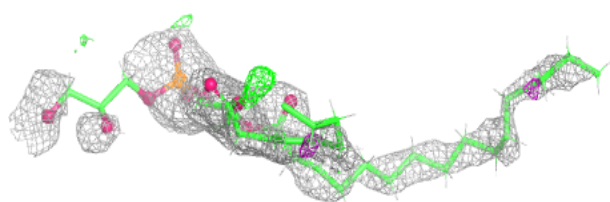
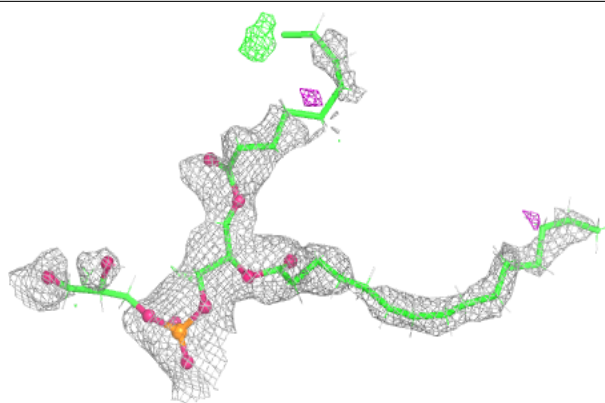
**Electron density around PL9 A 410:**

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

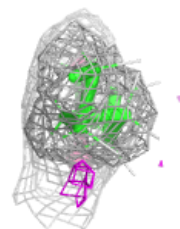
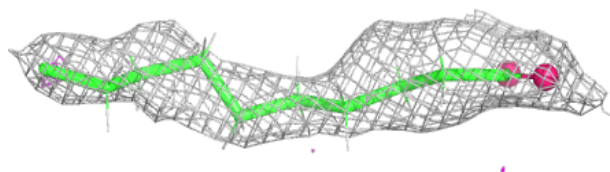
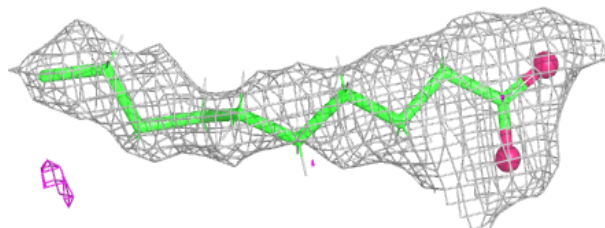


Electron density around LHG e 101:

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

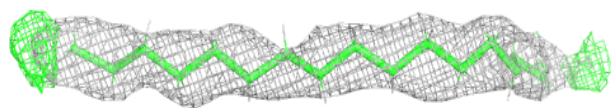
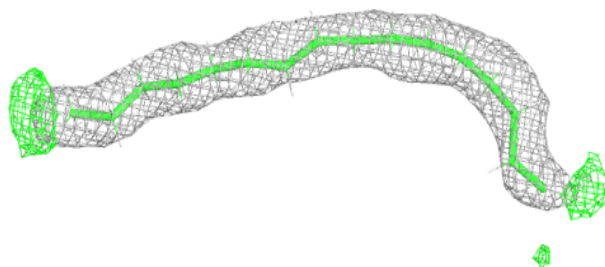
**Electron density around STE a 415:**

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

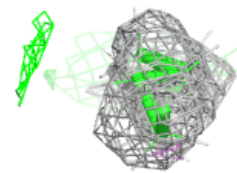
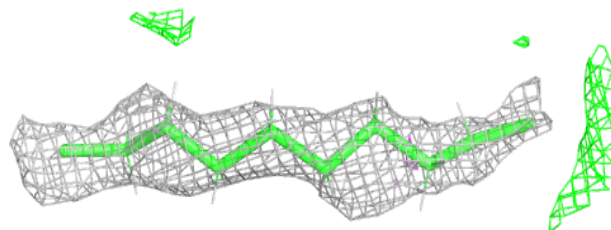
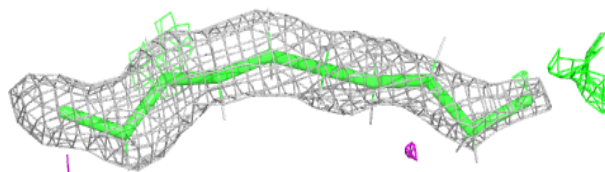


Electron density around STE C 519:

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

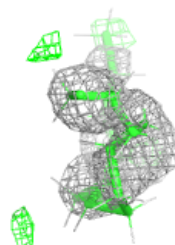
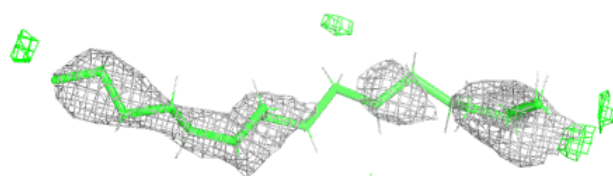
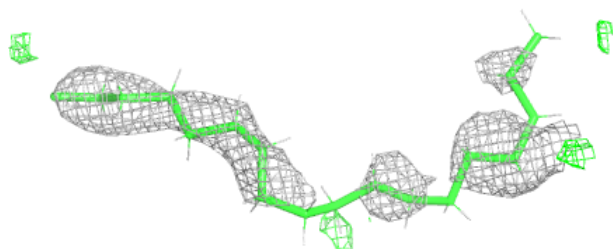
**Electron density around STE a 413:**

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

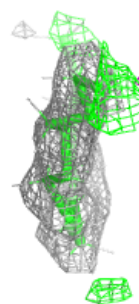
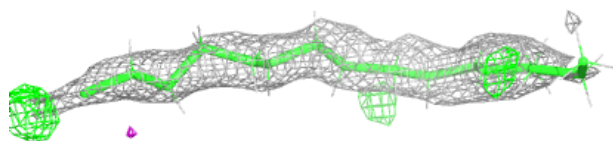


Electron density around STE H 103:

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

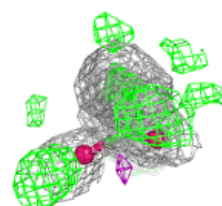
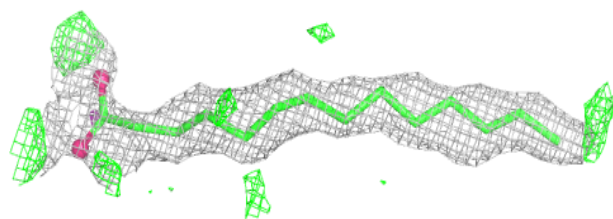
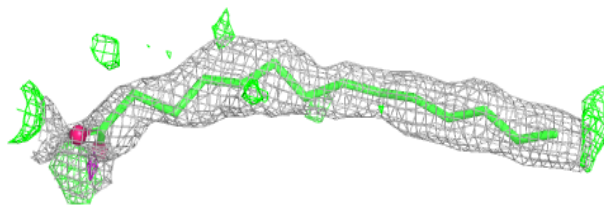
**Electron density around STE B 625:**

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

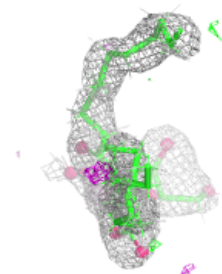
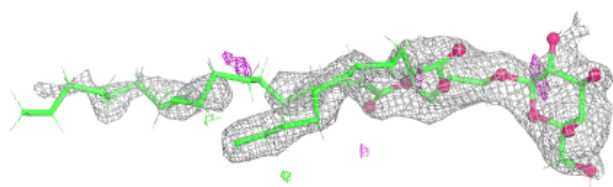
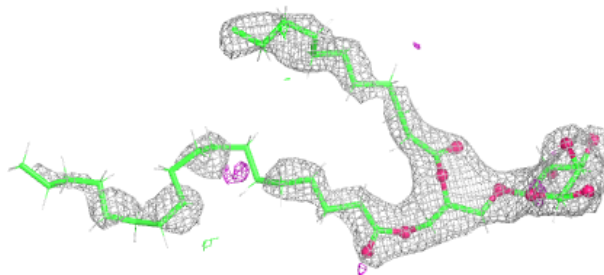


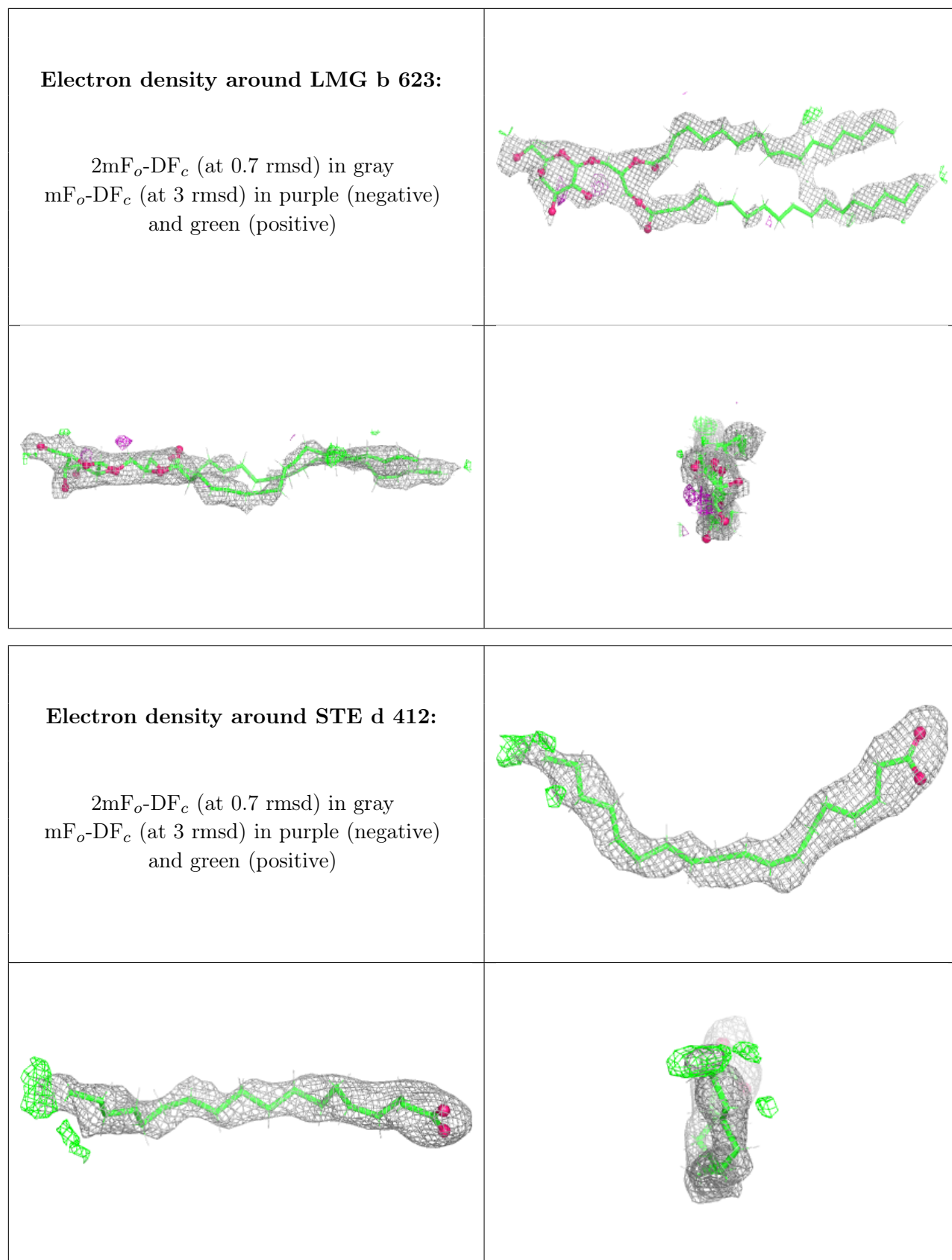
Electron density around STE B 627:

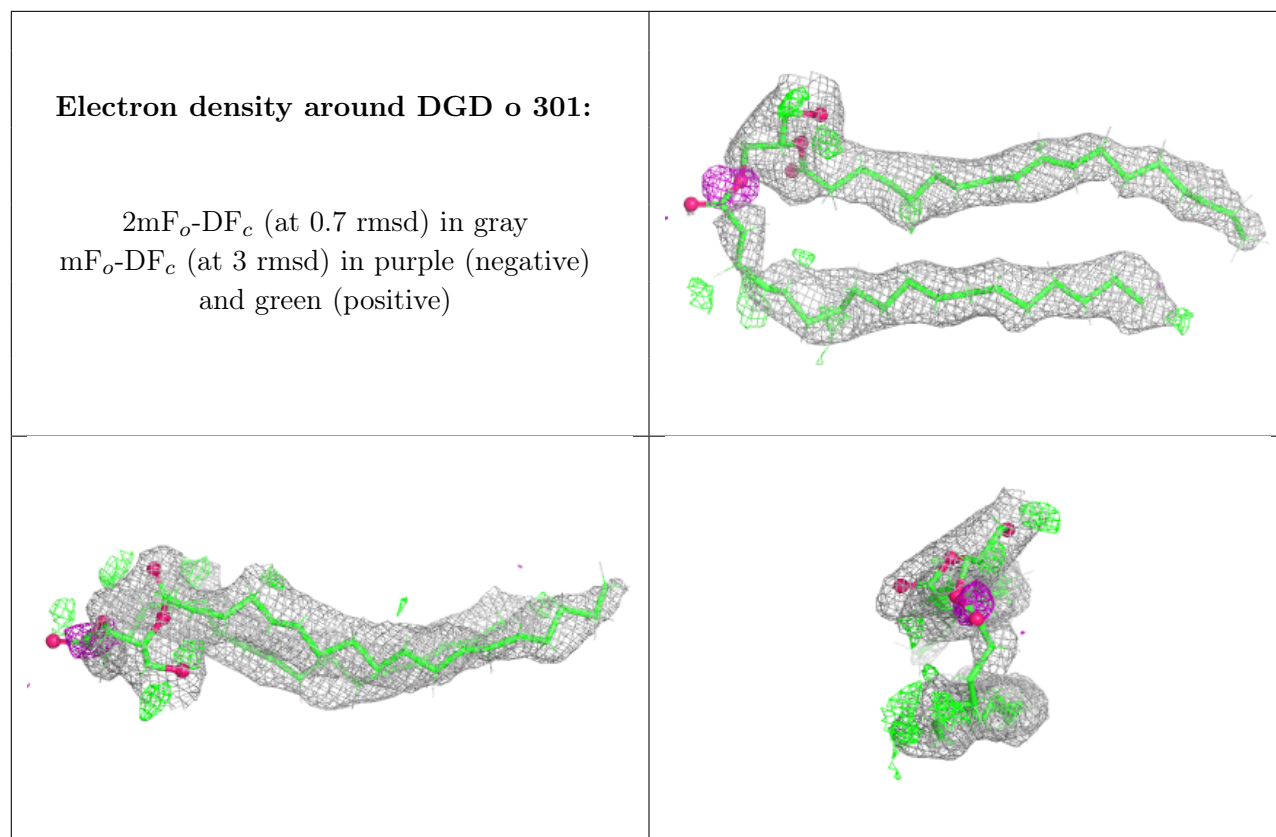
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around LMG c 521:**

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

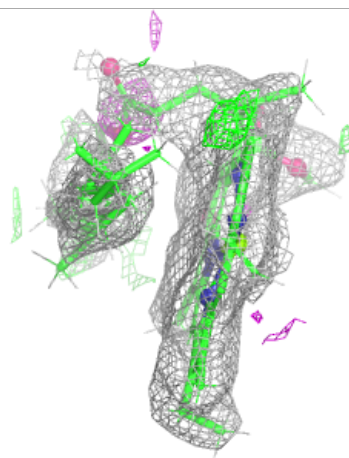
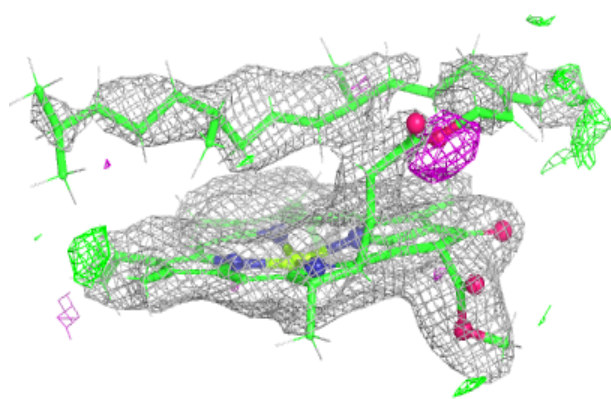
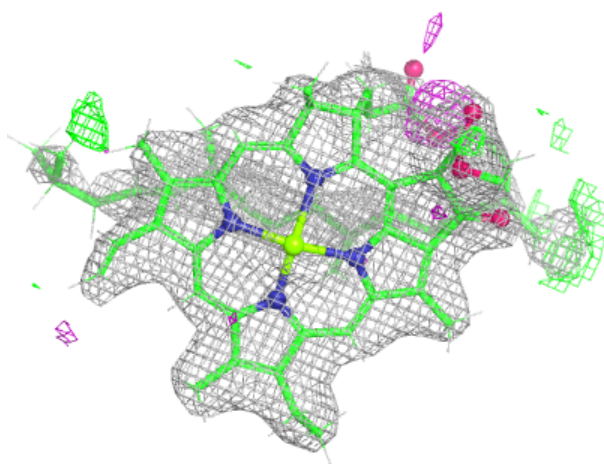






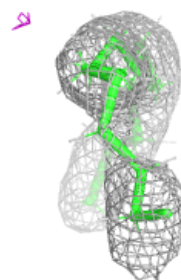
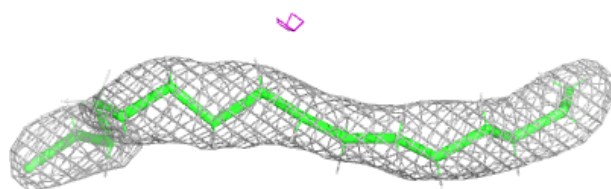
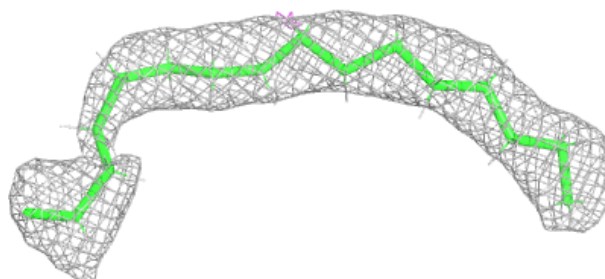
Electron density around CLA b 601:

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

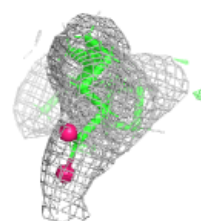
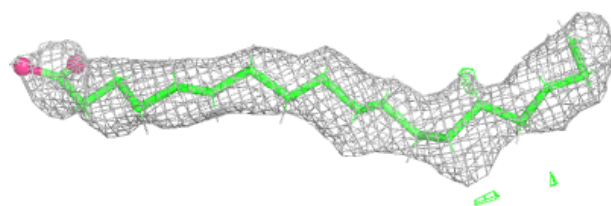
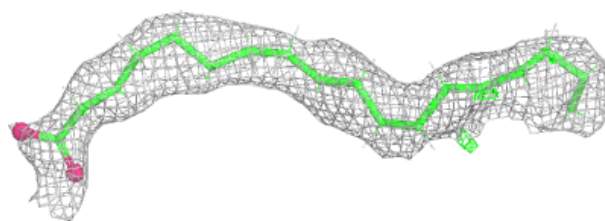


Electron density around STE b 621:

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

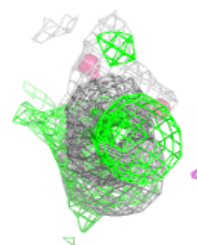
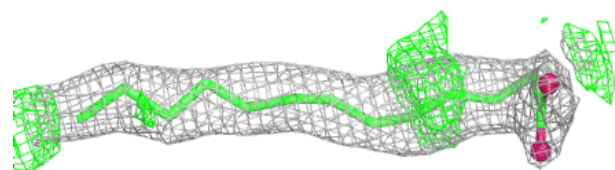
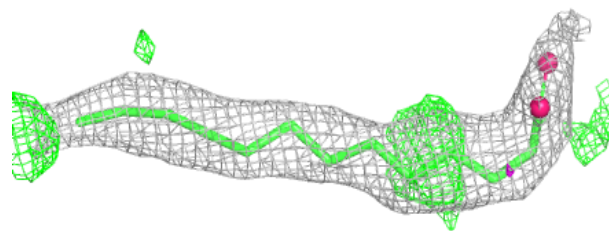
**Electron density around STE b 622:**

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

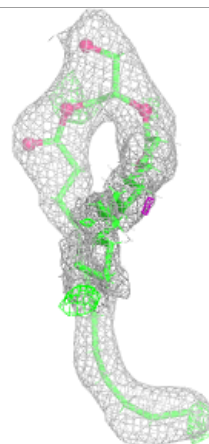
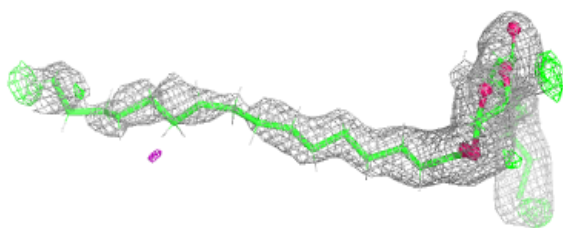
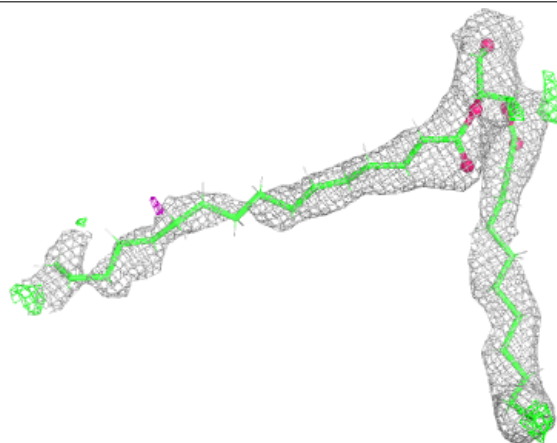


Electron density around STE D 413:

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

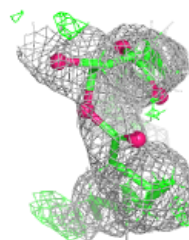
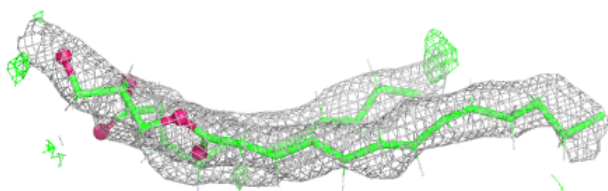
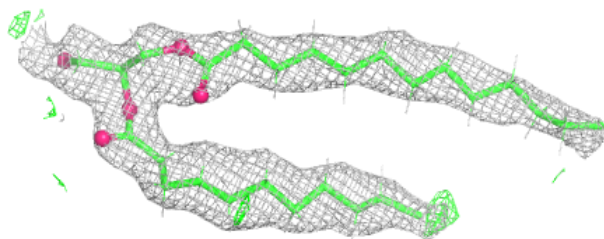
**Electron density around SQD a 412:**

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

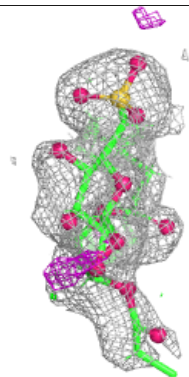
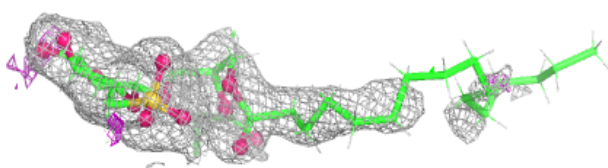
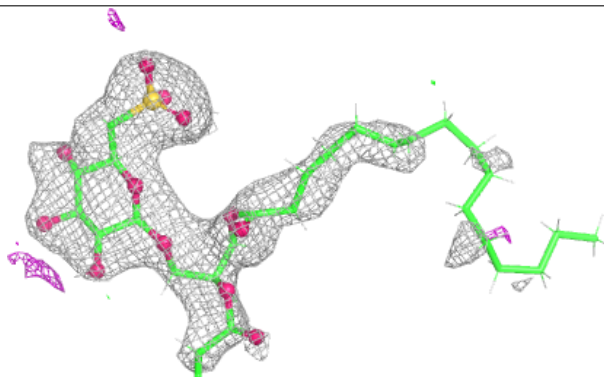


Electron density around LMG D 410:

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

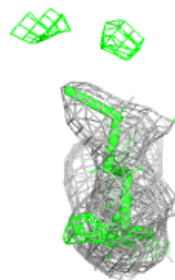
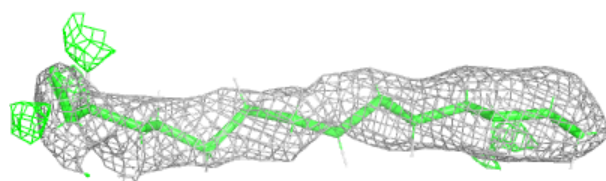
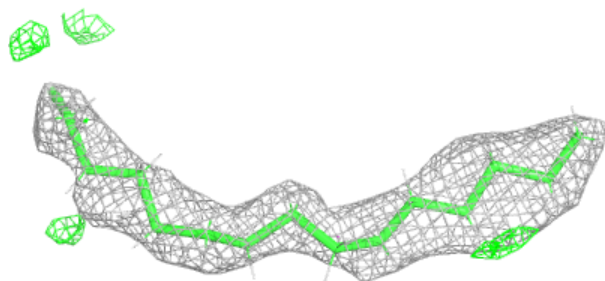
**Electron density around SQD f 102:**

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

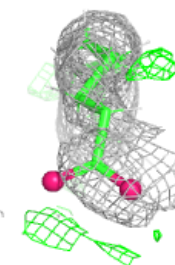
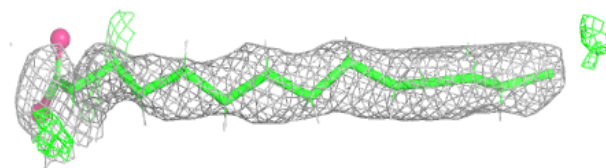
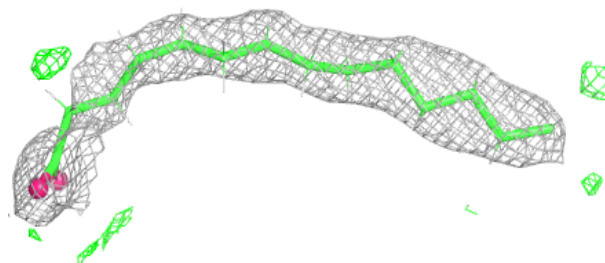


Electron density around STE T 102:

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

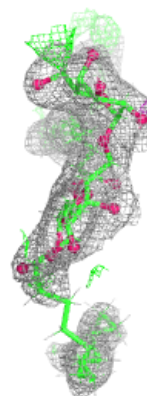
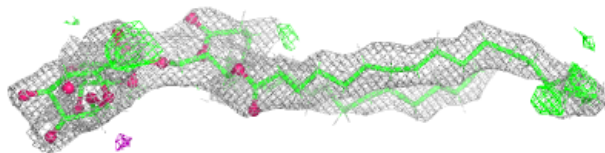
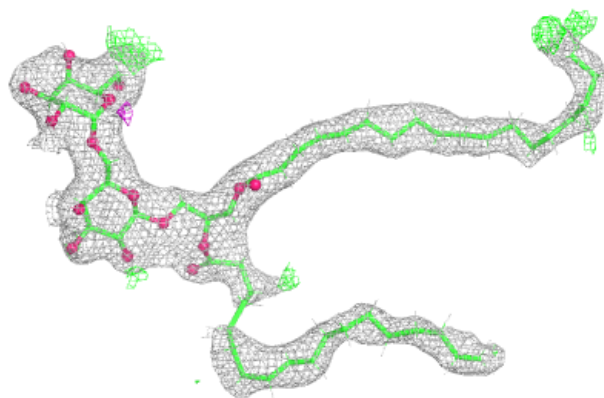
**Electron density around STE b 624:**

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

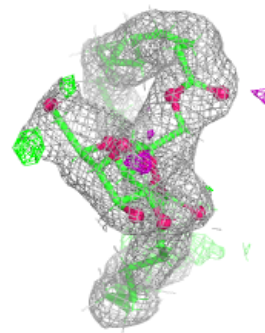
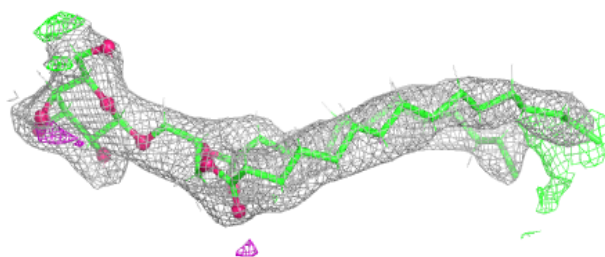
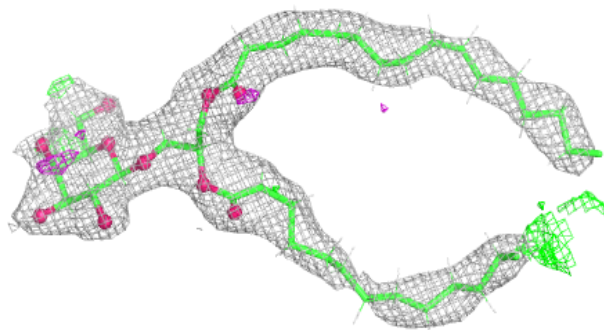


Electron density around DGD A 415:

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

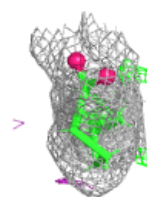
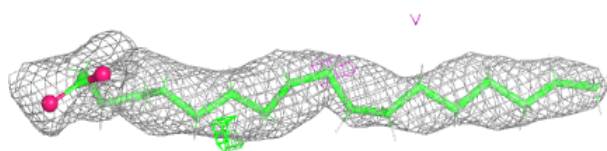
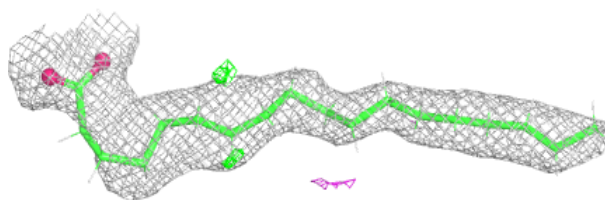
**Electron density around LMG A 411:**

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

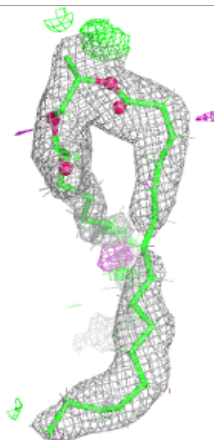
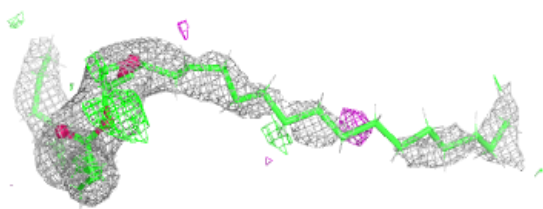
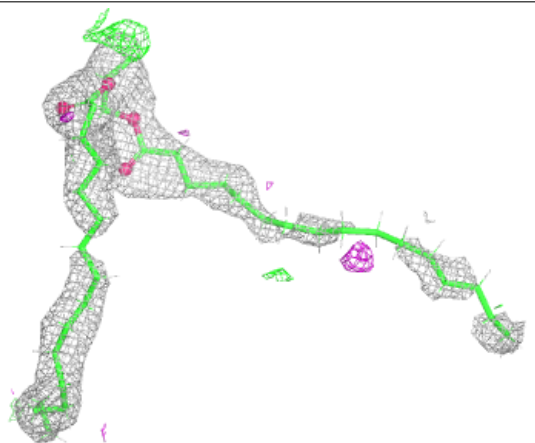


Electron density around STE c 520:

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

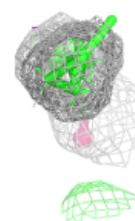
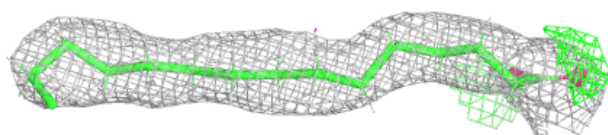
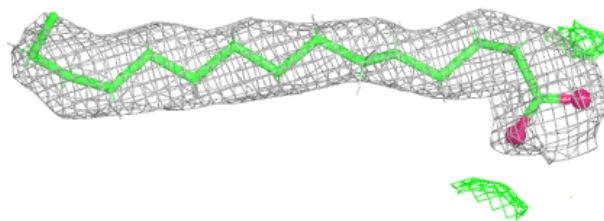
**Electron density around SQD A 414:**

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

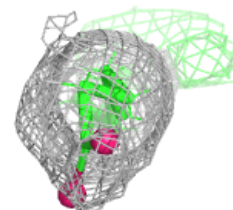
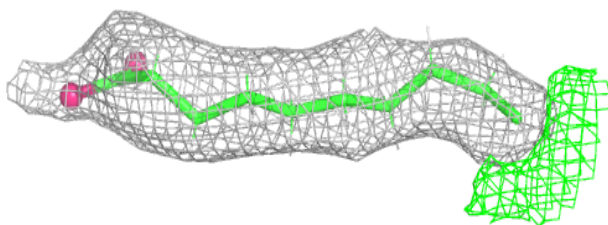
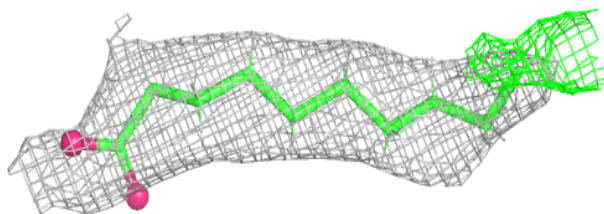


Electron density around STE d 411:

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

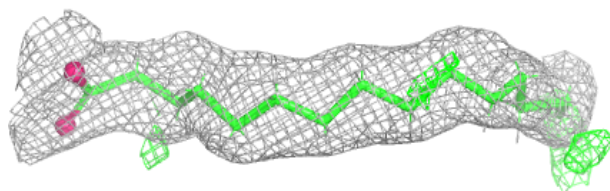
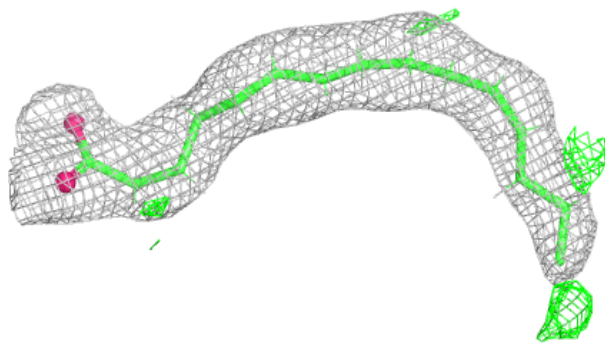
**Electron density around STE J 101:**

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



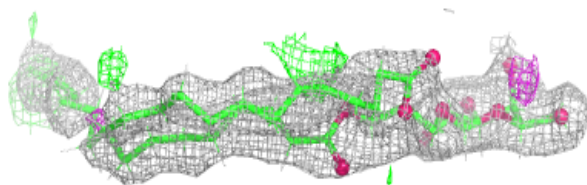
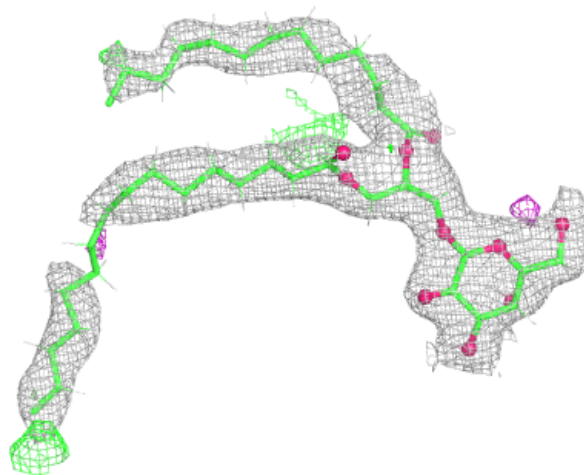
Electron density around STE B 620:

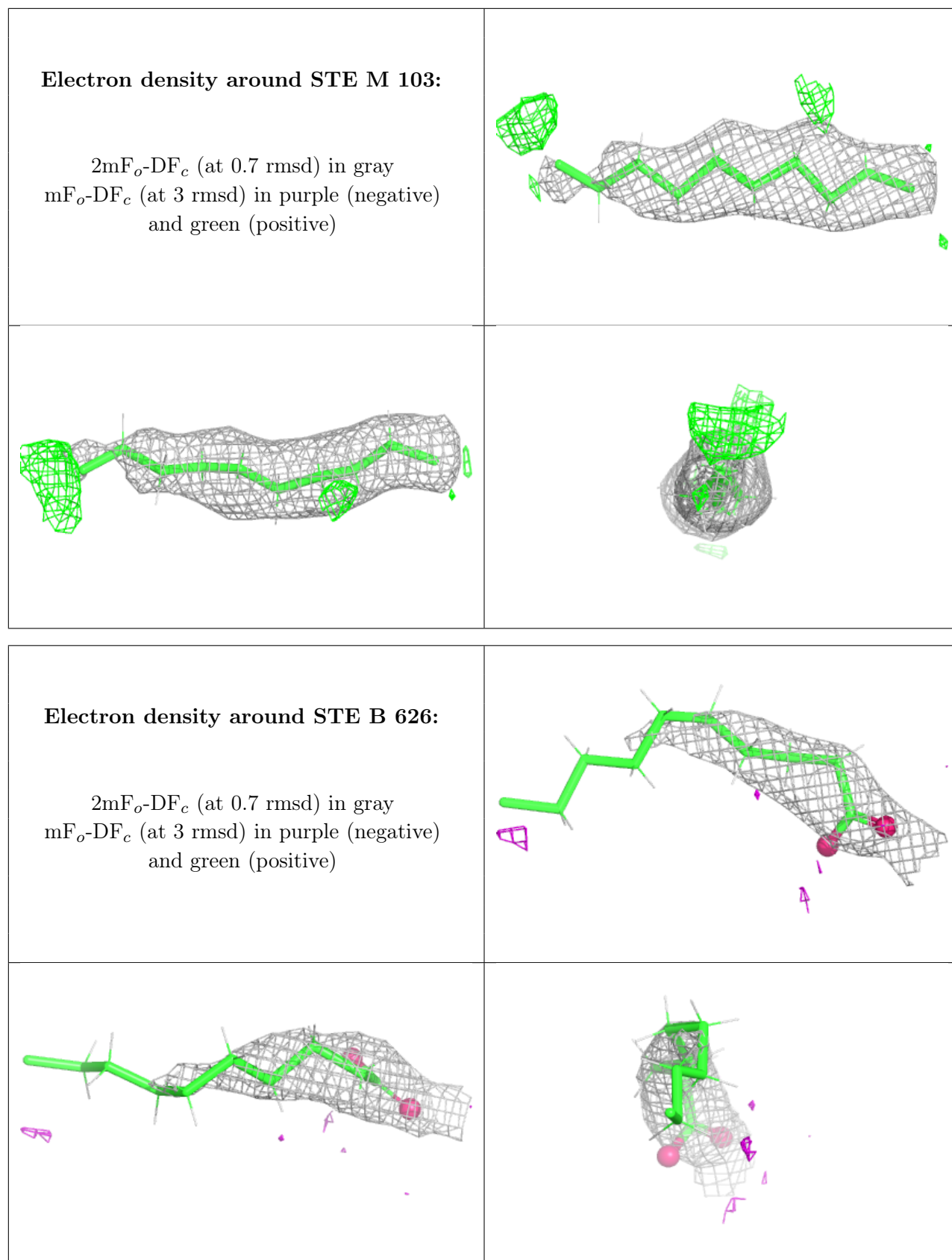
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMG Y 101:

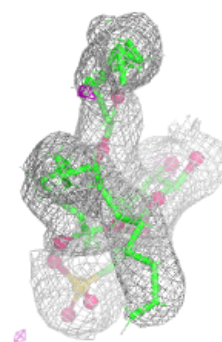
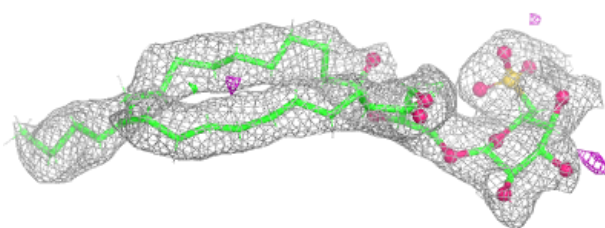
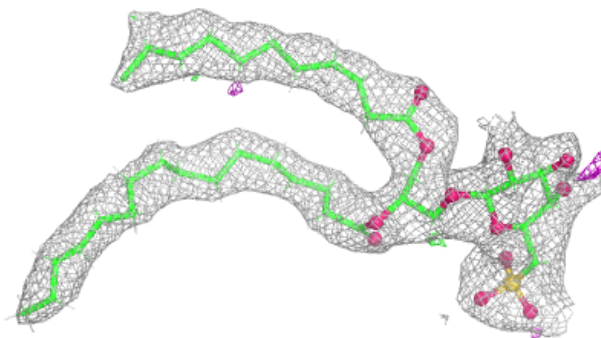
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



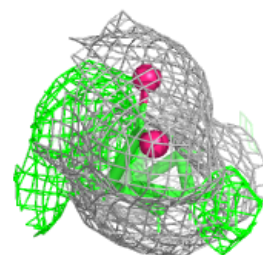
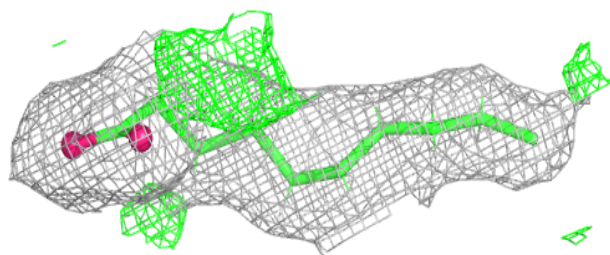
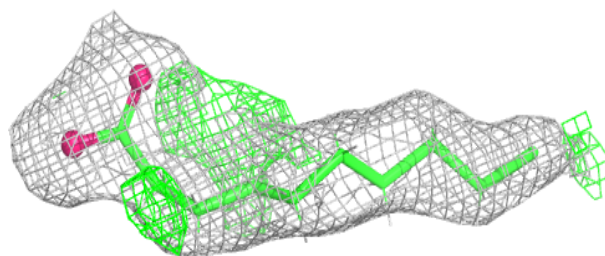


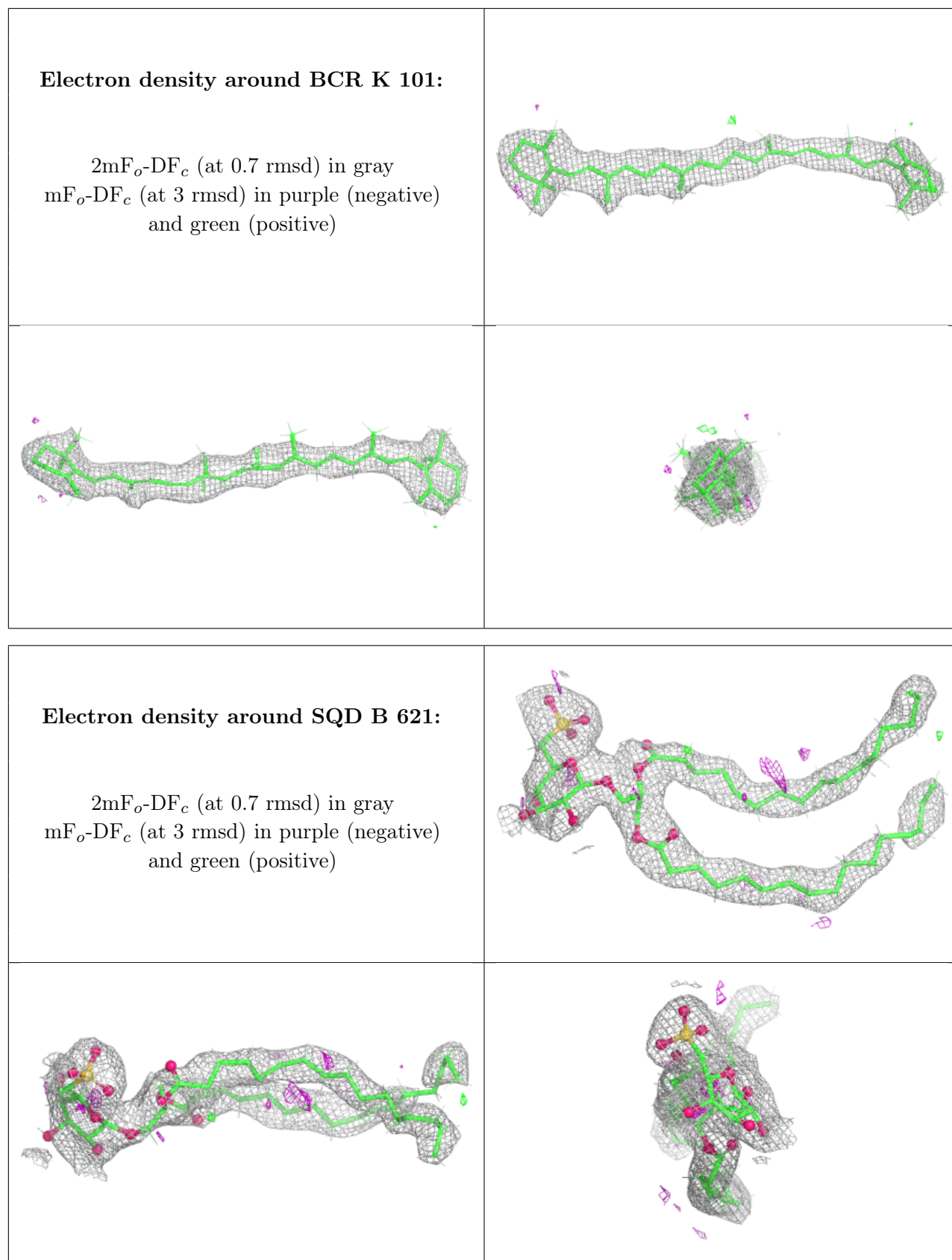
Electron density around SQD b 620:

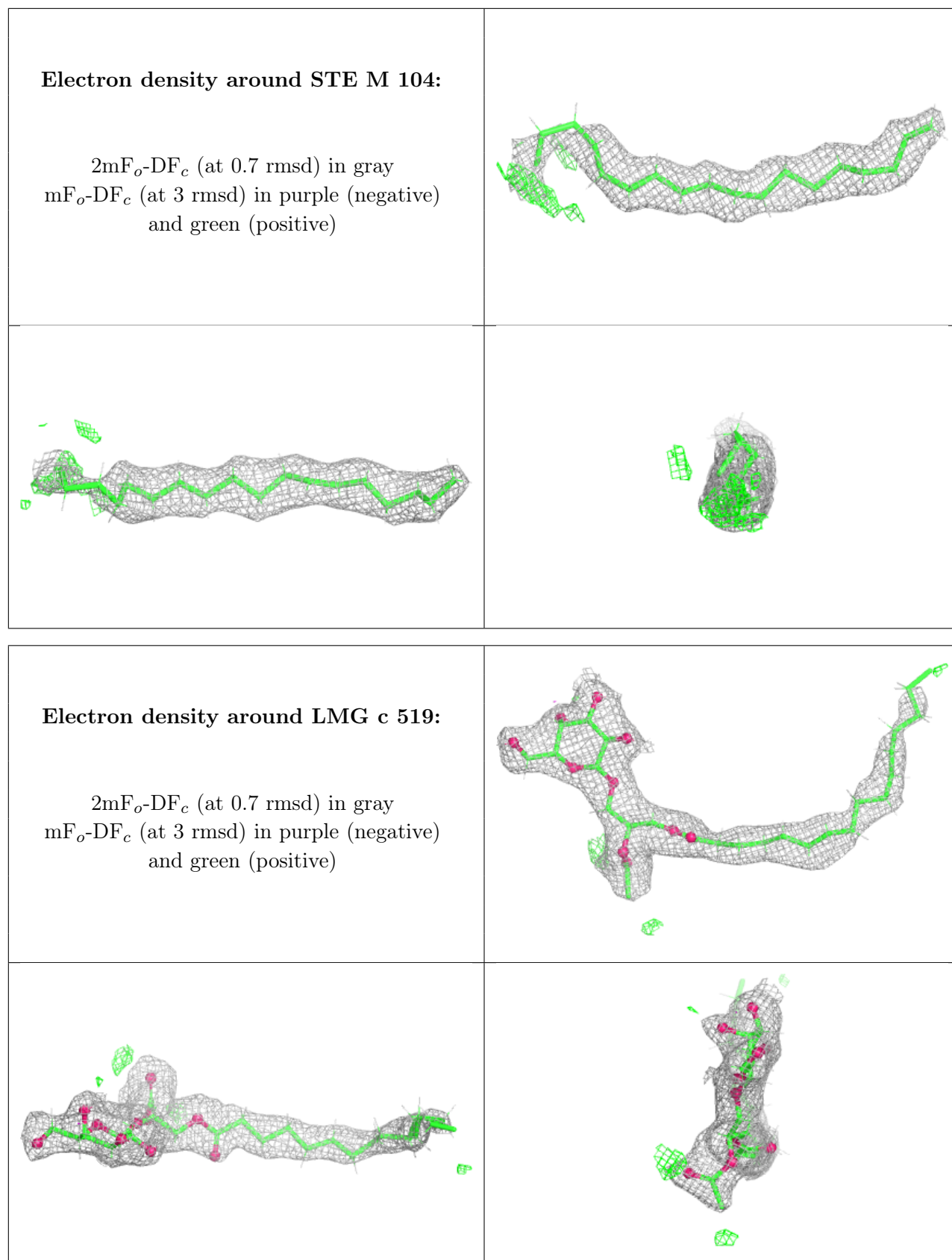
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around STE 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)

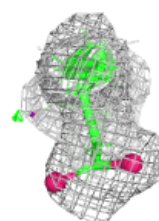
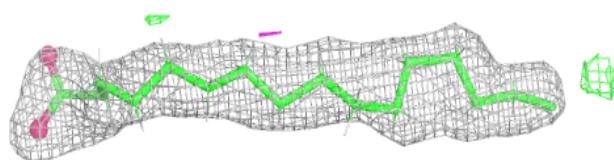
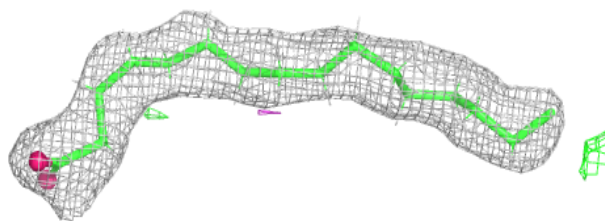




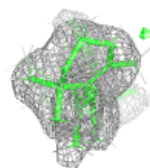
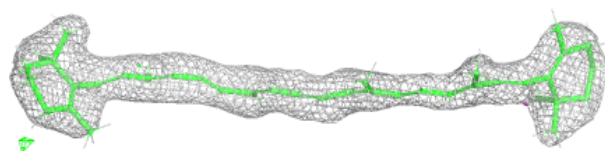
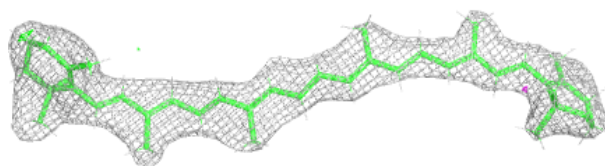


Electron density around STE B 624:

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

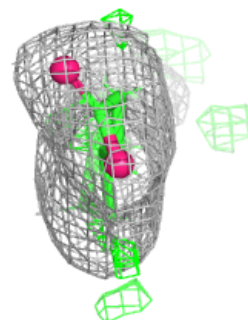
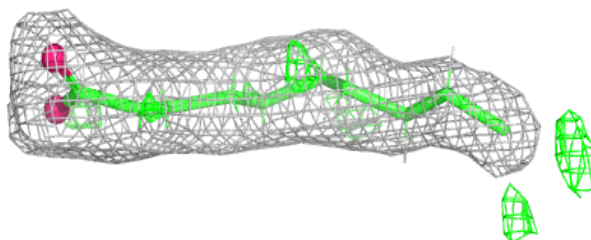
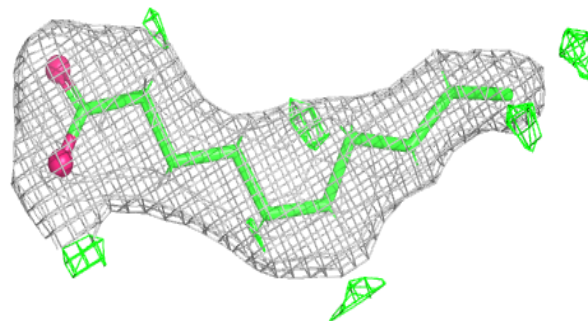
**Electron density around BCR k 101:**

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

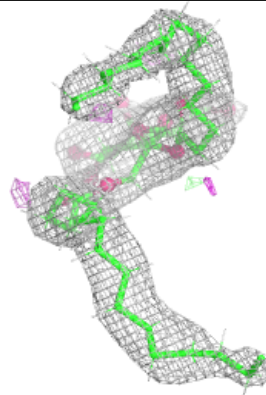
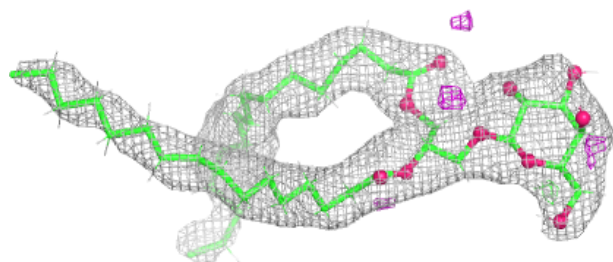
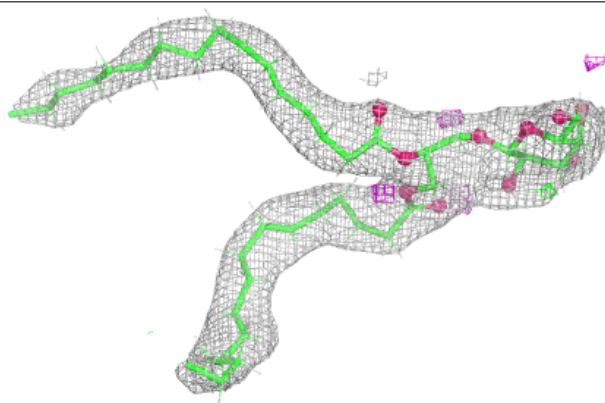


Electron density around STE C 520:

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

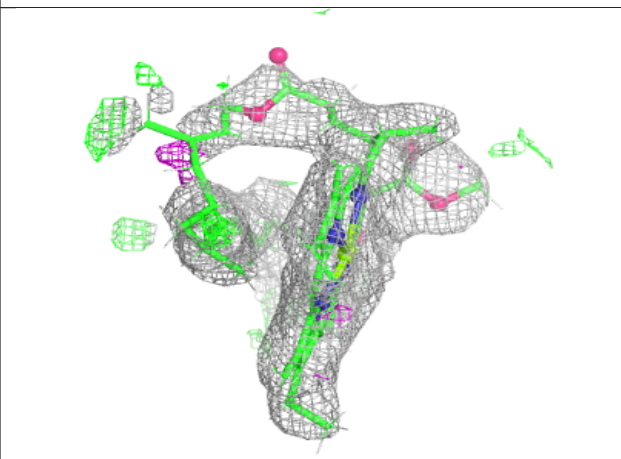
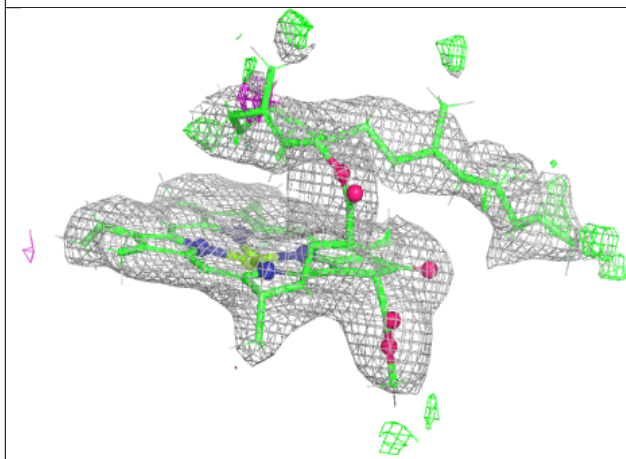
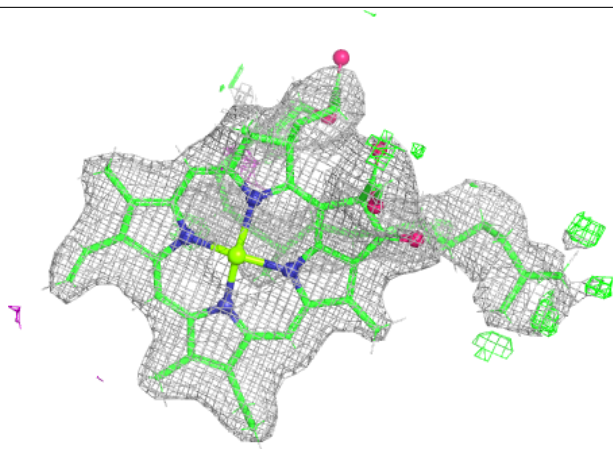
**Electron density around LMG m 101:**

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

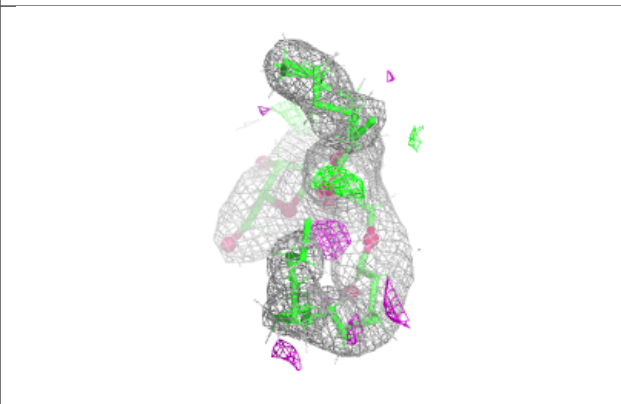
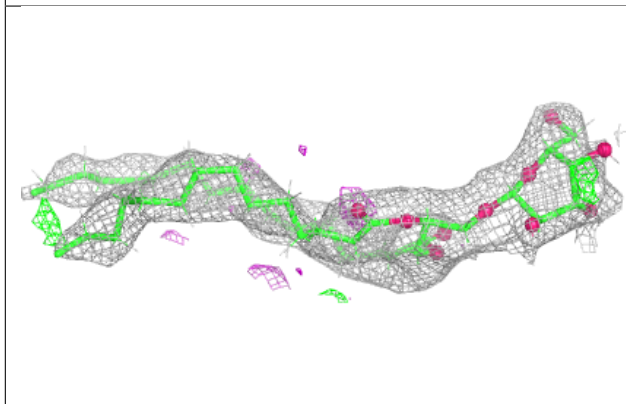
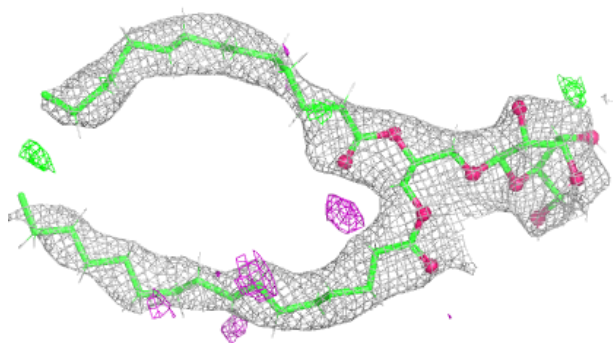


Electron density around CLA B 601:

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

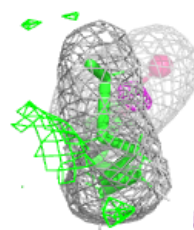
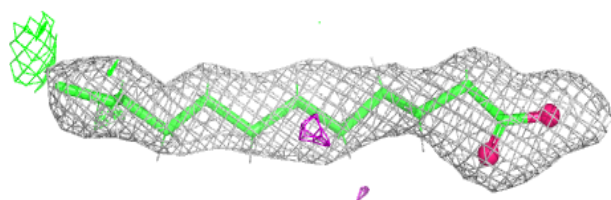
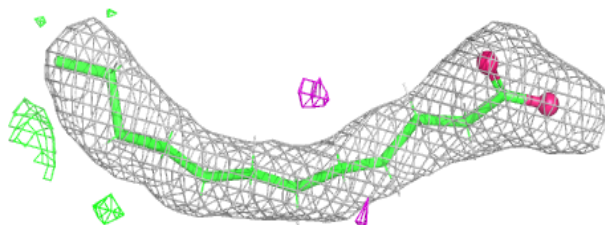
**Electron density around LMG a 414:**

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

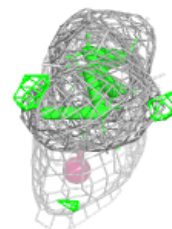
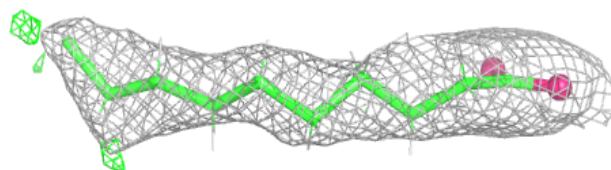
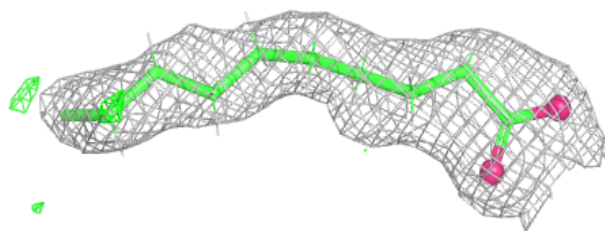


Electron density around STE B 622:

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

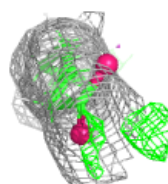
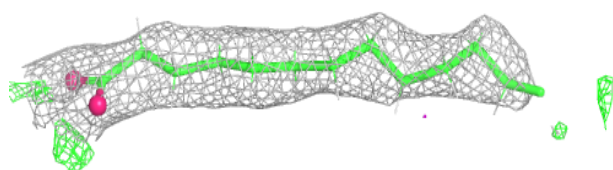
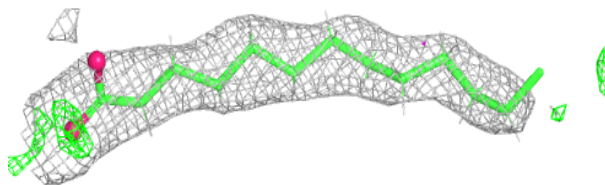
**Electron density around STE C 518:**

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

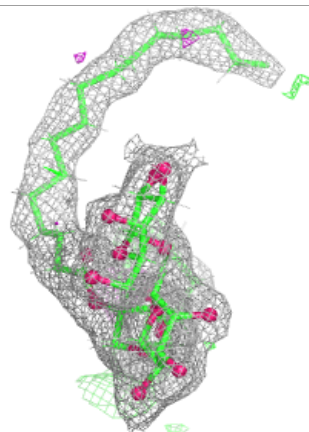
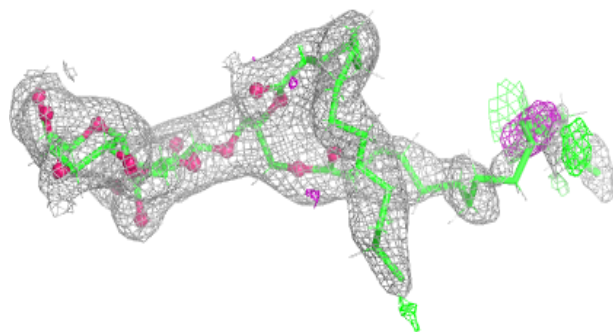
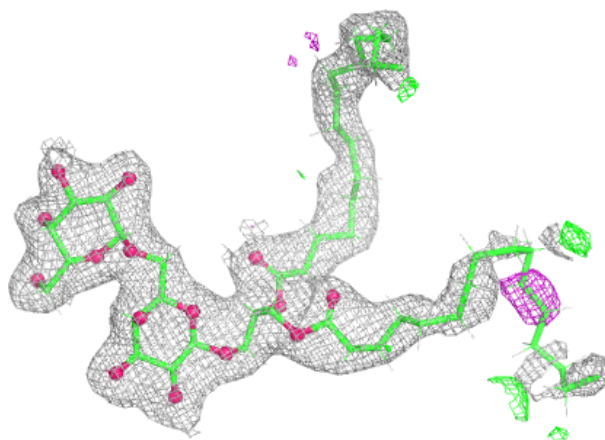


Electron density around STE M 102:

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

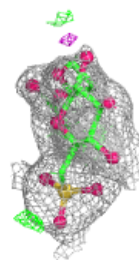
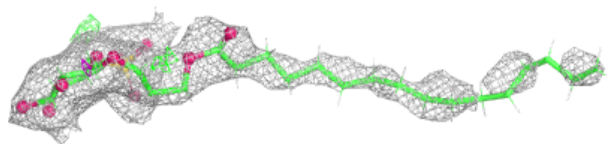
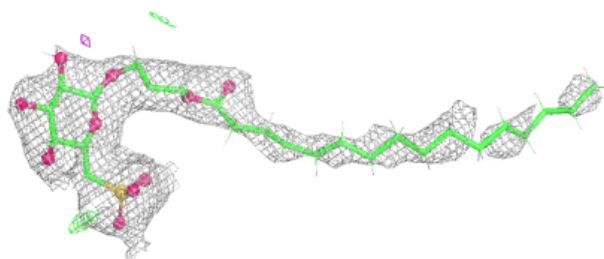
**Electron density around DGD C 516:**

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

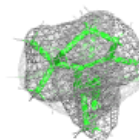
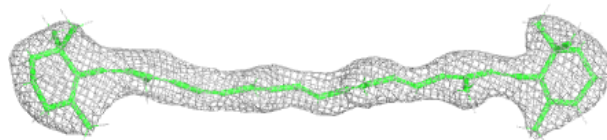
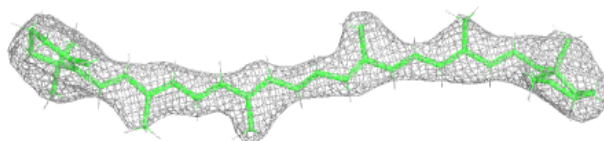


Electron density around SQD F 102:

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

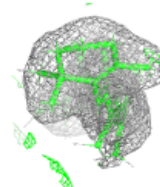
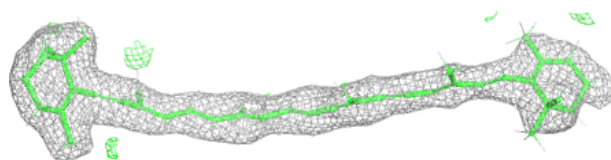
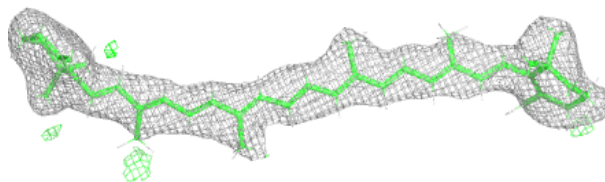
**Electron density around BCR c 514:**

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

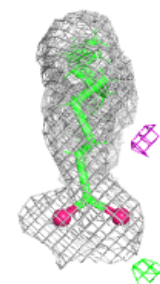
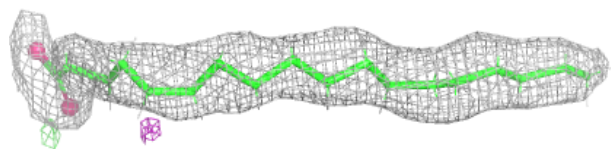
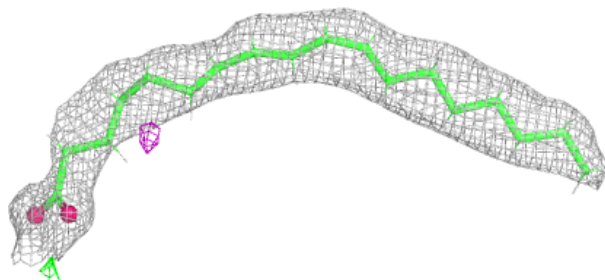


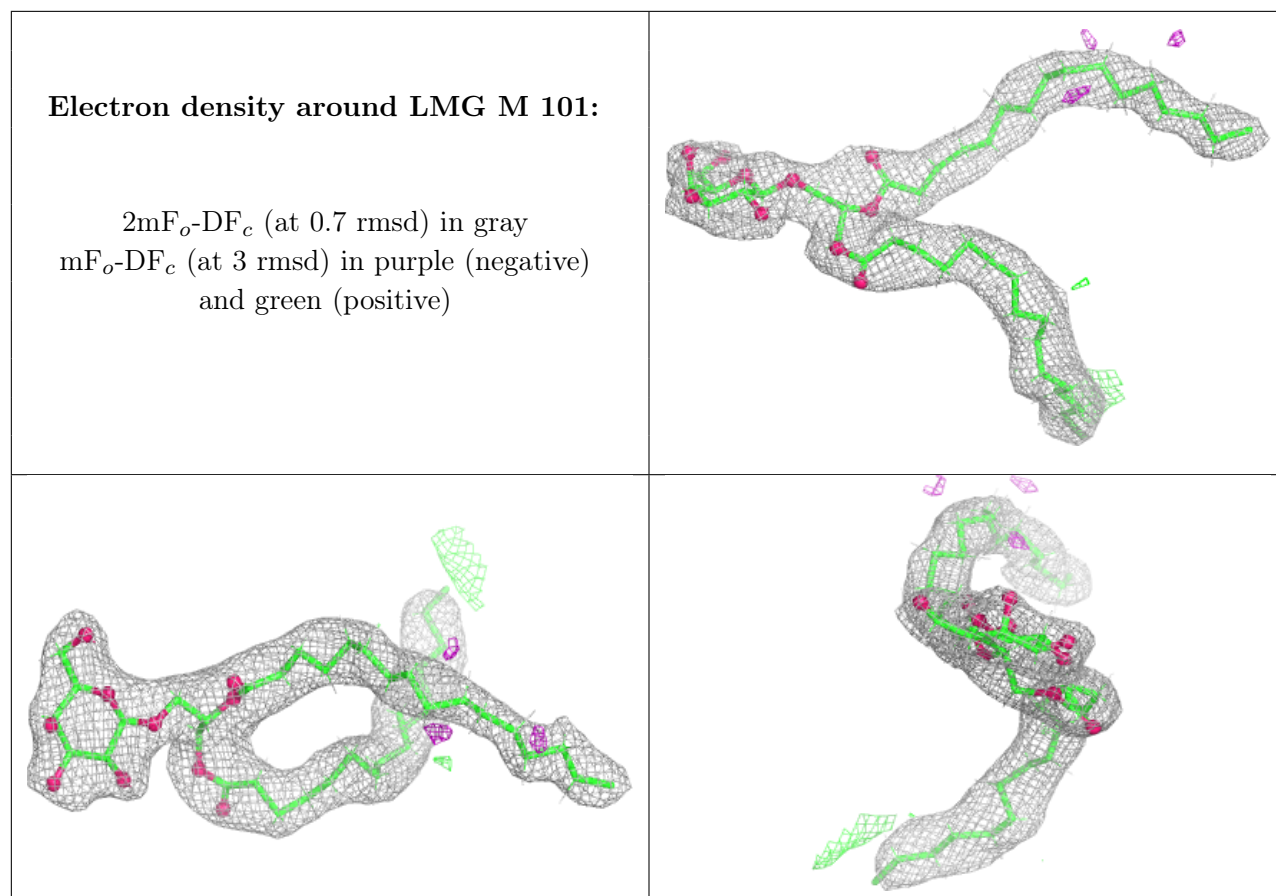
Electron density around BCR h 101:

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

**Electron density around STE D 412:**

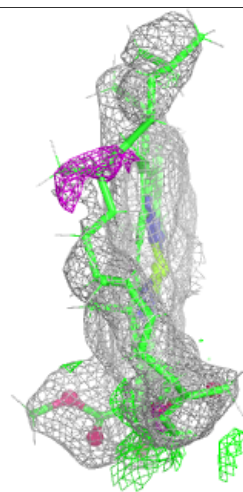
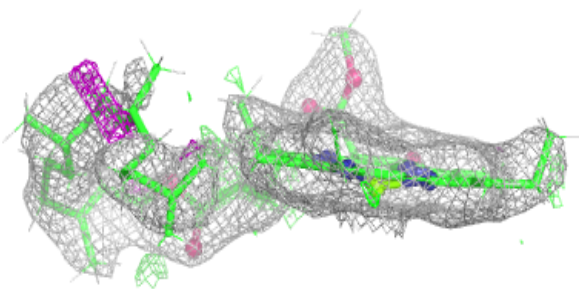
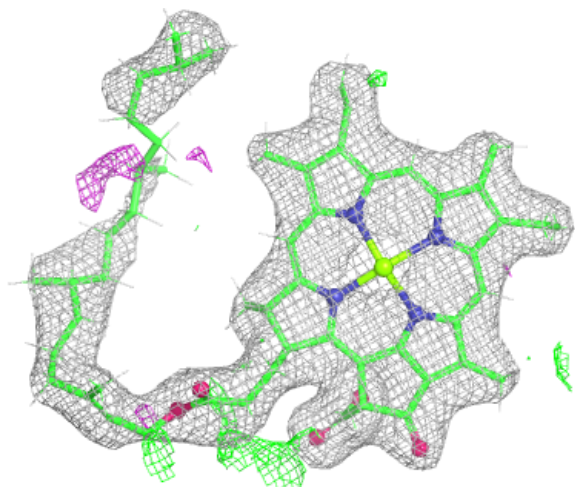
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





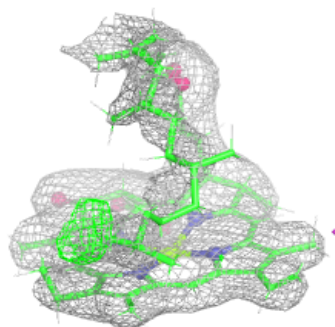
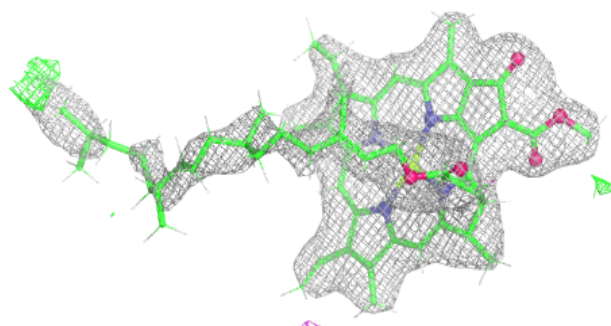
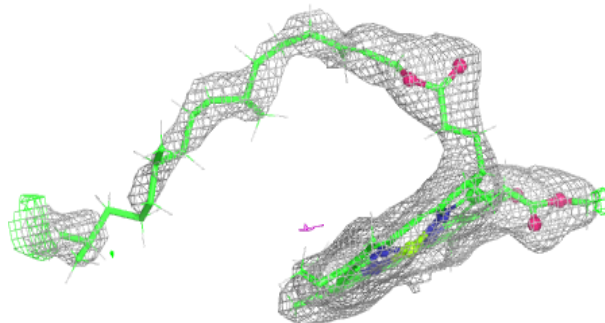
Electron density around CLA c 512:

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

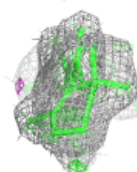
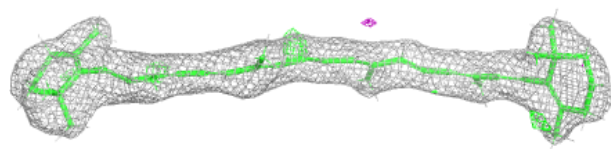
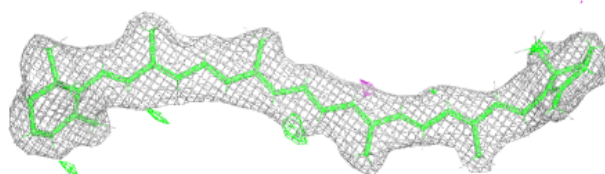


Electron density around CLA C 513:

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

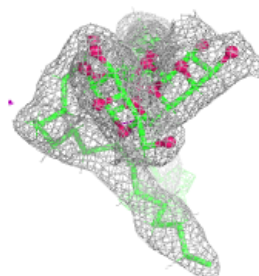
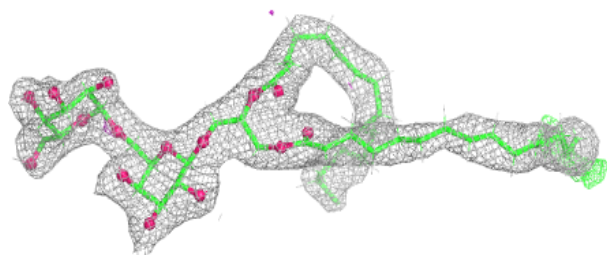
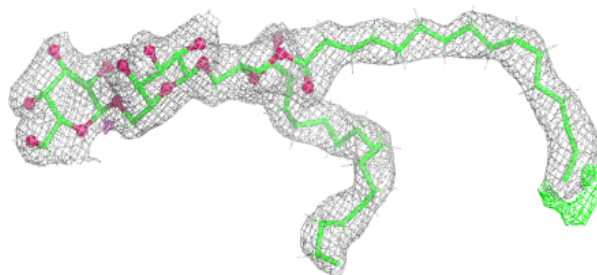
**Electron density around BCR K 102:**

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

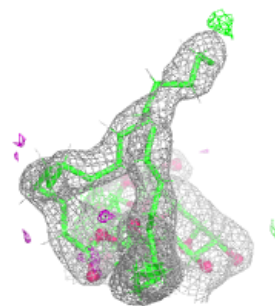
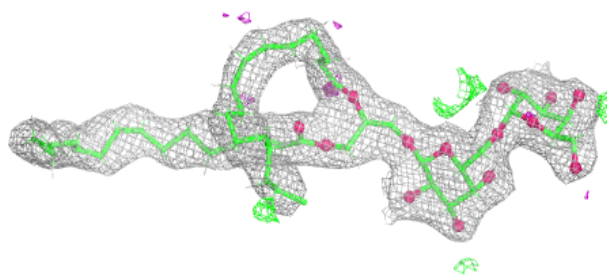
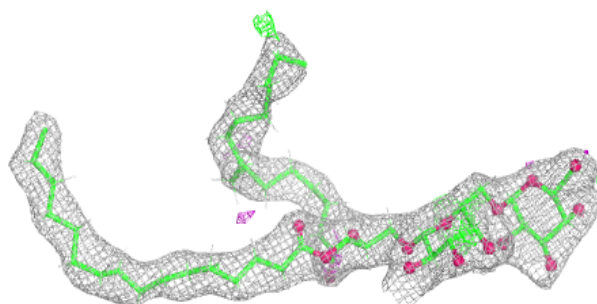


Electron density around DGD H 102:

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

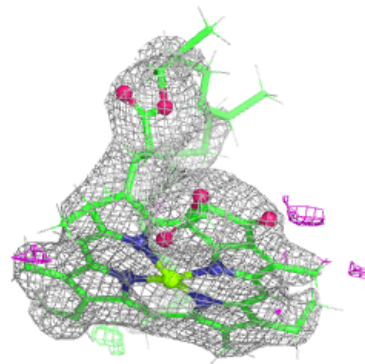
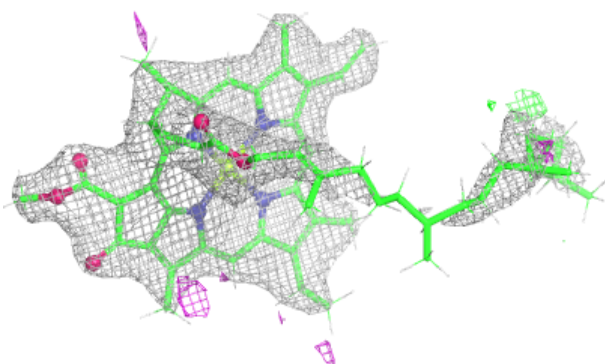
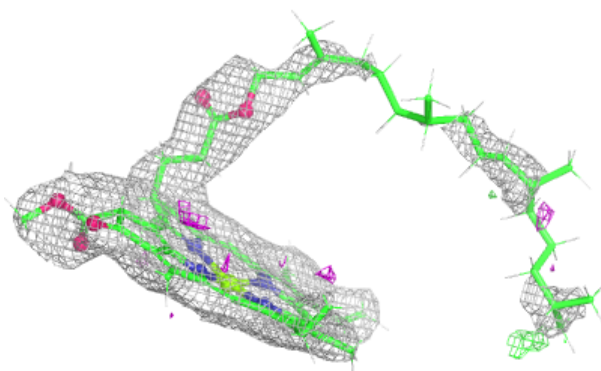
**Electron density around DGD h 103:**

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

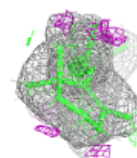
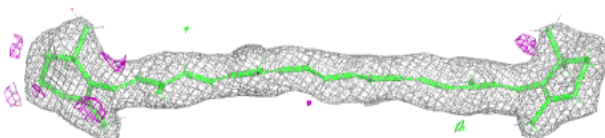
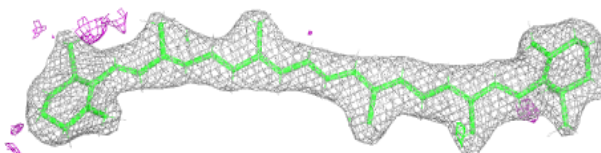


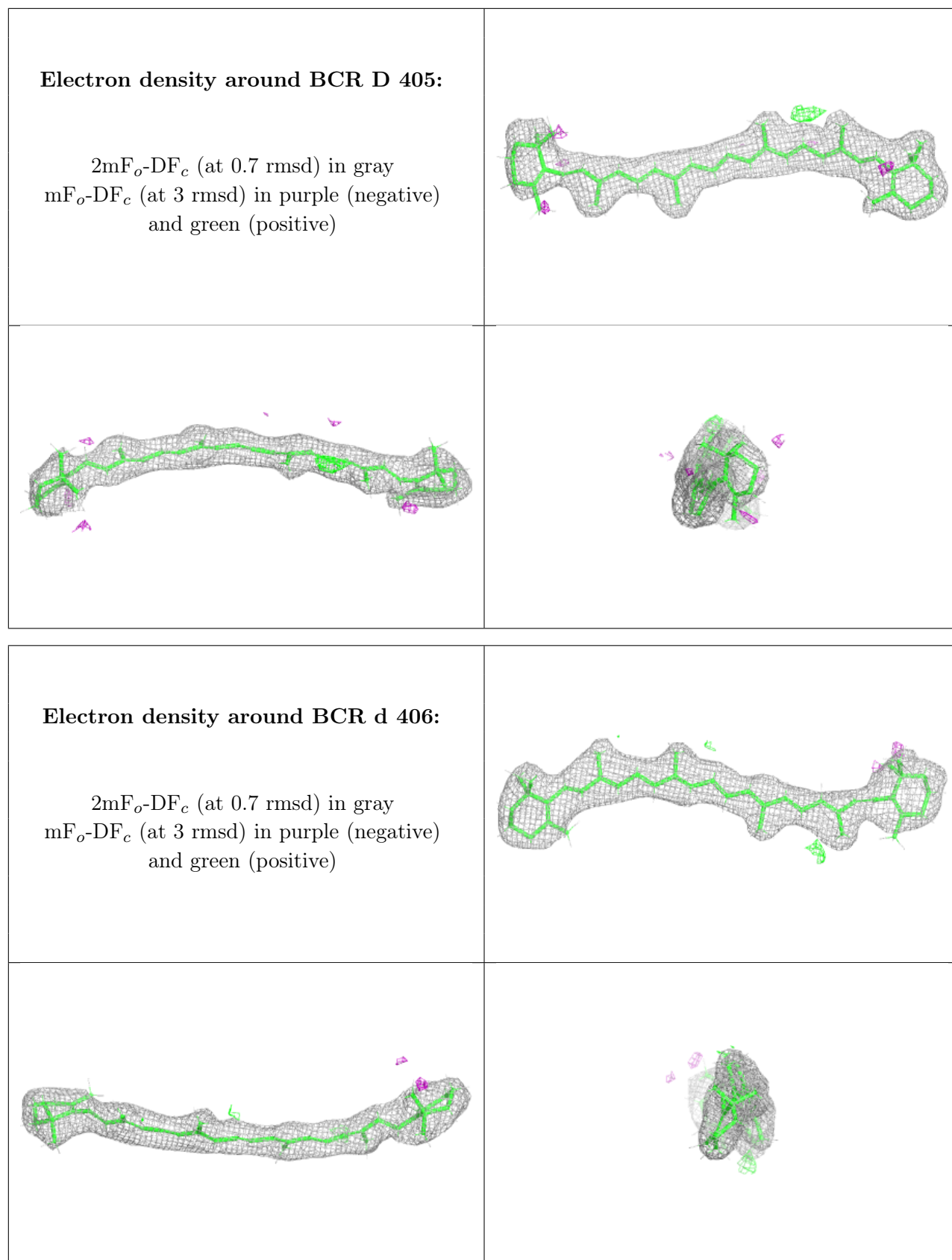
Electron density around CLA c 513:

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

**Electron density around BCR B 618:**

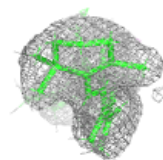
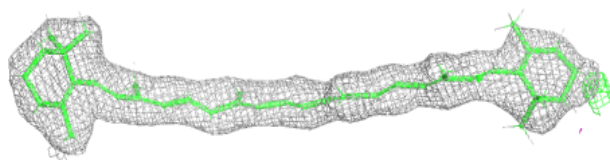
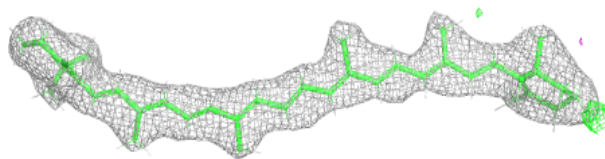
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



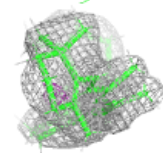
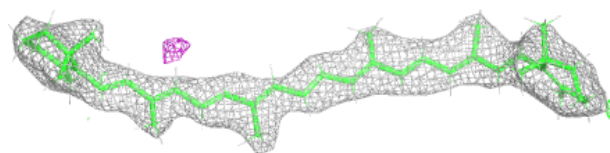
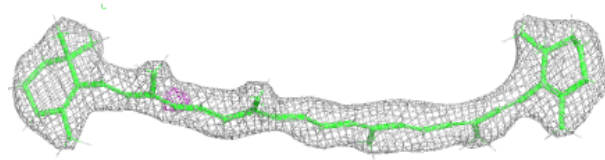


Electron density around BCR H 101:

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

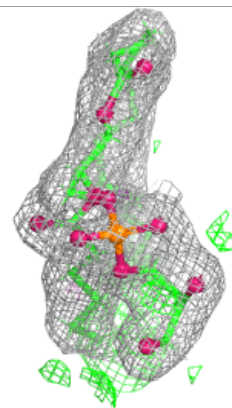
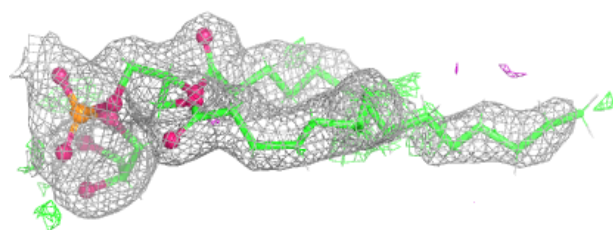
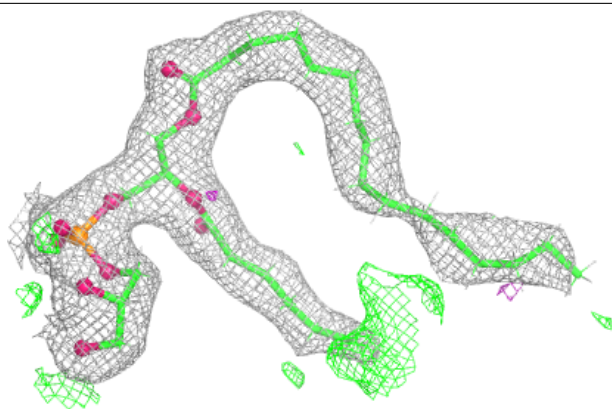
**Electron density around BCR K 103:**

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

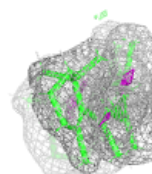
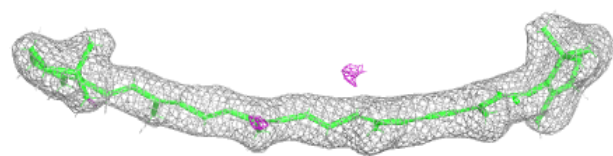
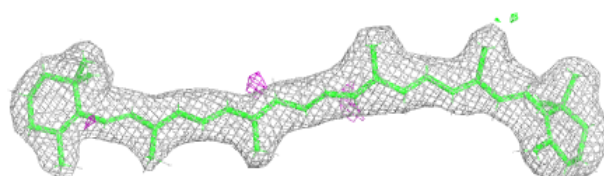


Electron density around LHG d 409:

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

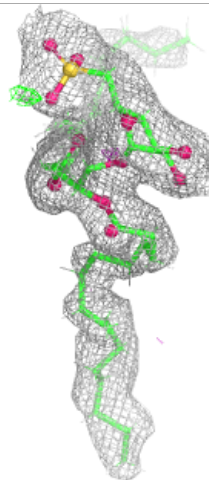
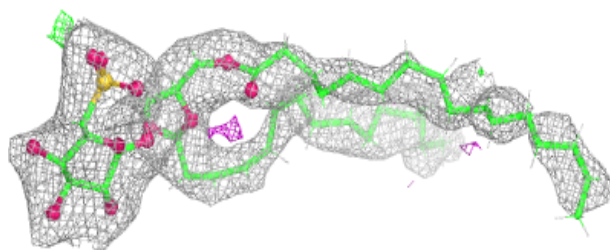
**Electron density around BCR T 101:**

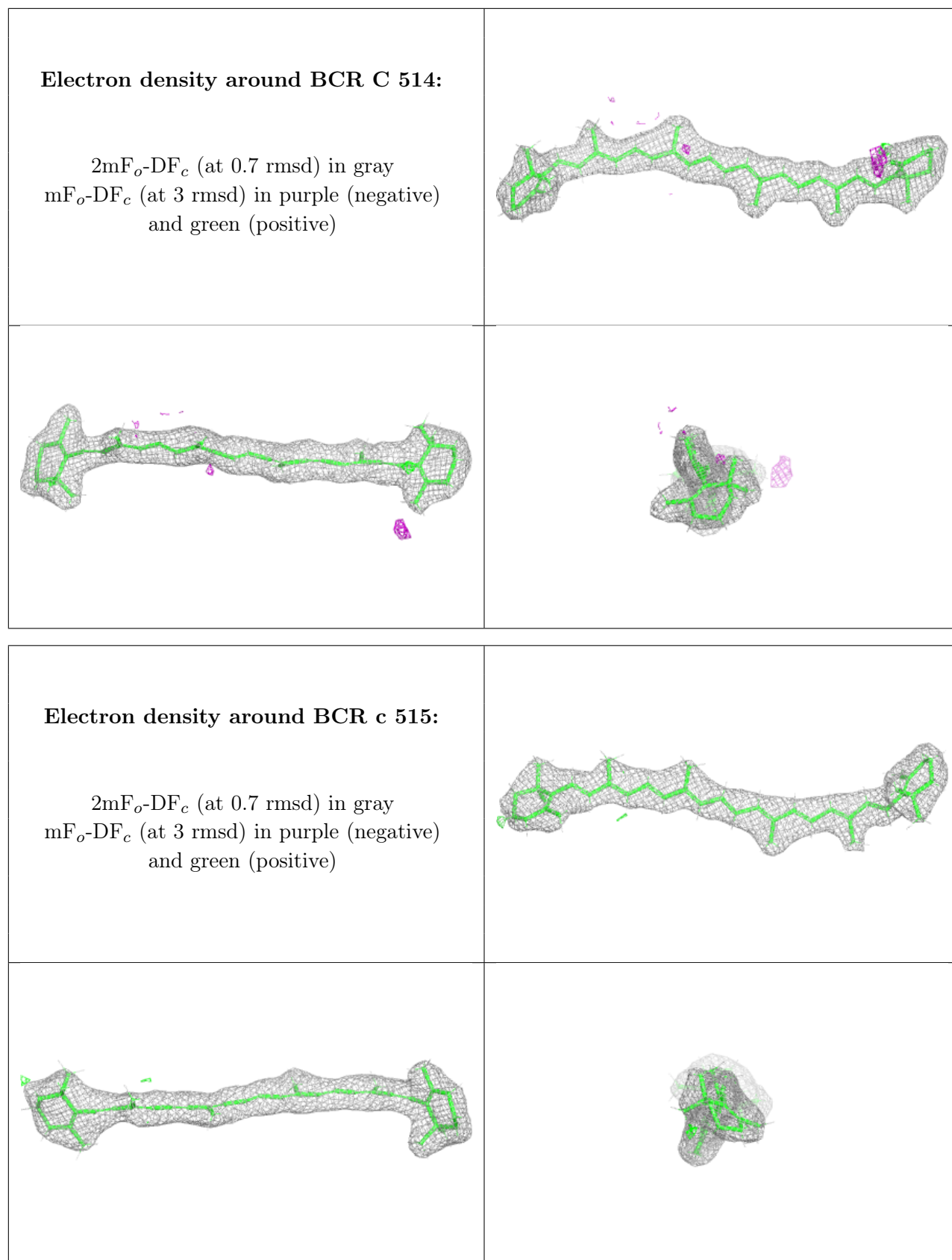
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD a 411:

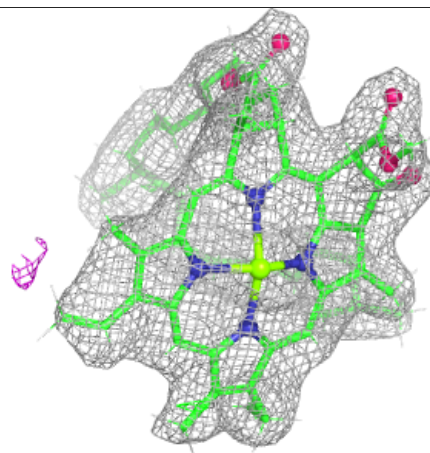
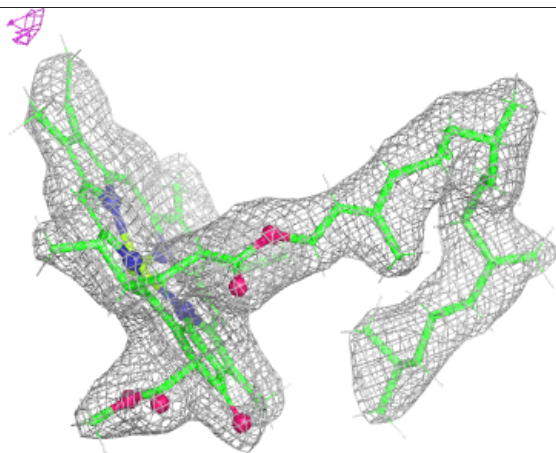
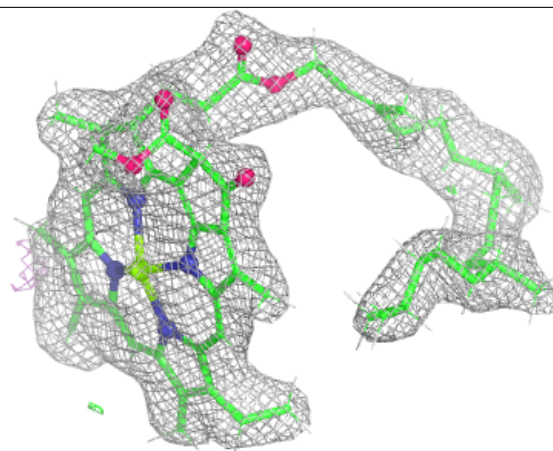
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



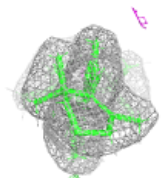
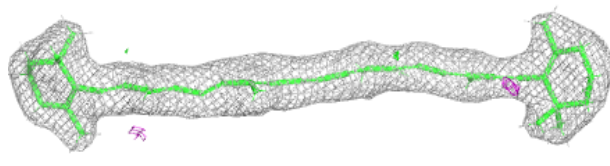
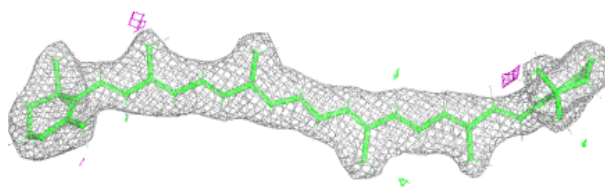


Electron density around CLA C 503:

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

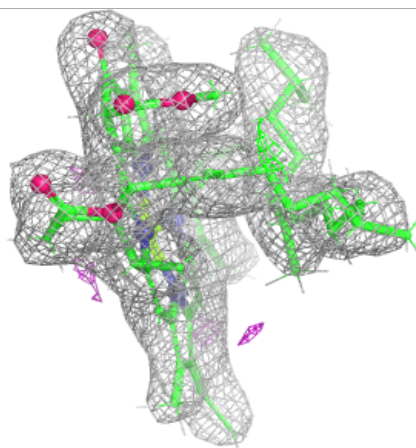
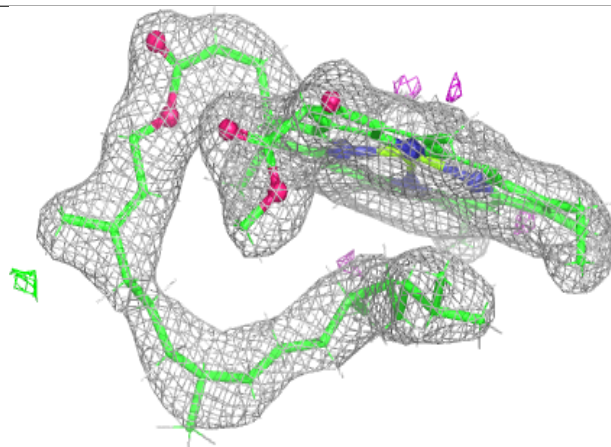
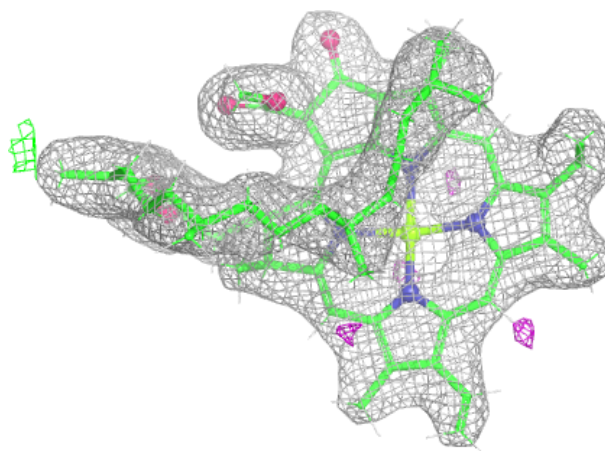
**Electron density around BCR A 407:**

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



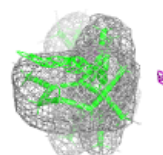
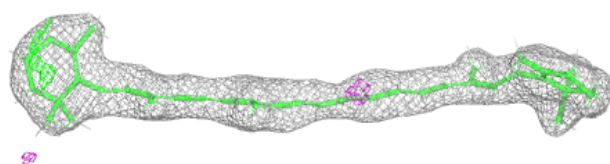
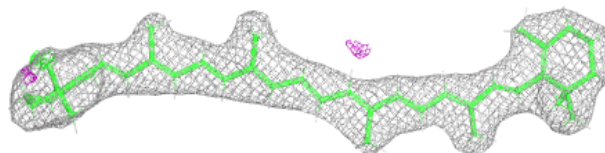
Electron density around CLA C 510:

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

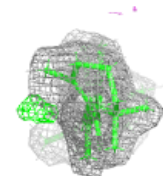
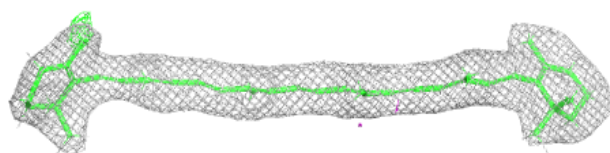
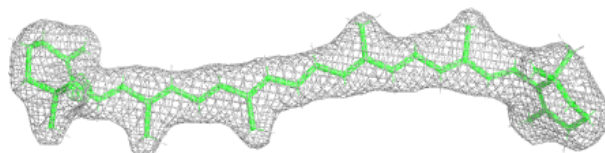


Electron density around BCR b 617:

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

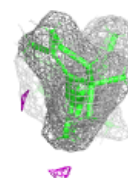
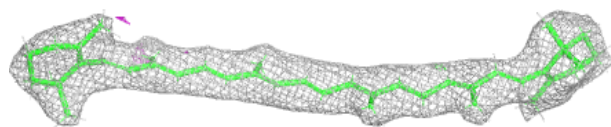
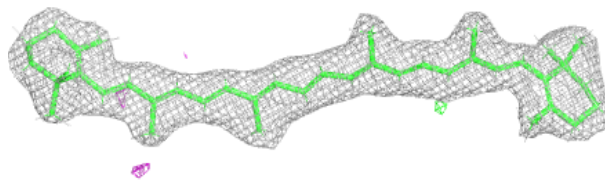
**Electron density around BCR b 618:**

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

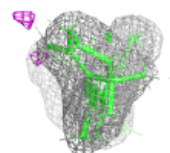
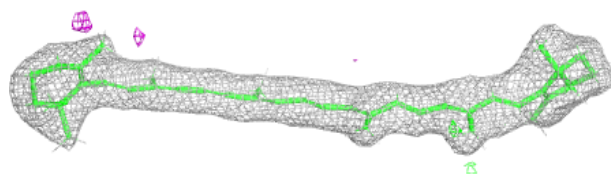
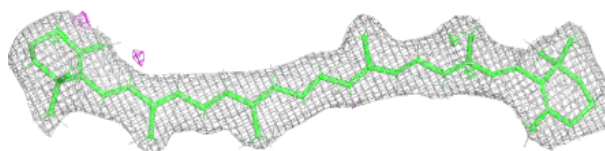


Electron density around BCR b 619:

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

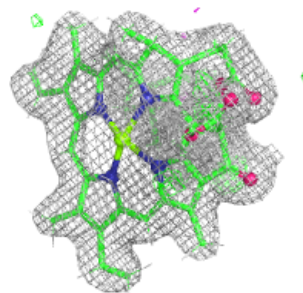
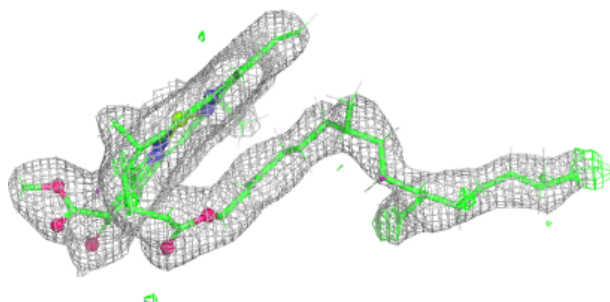
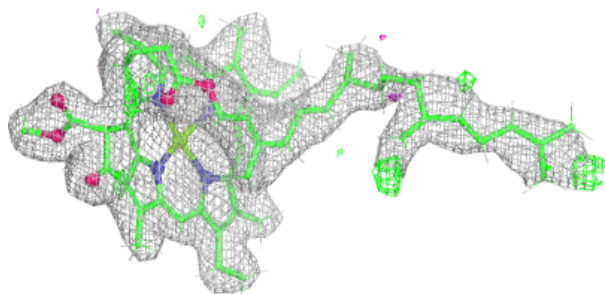
**Electron density around BCR B 619:**

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

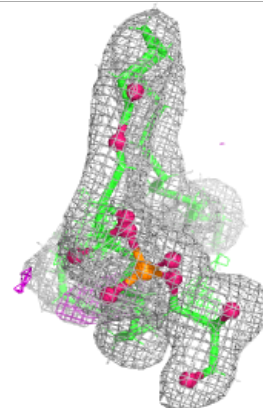
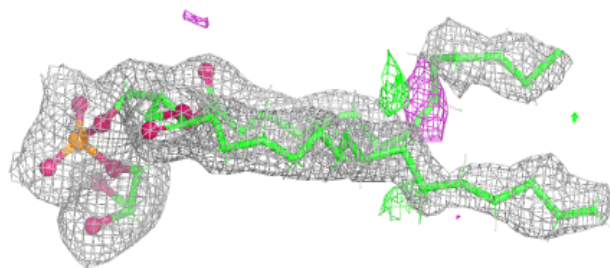
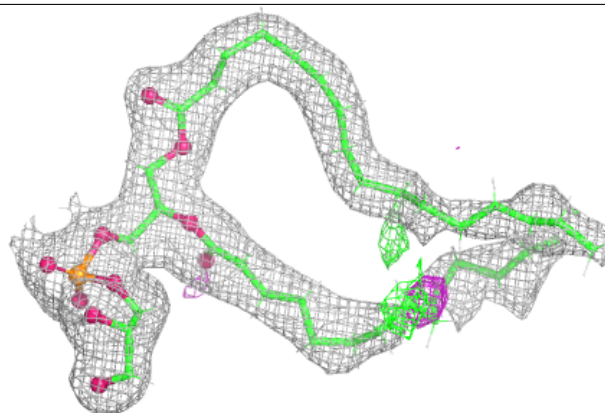


Electron density around CLA c 505:

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

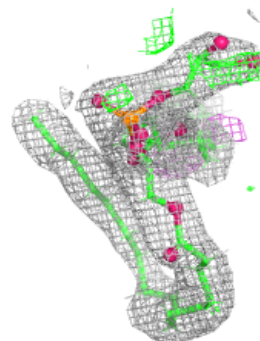
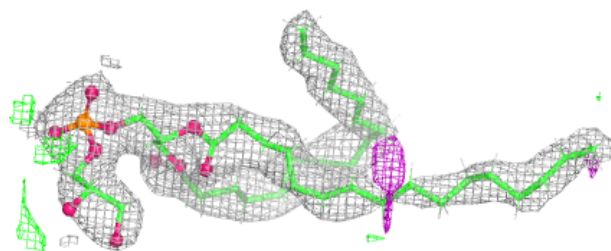
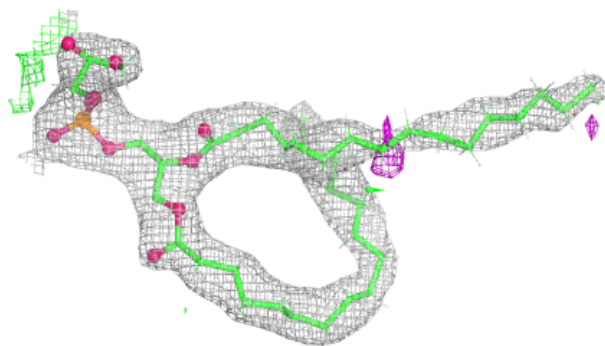
**Electron density around LHG D 409:**

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



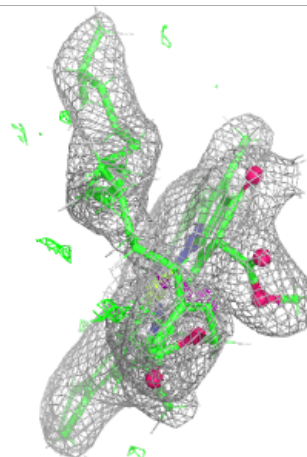
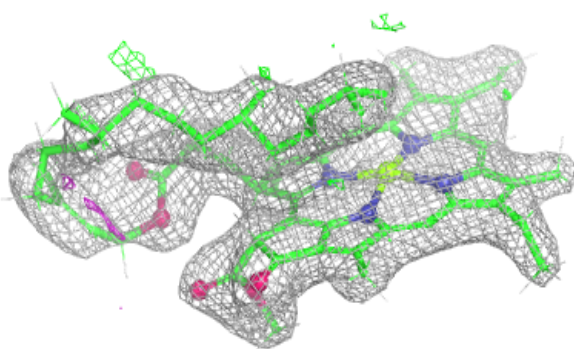
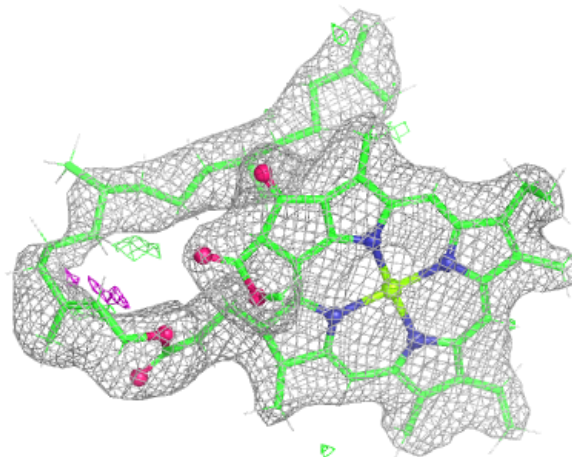
Electron density around LHG a 410:

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



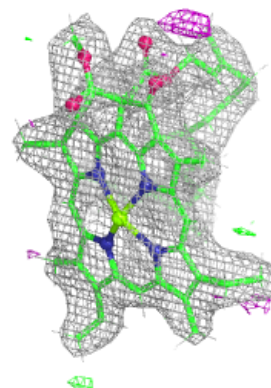
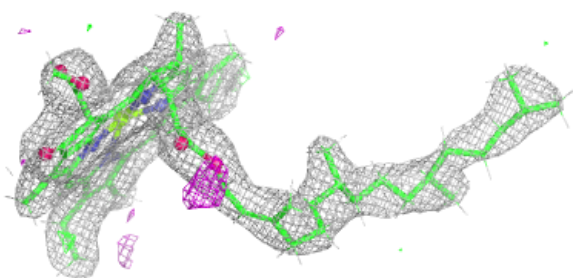
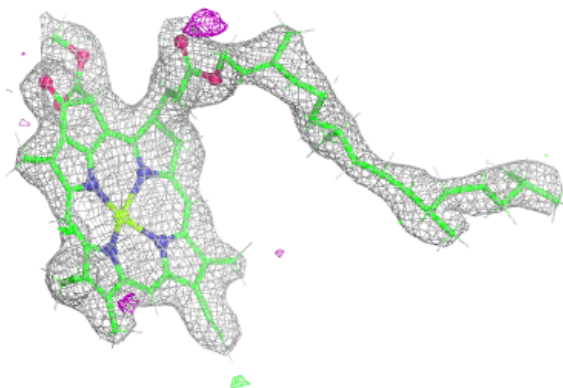
Electron density around CLA c 509:

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

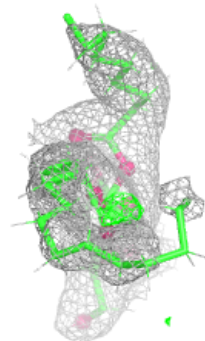
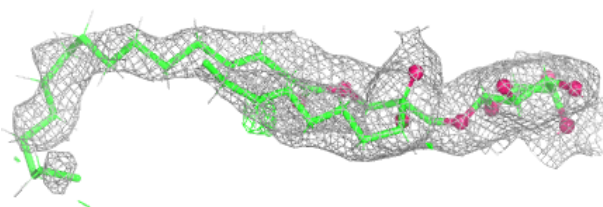
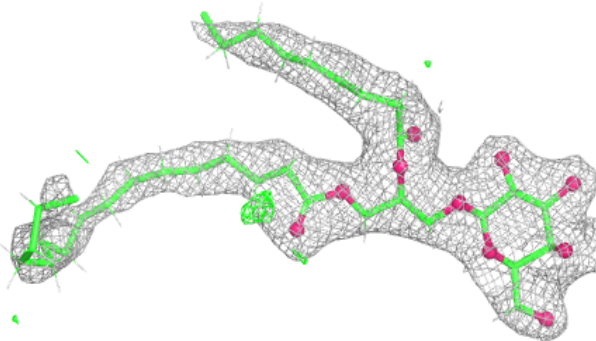


Electron density around CLA c 511:

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

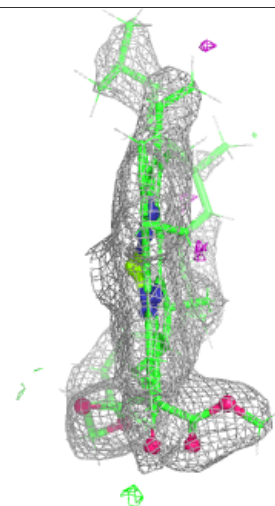
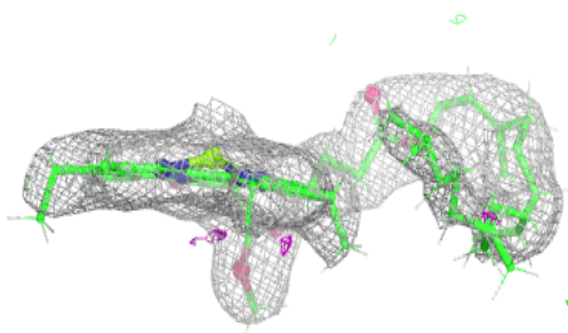
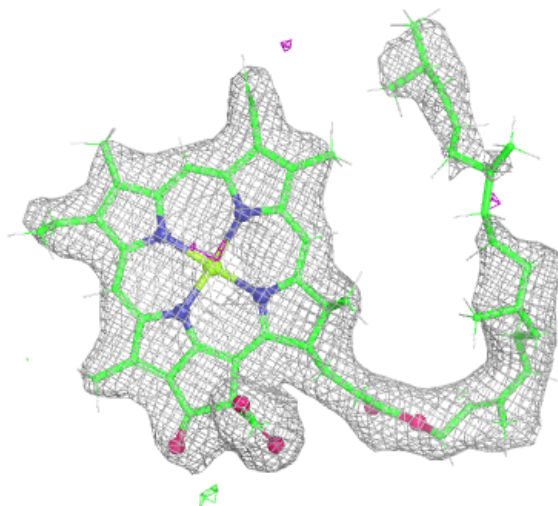
**Electron density around LMG d 410:**

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



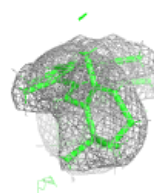
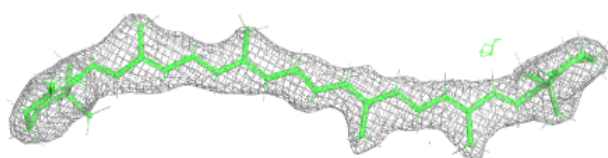
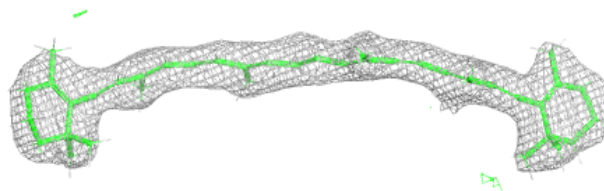
Electron density around CLA C 512:

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

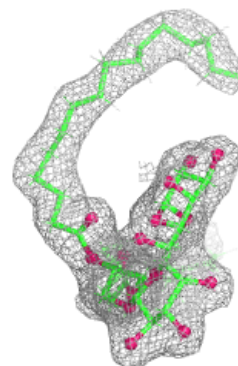
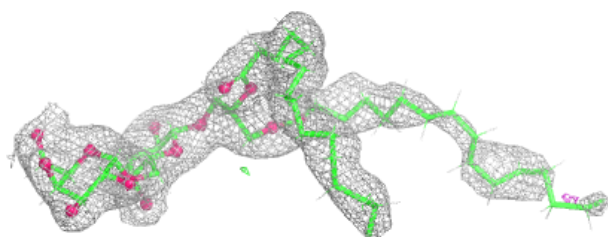
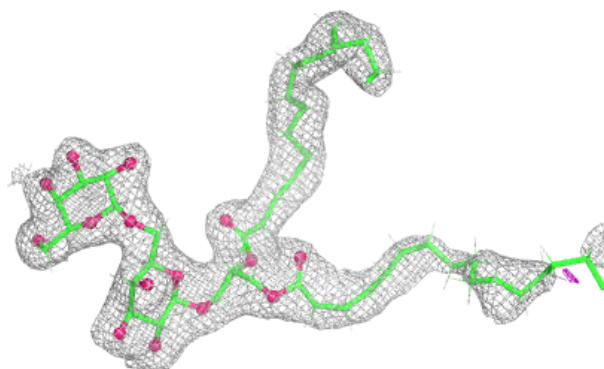


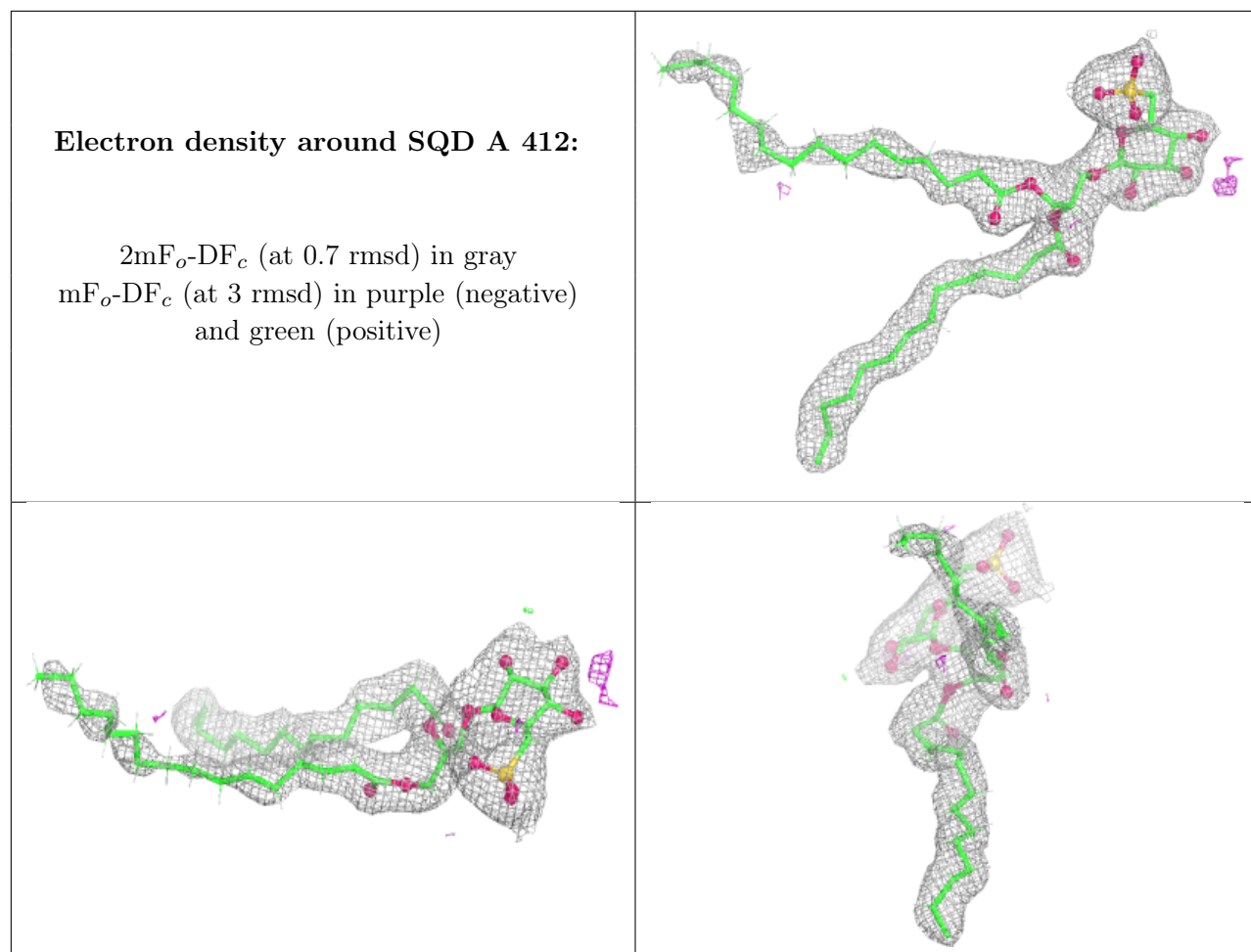
Electron density around BCR k 102:

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

**Electron density around DGD c 517:**

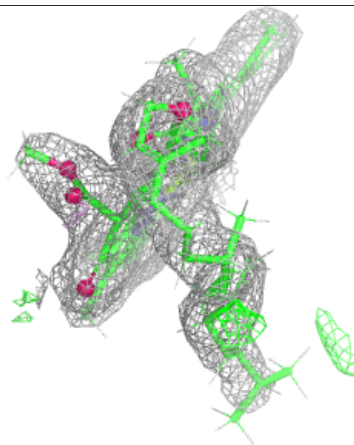
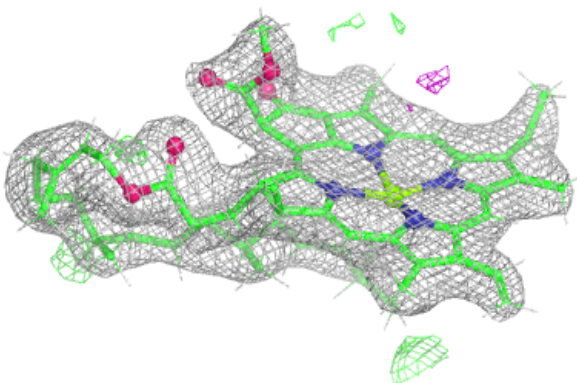
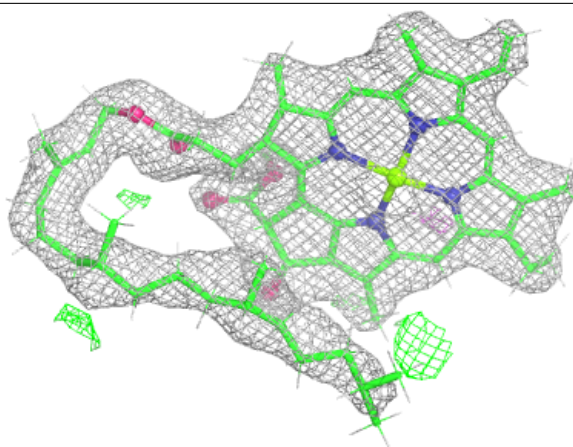
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



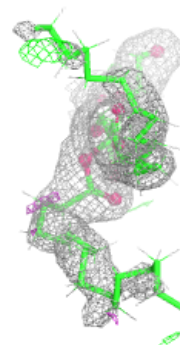
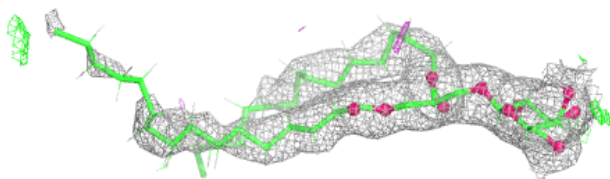
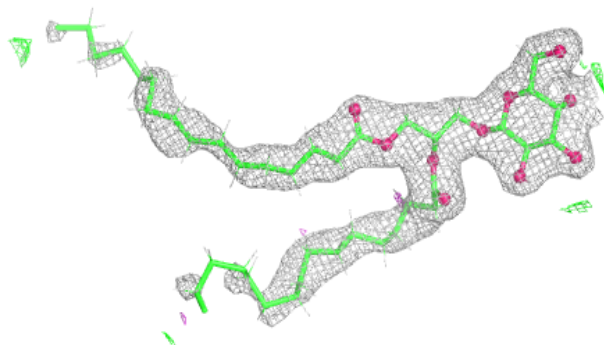


Electron density around CLA C 509:

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

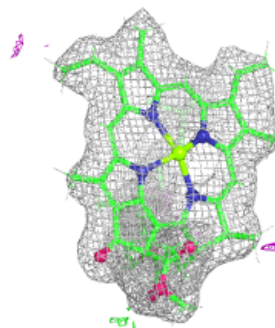
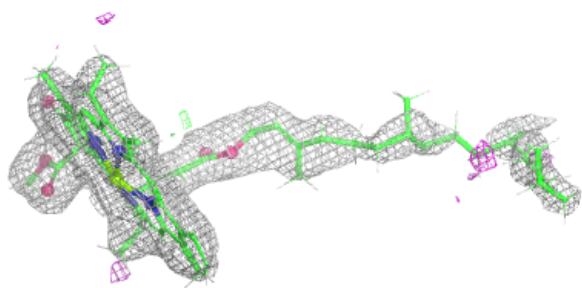
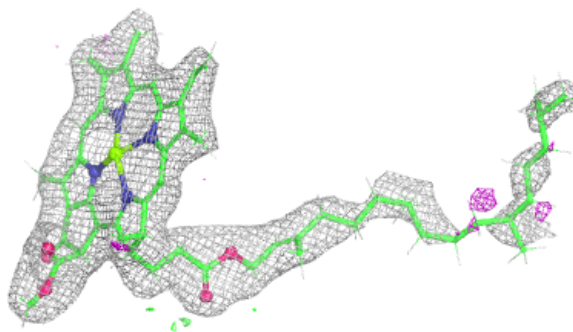
**Electron density around LMG D 407:**

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



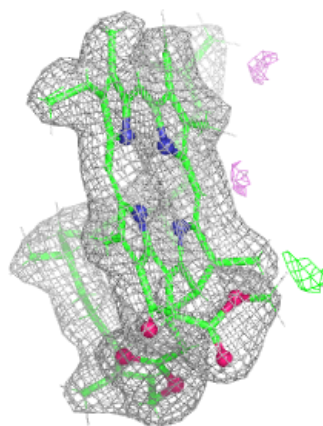
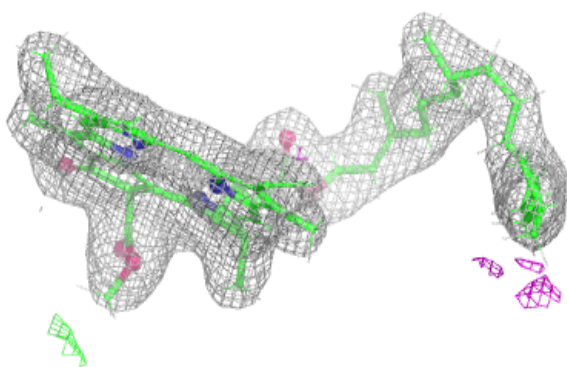
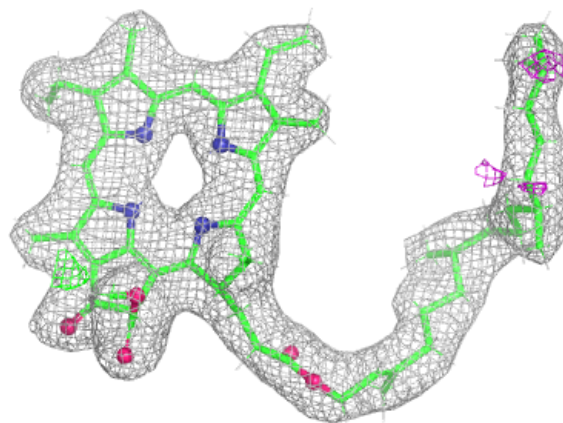
Electron density around CLA d 405:

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



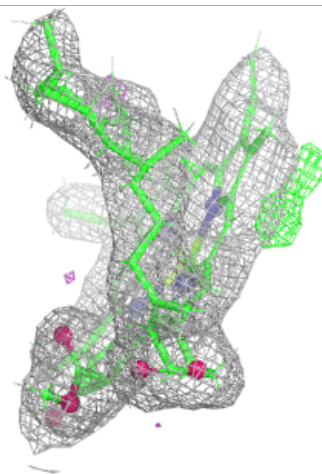
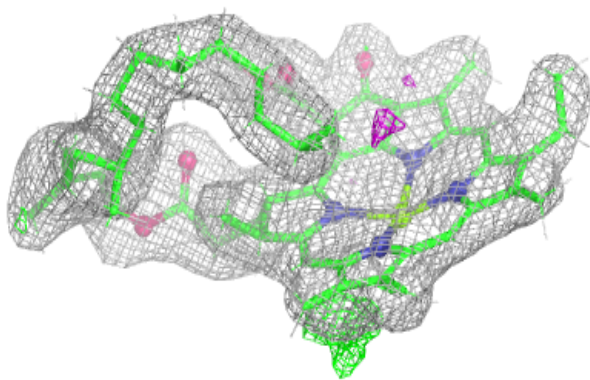
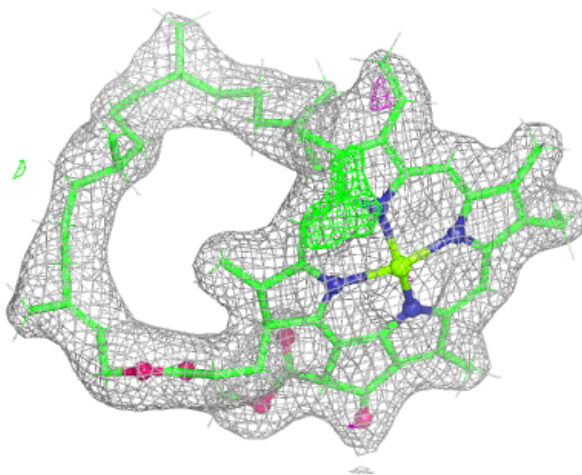
Electron density around PHO d 401:

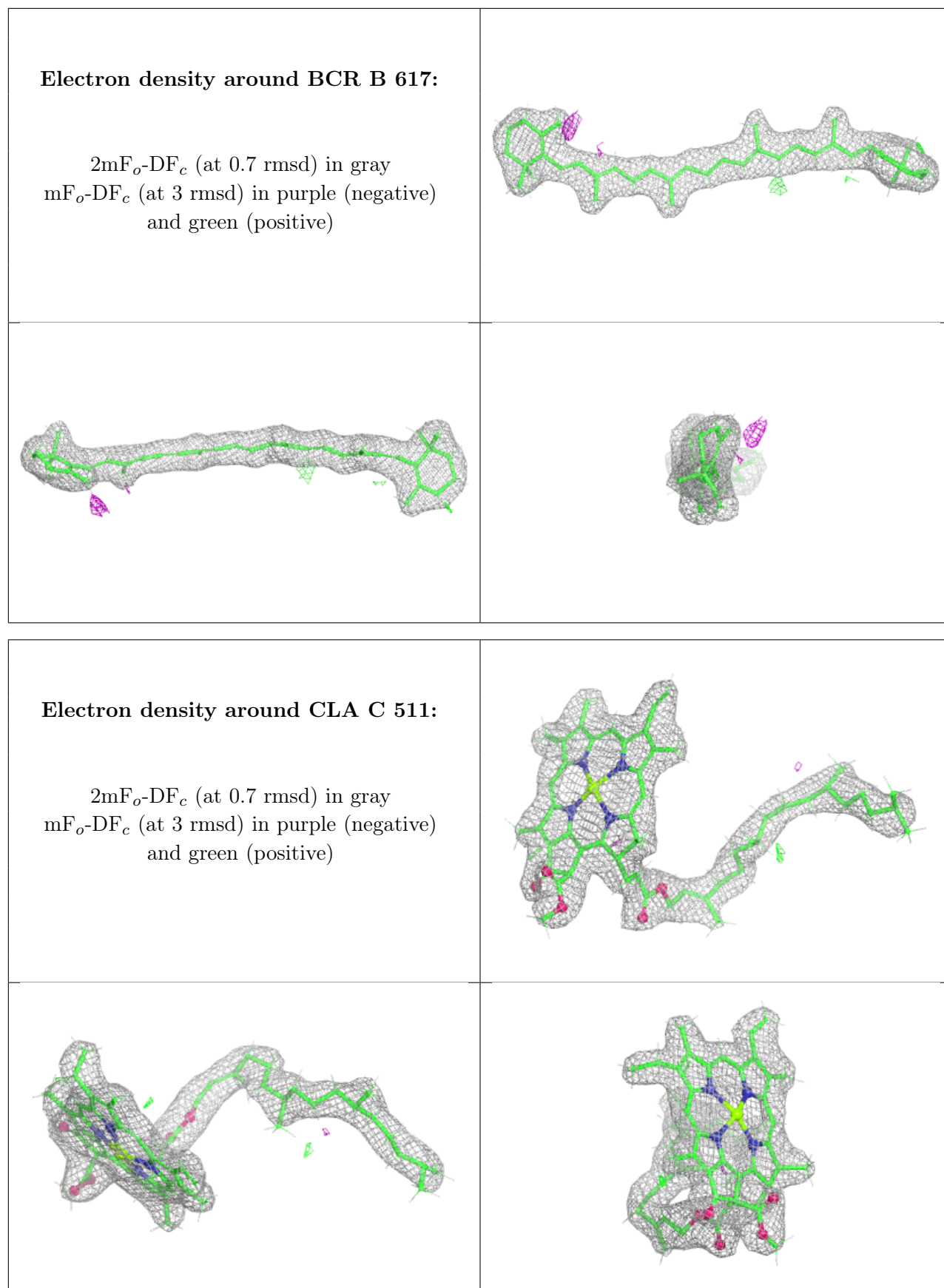
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 615:

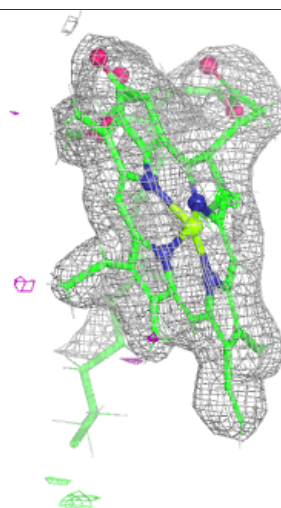
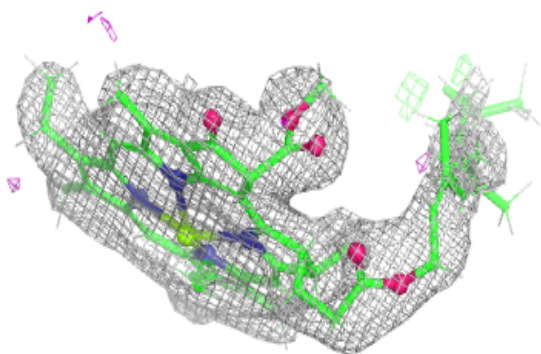
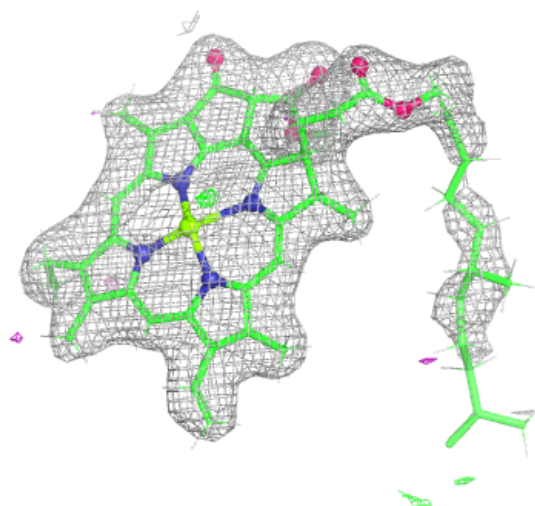
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





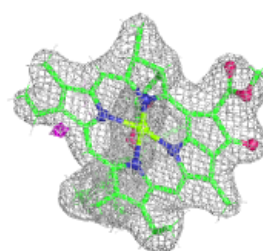
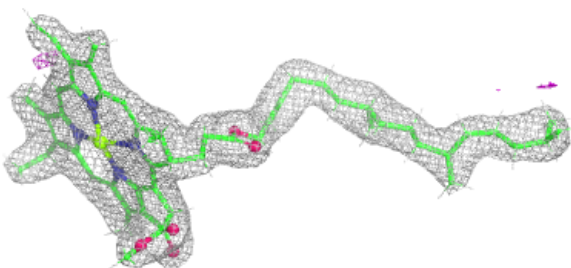
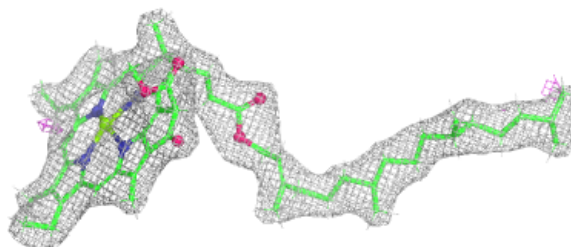
Electron density around CLA B 616:

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

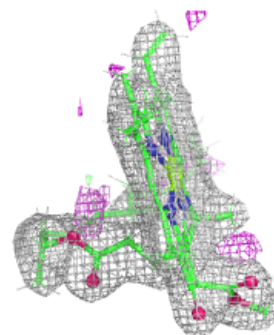
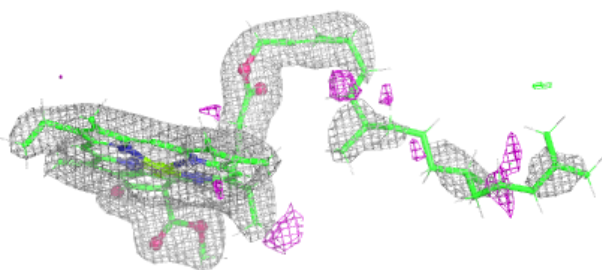
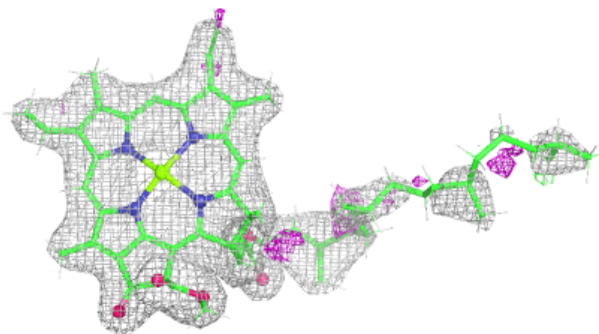


Electron density around CLA C 502:

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

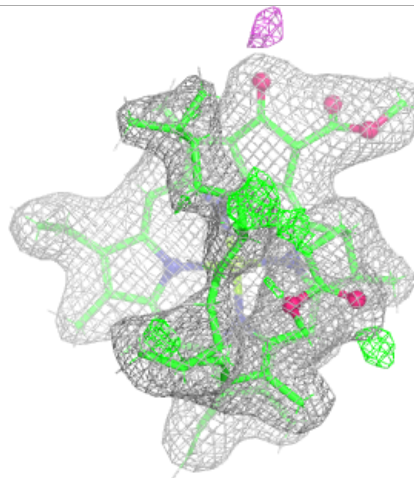
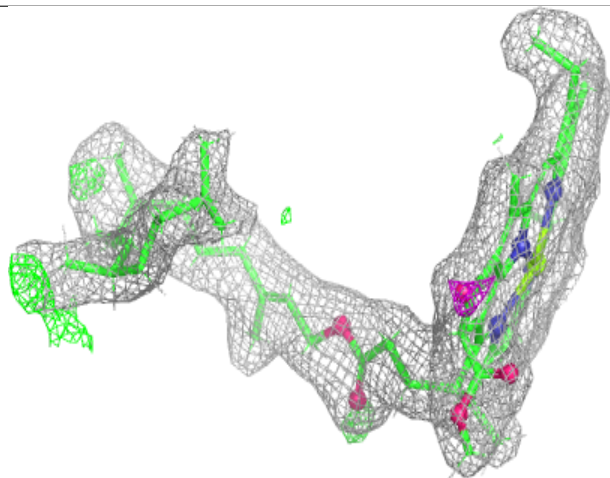
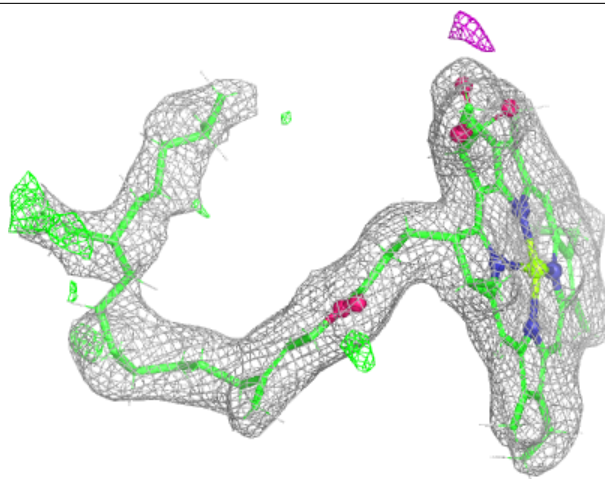
**Electron density around CLA a 403:**

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



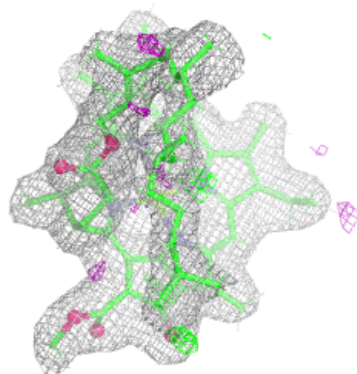
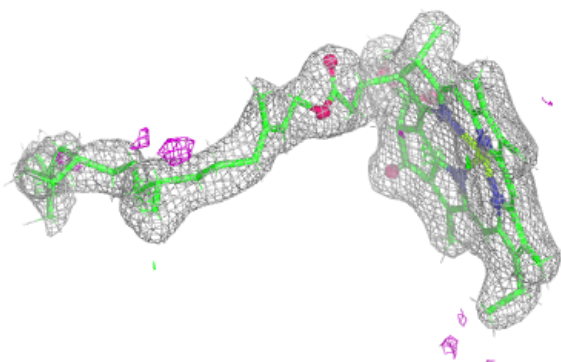
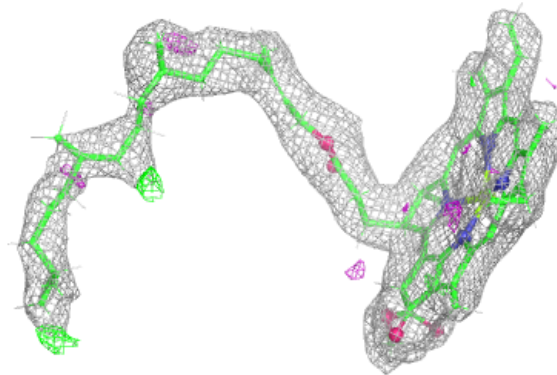
Electron density around CLA B 606:

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

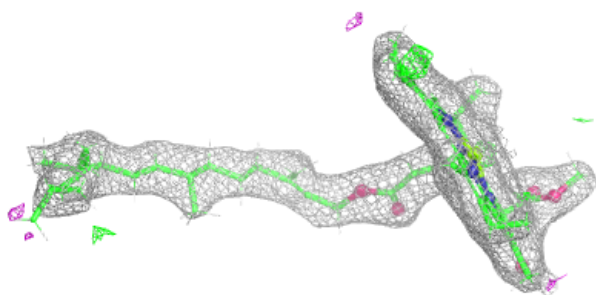
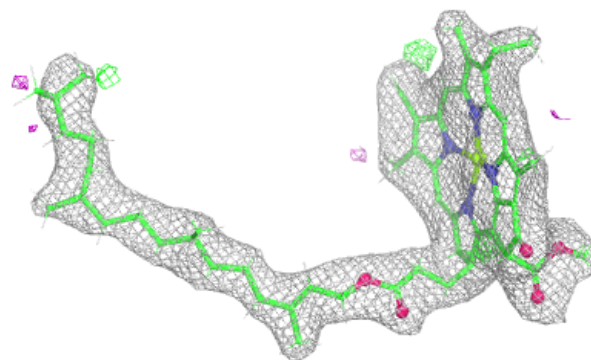


Electron density around CLA b 606:

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

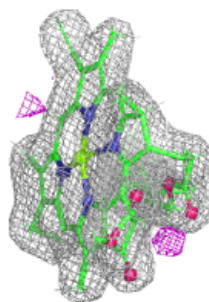
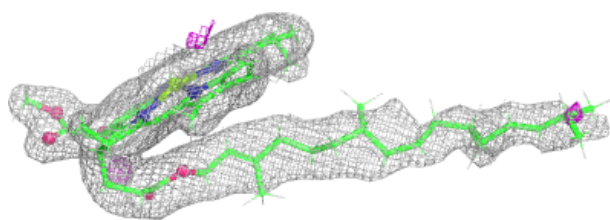
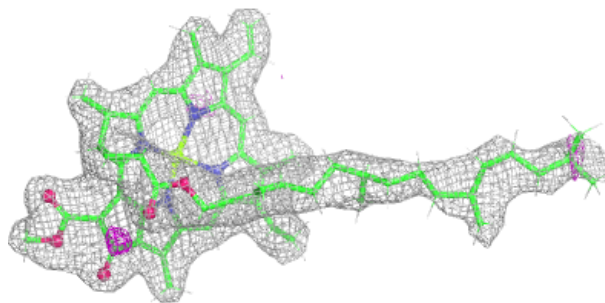
**Electron density around CLA b 609:**

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



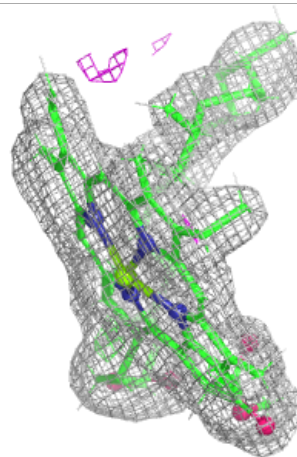
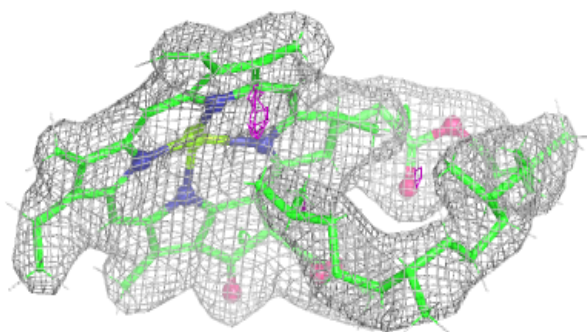
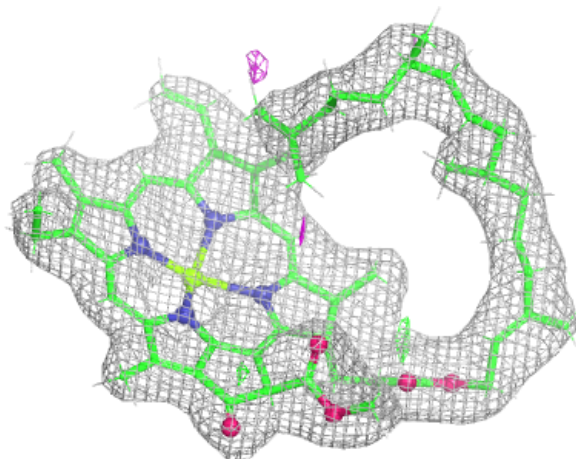
Electron density around CLA b 614:

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



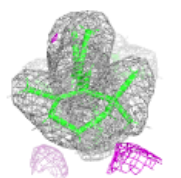
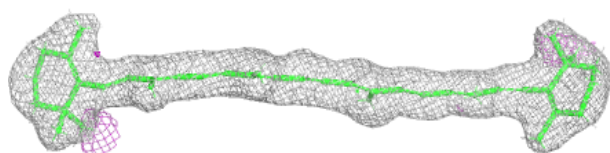
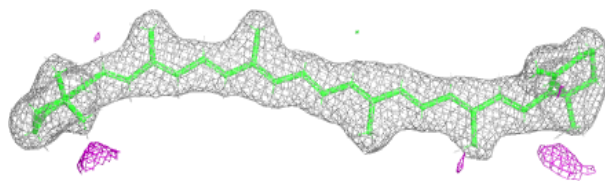
Electron density around CLA b 615:

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



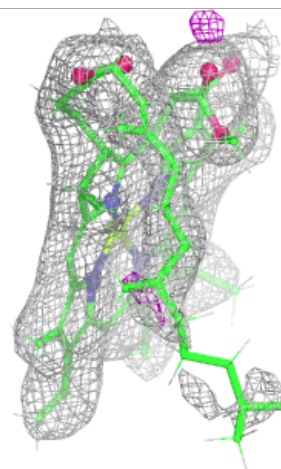
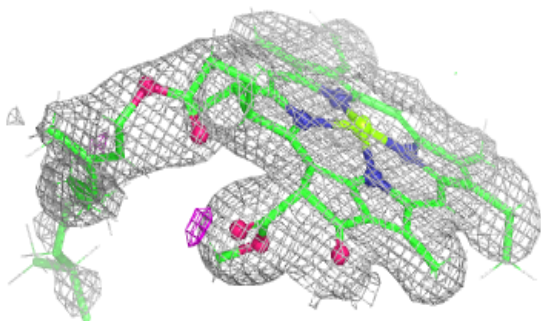
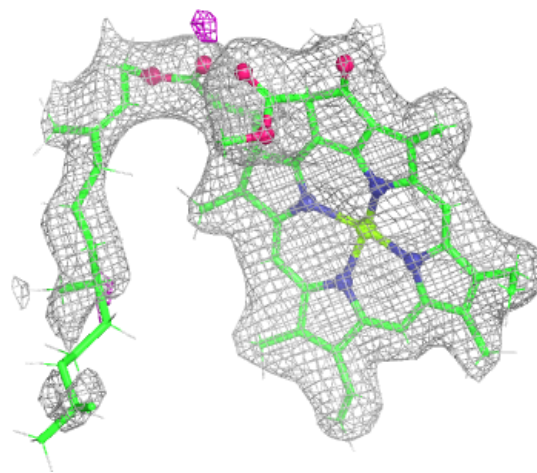
Electron density around BCR a 406:

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



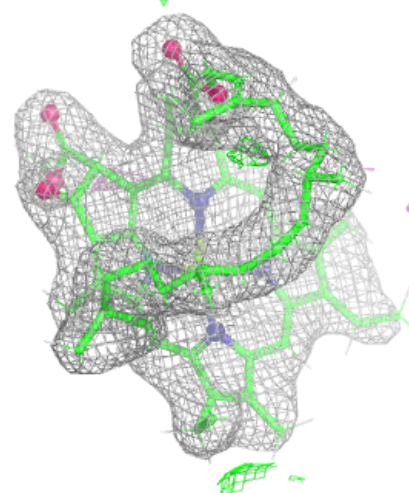
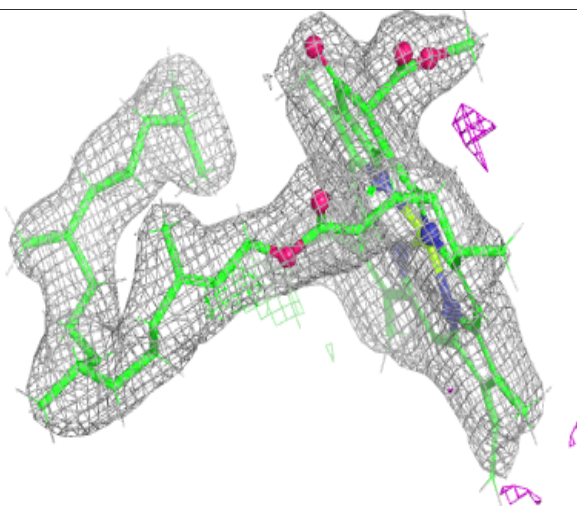
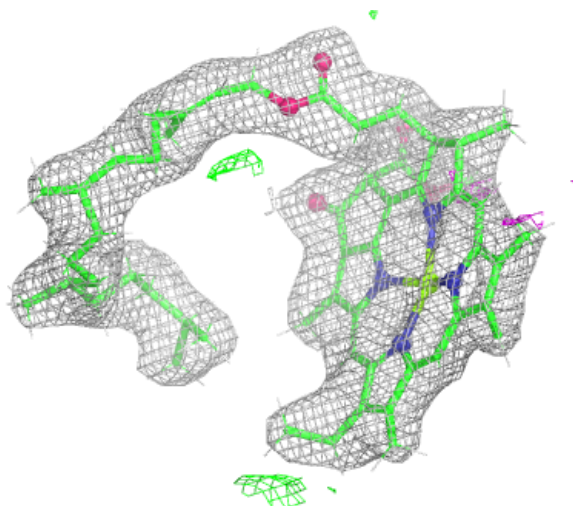
Electron density around CLA b 616:

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



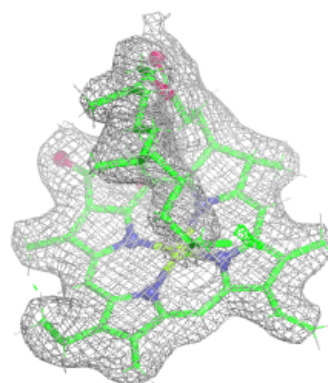
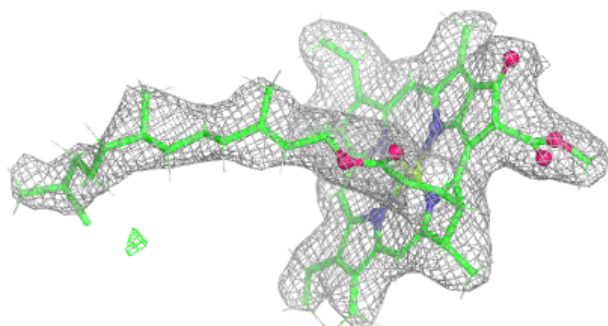
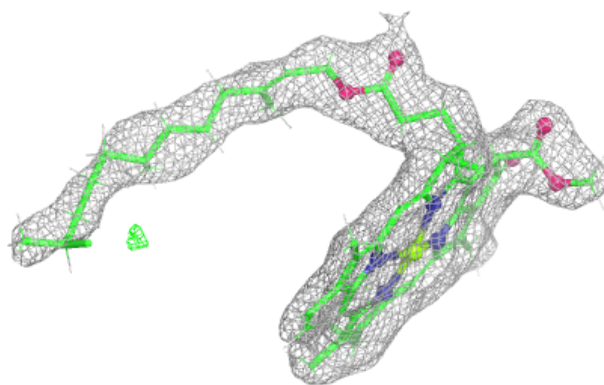
Electron density around CLA c 503:

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

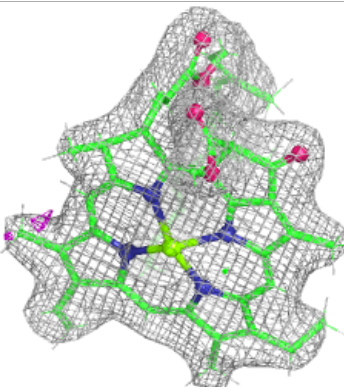
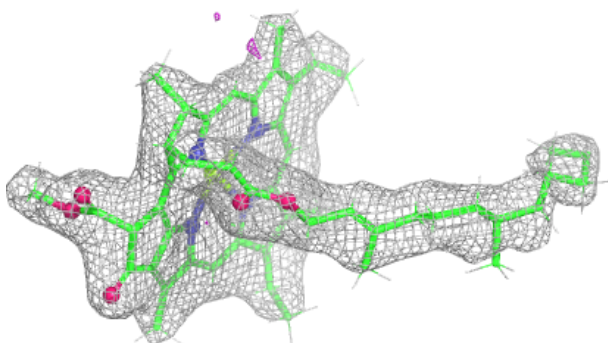
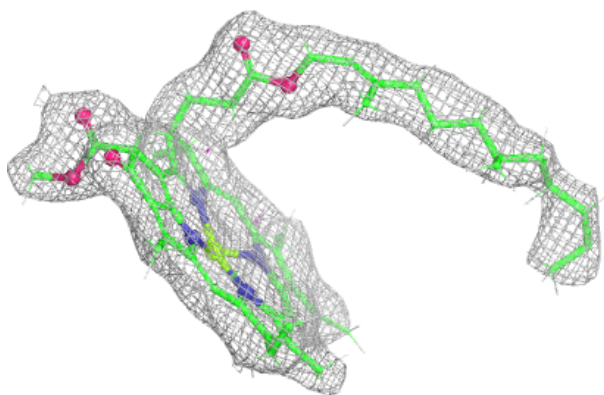


Electron density around CLA c 504:

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

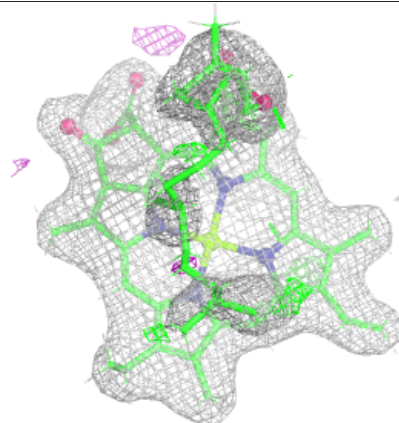
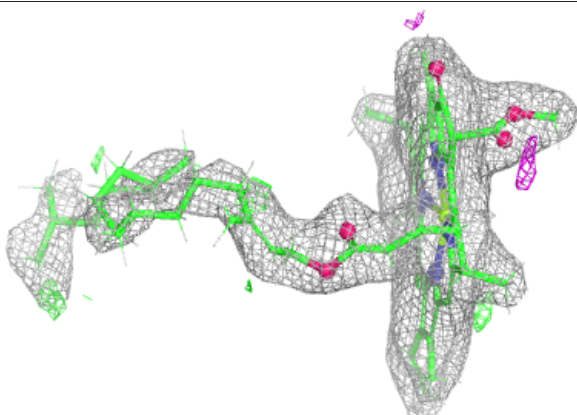
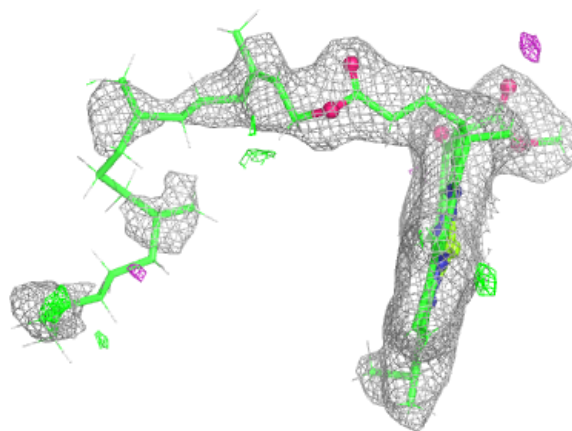
**Electron density around CLA C 504:**

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



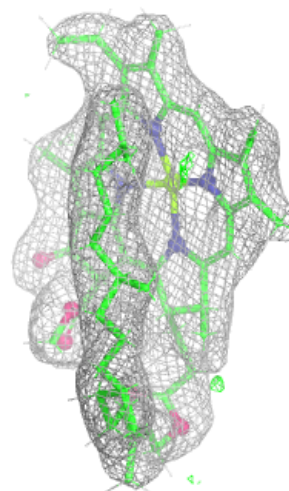
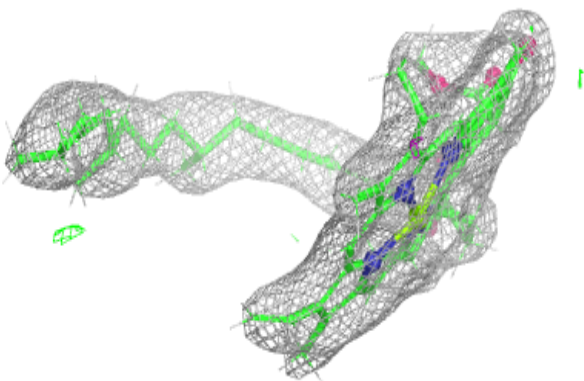
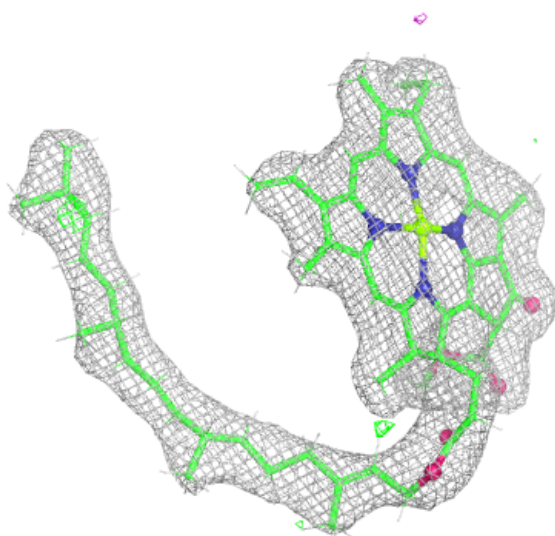
Electron density around CLA c 506:

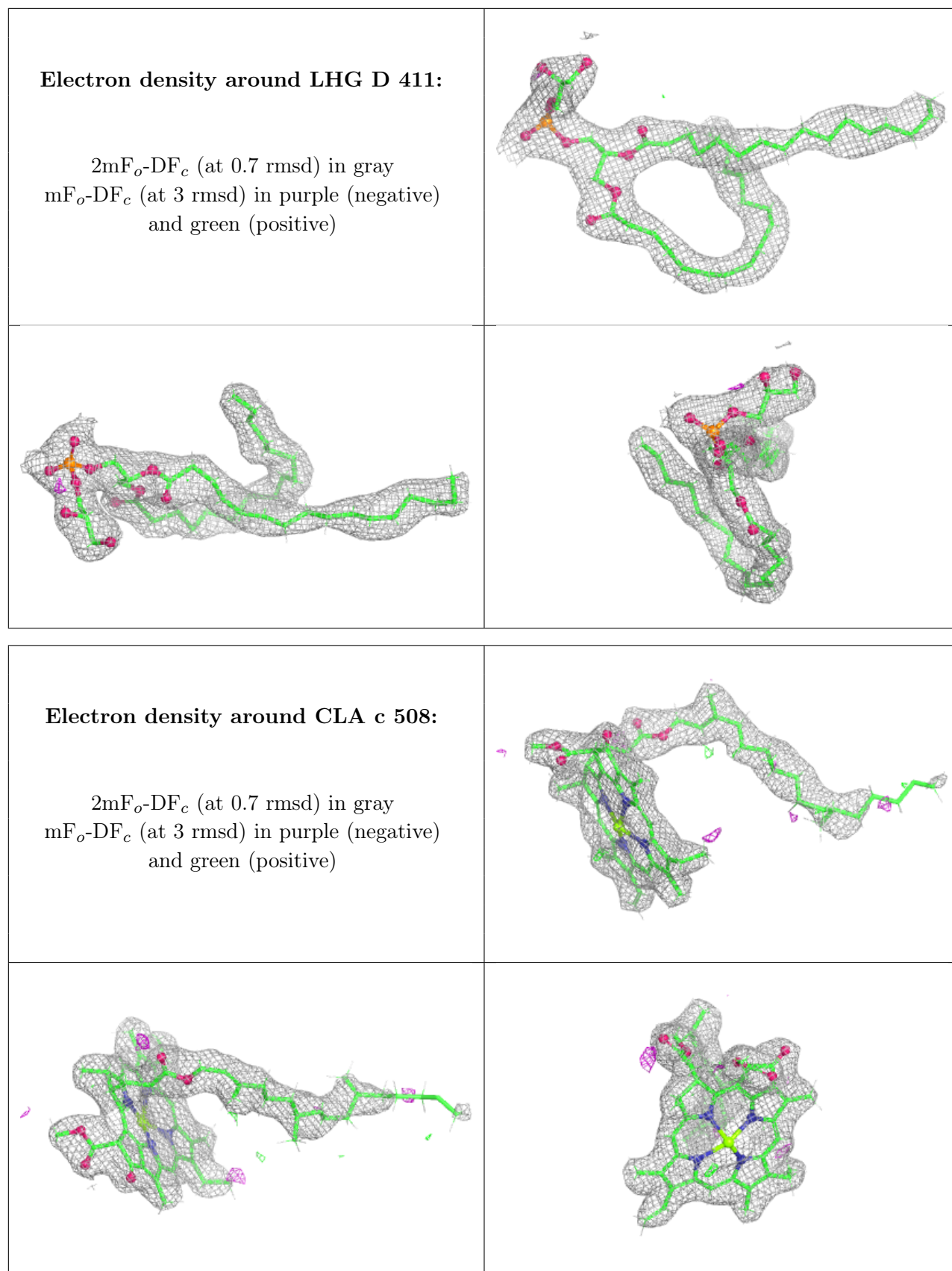
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 507:

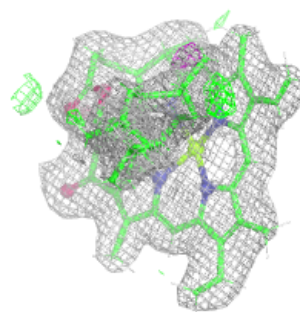
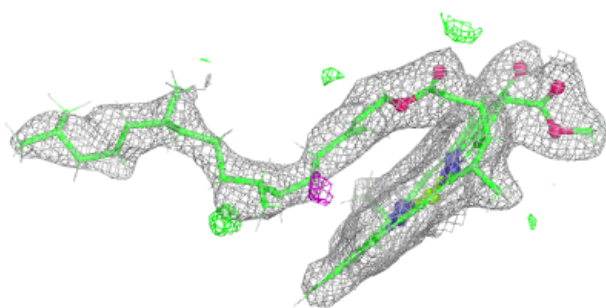
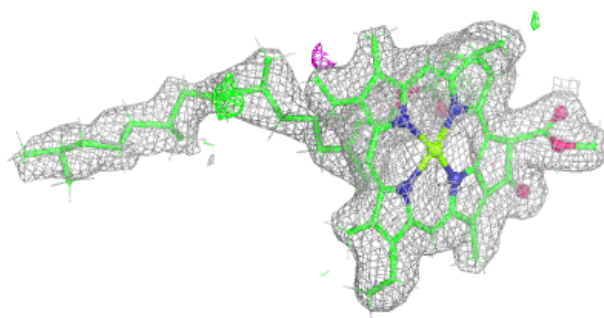
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





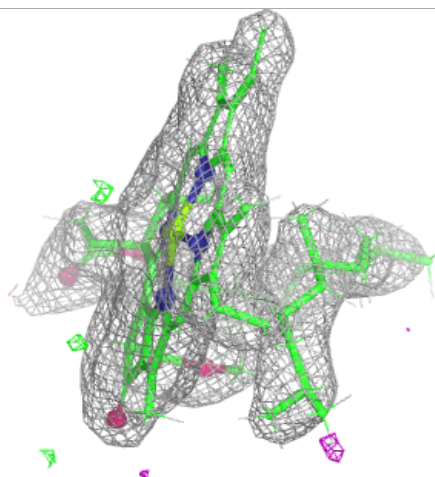
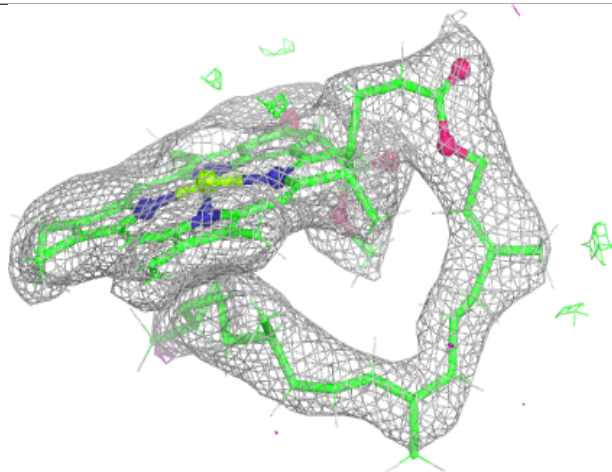
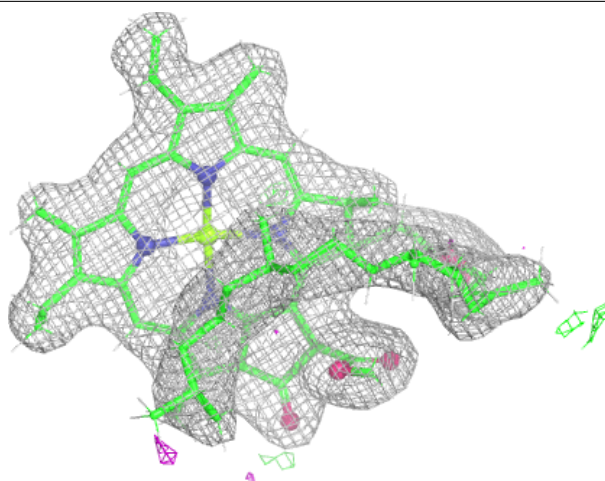
Electron density around CLA C 505:

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



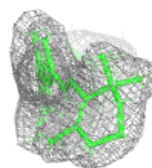
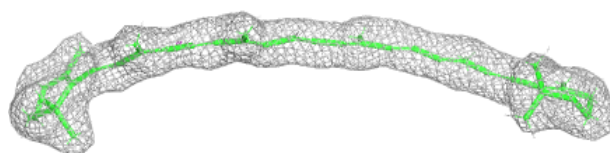
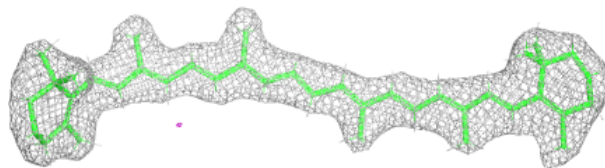
Electron density around CLA c 510:

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

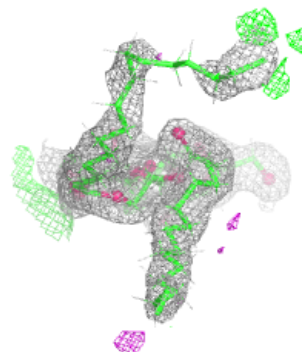
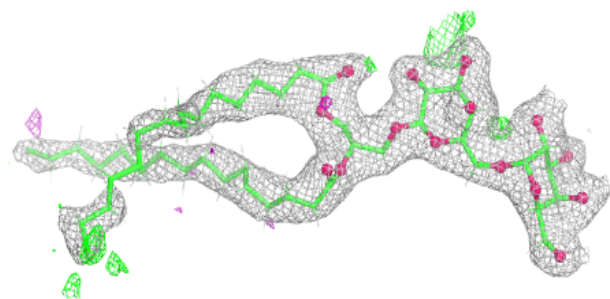
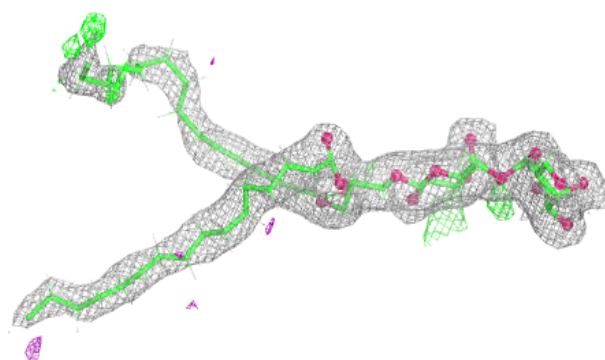


Electron density around BCR t 101:

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

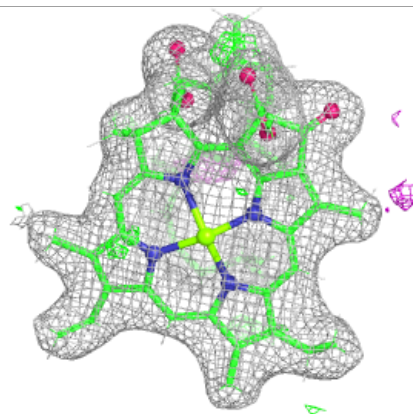
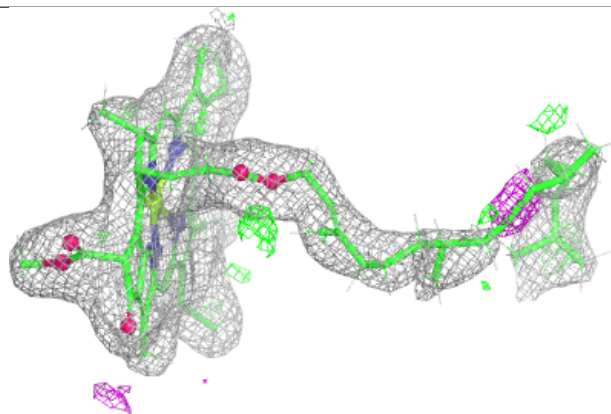
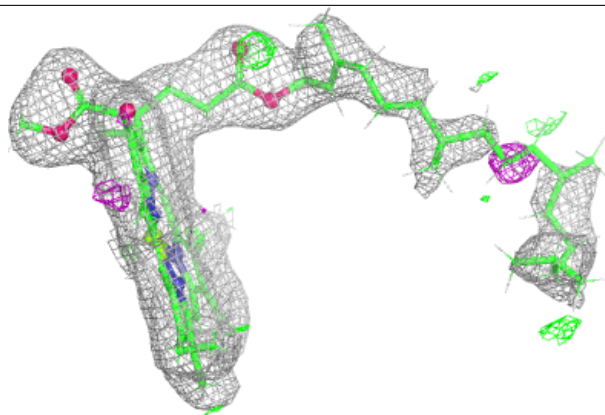
**Electron density around DGD C 515:**

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

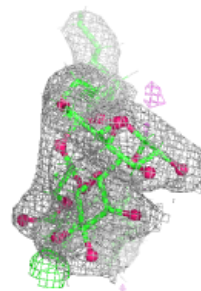
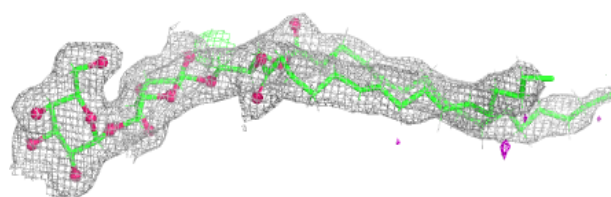
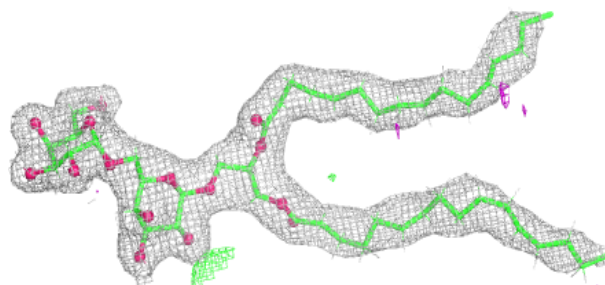


Electron density around CLA C 506:

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

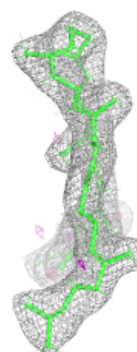
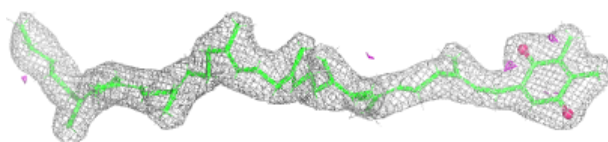
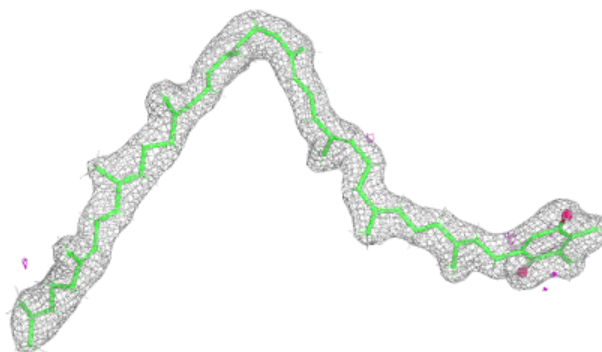
**Electron density around DGD C 517:**

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

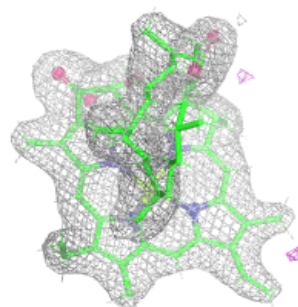
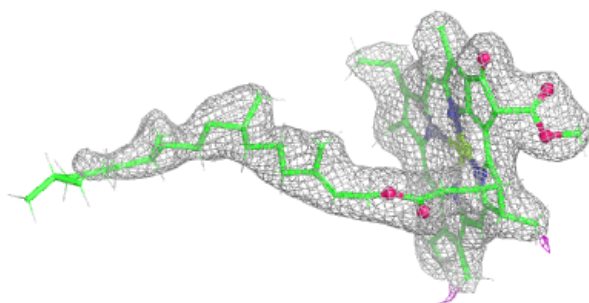
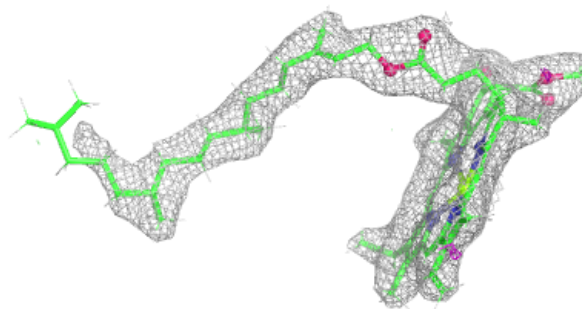


Electron density around PL9 D 406:

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

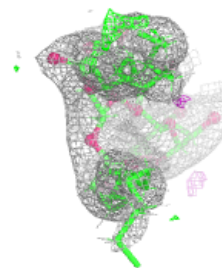
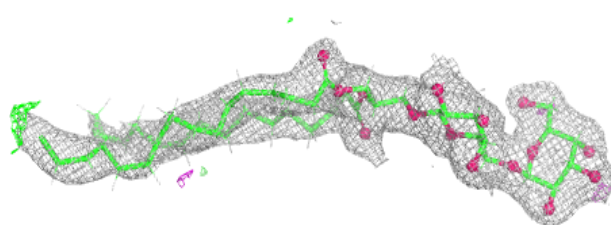
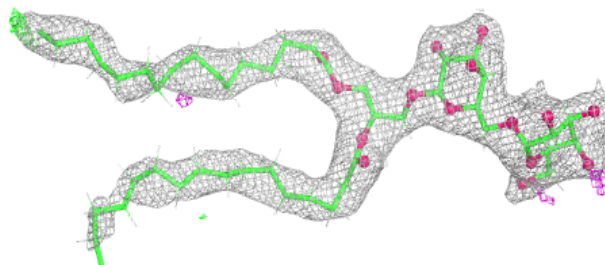
**Electron density around CLA C 508:**

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

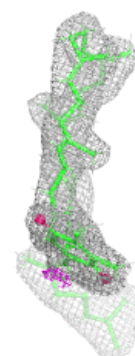
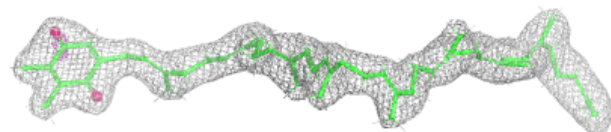
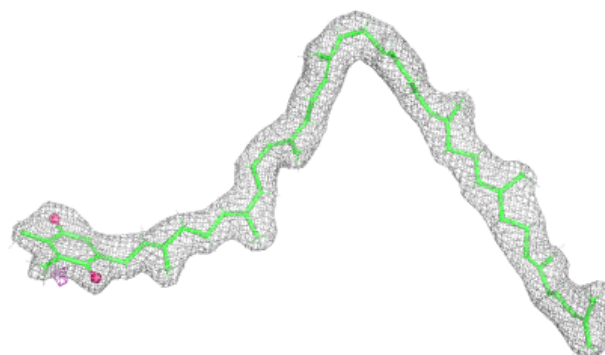


Electron density around DGD c 518:

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

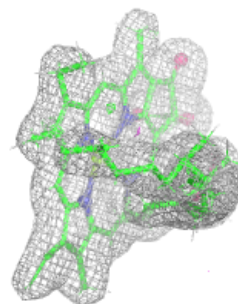
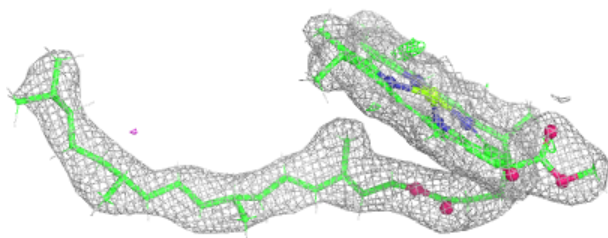
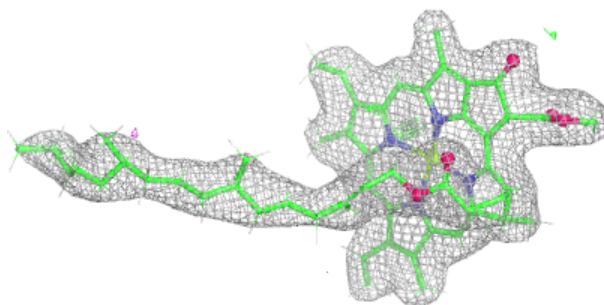
**Electron density around PL9 d 407:**

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

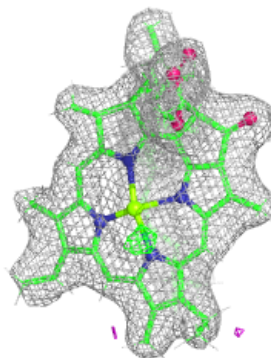
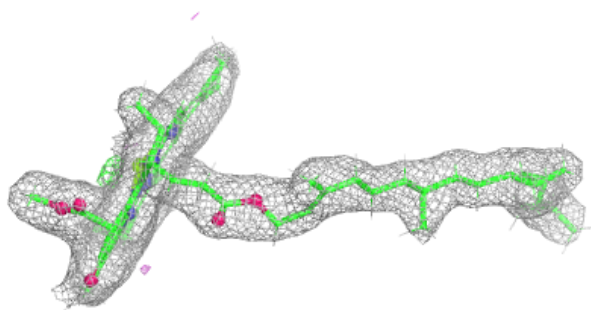
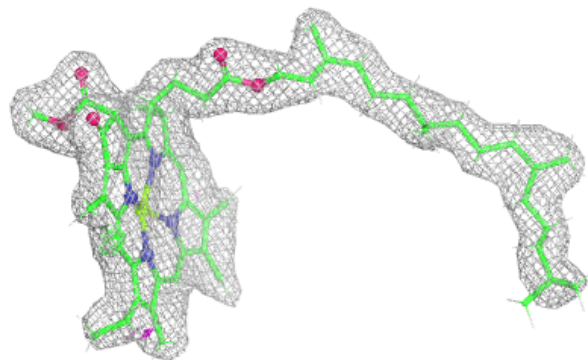


Electron density around CLA b 608:

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

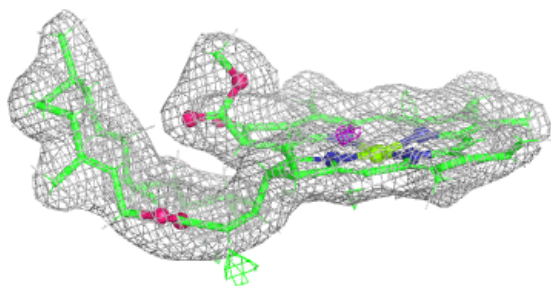
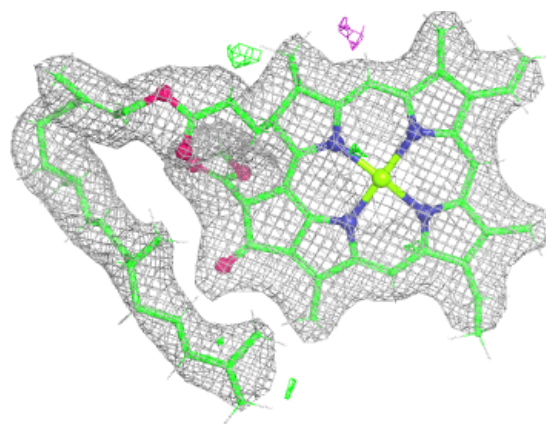
**Electron density around CLA B 609:**

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



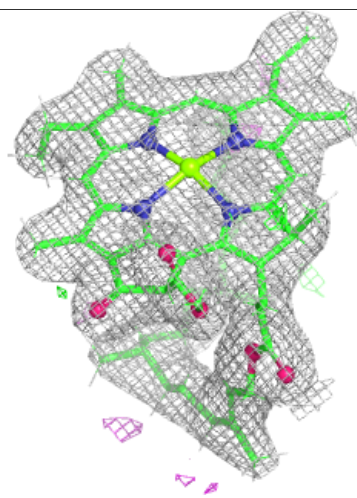
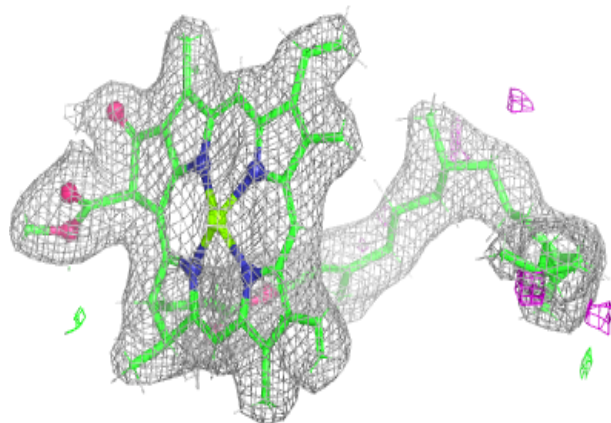
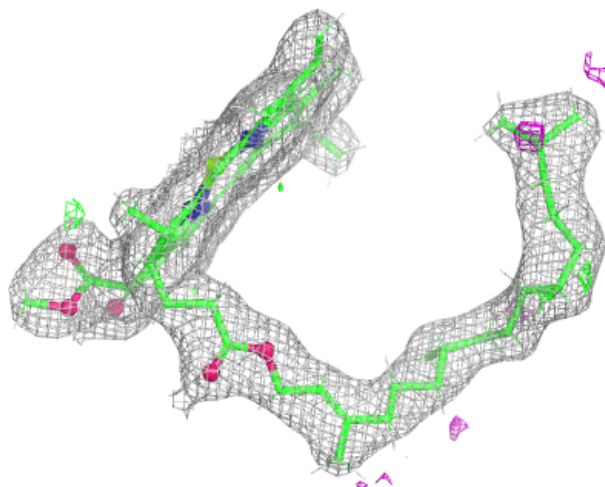
Electron density around CLA b 610:

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



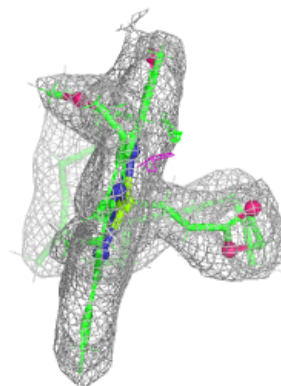
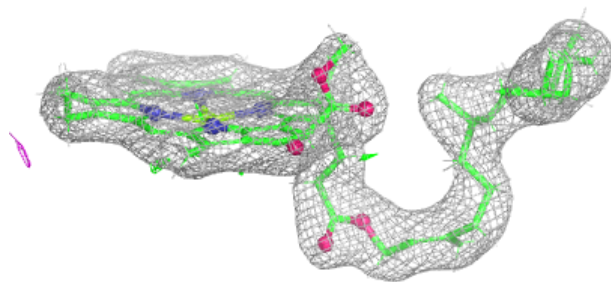
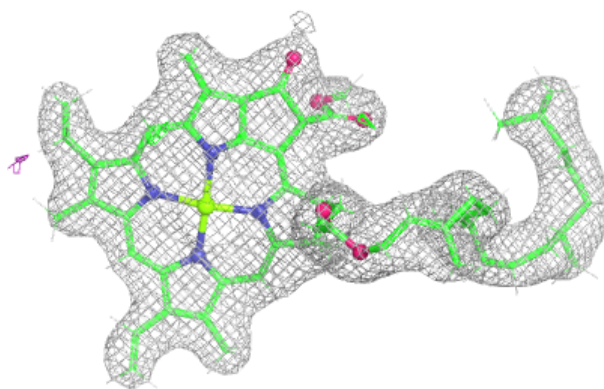
Electron density around CLA b 611:

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



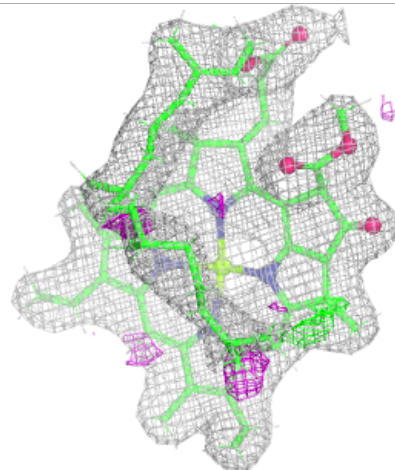
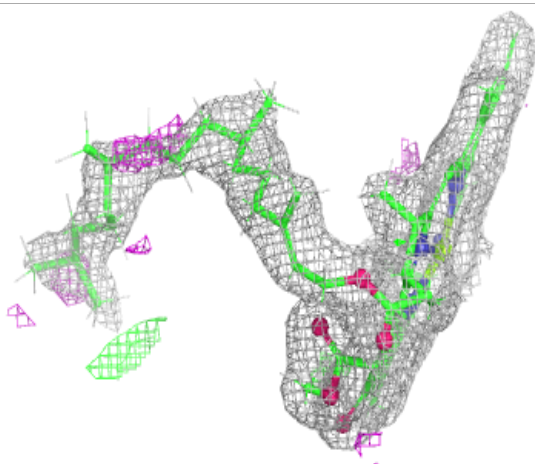
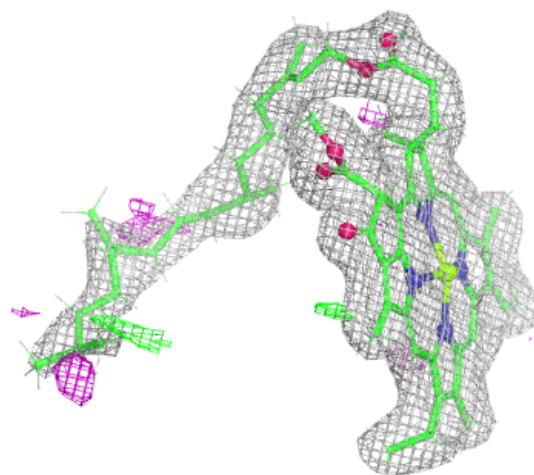
Electron density around CLA b 612:

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



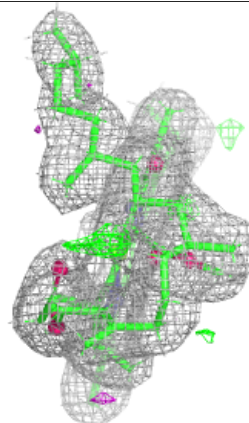
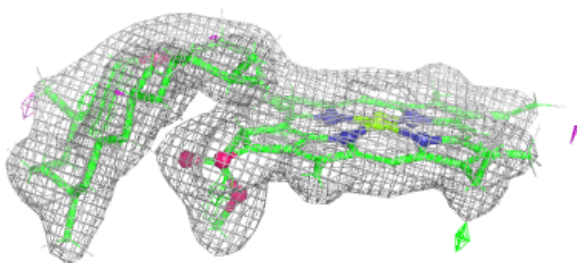
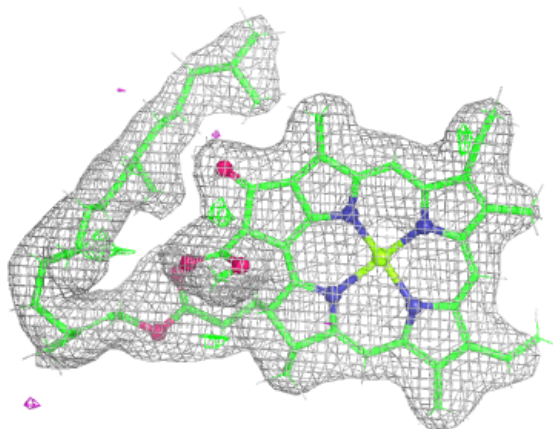
Electron density around CLA b 613:

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



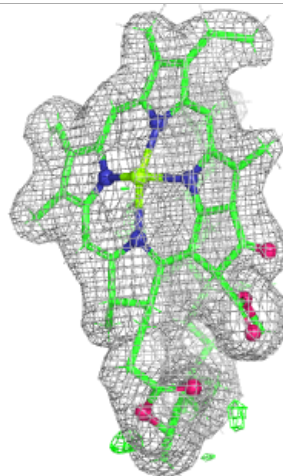
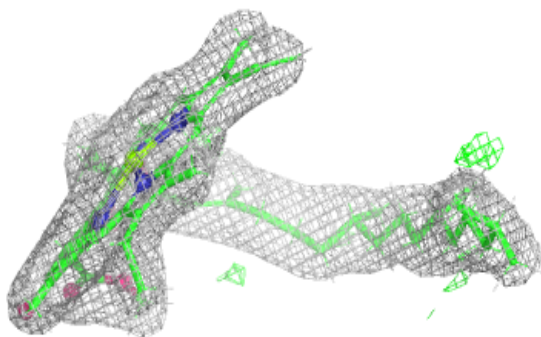
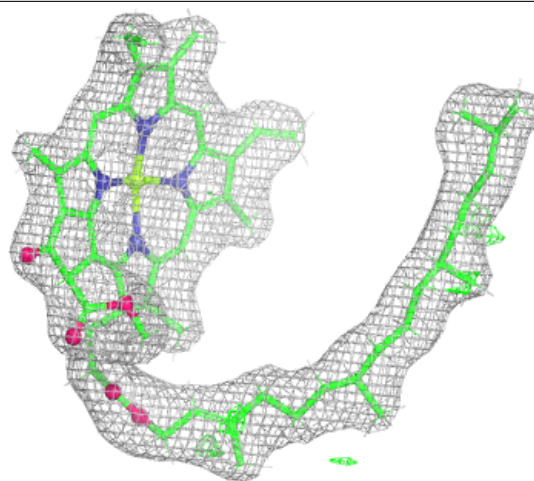
Electron density around CLA B 610:

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



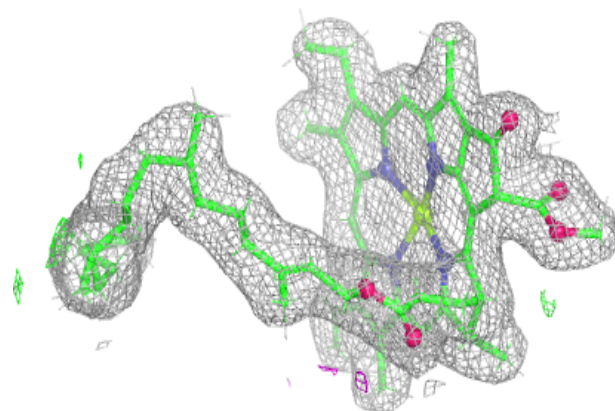
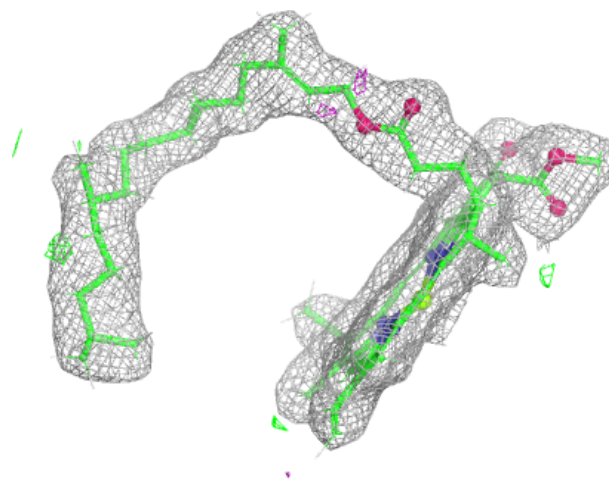
Electron density around CLA C 507:

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



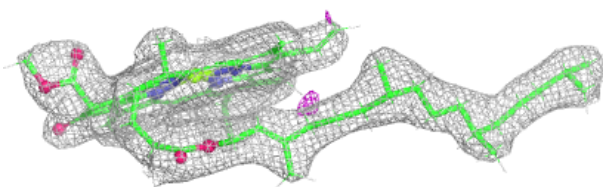
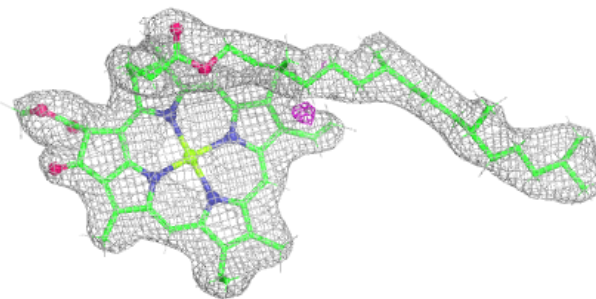
Electron density around CLA B 611:

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

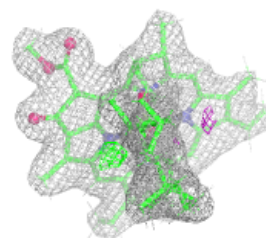
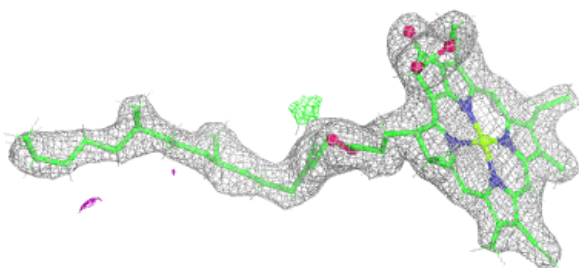
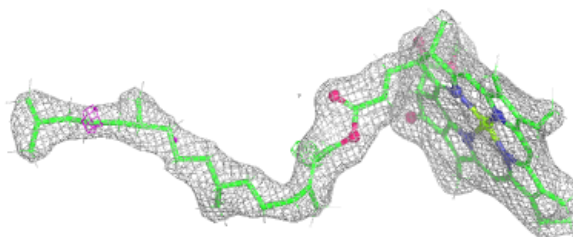


Electron density around CLA c 501:

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

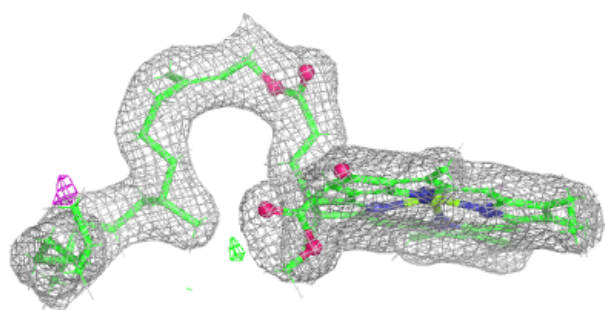
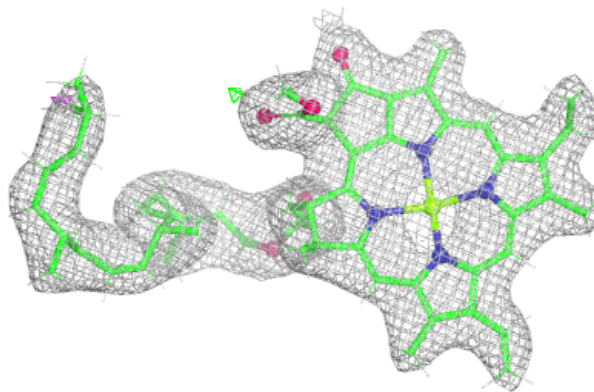
**Electron density around CLA c 502:**

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

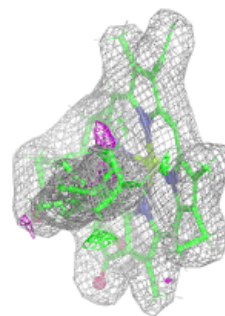
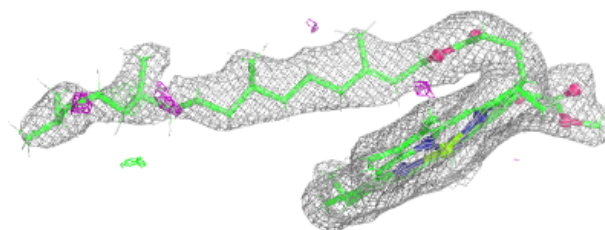
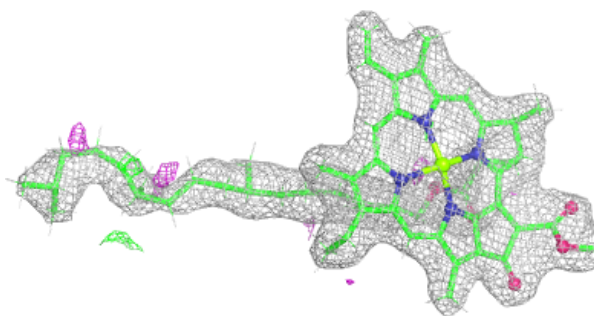


Electron density around CLA B 612:

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

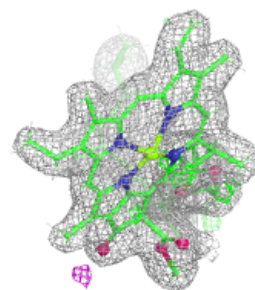
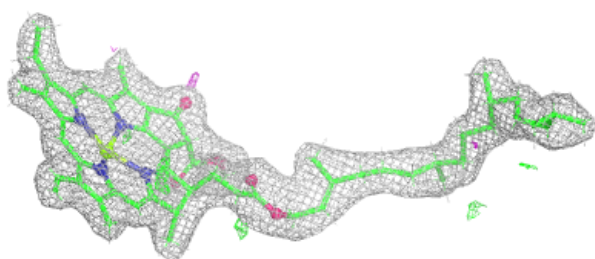
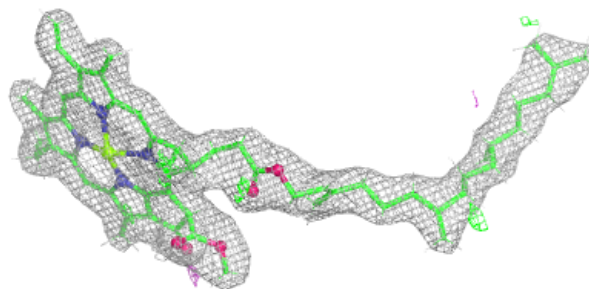
**Electron density around CLA B 614:**

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

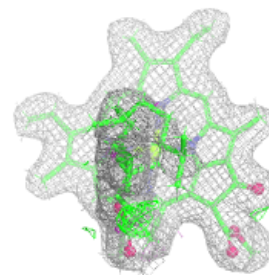
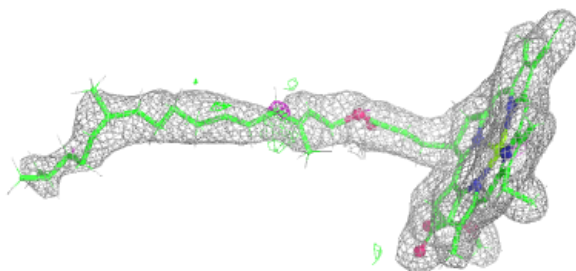
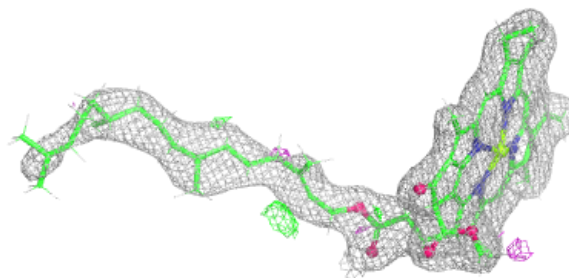


Electron density around CLA A 402:

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

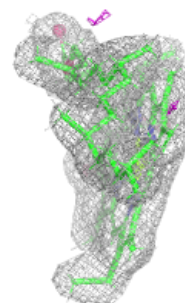
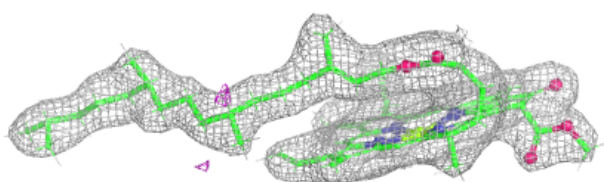
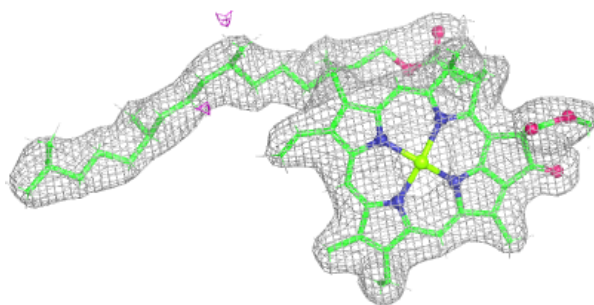
**Electron density around CLA B 604:**

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

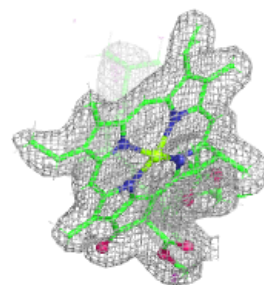
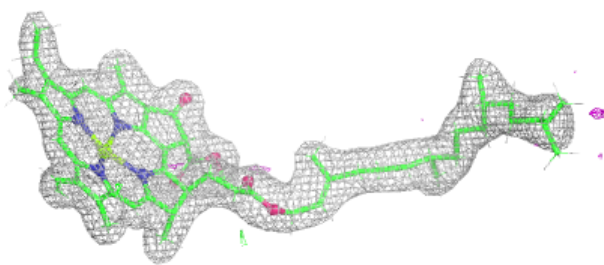
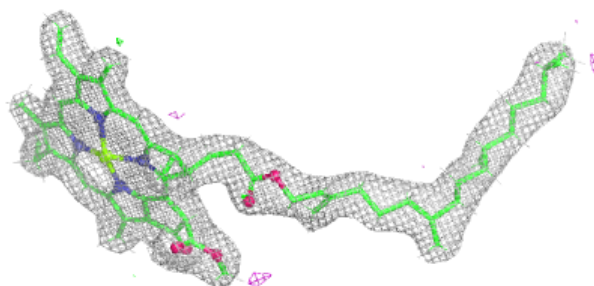


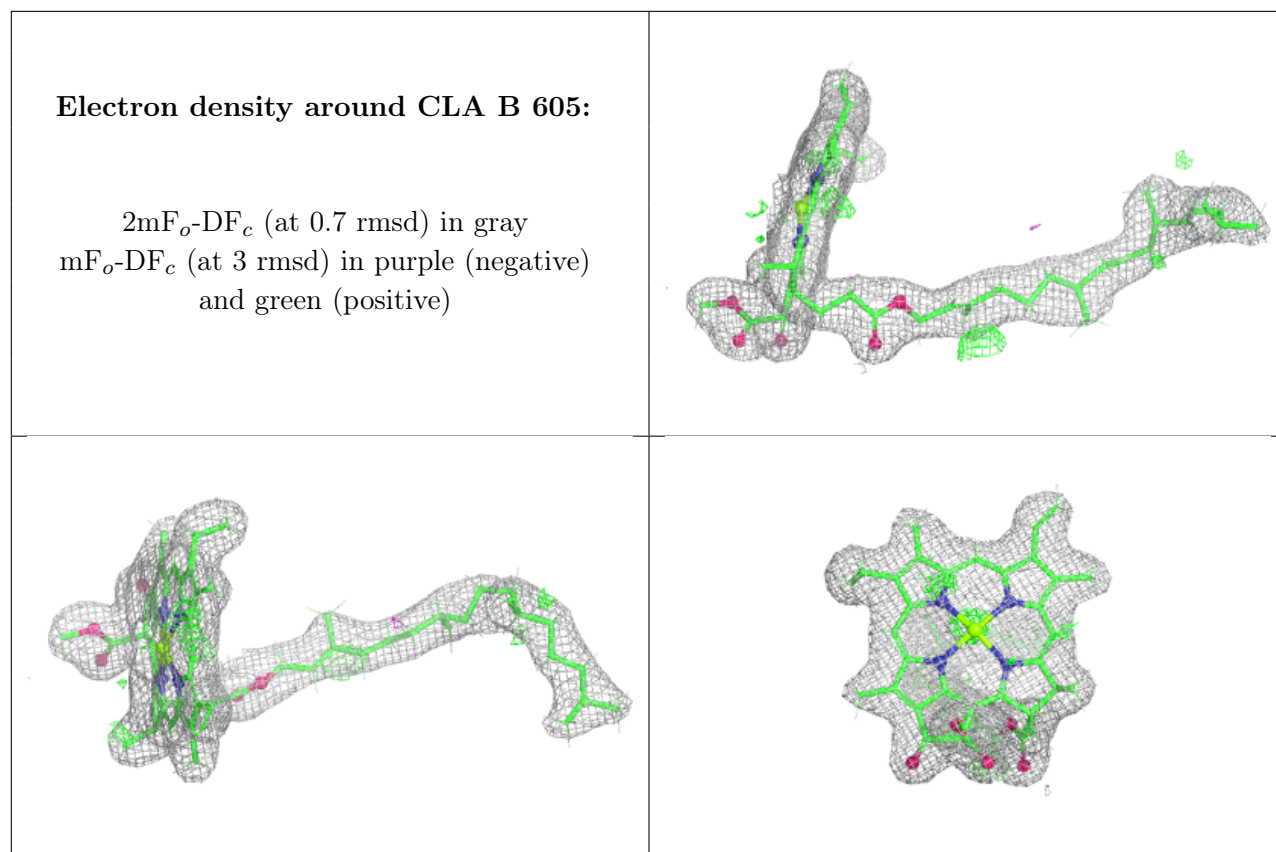
Electron density around CLA C 501:

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

**Electron density around CLA a 402:**

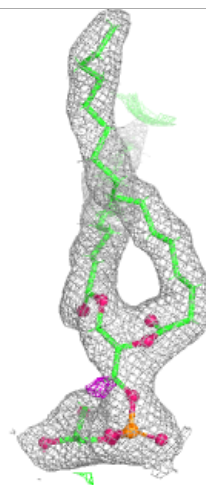
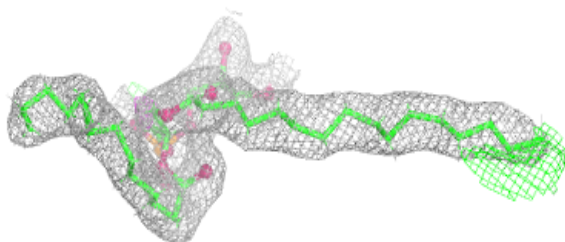
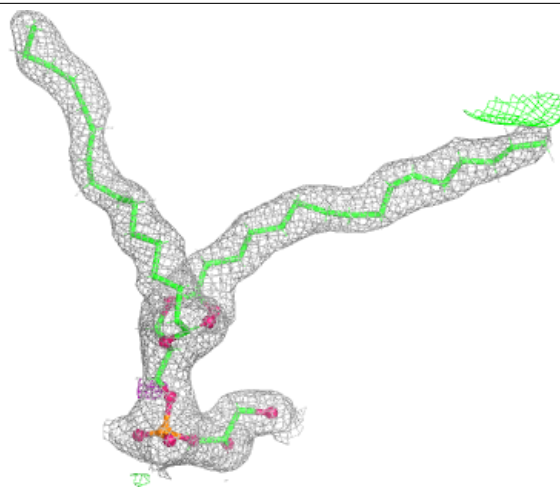
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





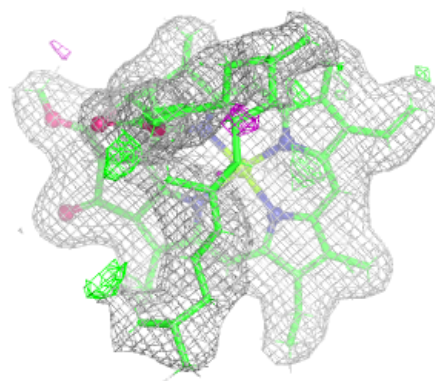
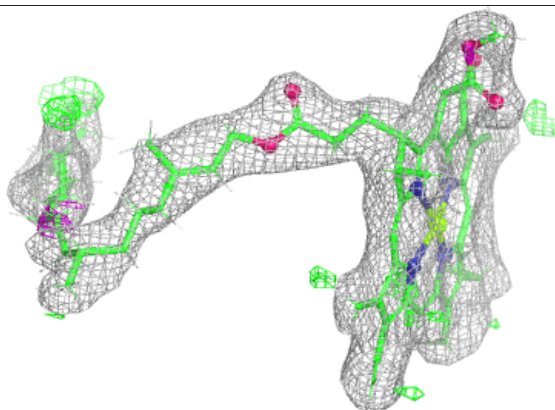
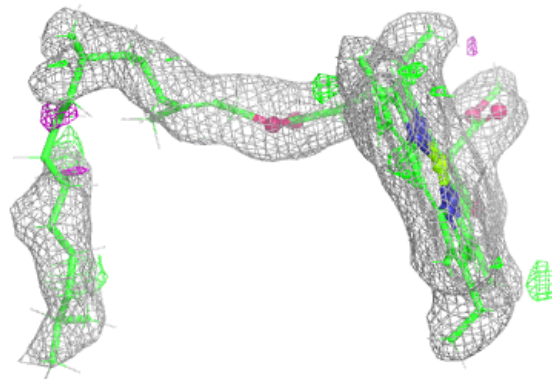
Electron density around LHG L 101:

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

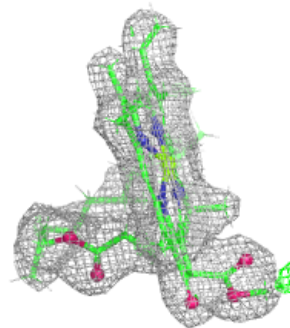
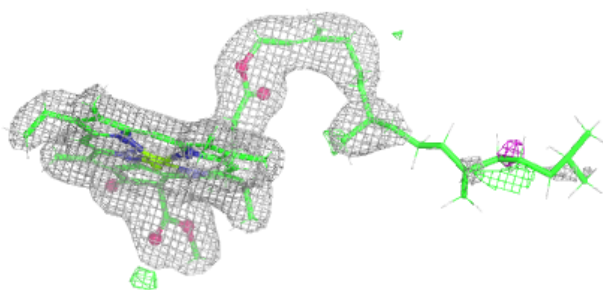
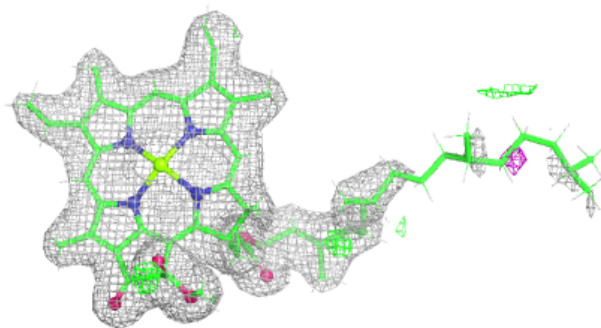


Electron density around CLA a 405:

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

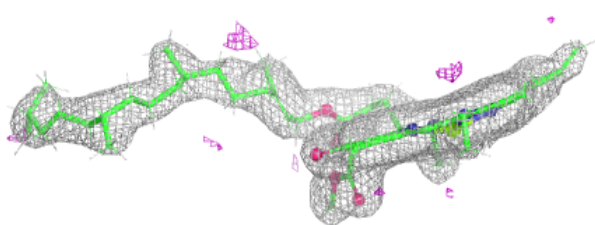
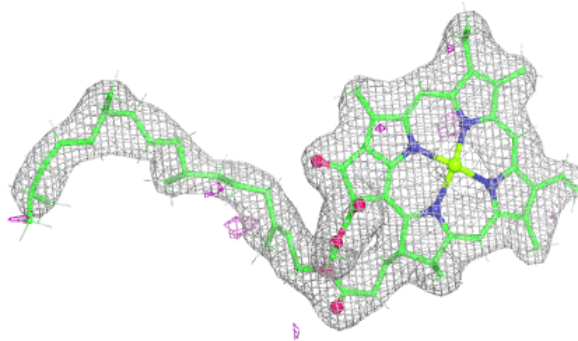
**Electron density around CLA A 403:**

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



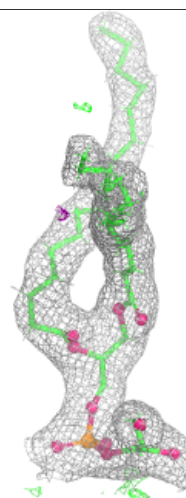
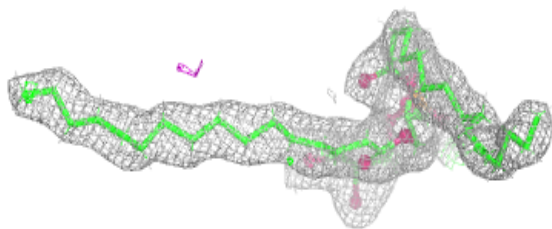
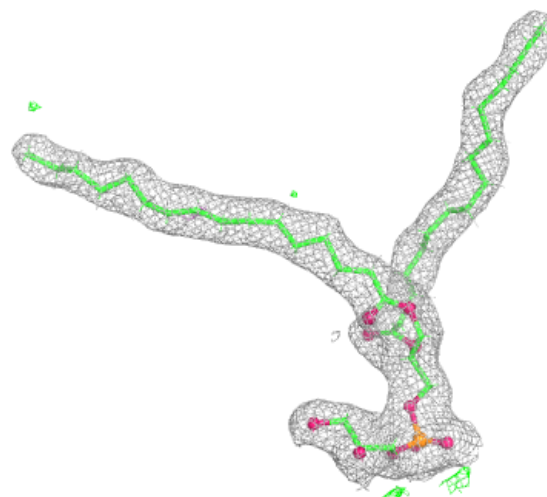
Electron density around CLA b 602:

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



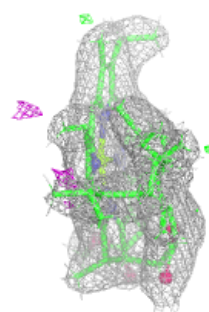
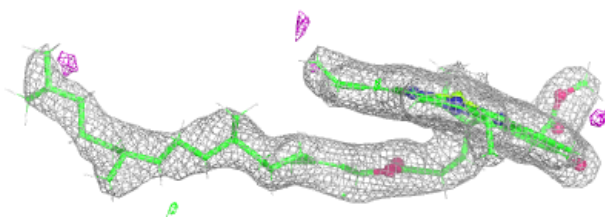
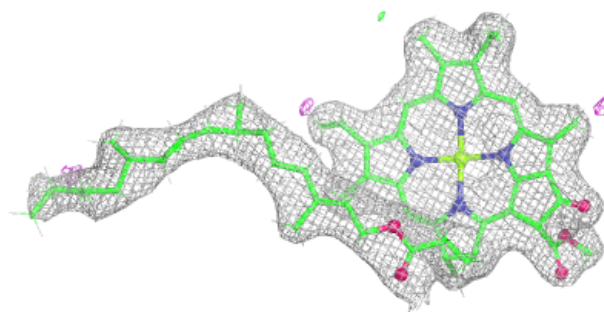
Electron density around LHG 1 101:

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

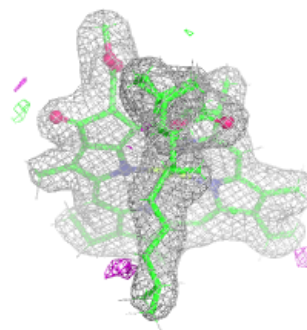
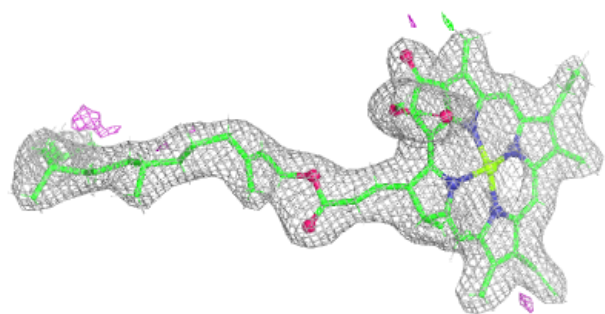
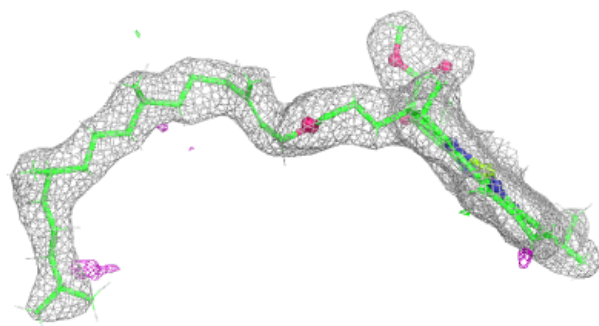


Electron density around CLA b 603:

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

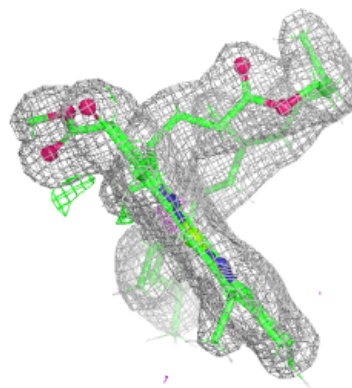
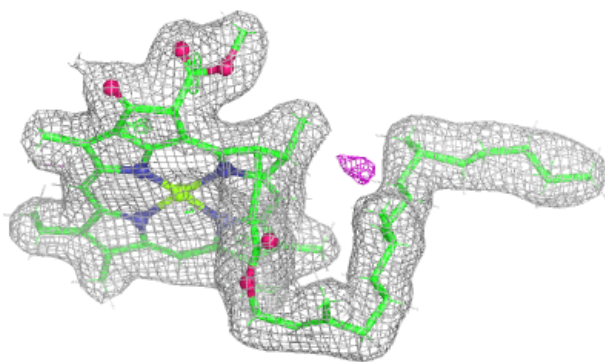
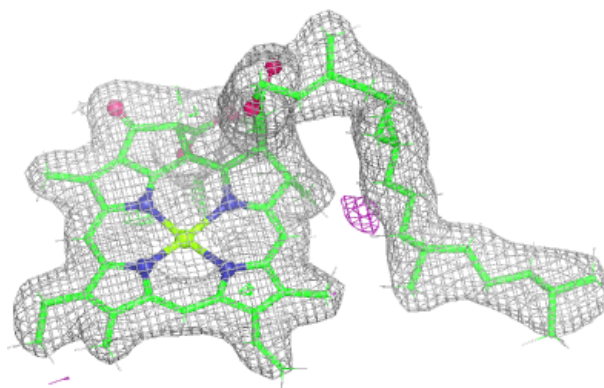
**Electron density around CLA d 403:**

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

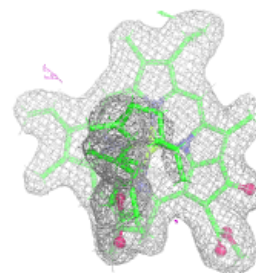
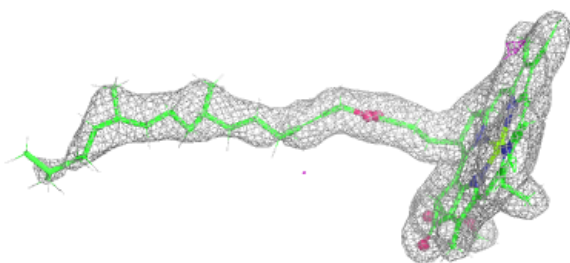
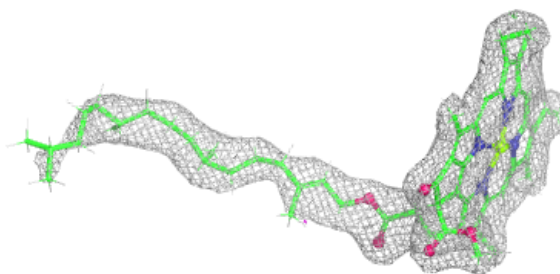


Electron density around CLA d 404:

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

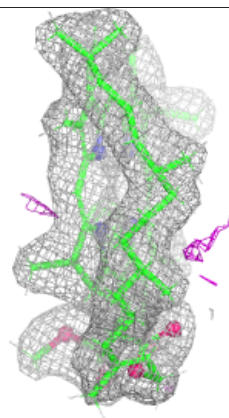
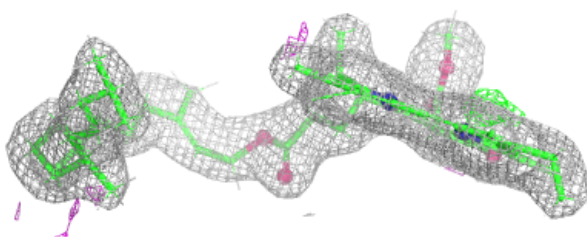
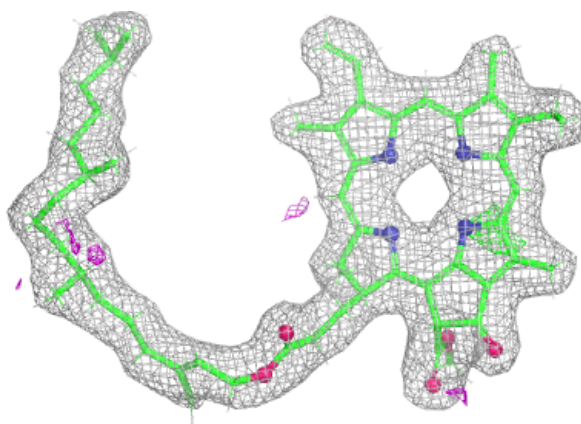
**Electron density around CLA b 604:**

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

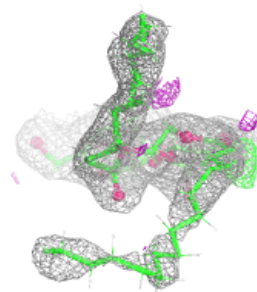
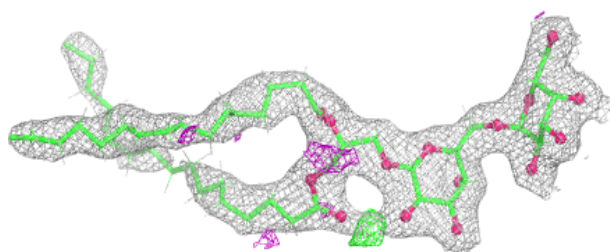
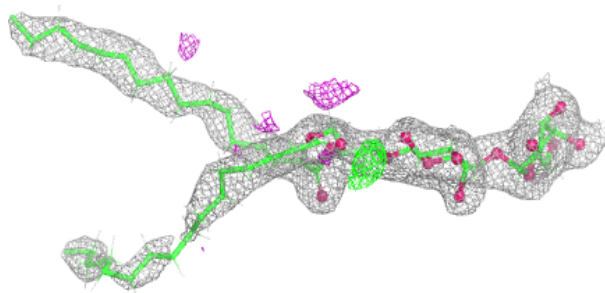


Electron density around PHO A 404:

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

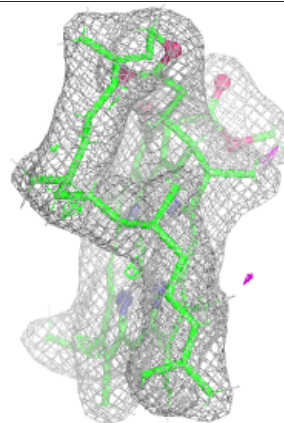
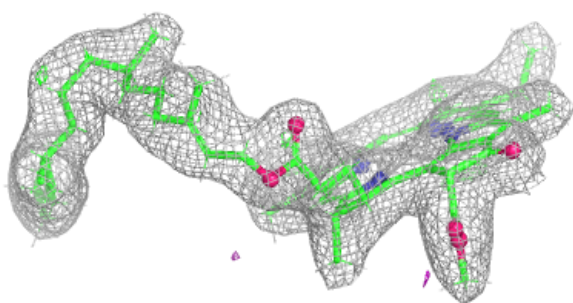
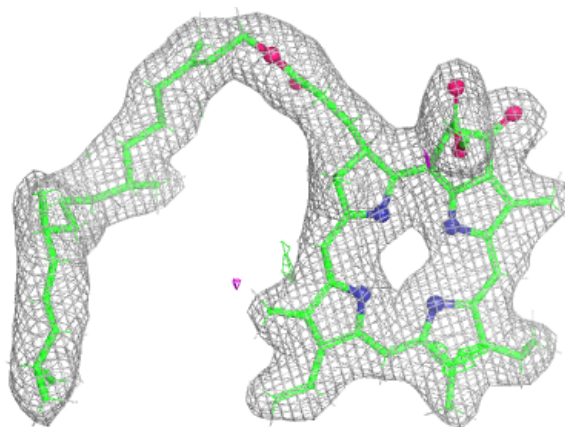
**Electron density around DGD c 516:**

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



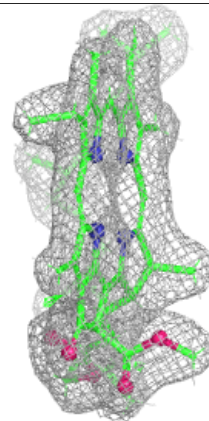
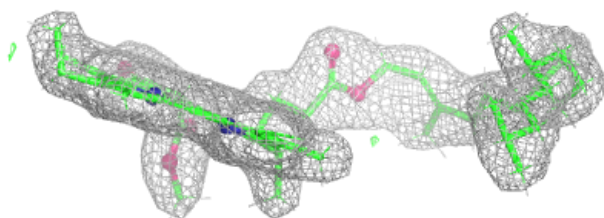
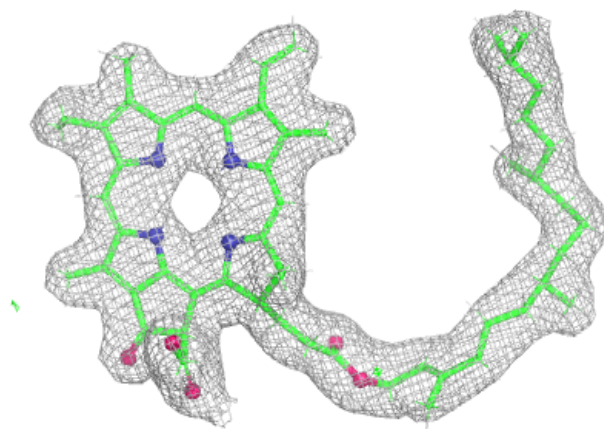
Electron density around PHO A 405:

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

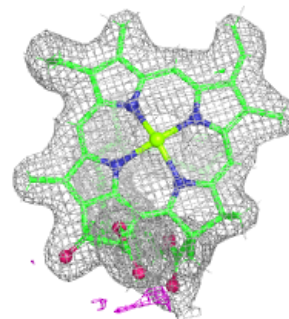
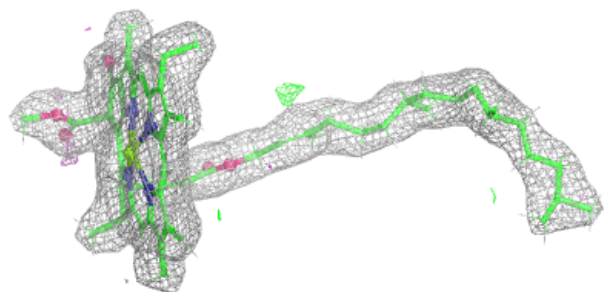
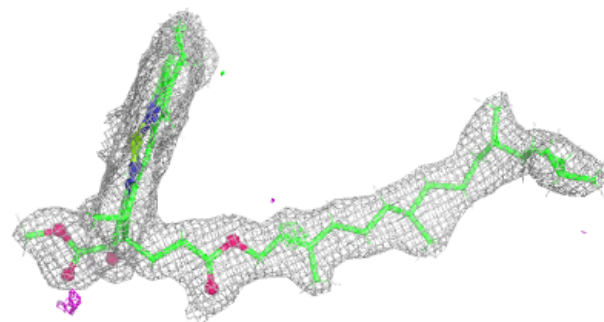


Electron density around PHO a 404:

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

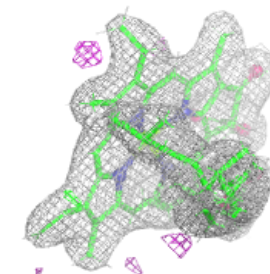
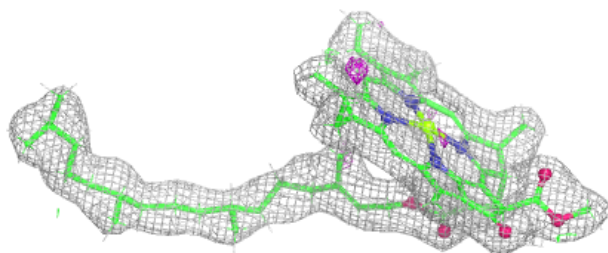
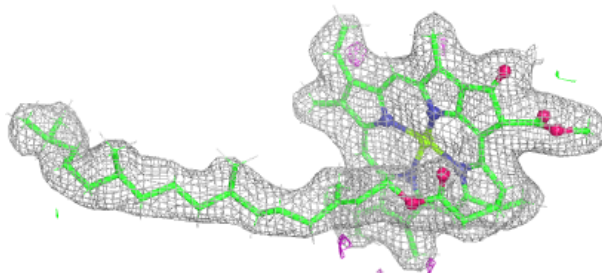
**Electron density around CLA b 605:**

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

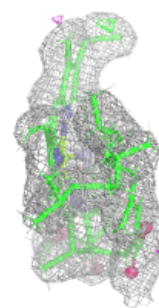
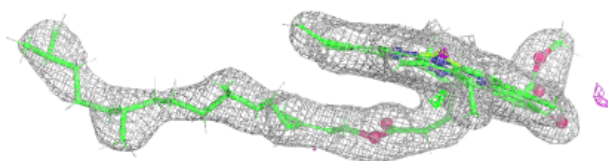
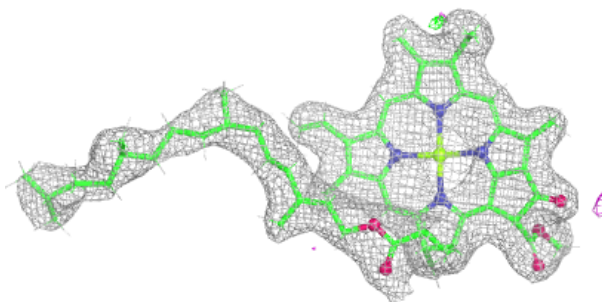


Electron density around CLA B 608:

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

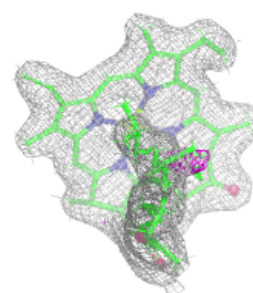
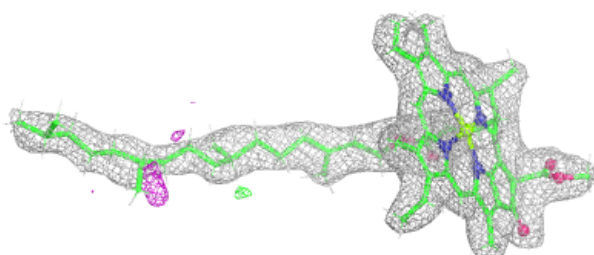
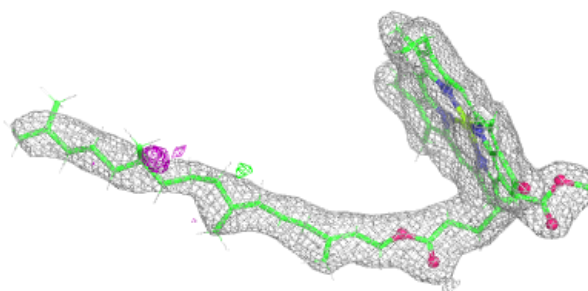
**Electron density around CLA B 603:**

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

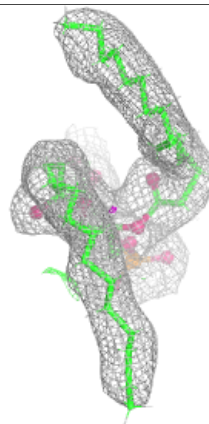
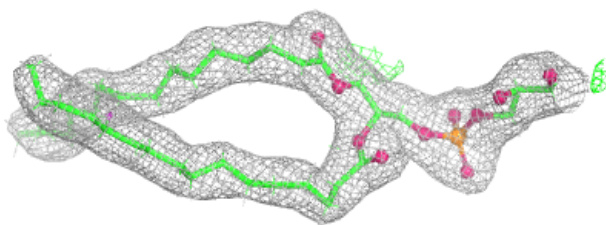
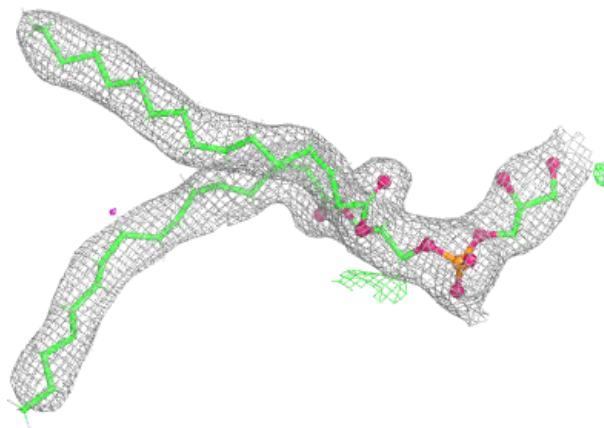


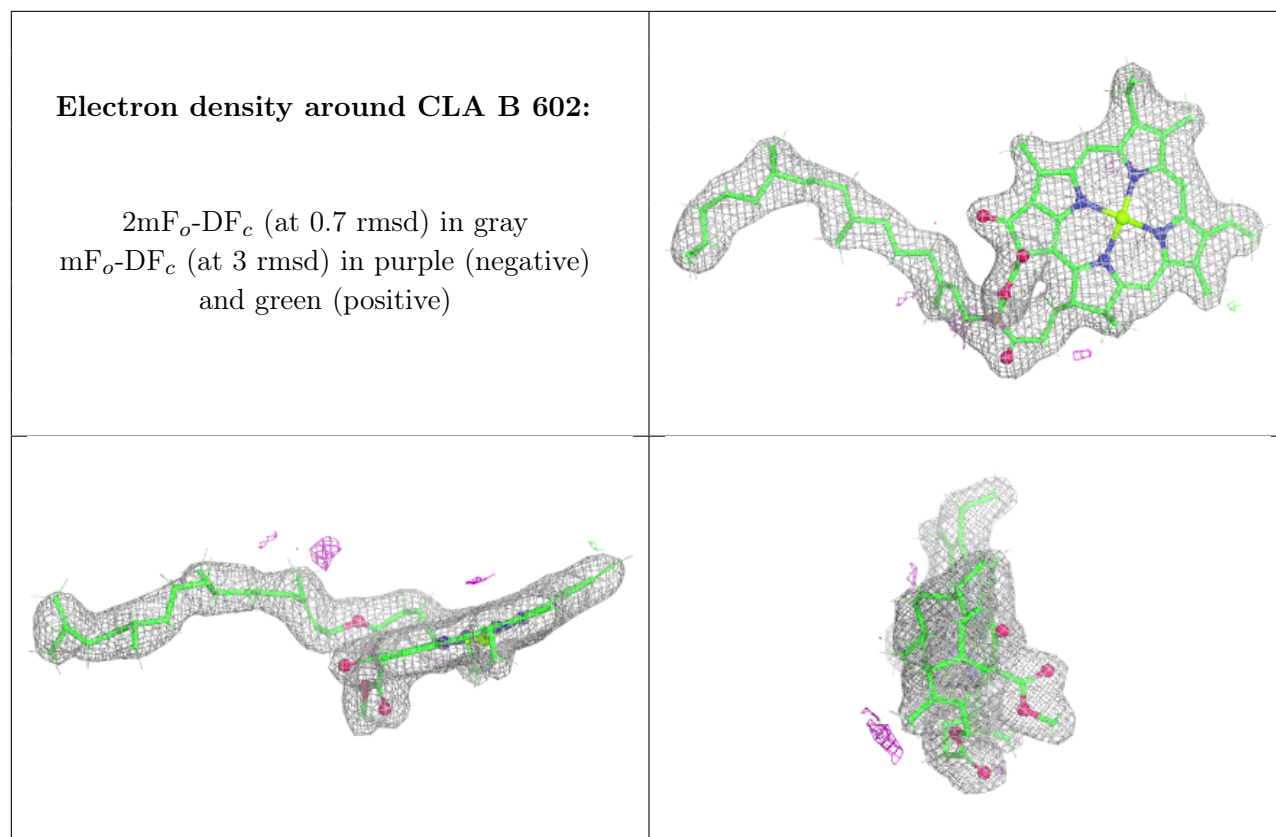
Electron density around CLA b 607:

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

**Electron density around LHG d 408:**

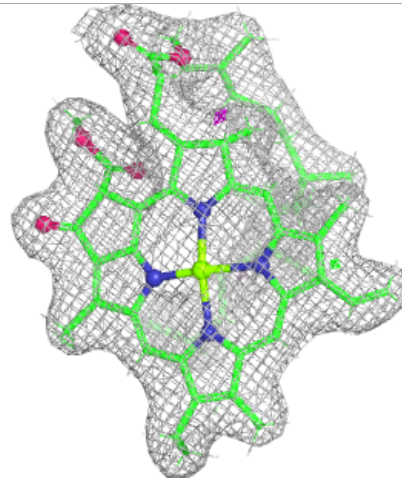
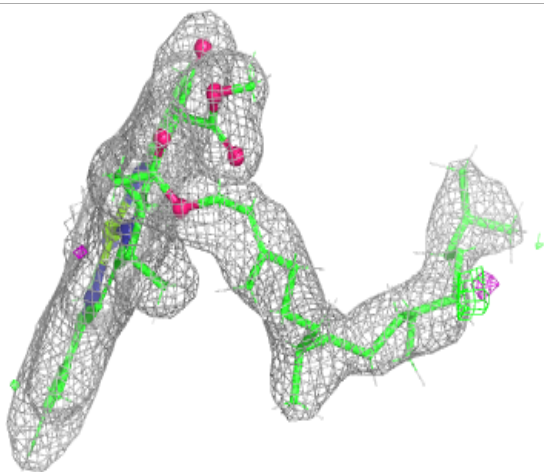
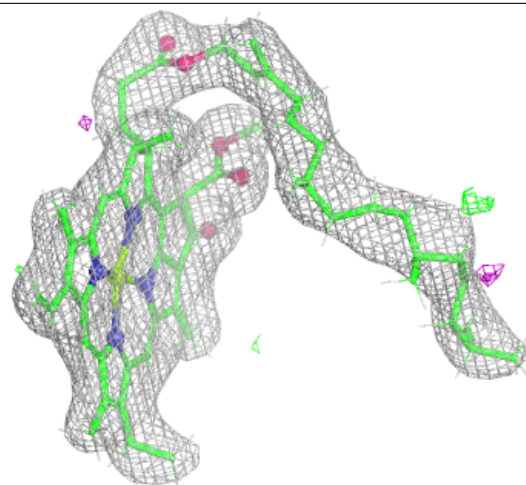
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





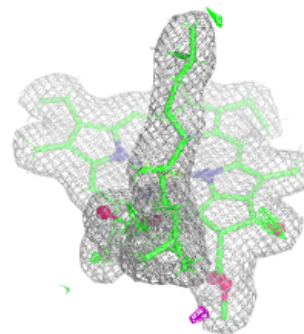
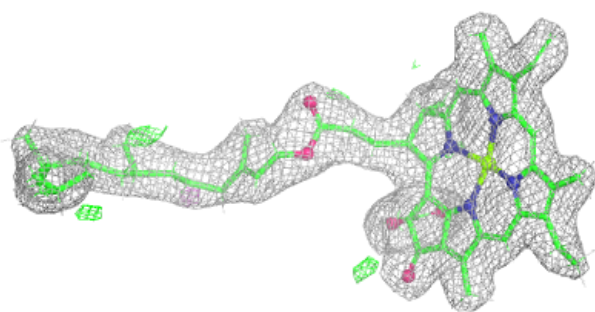
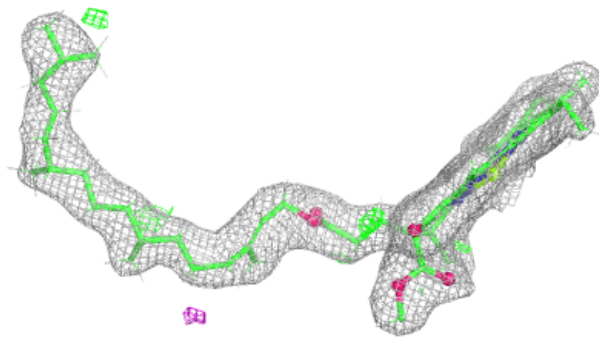
Electron density around CLA B 613:

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

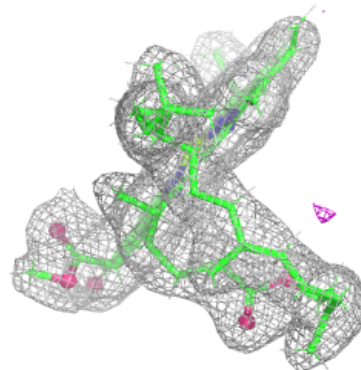
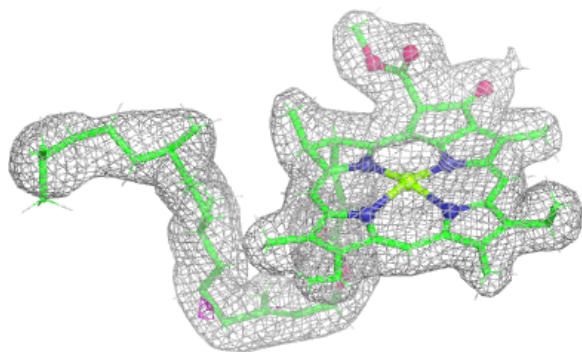
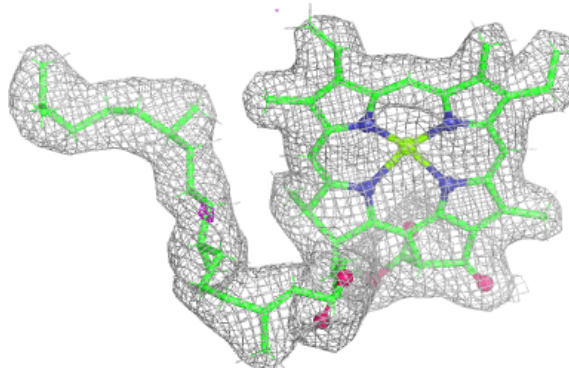


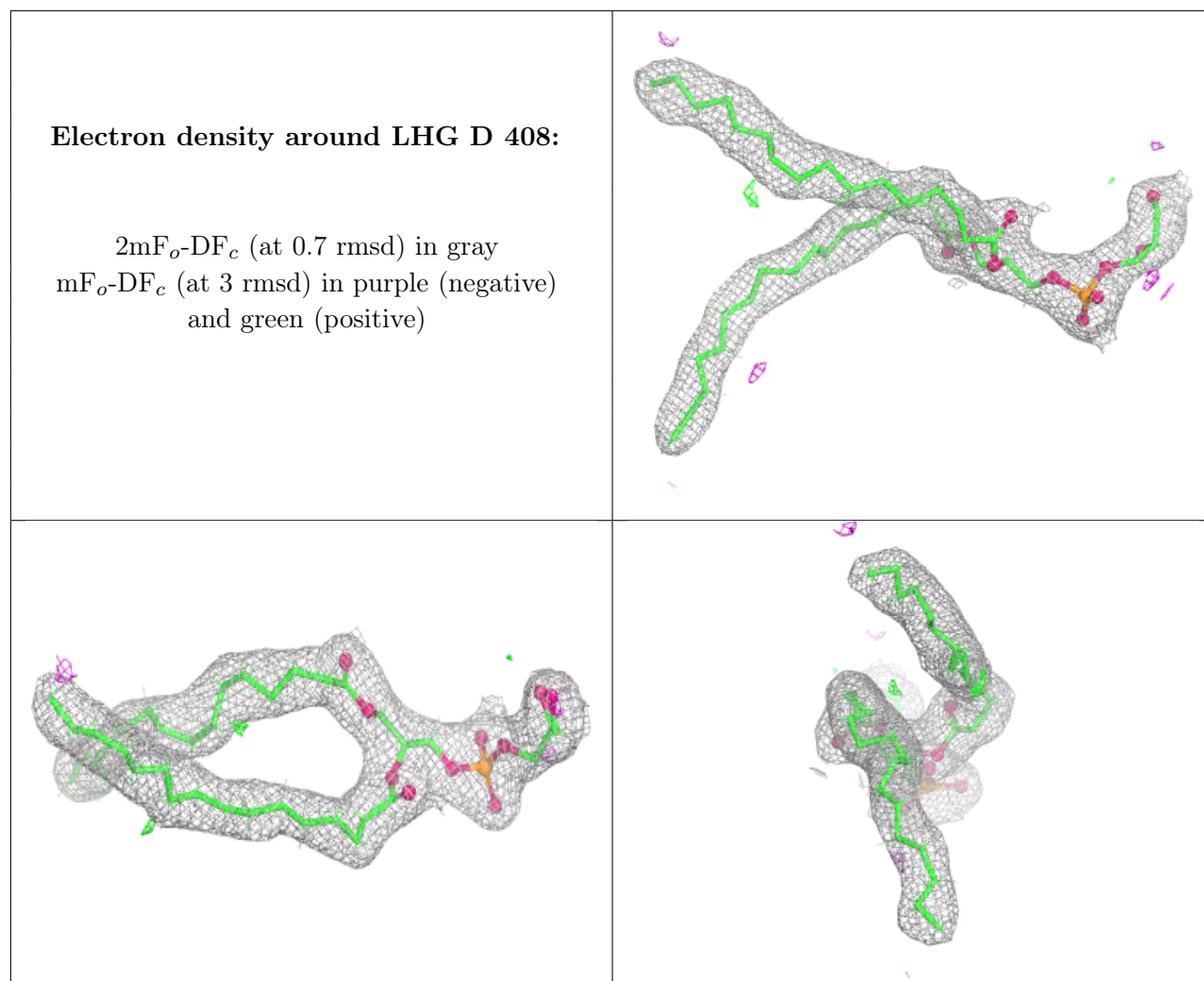
Electron density around CLA D 402:

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

**Electron density around CLA D 403:**

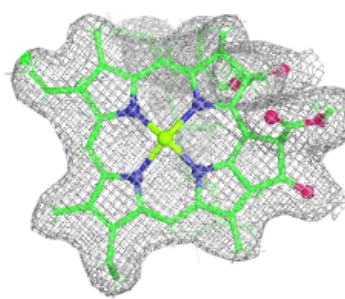
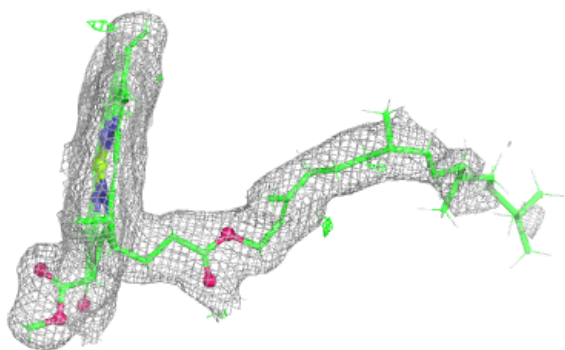
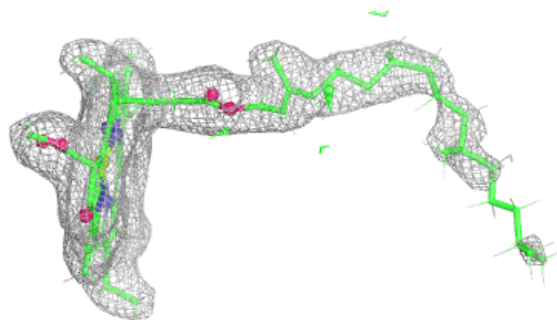
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



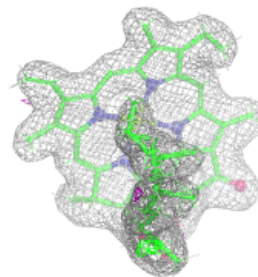
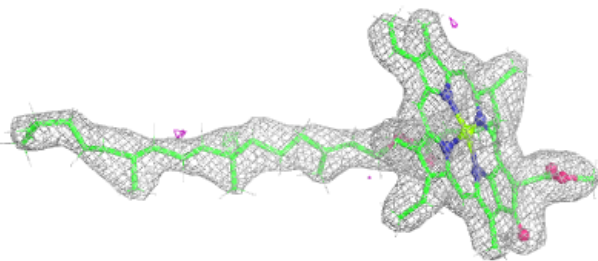
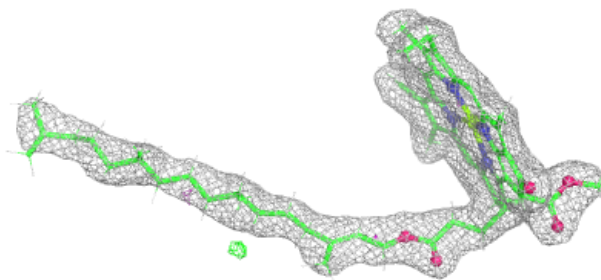


Electron density around CLA D 404:

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

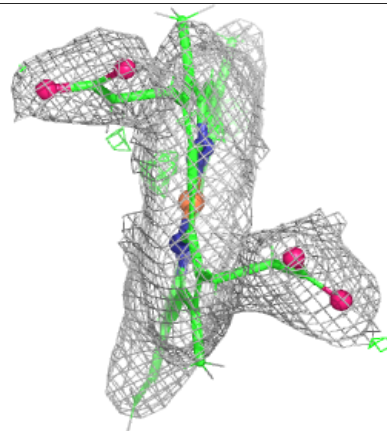
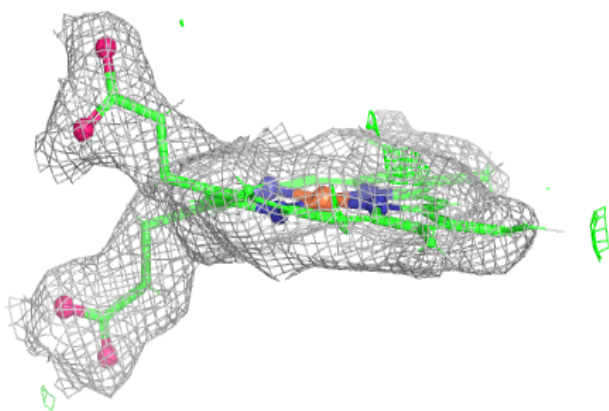
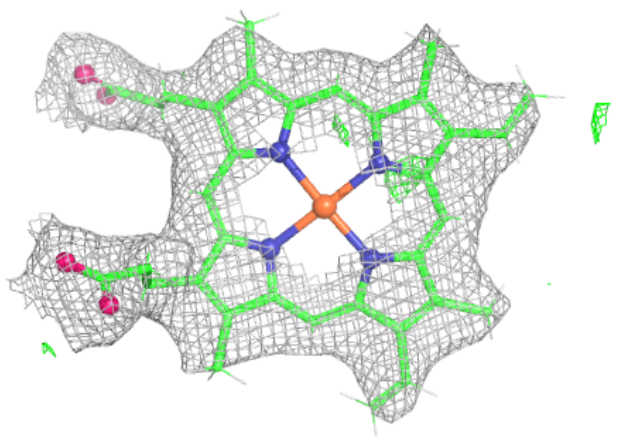
**Electron density around CLA B 607:**

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



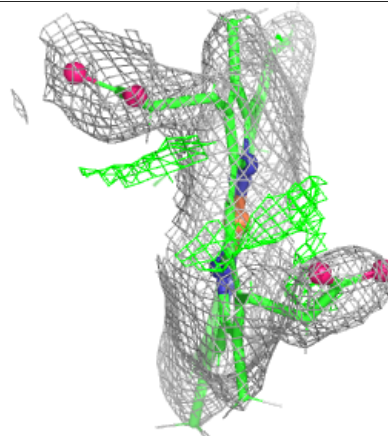
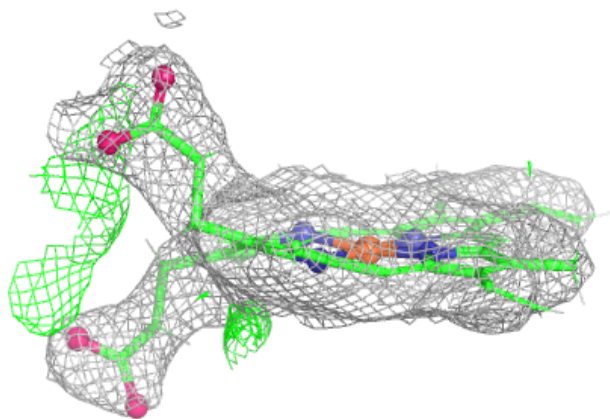
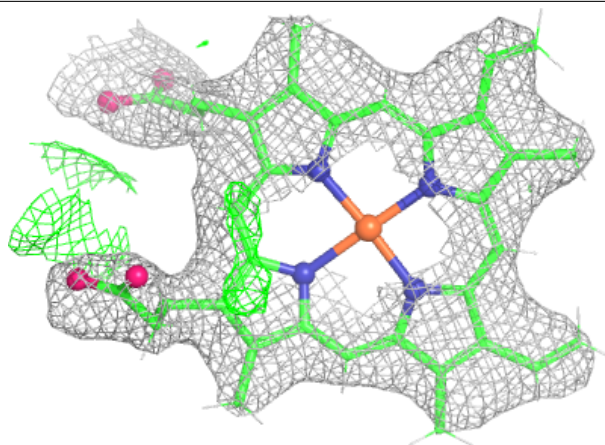
Electron density around HEM F 101:

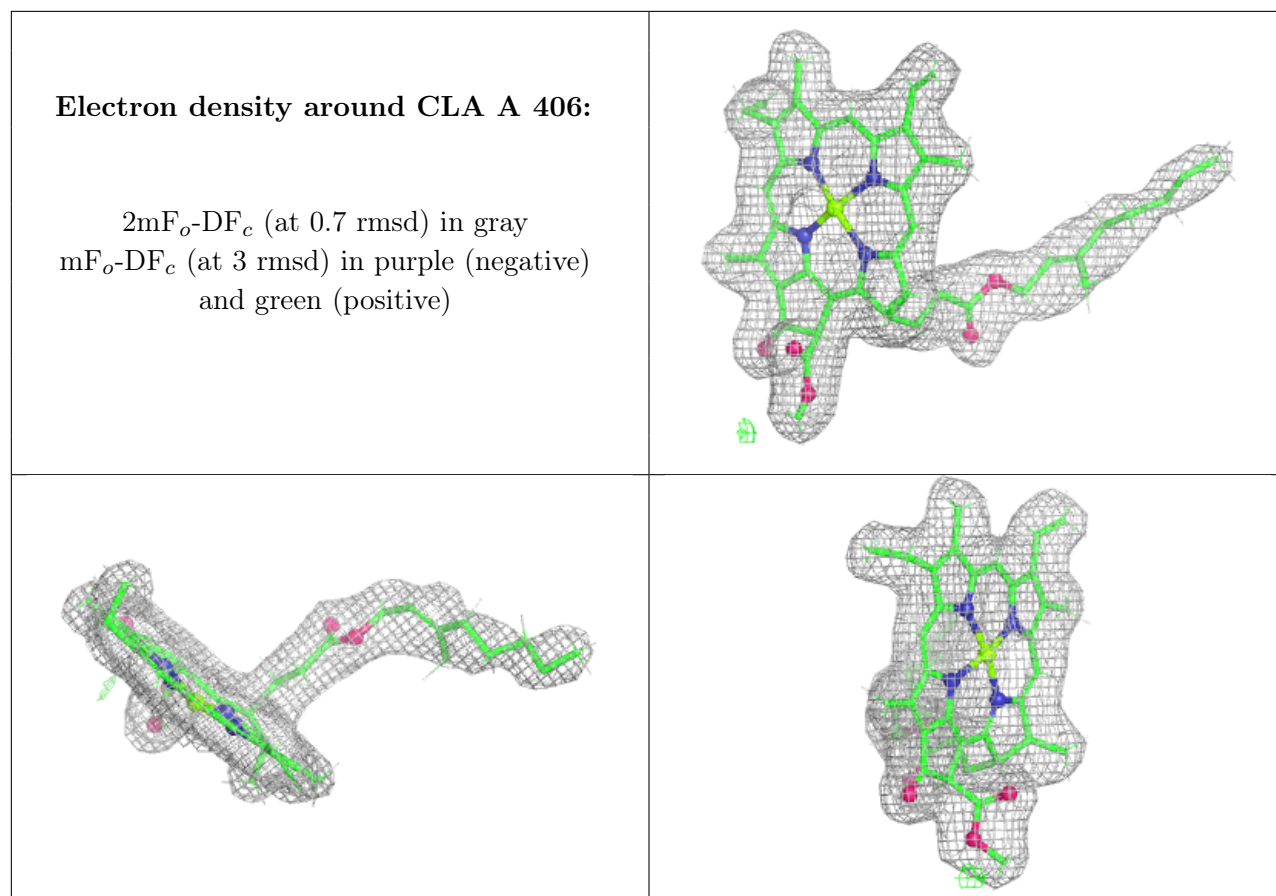
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM f 101:

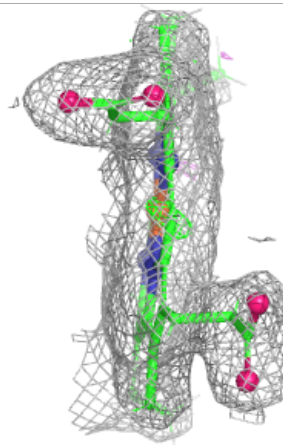
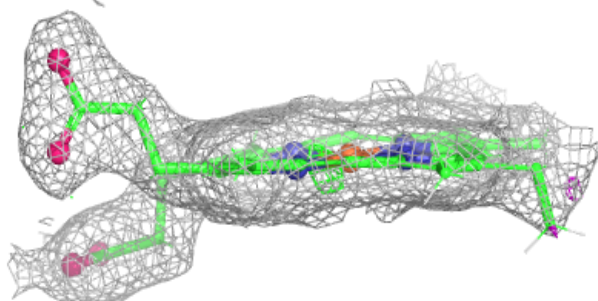
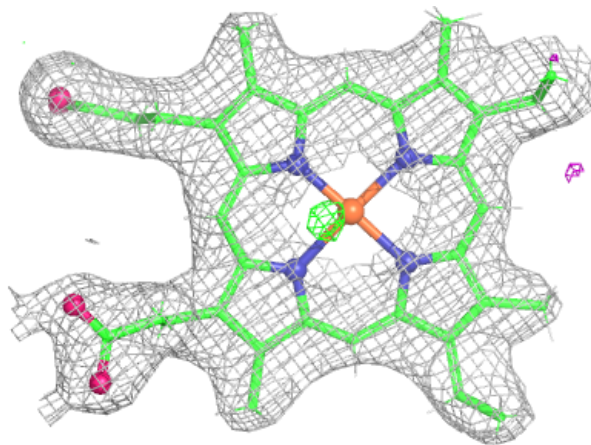
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





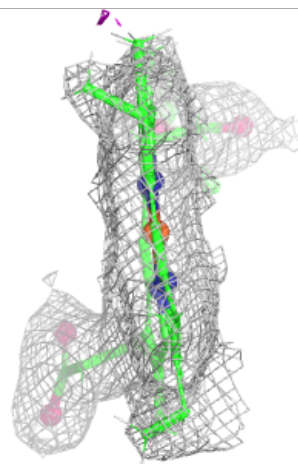
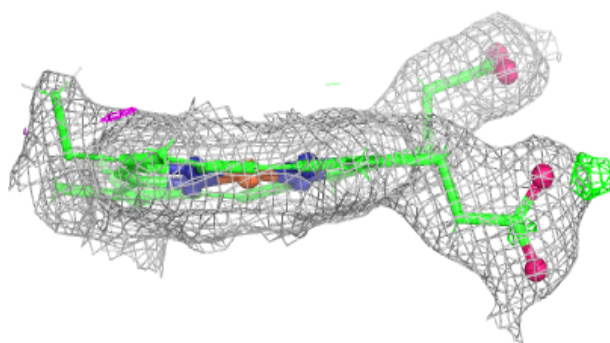
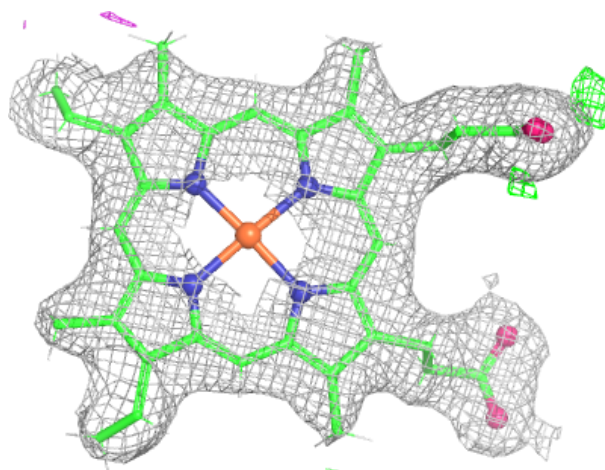
Electron density around HEC V 201:

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



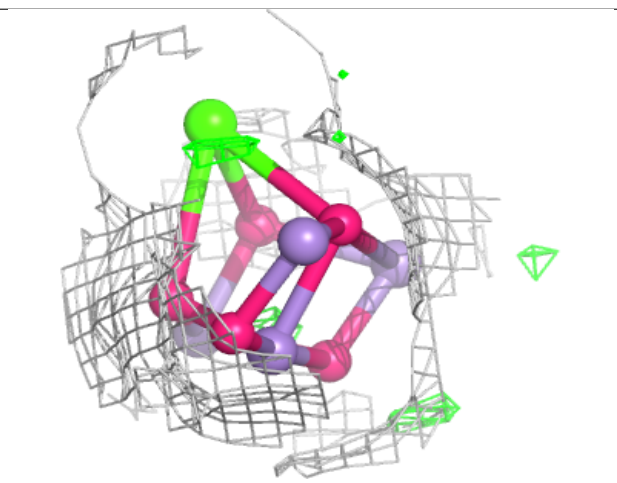
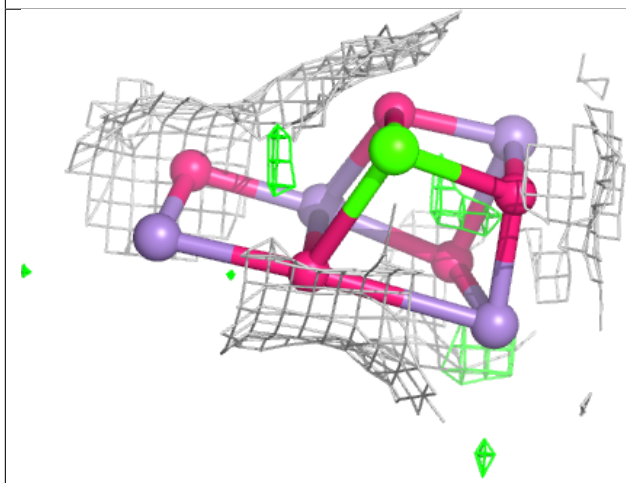
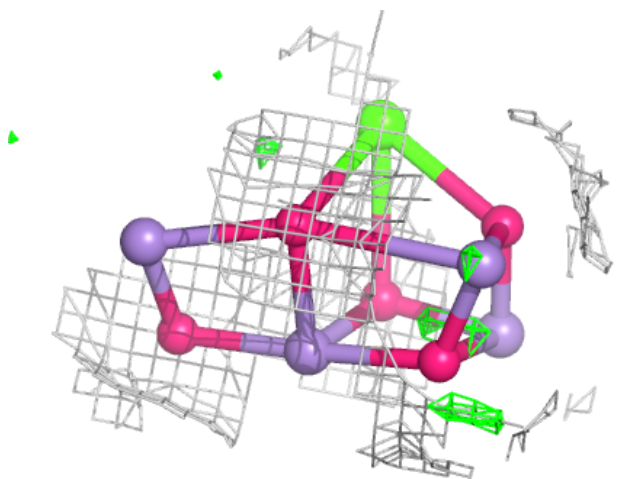
Electron density around HEC v 201:

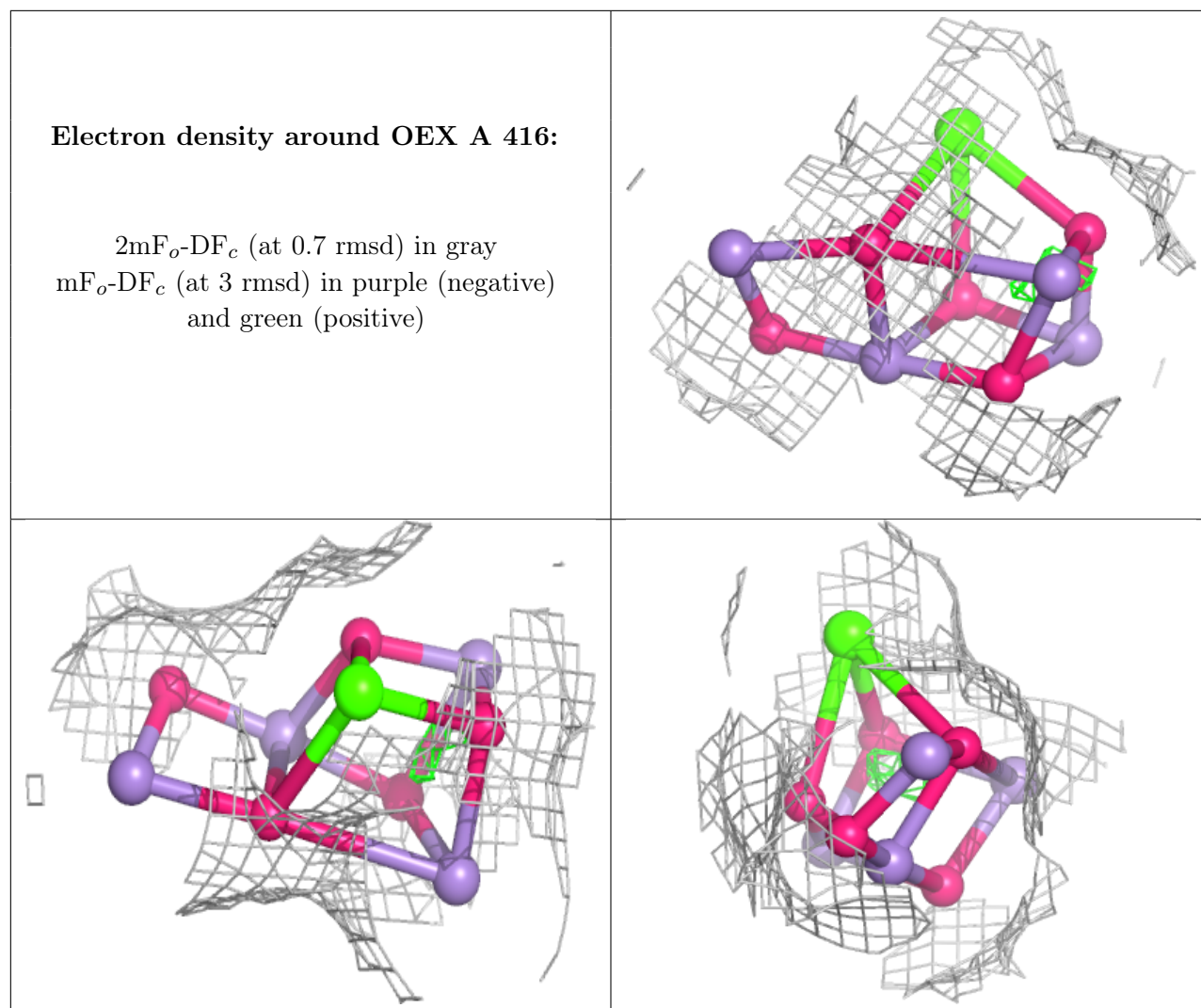
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OEX a 416:

$2mF_o-DF_c$ (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.