



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:33 PM UTC

PDB ID : 7RF8 / pdb\_00007rf8  
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution  
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 : 2.09 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)

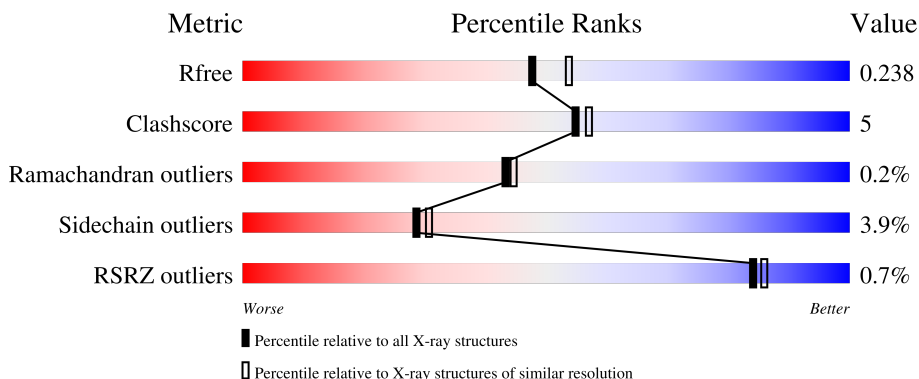
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


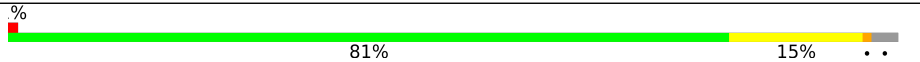
The reported resolution of this entry is 2.09 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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  $\geq 3$ , 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	 81% 15% ..

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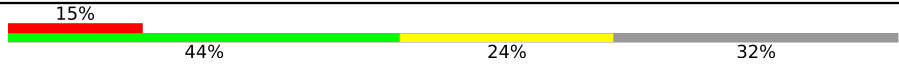








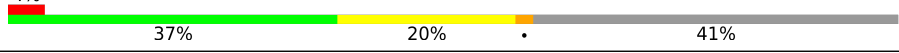
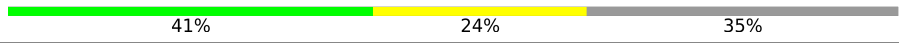


Density-Fitness : 1.0.12  
 Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	B	510	90% 9% ..
2	b	510	88% 10% ..
3	C	461	86% 9% .
3	c	461	87% 10% .
4	D	352	86% 11% .
4	d	352	82% 14% ..
5	E	84	80% 18% .
5	e	84	73% 25% .
6	F	45	60% 13% . 24%
6	f	45	60% 11% . 24%
7	H	66	89% 6% ..
7	h	66	80% 15% 5%
8	I	38	82% 13% 5%
8	i	38	84% 11% 5%
9	J	40	72% 18% 10%
9	j	40	68% 18% 5% 10%
10	K	46	63% 15% . 20%
10	k	46	52% 26% . 20%
11	L	37	92% 8%
11	l	37	84% 11% ..
12	M	36	72% 19% 8%
12	m	36	69% 19% 11%
13	O	272	78% 11% . 10%
13	o	272	78% 10% . 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	405	X	-	-	-
22	CLA	A	410	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	608	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	615	X	-	-	-
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	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	403	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	404	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	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	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	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
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 37 unique types of molecules in this entry. The entry contains 105937 atoms, of which 52685 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	6098	2030	2985	513	551	19	0	66	0
1	a	334	6086	2027	2976	513	551	19	0	66	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	6941	2302	3432	586	607	14	0	14	0
3	c	451	7086	2343	3503	602	624	14	0	14	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	5368	1809	2637	446	464	12	0	2	0
4	d	341	5380	1813	2643	446	466	12	0	3	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			

- 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
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0	0
			620	202	316	48	53	1			
11	l	36	Total	C	H	N	O	0	0	0	
			600	197	304	47	52				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	S	0	0	0
			525	171	269	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	36	46	1			

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
13	O	244	Total	C	H	N	O	S	0	1	0
			3700	1168	1830	313	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3720	1170	1846	317	383	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			
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
			2135	675	1071	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	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	
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

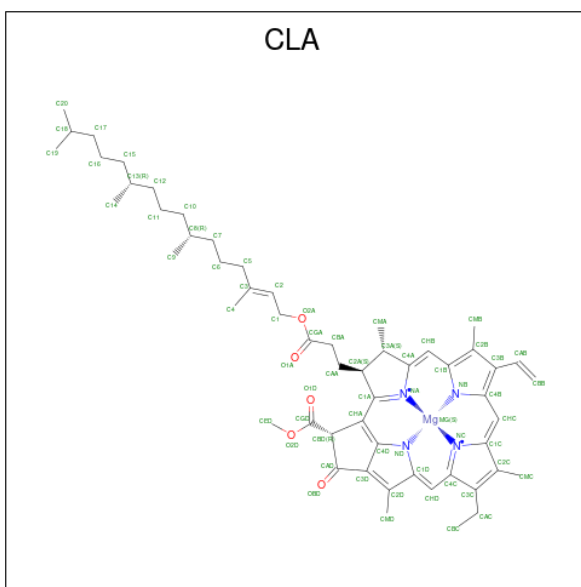
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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
			Total	Fe		
21	A	1	Total 1	Fe 1	0	0
21	a	1	Total 1	Fe 1	0	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
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		
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		

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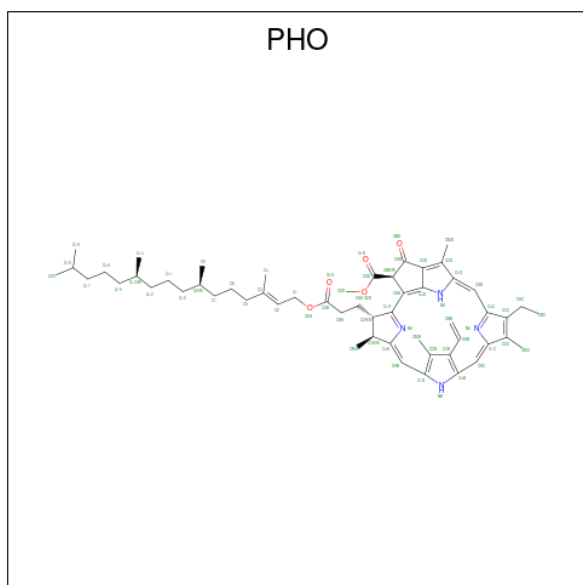
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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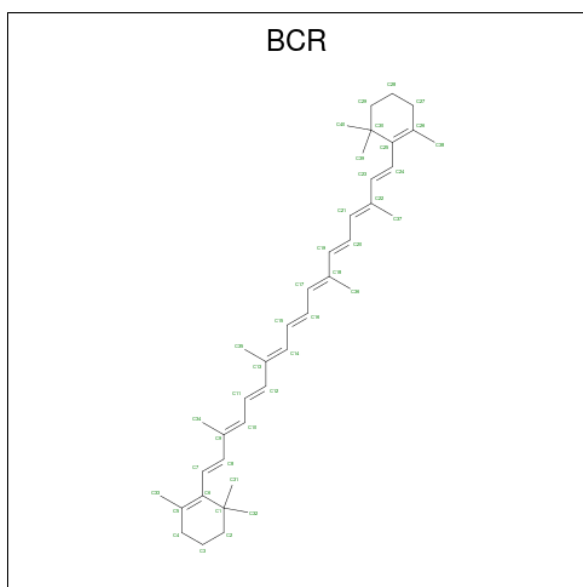
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	Mg	N			O
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



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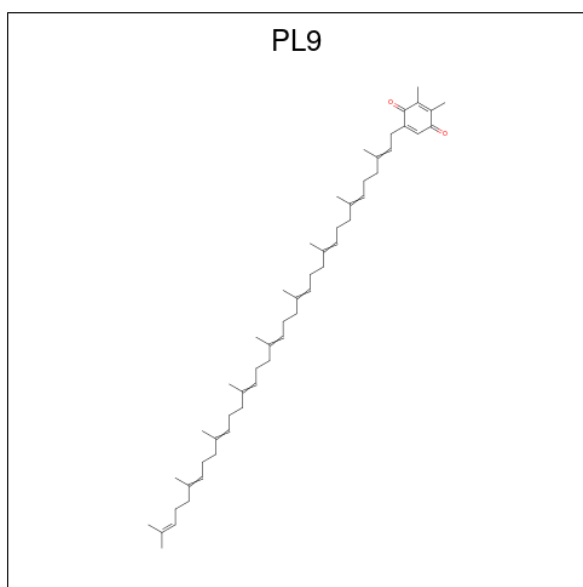
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40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

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

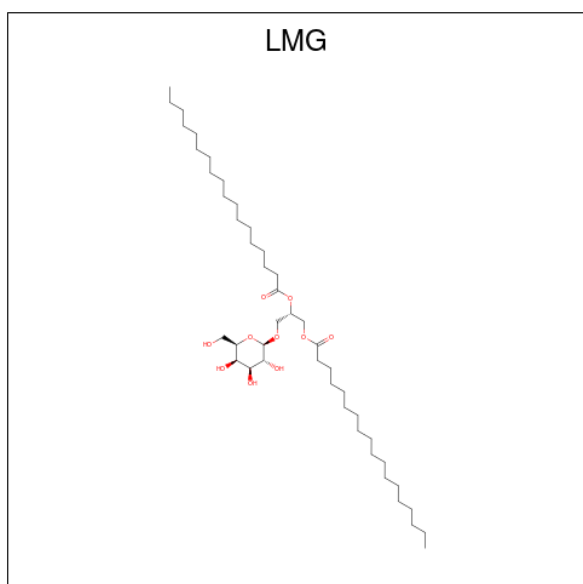
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- 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: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



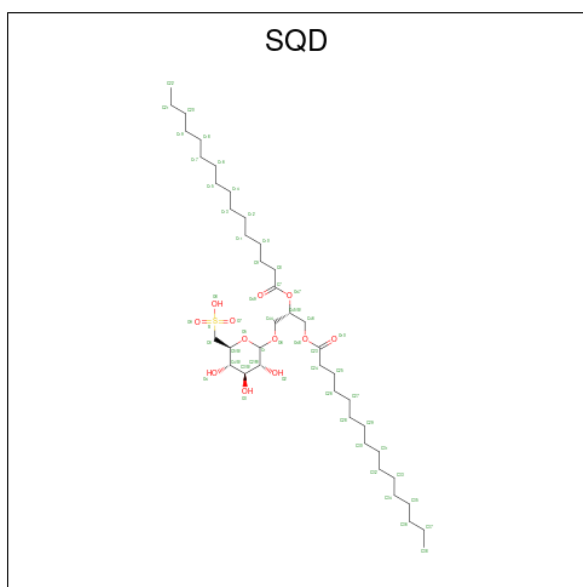
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
26	A	1	135	53	80	2	0	0
26	D	1	135	53	80	2	0	0
26	a	1	135	53	80	2	0	0
26	d	1	135	53	80	2	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



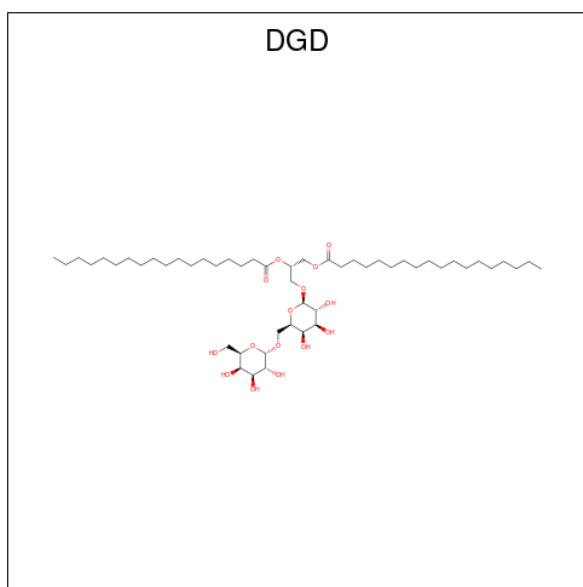
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			123	41	72	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	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			57	21	34	2		
27	d	1	Total	C	H	O	0	0
			102	34	58	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<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



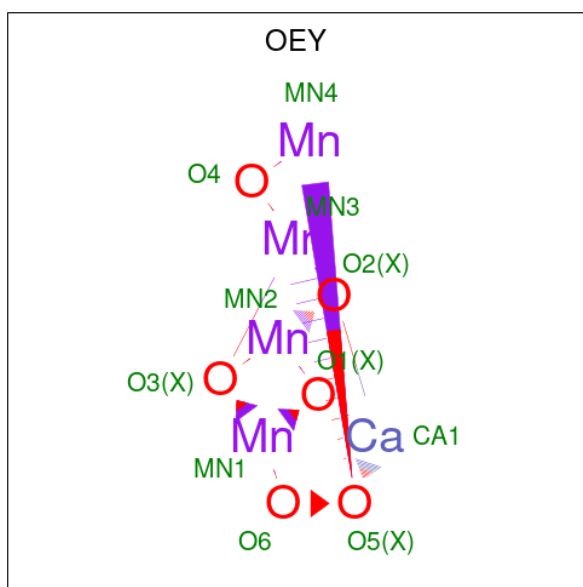
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
28	A	1	123	39	71	12	1	0	0
28	A	1	104	35	65	4		0	0
28	B	1	132	41	78	12	1	0	0
28	F	1	82	25	46	10	1	0	0
28	L	1	114	36	65	12	1	0	0
28	a	1	132	41	78	12	1	0	0
28	a	1	92	31	56	5		0	0
28	f	1	89	28	48	12	1	0	0

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



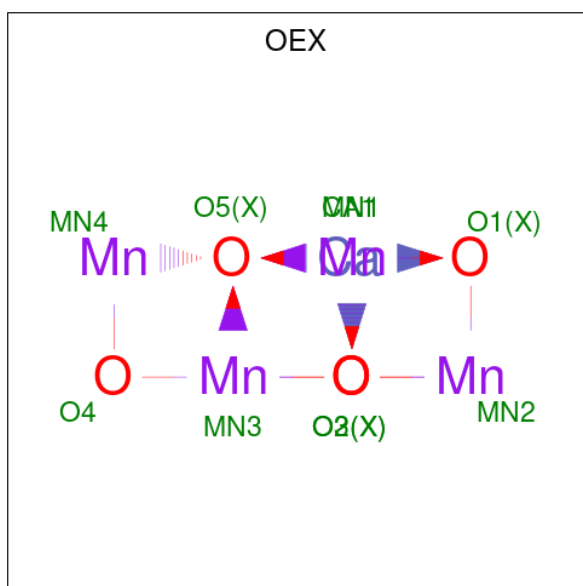
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
29	A	1	Total 162	C 51	H 96	O 15	0	0
29	C	1	Total 144	C 47	H 82	O 15	0	0
29	C	1	Total 144	C 47	H 82	O 15	0	0
29	C	1	Total 144	C 47	H 82	O 15	0	0
29	H	1	Total 144	C 47	H 82	O 15	0	0
29	a	1	Total 119	C 39	H 75	O 5	0	0
29	c	1	Total 144	C 47	H 82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

- Molecule 30 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



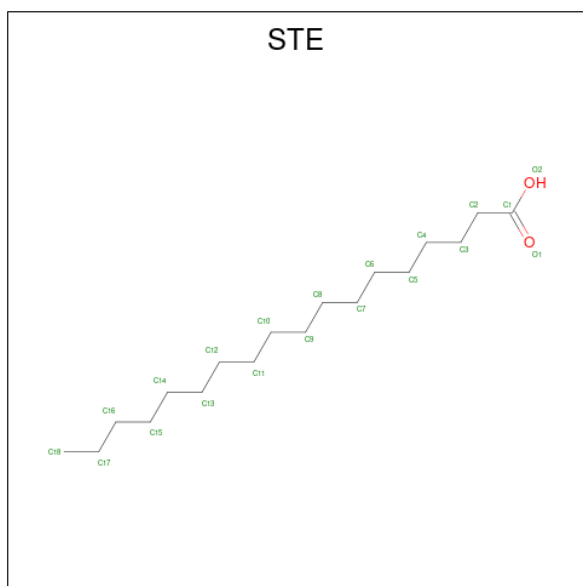
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
31	A	1	10	1	4	5	0	1

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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula:  $C_{18}H_{36}O_2$ ).



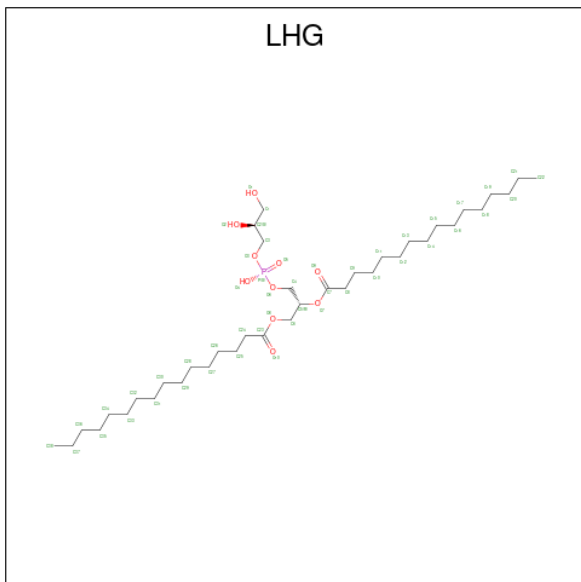
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
32	B	1	43	15	26	2	0	0
32	B	1	28	10	16	2	0	0
32	B	1	46	16	28	2	0	0
32	B	1	47	16	31		0	0
32	B	1	28	10	16	2	0	0
32	C	1	28	10	16	2	0	0
32	C	1	47	16	31		0	0
32	C	1	28	10	16	2	0	0
32	D	1	55	18	35	2	0	0
32	E	1	28	10	16	2	0	0

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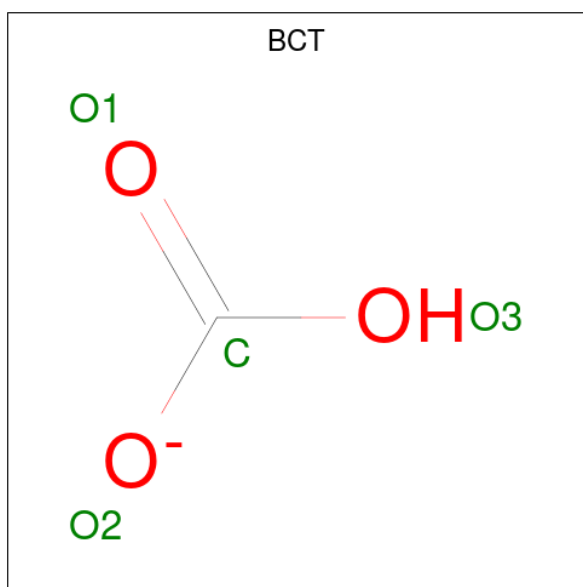
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	T	1	Total C H 47 16 31	0	0
32	T	1	Total C H 44 15 29	0	0
32	a	1	Total C H 26 10 16	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 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	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	m	1	Total C H O 28 10 16 2	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	x	1	Total C H O 55 18 35 2	0	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



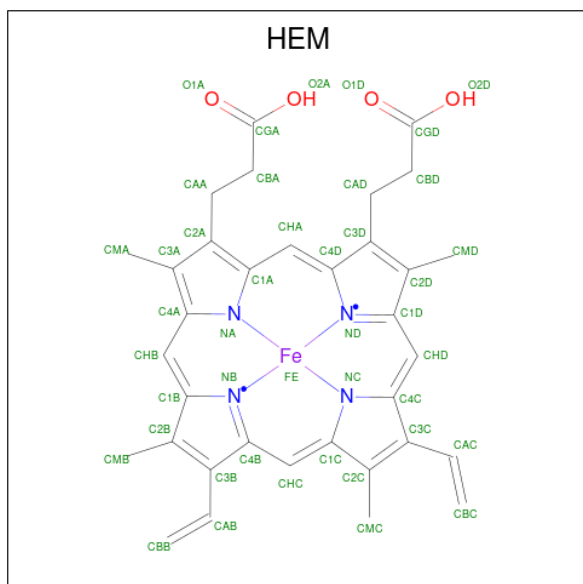
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
33	B	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	D	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	D	1	Total 114	C 36	H 67	O 10	P 1	0	0
33	E	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	L	1	Total 123	C 38	H 74	O 10	P 1	0	0
33	d	1	Total 123	C 38	H 74	O 10	P 1	0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

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula:  $CHO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	42	Total O 42 42	0	0
37	I	12	Total O 12 12	0	0
37	J	13	Total O 13 13	0	0
37	K	4	Total O 4 4	0	0
37	L	9	Total O 9 9	0	0
37	M	9	Total O 9 9	0	0
37	O	99	Total O 99 99	0	0
37	R	4	Total O 4 4	0	0
37	T	9	Total O 9 9	0	0
37	U	33	Total O 33 33	0	0
37	V	64	Total O 64 64	0	0
37	X	14	Total O 14 14	0	0
37	Y	4	Total O 4 4	0	0
37	Z	3	Total O 3 3	0	0
37	a	118	Total O 118 118	0	8
37	b	191	Total O 191 191	0	0
37	c	157	Total O 157 157	0	0
37	d	105	Total O 105 105	0	0
37	e	17	Total O 17 17	0	0
37	f	6	Total O 6 6	0	0
37	h	30	Total O 30 30	0	0

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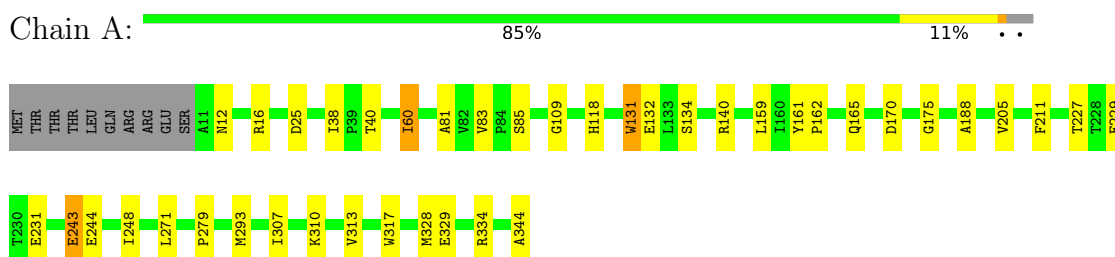
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
37	i	21	Total 21	O 21	0	0
37	j	6	Total 6	O 6	0	0
37	k	4	Total 4	O 4	0	0
37	l	12	Total 12	O 12	0	0
37	m	5	Total 5	O 5	0	0
37	o	93	Total 93	O 93	0	0
37	r	5	Total 5	O 5	0	0
37	t	8	Total 8	O 8	0	0
37	u	65	Total 65	O 65	0	0
37	v	59	Total 59	O 59	0	0
37	x	9	Total 9	O 9	0	0
37	y	4	Total 4	O 4	0	0

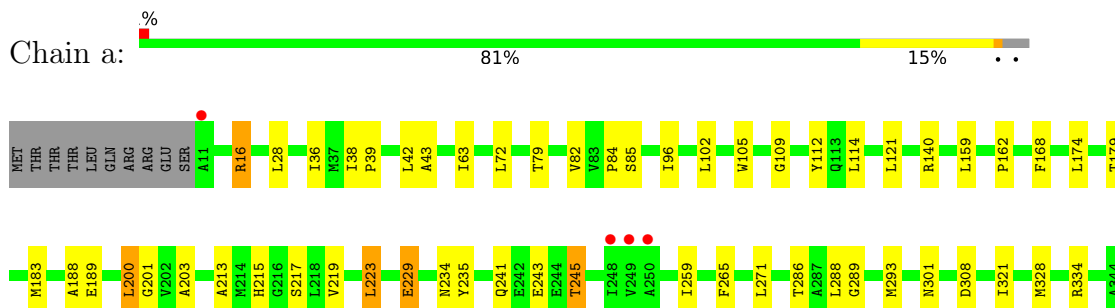
### 3 Residue-property plots [i](#)

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

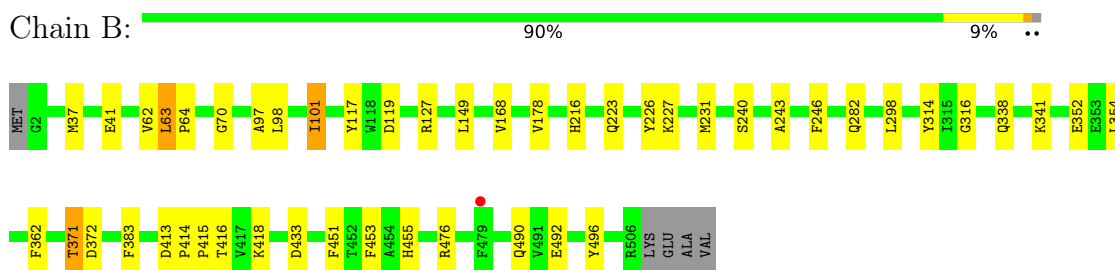
- Molecule 1: Photosystem II protein D1 1



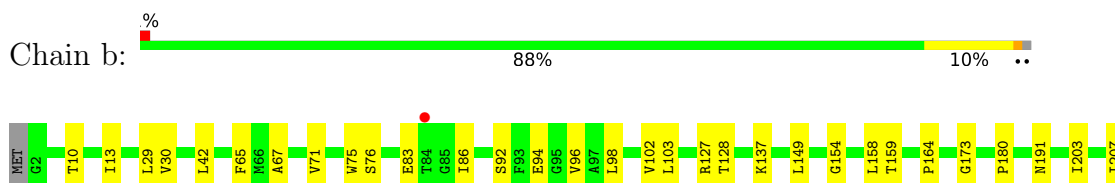
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



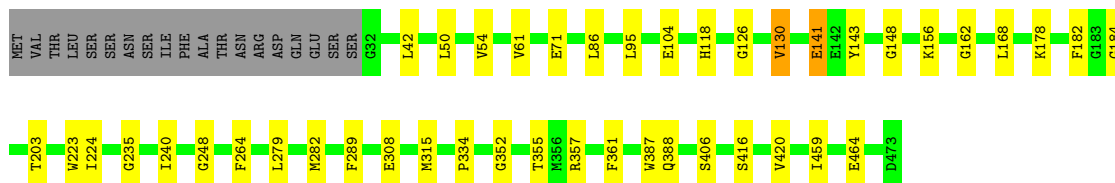
- Molecule 2: Photosystem II CP47 reaction center protein





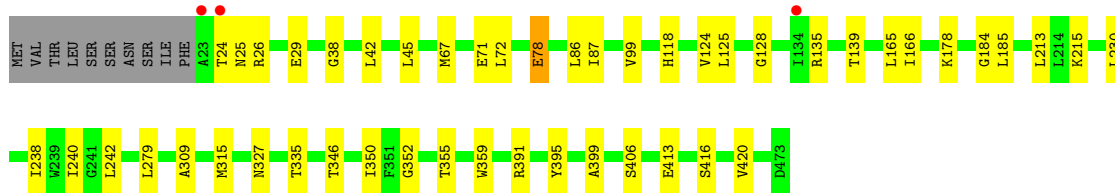
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 9% .



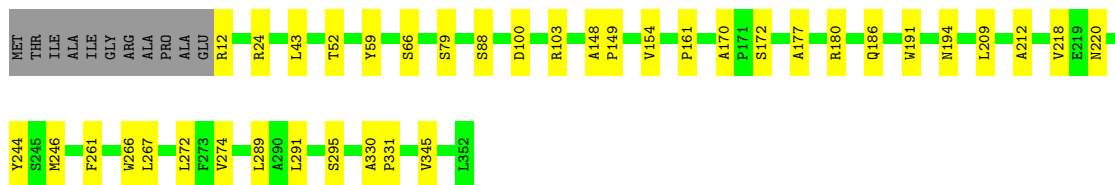
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 10% .



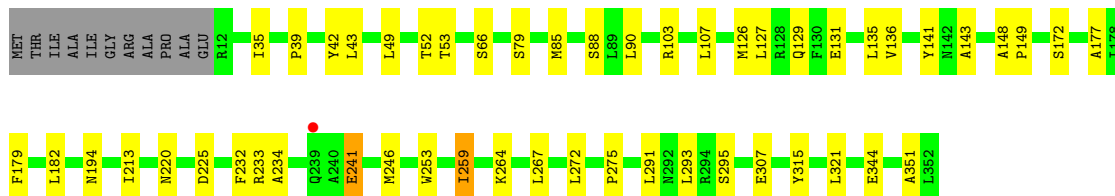
- Molecule 4: Photosystem II D2 protein

Chain D: 86% 11% .



- Molecule 4: Photosystem II D2 protein

Chain d: 82% 14% ..



- Molecule 5: Cytochrome b559 subunit alpha

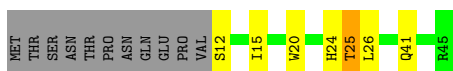
Chain E: 80% 18% .



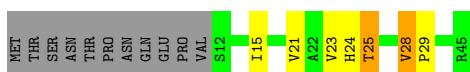
- Molecule 5: Cytochrome b559 subunit alpha



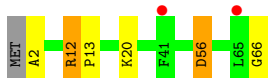
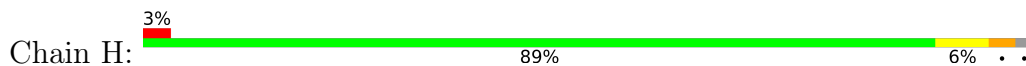
- Molecule 6: Cytochrome b559 subunit beta



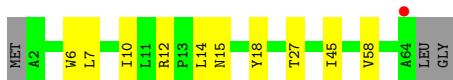
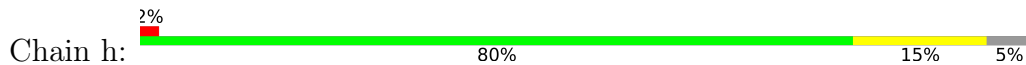
- Molecule 6: Cytochrome b559 subunit beta



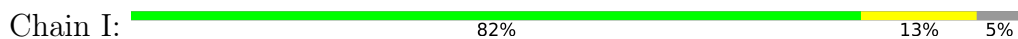
- Molecule 7: Photosystem II reaction center protein H



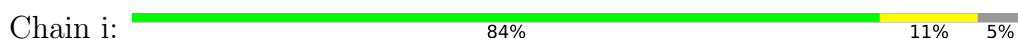
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





- Molecule 9: Photosystem II reaction center protein J



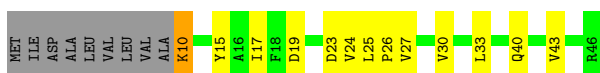
- Molecule 9: Photosystem II reaction center protein J



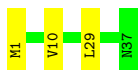
- Molecule 10: Photosystem II reaction center protein K



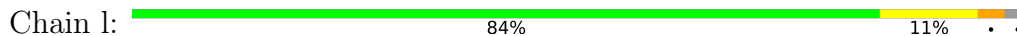
- Molecule 10: Photosystem II reaction center protein K



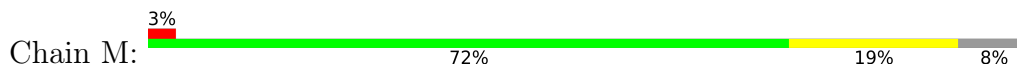
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

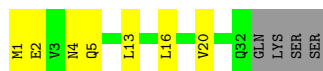


- Molecule 12: Photosystem II reaction center protein M

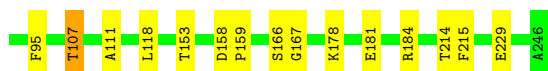
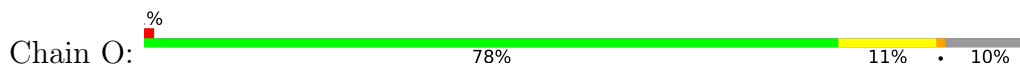




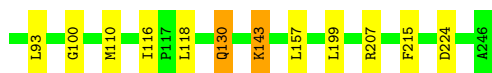
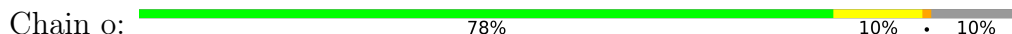
- Molecule 12: Photosystem II reaction center protein M



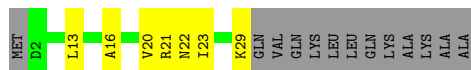
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



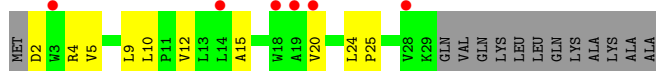
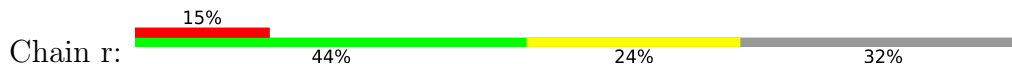
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



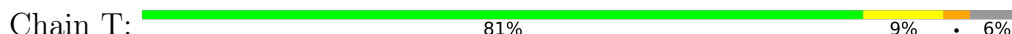
- Molecule 14: Photosystem II protein Y



- Molecule 14: Photosystem II protein Y

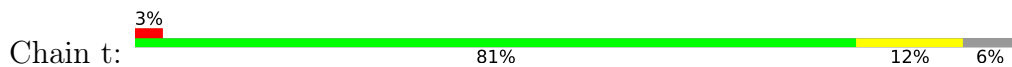


- Molecule 15: Photosystem II reaction center protein T

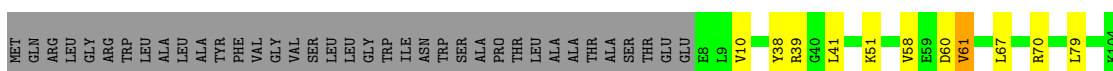




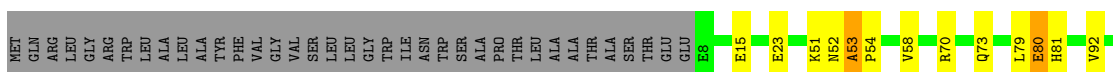
- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 12 kDa extrinsic protein



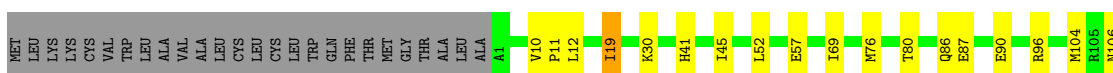
- Molecule 16: Photosystem II 12 kDa extrinsic protein



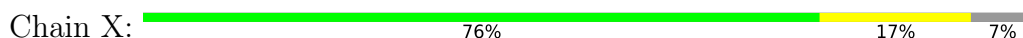
- Molecule 17: Cytochrome c-550



- Molecule 17: Cytochrome c-550



- Molecule 18: Photosystem II reaction center X protein





- Molecule 18: Photosystem II reaction center X protein



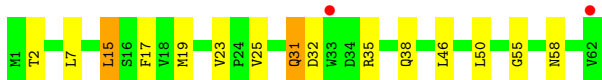
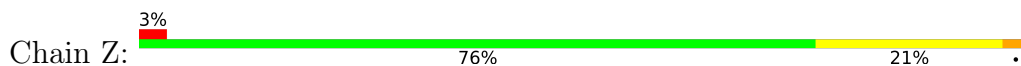
- Molecule 19: Photosystem II reaction center protein Ycf12



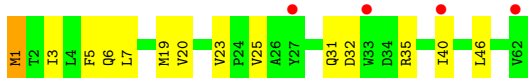
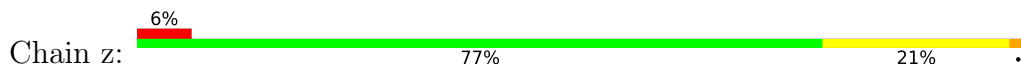
- Molecule 19: Photosystem II reaction center protein Ycf12



- 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, $\alpha$ , $\beta$ , $\gamma$	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.65-2.09) 85.3 (33.65-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.51 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.181 , 0.239 0.181 , 0.238	Depositor DCC
$R_{free}$ test set	4165 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	105937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OEX, PL9, BCR, FME, CLA, HEM, LMG, SQD, BCT, CL, STE, LHG, FE2, HEC, DGD, OEY, PHO

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	0.53	1/3227 (0.0%)	0.62	1/4397 (0.0%)
1	a	0.50	0/3224	0.59	0/4393
2	B	0.58	0/4161	0.63	0/5669
2	b	0.56	1/4118 (0.0%)	0.62	1/5611 (0.0%)
3	C	0.54	0/3647	0.60	0/4965
3	c	0.51	0/3719	0.59	0/5061
4	D	0.60	0/2825	0.64	0/3847
4	d	0.56	0/2834	0.64	0/3859
5	E	0.52	0/688	0.58	0/940
5	e	0.46	0/683	0.56	0/932
6	F	0.54	0/284	0.57	0/387
6	f	0.50	0/284	0.66	0/387
7	H	0.64	0/523	0.68	0/713
7	h	0.58	0/511	0.64	0/697
8	I	0.64	0/293	0.66	0/396
8	i	0.69	0/293	0.64	0/396
9	J	0.52	0/263	0.63	0/356
9	j	0.49	0/263	0.60	0/356
10	K	0.50	0/303	0.61	0/416
10	k	0.44	0/303	0.58	0/416
11	L	0.72	0/311	0.71	0/422
11	l	0.65	0/303	0.70	0/412
12	M	0.71	0/249	0.71	0/341
12	m	0.68	0/244	0.74	0/334
13	O	0.63	0/1904	0.70	0/2585
13	o	0.64	0/1905	0.68	0/2583
14	R	0.40	0/227	0.53	0/313
14	r	0.36	0/227	0.49	0/313
15	T	0.69	0/257	0.68	0/349
15	t	0.66	0/255	0.68	0/346
16	U	0.55	0/785	0.64	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	u	0.61	0/785	0.68	0/1064
17	V	0.62	0/1085	0.70	0/1473
17	v	0.57	0/1085	0.63	0/1473
18	X	0.50	0/284	0.59	0/384
18	x	0.42	0/289	0.51	0/391
19	Y	0.45	0/197	0.50	0/264
19	y	0.38	0/219	0.52	0/294
20	Z	0.58	1/490 (0.2%)	0.63	0/669
20	z	0.35	0/488	0.48	0/666
All	All	0.56	3/44035 (0.0%)	0.63	2/59934 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	V	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	221	PRO	CA-C	8.07	1.57	1.52
20	Z	23	VAL	CA-CB	7.58	1.58	1.54
1	A	38	ILE	CA-CB	-5.09	1.51	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	221	PRO	O-C-N	8.38	125.09	121.15
1	A	131	TRP	CA-CB-CG	-5.13	103.86	113.60

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	2985	2963	24	0
1	a	3110	2976	2954	38	0
2	B	4005	3873	3867	32	0
2	b	3978	3836	3836	33	0
3	C	3509	3432	3409	25	0
3	c	3583	3503	3492	26	0
4	D	2731	2637	2637	26	0
4	d	2737	2643	2643	35	0
5	E	666	651	651	11	0
5	e	664	648	648	15	0
6	F	275	282	282	6	0
6	f	275	282	282	4	0
7	H	510	532	532	5	0
7	h	498	518	518	7	0
8	I	296	311	311	2	0
8	i	296	311	311	1	0
9	J	257	268	268	11	0
9	j	257	268	268	8	0
10	K	293	305	305	4	0
10	k	293	305	305	10	0
11	L	304	316	316	3	0
11	l	296	304	304	3	0
12	M	256	269	269	5	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	21	0
13	o	1874	1846	1846	16	0
14	R	221	238	238	2	0
14	r	221	238	238	5	0
15	T	258	261	261	1	0
15	t	256	256	256	2	0
16	U	774	773	773	6	0
16	u	774	773	773	11	0
17	V	1064	1071	1073	11	0
17	v	1064	1071	1073	13	0
18	X	281	312	312	5	0
18	x	286	316	314	7	0
19	Y	196	217	217	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	y	218	241	241	6	0
20	Z	479	516	516	4	0
20	z	477	509	509	8	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	249	264	264	1	0
22	B	1035	1139	1139	22	0
22	C	839	922	922	12	0
22	D	130	144	144	3	0
22	a	195	216	216	1	0
22	b	1035	1139	1139	14	0
22	c	839	919	919	14	0
22	d	195	216	216	2	0
23	A	64	74	74	1	0
23	D	64	74	74	2	0
23	d	128	148	148	1	0
24	A	40	56	56	1	0
24	B	120	168	168	2	0
24	C	80	112	112	1	0
24	D	40	56	56	2	0
24	H	40	56	56	1	0
24	K	40	56	56	1	0
24	T	40	56	56	1	0
24	Y	40	56	56	2	0
24	a	40	56	56	1	0
24	b	120	168	168	1	0
24	c	120	168	168	3	0
24	d	40	56	56	2	0
24	h	40	56	56	0	0
24	k	40	56	56	0	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	3	0
26	D	55	80	80	2	0
26	a	55	80	80	5	0
26	d	55	80	80	1	0
27	A	48	66	66	0	0
27	B	28	40	40	0	0
27	C	48	66	66	1	0
27	D	84	117	116	2	0
27	M	51	72	71	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	b	106	158	158	1	0
27	c	134	181	181	1	0
27	d	67	92	92	0	0
28	A	91	136	135	0	0
28	B	54	78	78	0	0
28	F	36	46	45	1	0
28	L	49	65	64	1	0
28	a	90	134	132	4	0
28	f	41	48	47	2	0
29	A	66	96	96	5	0
29	C	186	246	243	1	0
29	H	62	82	80	0	0
29	a	44	75	75	4	0
29	c	186	246	243	2	0
29	h	62	82	81	0	0
30	A	11	0	0	2	0
30	a	11	0	0	1	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	B	75	117	117	1	0
32	C	40	63	63	1	0
32	D	20	35	35	2	0
32	E	12	16	16	0	0
32	H	18	35	35	2	0
32	I	15	26	26	3	0
32	J	12	16	16	0	0
32	M	25	38	38	0	0
32	T	31	60	60	1	0
32	a	22	32	32	2	0
32	b	66	110	110	1	0
32	c	32	51	51	1	0
32	d	17	26	26	2	0
32	j	12	16	16	0	0
32	l	18	35	35	1	0
32	m	12	16	16	0	0
32	t	14	20	20	1	0
32	x	20	35	35	3	0
33	B	49	74	74	1	0
33	D	96	141	141	2	0
33	E	49	74	74	1	0
33	L	49	74	74	1	0
33	d	137	199	199	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	e	42	57	57	2	0
33	l	49	74	74	2	0
34	D	4	1	1	0	0
34	a	4	1	1	0	0
35	E	43	30	30	2	0
35	f	43	30	30	4	0
36	V	43	30	31	1	0
36	v	43	30	30	1	0
37	A	136	0	0	11	0
37	B	213	0	0	6	0
37	C	159	0	0	0	0
37	D	130	0	0	1	0
37	E	40	0	0	3	0
37	F	8	0	0	1	0
37	H	42	0	0	2	0
37	I	12	0	0	0	0
37	J	13	0	0	6	0
37	K	4	0	0	0	0
37	L	9	0	0	0	0
37	M	9	0	0	1	0
37	O	99	0	0	2	0
37	R	4	0	0	0	0
37	T	9	0	0	0	0
37	U	33	0	0	1	0
37	V	64	0	0	0	0
37	X	14	0	0	0	0
37	Y	4	0	0	0	0
37	Z	3	0	0	0	0
37	a	118	0	0	4	0
37	b	191	0	0	8	0
37	c	157	0	0	5	0
37	d	105	0	0	0	0
37	e	17	0	0	1	0
37	f	6	0	0	0	0
37	h	30	0	0	1	0
37	i	21	0	0	0	0
37	j	6	0	0	3	0
37	k	4	0	0	3	0
37	l	12	0	0	1	0
37	m	5	0	0	1	0
37	o	93	0	0	2	0
37	r	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	t	8	0	0	0	0
37	u	65	0	0	4	0
37	v	59	0	0	1	0
37	x	9	0	0	0	0
37	y	4	0	0	2	0
All	All	53252	52685	52587	498	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 498 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)
5:E:3:GLY:N	37:E:201:HOH:O	1.79	1.11
1:A:344[A]:ALA:O	37:A:501[A]:HOH:O	1.69	1.07
1:A:165[A]:GLN:OE1	37:A:501[A]:HOH:O	1.76	1.03
16:u:53:ALA:O	37:u:201:HOH:O	1.80	0.98
30:A:415[B]:OEY:O4	37:A:502[B]:HOH:O	1.86	0.93

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/344 (115%)	390 (98%)	7 (2%)	0	100	100
1	a	397/344 (115%)	388 (98%)	8 (2%)	1 (0%)	36	36
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	492 (98%)	11 (2%)	0	100	100
3	C	454/461 (98%)	440 (97%)	13 (3%)	1 (0%)	43	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	463/461 (100%)	448 (97%)	14 (3%)	1 (0%)	43	44
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	7	4
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	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%)	227 (93%)	13 (5%)	3 (1%)	10	7
13	o	242/272 (89%)	231 (96%)	8 (3%)	3 (1%)	10	7
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	8
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	15
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
All	All	5387/5700 (94%)	5225 (97%)	150 (3%)	12 (0%)	43	44

5 of 12 Ramachandran outliers are listed below:

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

### 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	324/280 (116%)	314 (97%)	10 (3%)	35	39
1	a	323/280 (115%)	311 (96%)	12 (4%)	30	33
2	B	408/407 (100%)	397 (97%)	11 (3%)	39	45
2	b	402/407 (99%)	391 (97%)	11 (3%)	39	45
3	C	356/362 (98%)	350 (98%)	6 (2%)	53	62
3	c	364/362 (101%)	350 (96%)	14 (4%)	29	32
4	D	277/283 (98%)	273 (99%)	4 (1%)	59	67
4	d	278/283 (98%)	269 (97%)	9 (3%)	34	38
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	28
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	28
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	34
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	54/55 (98%)	52 (96%)	2 (4%)	30	33
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	32
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	14
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	8
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	5
10	k	30/37 (81%)	28 (93%)	2 (7%)	15	12
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	42
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	7
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	4
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	35
13	o	207/228 (91%)	198 (96%)	9 (4%)	26	27
14	R	22/33 (67%)	18 (82%)	4 (18%)	2	1
14	r	22/33 (67%)	19 (86%)	3 (14%)	3	2
15	T	26/28 (93%)	24 (92%)	2 (8%)	12	9
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	29
16	U	84/112 (75%)	80 (95%)	4 (5%)	23	23
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	34
17	V	117/138 (85%)	114 (97%)	3 (3%)	40	46
17	v	117/138 (85%)	112 (96%)	5 (4%)	26	27
18	X	31/34 (91%)	30 (97%)	1 (3%)	34	38
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	13
19	Y	19/37 (51%)	16 (84%)	3 (16%)	2	1
19	y	22/37 (60%)	21 (96%)	1 (4%)	24	25
20	Z	52/52 (100%)	43 (83%)	9 (17%)	2	1
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	5
All	All	4451/4654 (96%)	4278 (96%)	173 (4%)	28	31

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	90	LEU
12	m	16	LEU
4	d	259	ILE
6	f	28	VAL
13	o	130	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
16	U	78	ASN
20	z	31	GLN
2	b	274	GLN
13	o	124	ASN
2	b	179	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
15	FME	t	1	15	8,9,10	1.69	1 (12%)	8,9,11	0.95	0
15	FME	T	1	15	8,9,10	1.13	1 (12%)	8,9,11	1.07	0
12	FME	M	1	12	8,9,10	0.91	0	8,9,11	0.99	0
12	FME	m	1	12	8,9,10	1.07	1 (12%)	8,9,11	1.14	0
8	FME	I	1	8	8,9,10	0.97	1 (12%)	8,9,11	1.34	1 (12%)
8	FME	i	1	8	8,9,10	1.01	1 (12%)	8,9,11	1.36	1 (12%)

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

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	t	1	15	-	1/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
8	FME	i	1	8	-	4/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-4.26	1.40	1.46
12	m	1	FME	CA-N	-2.33	1.43	1.46
15	T	1	FME	CA-N	-2.28	1.43	1.46
8	I	1	FME	CA-N	-2.10	1.43	1.46
8	i	1	FME	CA-N	-2.08	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.57	114.46	109.50
8	I	1	FME	CA-N-CN	-2.47	119.02	122.82

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	i	1	FME	N-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE
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 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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$
35	HEM	f	101	6,5	50,50,50	1.47	8 (16%)	67,82,82	1.22	6 (8%)
22	CLA	C	504	37	63,67,73	1.23	8 (12%)	74,105,113	1.22	7 (9%)
22	CLA	c	512	-	69,73,73	1.26	12 (17%)	82,113,113	1.39	8 (9%)
22	CLA	b	612	-	69,73,73	1.34	7 (10%)	82,113,113	1.34	10 (12%)
24	BCR	T	101	-	41,41,41	1.34	4 (9%)	56,56,56	1.27	6 (10%)
22	CLA	b	615	-	69,73,73	1.45	11 (15%)	82,113,113	1.32	10 (12%)
22	CLA	B	602	-	69,73,73	1.31	10 (14%)	82,113,113	1.50	10 (12%)
22	CLA	B	606	-	69,73,73	1.33	11 (15%)	82,113,113	1.39	12 (14%)
29	DGD	C	516	-	63,63,67	1.36	11 (17%)	77,77,81	1.40	10 (12%)
32	STE	a	413	-	9,9,19	0.69	0	8,8,19	0.42	0
22	CLA	B	610	37	69,73,73	1.17	7 (10%)	82,113,113	1.41	11 (13%)
22	CLA	b	611	-	69,73,73	1.26	5 (7%)	82,113,113	1.38	6 (7%)
24	BCR	b	617	-	41,41,41	1.10	3 (7%)	56,56,56	1.46	11 (19%)
22	CLA	B	604	-	69,73,73	1.28	6 (8%)	82,113,113	1.66	14 (17%)
24	BCR	k	101	-	41,41,41	1.12	5 (12%)	56,56,56	1.13	3 (5%)
28	SQD	a	410	-	52,54,54	0.94	4 (7%)	62,65,65	2.02	13 (20%)
22	CLA	c	511	3	69,73,73	1.44	6 (8%)	82,113,113	1.49	8 (9%)
22	CLA	b	616	-	64,68,73	1.11	4 (6%)	76,107,113	1.49	10 (13%)
22	CLA	C	503	-	69,73,73	1.60	9 (13%)	82,113,113	1.43	10 (12%)
22	CLA	C	506	-	69,73,73	1.43	9 (13%)	82,113,113	1.33	8 (9%)
33	LHG	l	101	-	48,48,48	0.87	1 (2%)	51,54,54	1.16	5 (9%)
32	STE	C	520	-	11,11,19	0.74	0	11,11,19	1.54	2 (18%)
32	STE	b	625	-	9,9,19	0.64	0	8,8,19	0.48	0
22	CLA	C	505	-	69,73,73	1.35	8 (11%)	82,113,113	1.23	6 (7%)
22	CLA	b	607	37	69,73,73	1.37	8 (11%)	82,113,113	1.19	7 (8%)
32	STE	b	624	-	19,19,19	0.87	0	19,19,19	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	STE	l	102	-	17,17,19	0.47	0	16,16,19	0.80	0
22	CLA	B	609	-	69,73,73	1.13	6 (8%)	82,113,113	1.19	6 (7%)
22	CLA	d	405	-	69,73,73	1.43	11 (15%)	82,113,113	1.18	7 (8%)
31	OEX	A	416[A]	3,1,37	0,15,15	-	-	-	-	-
22	CLA	B	608	-	69,73,73	1.25	6 (8%)	82,113,113	1.55	11 (13%)
24	BCR	Y	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.21	4 (7%)
22	CLA	B	614	-	69,73,73	1.36	9 (13%)	82,113,113	1.25	9 (10%)
22	CLA	D	403	-	69,73,73	1.32	8 (11%)	82,113,113	1.29	9 (10%)
24	BCR	b	619	-	41,41,41	1.21	2 (4%)	56,56,56	1.42	11 (19%)
22	CLA	D	404	-	69,73,73	1.61	10 (14%)	82,113,113	1.43	8 (9%)
24	BCR	K	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.39	9 (16%)
22	CLA	c	503	-	69,73,73	1.26	11 (15%)	82,113,113	1.33	8 (9%)
22	CLA	c	508	-	68,72,73	1.25	10 (14%)	80,111,113	1.39	12 (15%)
32	STE	a	414	-	11,11,19	0.78	0	11,11,19	1.13	1 (9%)
33	LHG	B	622	-	48,48,48	1.05	4 (8%)	51,54,54	1.42	6 (11%)
22	CLA	B	603	-	69,73,73	1.32	12 (17%)	82,113,113	1.47	12 (14%)
22	CLA	d	403	-	69,73,73	1.24	6 (8%)	82,113,113	1.13	5 (6%)
22	CLA	c	510	-	69,73,73	1.19	9 (13%)	82,113,113	1.39	8 (9%)
29	DGD	C	518	-	63,63,67	1.17	10 (15%)	77,77,81	1.36	9 (11%)
32	STE	J	101	-	11,11,19	0.69	0	11,11,19	1.39	1 (9%)
22	CLA	B	612	-	69,73,73	1.17	7 (10%)	82,113,113	1.36	10 (12%)
22	CLA	B	601	37	69,73,73	1.53	11 (15%)	82,113,113	1.39	7 (8%)
22	CLA	B	607	37	69,73,73	1.56	9 (13%)	82,113,113	1.53	7 (8%)
32	STE	c	524	-	11,11,19	0.75	0	11,11,19	1.20	1 (9%)
22	CLA	C	511	3	69,73,73	1.37	8 (11%)	82,113,113	1.17	5 (6%)
32	STE	t	102	-	13,13,19	0.71	0	13,13,19	1.15	1 (7%)
23	PHO	d	402	-	58,69,69	2.12	9 (15%)	55,99,99	1.66	10 (18%)
32	STE	I	101	-	14,14,19	0.64	0	13,13,19	0.40	0
32	STE	E	103	-	11,11,19	0.98	0	11,11,19	0.83	0
24	BCR	c	515	-	41,41,41	1.26	3 (7%)	56,56,56	1.41	9 (16%)
30	OEY	A	415[B]	3,1,37	0,16,16	-	-	-	-	-
24	BCR	a	405	-	41,41,41	1.17	4 (9%)	56,56,56	1.43	8 (14%)
28	SQD	B	623	-	52,54,54	1.00	2 (3%)	62,65,65	1.82	11 (17%)
29	DGD	H	102	-	63,63,67	1.40	9 (14%)	77,77,81	1.43	8 (10%)
27	LMG	A	411	-	48,48,55	0.99	3 (6%)	56,56,63	1.32	7 (12%)
22	CLA	C	513	-	69,73,73	1.22	8 (11%)	82,113,113	1.43	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	D	410	-	31,31,55	1.18	3 (9%)	33,33,63	1.11	2 (6%)
24	BCR	C	514	-	41,41,41	1.25	4 (9%)	56,56,56	1.30	6 (10%)
24	BCR	B	617	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	6 (10%)
29	DGD	A	414	-	67,67,67	1.39	7 (10%)	81,81,81	1.48	11 (13%)
32	STE	x	101	-	19,19,19	0.82	0	19,19,19	0.65	0
22	CLA	b	606	-	69,73,73	1.23	7 (10%)	82,113,113	1.55	9 (10%)
22	CLA	C	508	-	69,73,73	1.37	10 (14%)	82,113,113	1.38	9 (10%)
24	BCR	B	619	-	41,41,41	1.13	3 (7%)	56,56,56	1.39	4 (7%)
29	DGD	C	517	-	63,63,67	1.40	7 (11%)	77,77,81	1.55	14 (18%)
29	DGD	c	518	-	63,63,67	1.31	9 (14%)	77,77,81	1.52	9 (11%)
34	BCT	D	402	21	3,3,3	1.02	0	2,3,3	3.66	2 (100%)
22	CLA	a	404	-	69,73,73	1.41	10 (14%)	82,113,113	1.19	7 (8%)
22	CLA	C	510	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	9 (10%)
24	BCR	b	618	-	41,41,41	1.37	4 (9%)	56,56,56	1.22	5 (8%)
26	PL9	a	409	-	55,55,55	0.94	2 (3%)	68,69,69	1.66	16 (23%)
32	STE	c	521	-	19,19,19	0.79	1 (5%)	19,19,19	0.94	0
27	LMG	D	407	-	51,51,55	1.18	4 (7%)	59,59,63	1.34	9 (15%)
26	PL9	A	409	-	55,55,55	1.14	5 (9%)	68,69,69	1.57	13 (19%)
22	CLA	c	509	-	69,73,73	1.38	8 (11%)	82,113,113	1.61	9 (10%)
29	DGD	h	102	-	63,63,67	1.29	11 (17%)	77,77,81	1.54	13 (16%)
27	LMG	M	101	-	51,51,55	1.11	5 (9%)	59,59,63	1.41	7 (11%)
22	CLA	c	506	-	69,73,73	1.26	8 (11%)	82,113,113	1.25	8 (9%)
32	STE	B	620	-	16,16,19	0.71	0	16,16,19	1.05	1 (6%)
24	BCR	t	101	-	41,41,41	1.17	4 (9%)	56,56,56	1.48	9 (16%)
32	STE	B	626	-	15,15,19	0.49	0	14,14,19	0.73	0
24	BCR	d	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	6 (10%)
32	STE	b	623	-	15,15,19	0.94	1 (6%)	15,15,19	0.94	1 (6%)
36	HEC	V	201	17	46,50,50	1.75	5 (10%)	58,82,82	2.01	5 (8%)
33	LHG	e	101	-	41,41,48	0.88	1 (2%)	44,47,54	1.29	4 (9%)
22	CLA	b	613	-	69,73,73	1.45	11 (15%)	82,113,113	1.43	10 (12%)
22	CLA	c	504	37	64,68,73	1.33	8 (12%)	76,107,113	1.34	6 (7%)
32	STE	H	103	-	17,17,19	0.59	0	16,16,19	0.59	0
27	LMG	b	620	-	51,51,55	1.14	6 (11%)	59,59,63	1.51	11 (18%)
27	LMG	b	622	-	55,55,55	1.04	7 (12%)	63,63,63	1.44	7 (11%)
27	LMG	d	411	-	21,21,55	0.83	0	20,20,63	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LHG	D	408	-	48,48,48	1.00	5 (10%)	51,54,54	1.29	5 (9%)
33	LHG	L	102	-	48,48,48	1.02	2 (4%)	51,54,54	1.25	2 (3%)
22	CLA	C	502	-	69,73,73	1.18	8 (11%)	82,113,113	1.19	5 (6%)
28	SQD	L	101	-	47,49,54	0.99	3 (6%)	57,60,65	2.25	16 (28%)
28	SQD	A	412	-	50,52,54	1.02	4 (8%)	60,63,65	2.04	12 (20%)
29	DGD	c	517	-	63,63,67	1.10	6 (9%)	77,77,81	1.35	7 (9%)
30	OEY	a	415[B]	3,1,37	0,16,16	-	-	-	-	-
33	LHG	D	409	-	46,46,48	1.13	3 (6%)	49,52,54	1.14	3 (6%)
28	SQD	a	411	-	35,35,54	1.13	2 (5%)	37,37,65	1.19	5 (13%)
32	STE	b	621	-	19,19,19	0.71	0	19,19,19	0.90	0
27	LMG	C	519	-	48,48,55	1.19	7 (14%)	56,56,63	1.43	7 (12%)
22	CLA	a	403	37	69,73,73	1.33	6 (8%)	82,113,113	1.41	11 (13%)
24	BCR	D	405	-	41,41,41	1.22	3 (7%)	56,56,56	1.16	6 (10%)
33	LHG	d	408	-	48,48,48	1.06	4 (8%)	51,54,54	1.47	8 (15%)
22	CLA	A	410	37	69,73,73	1.17	7 (10%)	82,113,113	1.24	8 (9%)
27	LMG	c	522	-	48,48,55	1.20	6 (12%)	56,56,63	1.37	8 (14%)
22	CLA	c	505	-	69,73,73	1.03	5 (7%)	82,113,113	1.34	7 (8%)
23	PHO	D	401	-	58,69,69	1.96	11 (18%)	55,99,99	1.54	10 (18%)
22	CLA	A	405	-	58,62,73	1.48	8 (13%)	68,99,113	1.42	10 (14%)
22	CLA	A	403	37	69,73,73	1.38	7 (10%)	82,113,113	1.18	10 (12%)
22	CLA	C	512	-	69,73,73	1.55	12 (17%)	82,113,113	1.28	8 (9%)
22	CLA	B	605	-	69,73,73	1.29	9 (13%)	82,113,113	1.33	5 (6%)
22	CLA	b	604	-	69,73,73	1.17	9 (13%)	82,113,113	1.55	11 (13%)
28	SQD	F	101	-	34,36,54	1.01	3 (8%)	42,45,65	1.84	9 (21%)
24	BCR	B	618	-	41,41,41	1.27	4 (9%)	56,56,56	1.19	9 (16%)
22	CLA	c	513	-	69,73,73	1.28	11 (15%)	82,113,113	1.28	11 (13%)
22	CLA	b	614	-	69,73,73	1.39	11 (15%)	82,113,113	1.24	9 (10%)
32	STE	B	625	-	17,17,19	0.65	0	17,17,19	0.99	0
32	STE	C	521	-	15,15,19	0.57	0	14,14,19	0.51	0
32	STE	M	102	-	14,14,19	0.84	0	14,14,19	1.06	0
22	CLA	b	609	-	69,73,73	1.20	8 (11%)	82,113,113	1.23	7 (8%)
22	CLA	C	501	-	69,73,73	1.31	10 (14%)	82,113,113	1.48	7 (8%)
32	STE	B	627	-	11,11,19	1.05	1 (9%)	11,11,19	0.71	0
32	STE	T	102	-	15,15,19	0.53	0	14,14,19	0.70	0
32	STE	D	411	-	19,19,19	0.67	1 (5%)	19,19,19	1.06	0
33	LHG	d	410	-	38,38,48	0.89	3 (7%)	41,44,54	1.15	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	b	608	-	69,73,73	1.12	7 (10%)	82,113,113	1.46	11 (13%)
24	BCR	h	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	9 (16%)
27	LMG	c	523	-	49,49,55	1.04	3 (6%)	57,57,63	1.28	7 (12%)
26	PL9	d	407	-	55,55,55	1.44	6 (10%)	68,69,69	1.81	16 (23%)
32	STE	M	103	-	9,9,19	0.53	0	8,8,19	0.61	0
36	HEC	v	201	17	46,50,50	1.93	6 (13%)	58,82,82	1.79	4 (6%)
22	CLA	C	507	37	69,73,73	1.17	7 (10%)	82,113,113	1.59	8 (9%)
23	PHO	A	404	-	58,69,69	1.77	9 (15%)	55,99,99	1.67	12 (21%)
24	BCR	c	514	-	41,41,41	1.24	2 (4%)	56,56,56	1.32	8 (14%)
23	PHO	d	401	-	58,69,69	2.14	11 (18%)	55,99,99	1.49	11 (20%)
35	HEM	E	101	6,5	50,50,50	1.34	5 (10%)	67,82,82	1.16	5 (7%)
24	BCR	C	515	-	41,41,41	1.21	5 (12%)	56,56,56	1.13	4 (7%)
22	CLA	A	402	-	69,73,73	1.25	7 (10%)	82,113,113	1.33	10 (12%)
22	CLA	B	611	-	69,73,73	1.10	6 (8%)	82,113,113	1.40	15 (18%)
33	LHG	E	102	-	48,48,48	0.88	3 (6%)	51,54,54	1.20	3 (5%)
32	STE	m	101	-	11,11,19	0.70	0	11,11,19	1.69	2 (18%)
29	DGD	a	412	-	43,43,67	1.15	3 (6%)	45,45,81	1.47	7 (15%)
27	LMG	c	520	-	37,37,55	1.25	5 (13%)	45,45,63	1.31	6 (13%)
22	CLA	b	601	37	69,73,73	1.33	7 (10%)	82,113,113	1.50	6 (7%)
22	CLA	b	605	-	69,73,73	1.15	9 (13%)	82,113,113	1.42	17 (20%)
22	CLA	b	610	37	69,73,73	1.34	9 (13%)	82,113,113	1.28	11 (13%)
28	SQD	A	413	-	38,38,54	1.04	3 (7%)	40,40,65	1.45	6 (15%)
27	LMG	B	621	-	26,26,55	0.96	1 (3%)	26,26,63	1.14	1 (3%)
22	CLA	B	615	-	69,73,73	1.36	7 (10%)	82,113,113	1.45	9 (10%)
24	BCR	c	516	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	7 (12%)
22	CLA	c	501	-	69,73,73	1.17	9 (13%)	82,113,113	1.40	10 (12%)
22	CLA	B	616	-	64,68,73	1.31	6 (9%)	76,107,113	1.68	9 (11%)
27	LMG	d	412	-	44,44,55	1.23	6 (13%)	52,52,63	1.39	8 (15%)
32	STE	T	103	-	14,14,19	0.44	0	13,13,19	0.89	0
26	PL9	D	406	-	55,55,55	1.51	5 (9%)	68,69,69	1.60	15 (22%)
31	OEX	a	416[A]	3,1,37	0,15,15	-	-	-	-	-
22	CLA	a	402	-	69,73,73	1.38	10 (14%)	82,113,113	1.32	11 (13%)
32	STE	C	522	-	11,11,19	0.59	0	11,11,19	1.65	3 (27%)
33	LHG	d	409	-	48,48,48	0.78	2 (4%)	51,54,54	1.15	3 (5%)
32	STE	B	624	-	11,11,19	0.86	0	11,11,19	0.96	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	C	509	-	69,73,73	1.41	13 (18%)	82,113,113	1.37	12 (14%)
24	BCR	A	406	-	41,41,41	1.19	2 (4%)	56,56,56	1.46	10 (17%)
32	STE	d	413	-	16,16,19	0.76	0	16,16,19	1.13	1 (6%)
22	CLA	b	602	-	69,73,73	1.12	9 (13%)	82,113,113	1.37	9 (10%)
34	BCT	a	408	21	3,3,3	1.10	0	2,3,3	3.45	2 (100%)
29	DGD	c	519	-	63,63,67	1.40	9 (14%)	77,77,81	1.43	12 (15%)
22	CLA	c	502	-	69,73,73	1.24	9 (13%)	82,113,113	1.28	8 (9%)
32	STE	j	101	-	11,11,19	0.84	0	11,11,19	1.65	3 (27%)
22	CLA	d	404	37	69,73,73	1.37	5 (7%)	82,113,113	1.50	10 (12%)
22	CLA	B	613	-	69,73,73	1.29	11 (15%)	82,113,113	1.41	10 (12%)
24	BCR	H	101	-	41,41,41	1.16	1 (2%)	56,56,56	1.28	8 (14%)
22	CLA	b	603	-	69,73,73	1.37	10 (14%)	82,113,113	1.39	7 (8%)
28	SQD	f	102	-	39,41,54	1.18	4 (10%)	49,52,65	1.76	11 (22%)
22	CLA	c	507	37	69,73,73	1.24	7 (10%)	82,113,113	1.17	7 (8%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	f	101	6,5	-	4/14/54/54	-
22	CLA	C	504	37	1/1/18/20	6/32/108/115	-
22	CLA	c	512	-	1/1/20/20	22/39/115/115	-
22	CLA	b	612	-	1/1/20/20	6/39/115/115	-
24	BCR	T	101	-	-	9/29/63/63	0/2/2/2
22	CLA	b	615	-	1/1/20/20	11/39/115/115	-
22	CLA	B	606	-	1/1/20/20	11/39/115/115	-
22	CLA	B	602	-	-	9/39/115/115	-
29	DGD	C	516	-	-	21/51/91/95	0/2/2/2
32	STE	a	413	-	-	3/7/7/17	-
22	CLA	B	610	37	1/1/20/20	6/39/115/115	-
22	CLA	b	611	-	1/1/20/20	6/39/115/115	-
24	BCR	b	617	-	-	8/29/63/63	0/2/2/2
22	CLA	B	604	-	1/1/20/20	13/39/115/115	-
24	BCR	k	101	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	a	410	-	-	20/49/69/69	0/1/1/1
22	CLA	c	511	3	1/1/20/20	11/39/115/115	-
22	CLA	b	616	-	1/1/19/20	6/33/109/115	-
22	CLA	C	503	-	1/1/20/20	8/39/115/115	-
22	CLA	C	506	-	1/1/20/20	11/39/115/115	-
33	LHG	l	101	-	-	26/53/53/53	-
32	STE	C	520	-	-	5/9/9/17	-
32	STE	b	625	-	-	5/7/7/17	-
22	CLA	C	505	-	1/1/20/20	18/39/115/115	-
22	CLA	b	607	37	1/1/20/20	15/39/115/115	-
32	STE	b	624	-	-	8/17/17/17	-
32	STE	l	102	-	-	9/15/15/17	-
22	CLA	B	609	-	-	4/39/115/115	-
22	CLA	d	405	-	1/1/20/20	10/39/115/115	-
22	CLA	B	608	-	1/1/20/20	3/39/115/115	-
24	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
22	CLA	B	614	-	1/1/20/20	12/39/115/115	-
22	CLA	D	403	-	1/1/20/20	6/39/115/115	-
24	BCR	b	619	-	-	5/29/63/63	0/2/2/2
22	CLA	D	404	-	-	8/39/115/115	-
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2
22	CLA	c	503	-	1/1/20/20	8/39/115/115	-
22	CLA	c	508	-	-	5/38/114/115	-
32	STE	a	414	-	-	7/9/9/17	-
33	LHG	B	622	-	-	18/53/53/53	-
22	CLA	B	603	-	1/1/20/20	11/39/115/115	-
22	CLA	d	403	-	-	11/39/115/115	-
22	CLA	c	510	-	1/1/20/20	14/39/115/115	-
29	DGD	C	518	-	-	12/51/91/95	0/2/2/2
32	STE	J	101	-	-	2/9/9/17	-
22	CLA	B	612	-	1/1/20/20	10/39/115/115	-
22	CLA	B	601	37	1/1/20/20	16/39/115/115	-
22	CLA	B	607	37	1/1/20/20	11/39/115/115	-
32	STE	c	524	-	-	5/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	511	3	1/1/20/20	6/39/115/115	-
32	STE	t	102	-	-	4/11/11/17	-
23	PHO	d	402	-	-	7/37/103/103	0/5/6/6
32	STE	I	101	-	-	8/12/12/17	-
32	STE	E	103	-	-	6/9/9/17	-
24	BCR	c	515	-	-	3/29/63/63	0/2/2/2
24	BCR	a	405	-	-	4/29/63/63	0/2/2/2
28	SQD	B	623	-	-	24/49/69/69	0/1/1/1
29	DGD	H	102	-	-	22/51/91/95	0/2/2/2
27	LMG	A	411	-	-	23/43/63/70	0/1/1/1
22	CLA	C	513	-	1/1/20/20	16/39/115/115	-
27	LMG	D	410	-	-	17/33/33/70	-
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2
24	BCR	B	617	-	-	2/29/63/63	0/2/2/2
29	DGD	A	414	-	-	25/55/95/95	0/2/2/2
32	STE	x	101	-	-	9/17/17/17	-
22	CLA	b	606	-	1/1/20/20	13/39/115/115	-
22	CLA	C	508	-	-	7/39/115/115	-
24	BCR	B	619	-	-	1/29/63/63	0/2/2/2
29	DGD	C	517	-	-	19/51/91/95	0/2/2/2
29	DGD	c	518	-	-	21/51/91/95	0/2/2/2
22	CLA	a	404	-	1/1/20/20	8/39/115/115	-
22	CLA	C	510	-	1/1/20/20	10/39/115/115	-
24	BCR	b	618	-	-	7/29/63/63	0/2/2/2
26	PL9	a	409	-	-	18/53/73/73	0/1/1/1
32	STE	c	521	-	-	10/17/17/17	-
27	LMG	D	407	-	-	17/46/66/70	0/1/1/1
26	PL9	A	409	-	-	22/53/73/73	0/1/1/1
22	CLA	c	509	-	1/1/20/20	10/39/115/115	-
29	DGD	h	102	-	-	15/51/91/95	0/2/2/2
27	LMG	M	101	-	-	24/46/66/70	0/1/1/1
22	CLA	c	506	-	1/1/20/20	11/39/115/115	-
32	STE	B	620	-	-	8/14/14/17	-
24	BCR	t	101	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	B	626	-	-	6/13/13/17	-
24	BCR	d	406	-	-	7/29/63/63	0/2/2/2
32	STE	b	623	-	-	6/13/13/17	-
36	HEC	V	201	17	-	6/14/54/54	-
33	LHG	e	101	-	-	22/46/46/53	-
22	CLA	b	613	-	1/1/20/20	4/39/115/115	-
22	CLA	c	504	37	1/1/19/20	4/33/109/115	-
32	STE	H	103	-	-	6/15/15/17	-
27	LMG	b	620	-	-	14/46/66/70	0/1/1/1
27	LMG	b	622	-	-	29/50/70/70	0/1/1/1
27	LMG	d	411	-	-	10/17/17/70	-
33	LHG	D	408	-	-	26/53/53/53	-
33	LHG	L	102	-	-	20/53/53/53	-
22	CLA	C	502	-	1/1/20/20	10/39/115/115	-
28	SQD	L	101	-	-	22/44/64/69	0/1/1/1
28	SQD	A	412	-	-	15/47/67/69	0/1/1/1
29	DGD	c	517	-	-	27/51/91/95	0/2/2/2
33	LHG	D	409	-	-	16/51/51/53	-
28	SQD	a	411	-	-	17/37/37/69	-
32	STE	b	621	-	-	12/17/17/17	-
27	LMG	C	519	-	-	19/43/63/70	0/1/1/1
22	CLA	a	403	37	-	9/39/115/115	-
24	BCR	D	405	-	-	5/29/63/63	0/2/2/2
33	LHG	d	408	-	-	24/53/53/53	-
22	CLA	A	410	37	1/1/20/20	9/39/115/115	-
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1
22	CLA	c	505	-	1/1/20/20	9/39/115/115	-
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
22	CLA	A	405	-	1/1/17/20	3/26/102/115	-
22	CLA	C	512	-	1/1/20/20	14/39/115/115	-
22	CLA	b	604	-	1/1/20/20	8/39/115/115	-
22	CLA	B	605	-	1/1/20/20	11/39/115/115	-
22	CLA	A	403	37	-	13/39/115/115	-
28	SQD	F	101	-	-	10/28/48/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	618	-	-	5/29/63/63	0/2/2/2
22	CLA	c	513	-	1/1/20/20	6/39/115/115	-
22	CLA	b	614	-	1/1/20/20	15/39/115/115	-
32	STE	B	625	-	-	11/15/15/17	-
32	STE	C	521	-	-	5/13/13/17	-
32	STE	M	102	-	-	4/12/12/17	-
22	CLA	b	609	-	1/1/20/20	8/39/115/115	-
22	CLA	C	501	-	1/1/20/20	4/39/115/115	-
32	STE	B	627	-	-	4/9/9/17	-
32	STE	T	102	-	-	5/13/13/17	-
32	STE	D	411	-	-	12/17/17/17	-
33	LHG	d	410	-	-	13/43/43/53	-
22	CLA	b	608	-	1/1/20/20	9/39/115/115	-
24	BCR	h	101	-	-	10/29/63/63	0/2/2/2
27	LMG	c	523	-	-	23/44/64/70	0/1/1/1
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
32	STE	M	103	-	-	2/7/7/17	-
36	HEC	v	201	17	-	6/14/54/54	-
22	CLA	C	507	37	1/1/20/20	6/39/115/115	-
23	PHO	A	404	-	-	5/37/103/103	0/5/6/6
24	BCR	c	514	-	-	9/29/63/63	0/2/2/2
23	PHO	d	401	-	-	3/37/103/103	0/5/6/6
35	HEM	E	101	6,5	-	2/14/54/54	-
24	BCR	C	515	-	-	13/29/63/63	0/2/2/2
22	CLA	A	402	-	1/1/20/20	5/39/115/115	-
22	CLA	B	611	-	1/1/20/20	7/39/115/115	-
33	LHG	E	102	-	-	24/53/53/53	-
32	STE	m	101	-	-	5/9/9/17	-
29	DGD	a	412	-	-	27/45/45/95	-
27	LMG	c	520	-	-	8/31/51/70	0/1/1/1
22	CLA	b	601	37	1/1/20/20	15/39/115/115	-
22	CLA	b	605	-	1/1/20/20	8/39/115/115	-
22	CLA	b	610	37	1/1/20/20	3/39/115/115	-
28	SQD	A	413	-	-	13/39/39/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	B	621	-	-	14/22/22/70	-
22	CLA	B	615	-	1/1/20/20	9/39/115/115	-
24	BCR	c	516	-	-	4/29/63/63	0/2/2/2
22	CLA	c	501	-	1/1/20/20	3/39/115/115	-
22	CLA	B	616	-	1/1/19/20	10/33/109/115	-
27	LMG	d	412	-	-	11/39/59/70	0/1/1/1
32	STE	T	103	-	-	7/12/12/17	-
26	PL9	D	406	-	-	7/53/73/73	0/1/1/1
22	CLA	a	402	-	1/1/20/20	6/39/115/115	-
32	STE	C	522	-	-	4/9/9/17	-
33	LHG	d	409	-	-	17/53/53/53	-
32	STE	B	624	-	-	6/9/9/17	-
22	CLA	C	509	-	1/1/20/20	14/39/115/115	-
24	BCR	A	406	-	-	3/29/63/63	0/2/2/2
32	STE	d	413	-	-	11/14/14/17	-
22	CLA	b	602	-	-	11/39/115/115	-
29	DGD	c	519	-	-	19/51/91/95	0/2/2/2
22	CLA	c	502	-	1/1/20/20	9/39/115/115	-
32	STE	j	101	-	-	3/9/9/17	-
22	CLA	d	404	37	1/1/20/20	6/39/115/115	-
22	CLA	B	613	-	1/1/20/20	11/39/115/115	-
24	BCR	H	101	-	-	7/29/63/63	0/2/2/2
22	CLA	b	603	-	1/1/20/20	5/39/115/115	-
28	SQD	f	102	-	-	11/36/56/69	0/1/1/1
22	CLA	c	507	37	1/1/20/20	10/39/115/115	-

The worst 5 of 934 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	PHO	C1B-C2B	10.16	1.50	1.39
23	d	401	PHO	C1B-C2B	9.28	1.49	1.39
23	d	401	PHO	C3B-C4B	8.71	1.50	1.41
23	D	401	PHO	C3B-C4B	8.45	1.50	1.41
22	D	404	CLA	MG-NB	-8.06	1.89	2.05

The worst 5 of 1235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C4A-NA-C1A	9.84	111.17	106.68
36	V	201	HEC	CBB-CAB-C3B	-9.82	107.80	127.43
28	L	101	SQD	O6-C1-C2	9.53	122.74	108.27
22	c	511	CLA	C4A-NA-C1A	9.36	110.95	106.68
22	B	616	CLA	C4A-NA-C1A	9.28	110.91	106.68

5 of 61 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	405	CLA	ND
22	A	410	CLA	ND
22	B	601	CLA	ND
22	B	603	CLA	ND

5 of 1853 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	CAD-CBD-CGD-O1D
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

112 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	f	101	HEM	4	0
22	c	512	CLA	1	0
24	T	101	BCR	1	0
22	b	615	CLA	2	0
22	B	606	CLA	2	0
29	C	516	DGD	1	0
24	b	617	BCR	1	0
22	B	604	CLA	3	0
28	a	410	SQD	2	0
22	c	511	CLA	2	0
22	b	616	CLA	2	0
22	C	503	CLA	2	0
22	C	506	CLA	1	0
33	l	101	LHG	2	0
22	b	607	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	l	102	STE	1	0
22	B	609	CLA	1	0
22	d	405	CLA	2	0
24	Y	101	BCR	2	0
22	B	614	CLA	2	0
22	D	403	CLA	2	0
22	D	404	CLA	1	0
24	K	101	BCR	1	0
22	c	503	CLA	2	0
22	c	508	CLA	1	0
32	a	414	STE	2	0
33	B	622	LHG	1	0
22	B	603	CLA	3	0
22	c	510	CLA	2	0
22	B	612	CLA	1	0
22	B	601	CLA	3	0
22	B	607	CLA	2	0
22	C	511	CLA	1	0
32	t	102	STE	1	0
23	d	402	PHO	1	0
32	I	101	STE	3	0
24	c	515	BCR	2	0
30	A	415[B]	OEY	2	0
24	a	405	BCR	1	0
22	C	513	CLA	2	0
27	D	410	LMG	1	0
24	C	514	BCR	1	0
29	A	414	DGD	5	0
32	x	101	STE	3	0
22	b	606	CLA	4	0
22	C	508	CLA	1	0
24	B	619	BCR	2	0
22	a	404	CLA	1	0
22	C	510	CLA	2	0
26	a	409	PL9	5	0
32	c	521	STE	1	0
27	D	407	LMG	1	0
26	A	409	PL9	3	0
27	M	101	LMG	2	0
22	c	506	CLA	1	0
24	t	101	BCR	2	0
24	d	406	BCR	2	0

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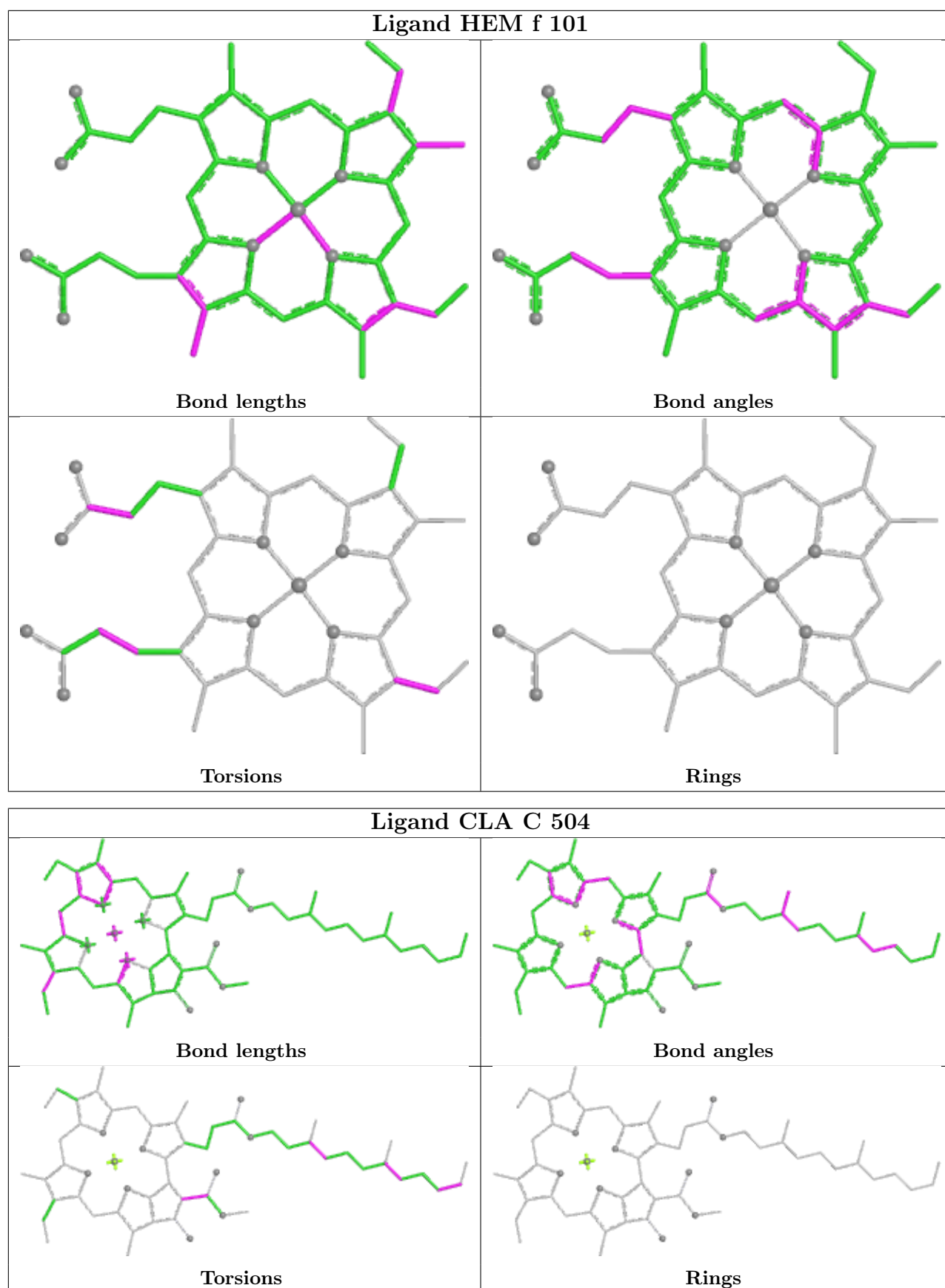
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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33	e	101	LHG	2	0
32	H	103	STE	2	0
27	b	620	LMG	1	0
33	D	408	LHG	2	0
33	L	102	LHG	1	0
22	C	502	CLA	1	0
28	L	101	SQD	1	0
30	a	415[B]	OEY	1	0
28	a	411	SQD	2	0
32	b	621	STE	1	0
27	C	519	LMG	1	0
24	D	405	BCR	2	0
33	d	408	LHG	3	0
22	c	505	CLA	2	0
23	D	401	PHO	2	0
22	A	405	CLA	1	0
22	B	605	CLA	5	0
22	b	604	CLA	1	0
28	F	101	SQD	1	0
22	c	513	CLA	1	0
32	B	625	STE	1	0
32	C	521	STE	1	0
22	b	609	CLA	1	0
22	C	501	CLA	1	0
32	T	102	STE	1	0
32	D	411	STE	2	0
33	d	410	LHG	1	0
22	b	608	CLA	1	0
27	c	523	LMG	1	0
26	d	407	PL9	1	0
36	v	201	HEC	1	0
23	A	404	PHO	1	0
35	E	101	HEM	2	0
22	B	611	CLA	1	0
33	E	102	LHG	1	0
29	a	412	DGD	4	0
22	b	605	CLA	2	0
22	b	610	CLA	1	0
22	B	615	CLA	2	0
24	c	516	BCR	1	0
22	c	501	CLA	2	0

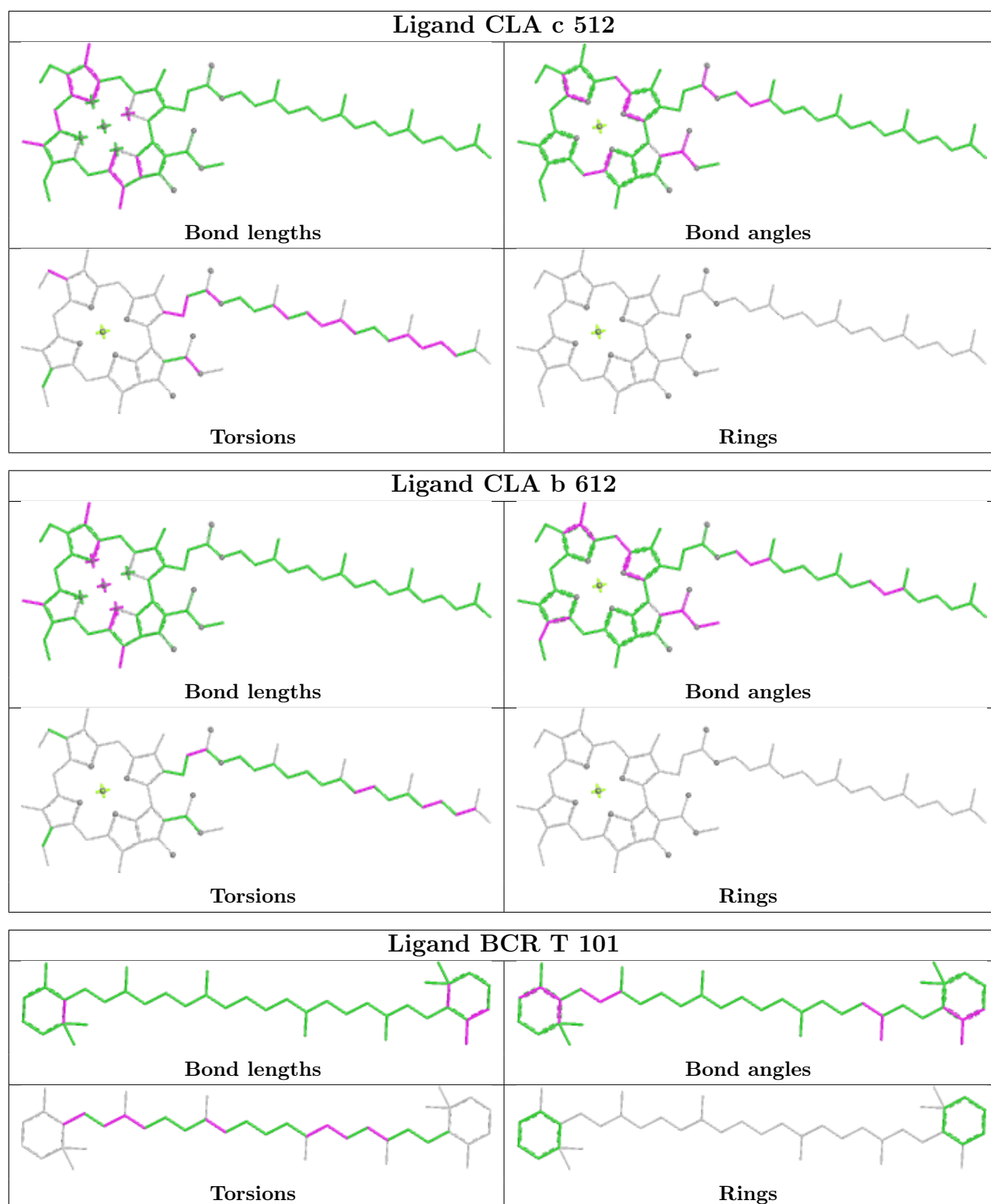
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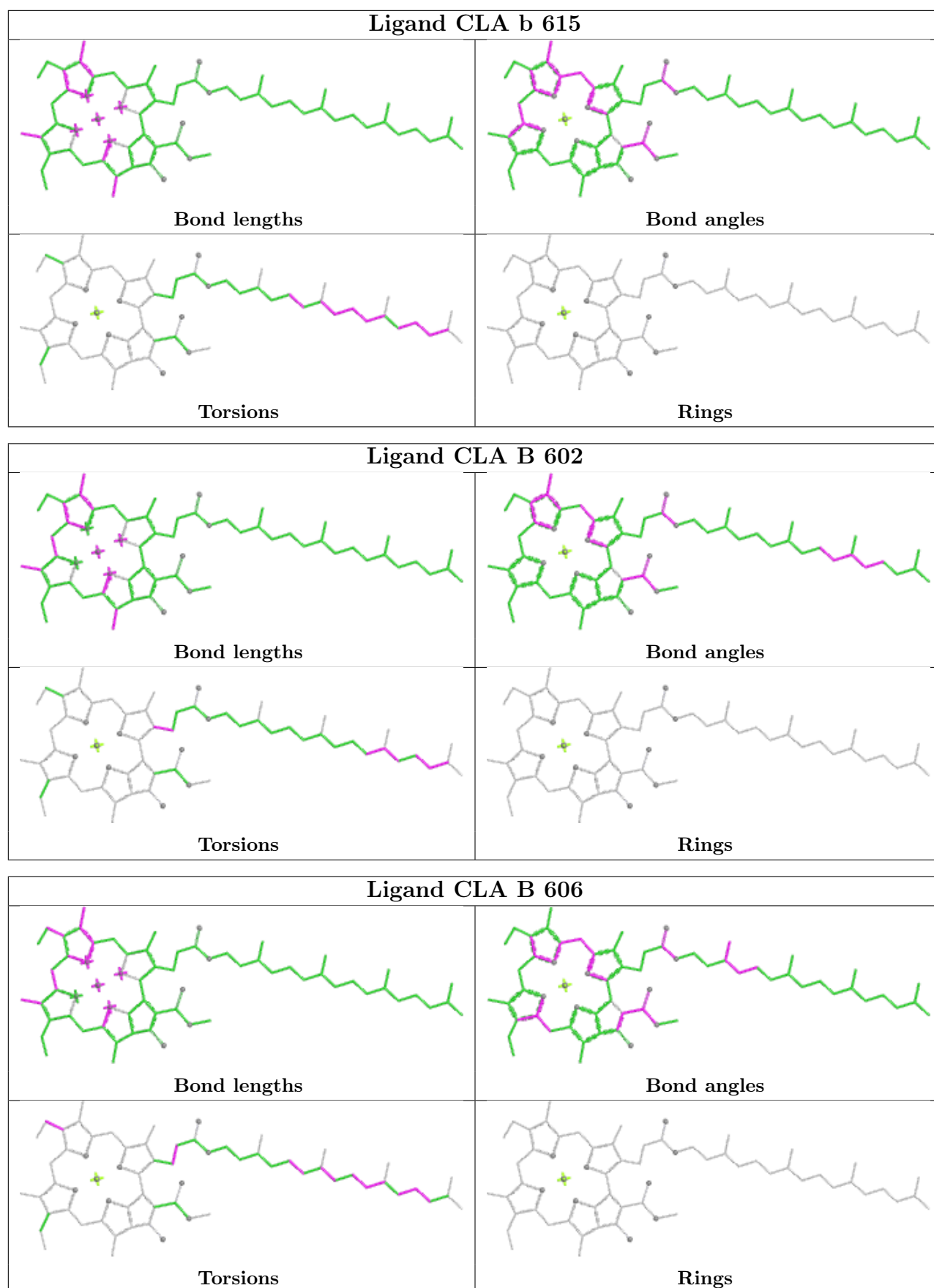
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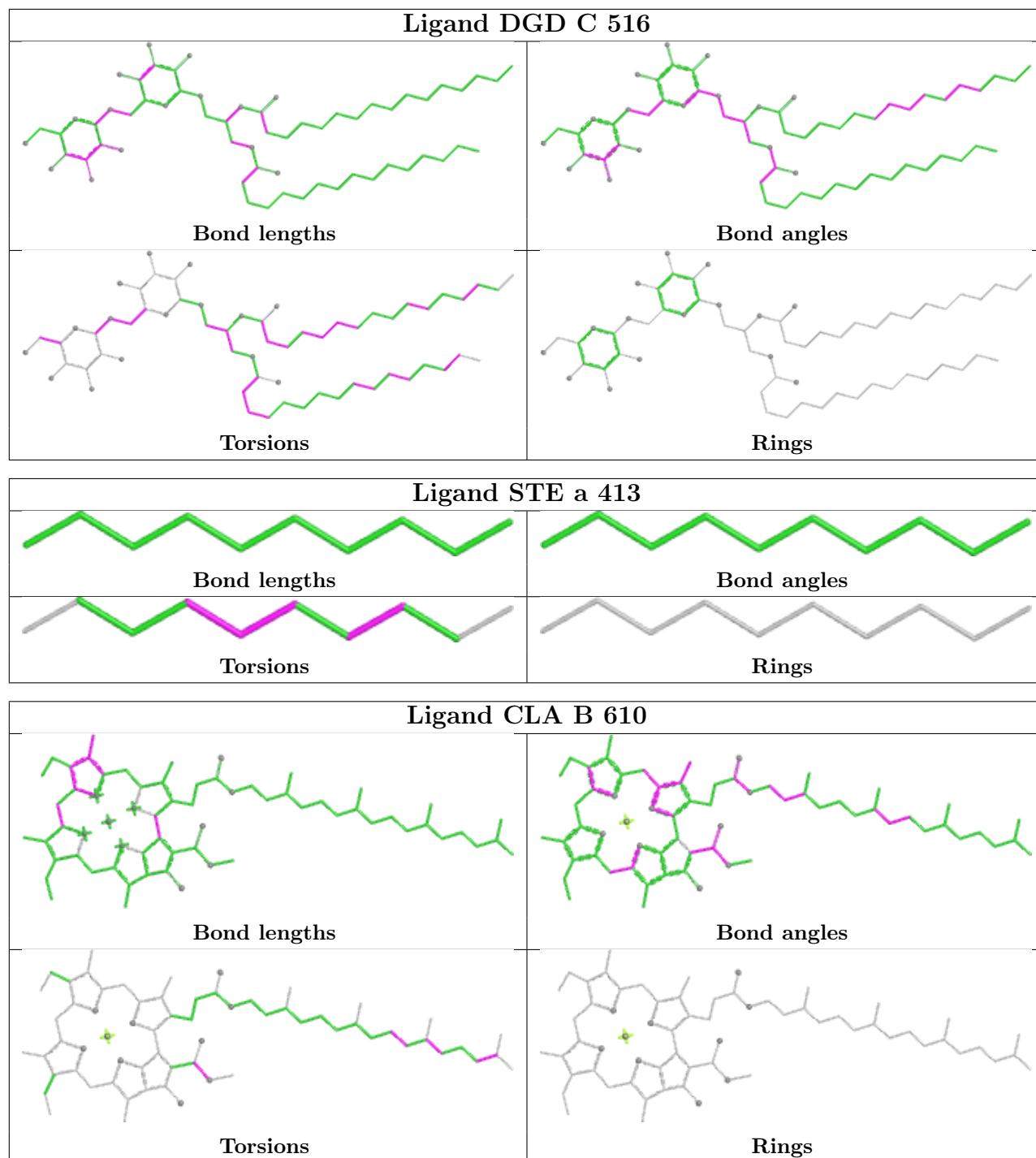
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	616	CLA	2	0
26	D	406	PL9	2	0
33	d	409	LHG	4	0
22	C	509	CLA	3	0
24	A	406	BCR	1	0
32	d	413	STE	2	0
22	b	602	CLA	1	0
29	c	519	DGD	2	0
22	c	502	CLA	1	0
24	H	101	BCR	1	0
22	b	603	CLA	1	0
28	f	102	SQD	2	0
22	c	507	CLA	2	0

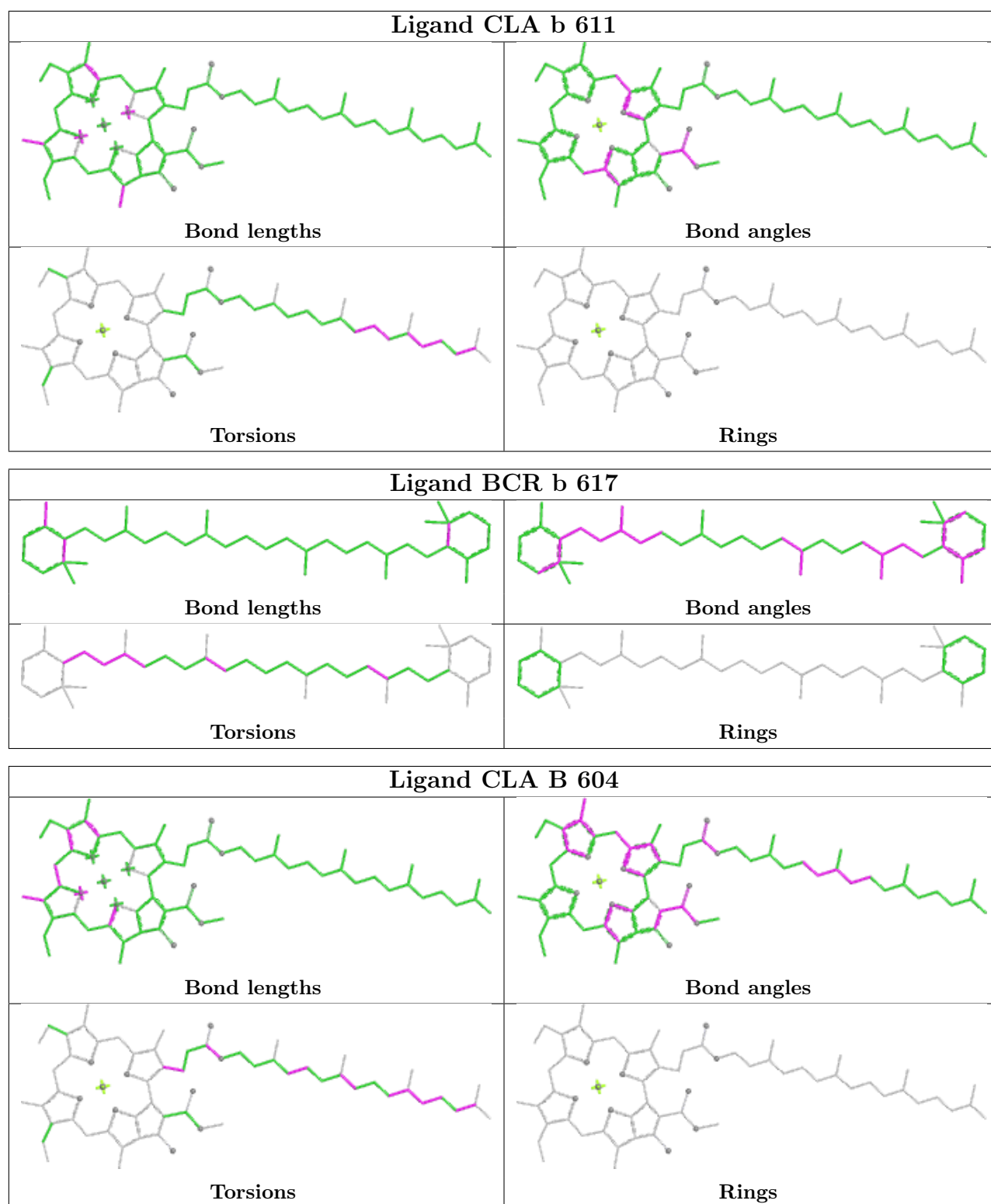
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

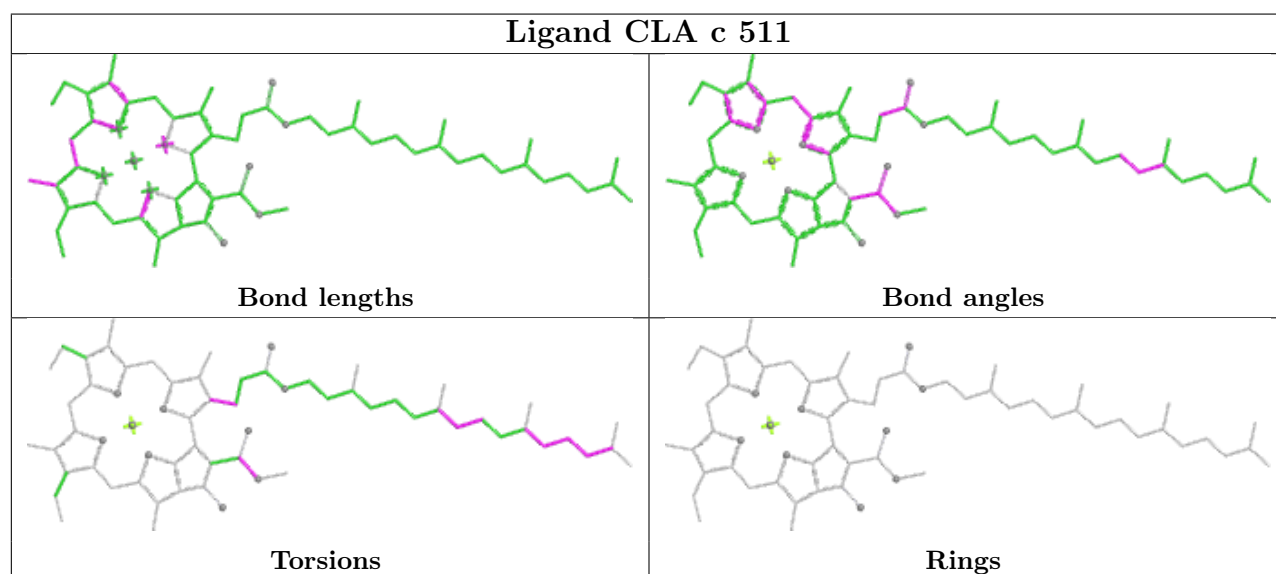
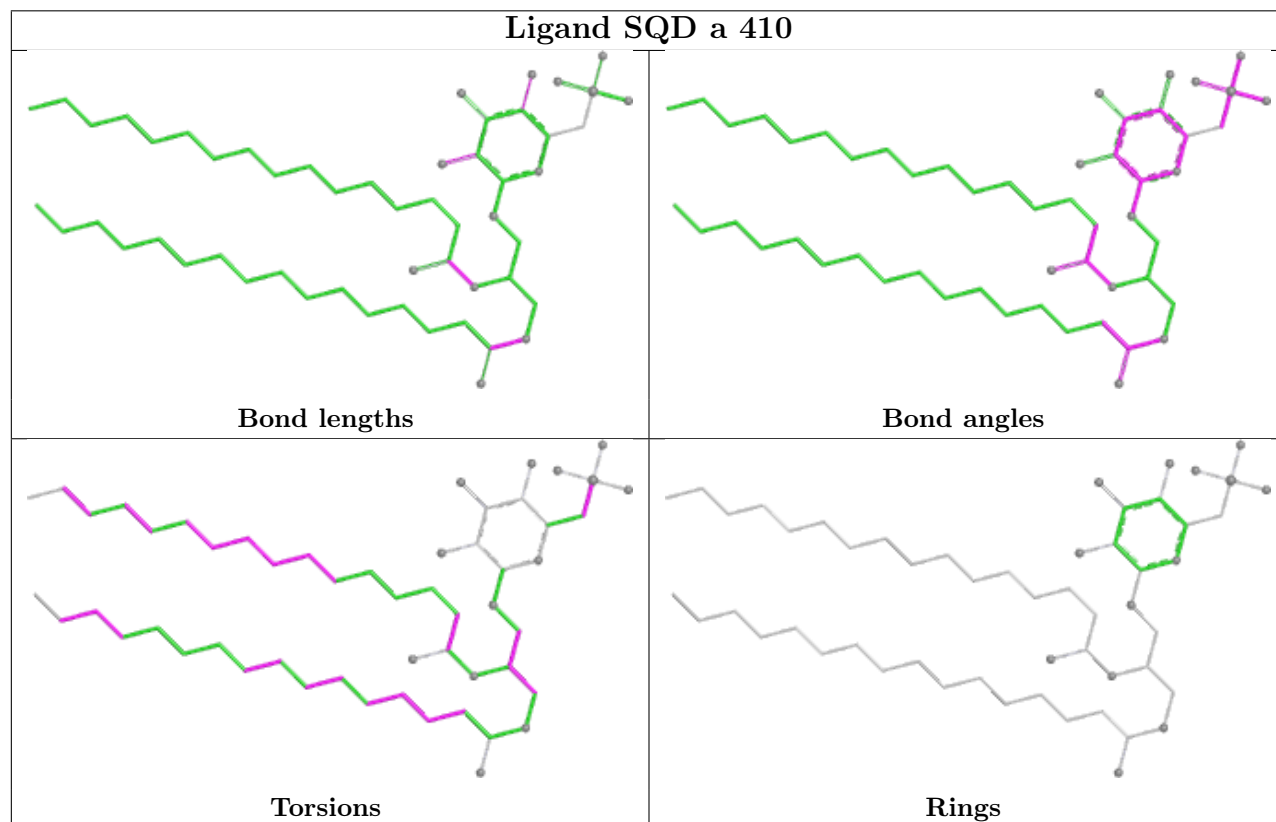
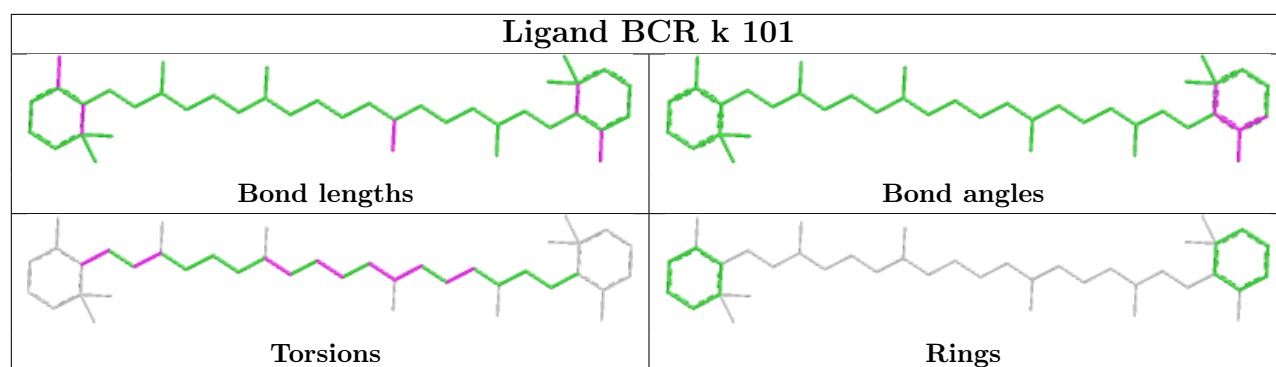


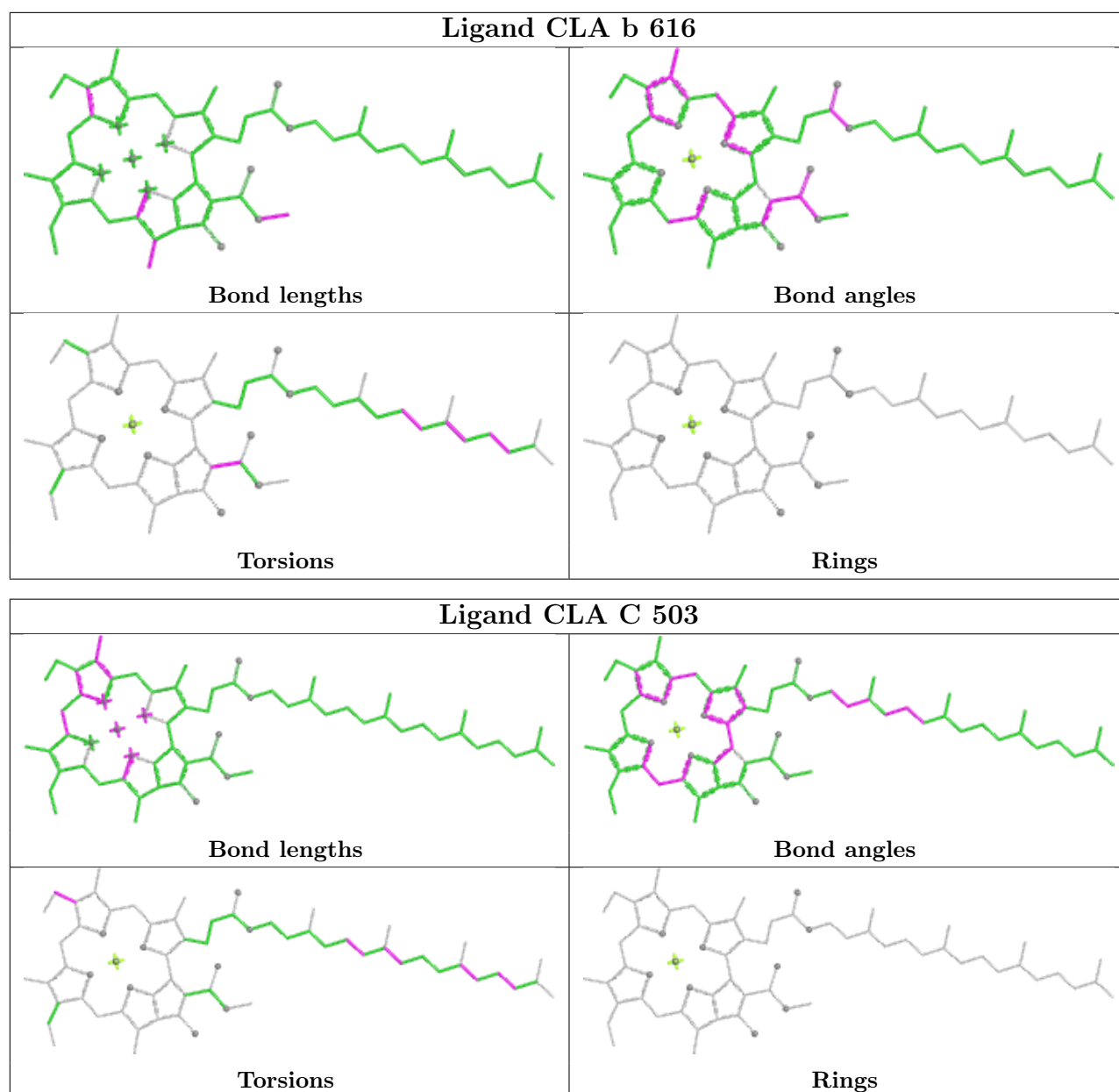


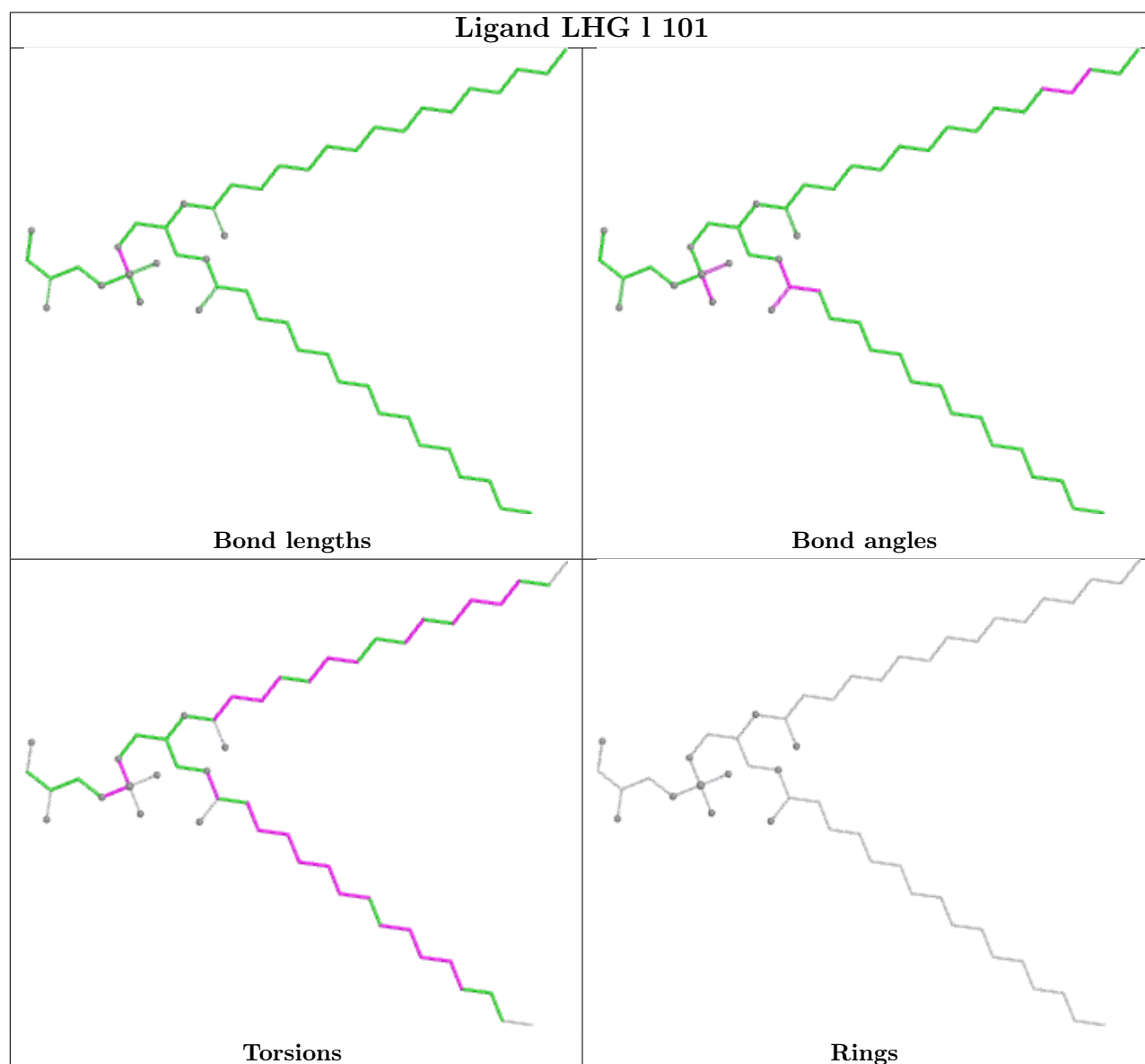
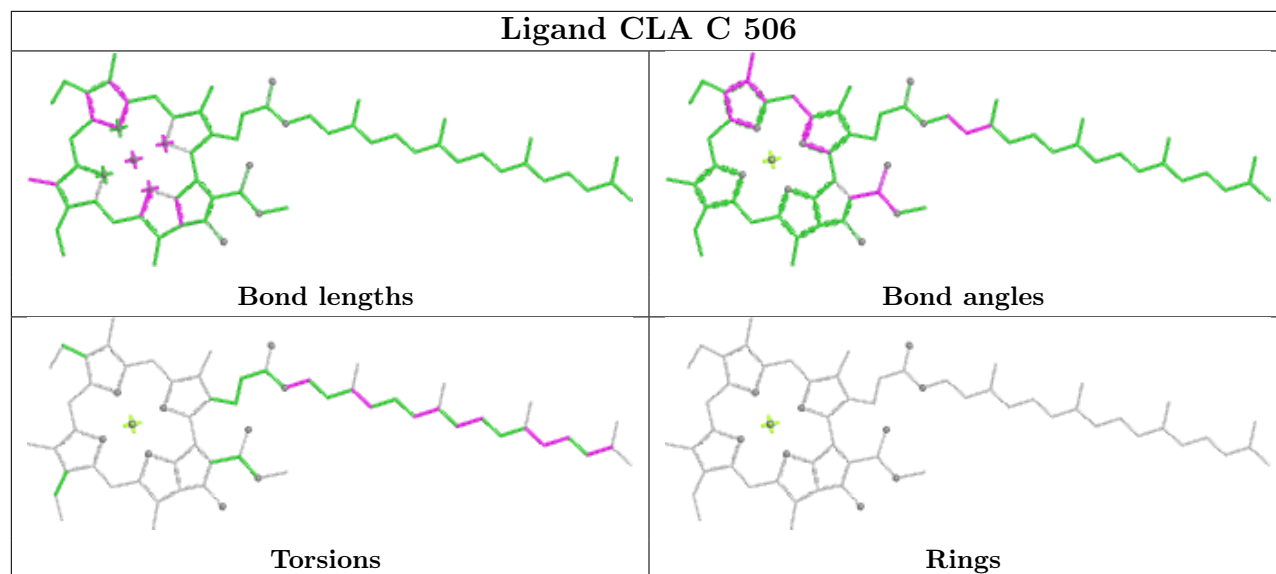


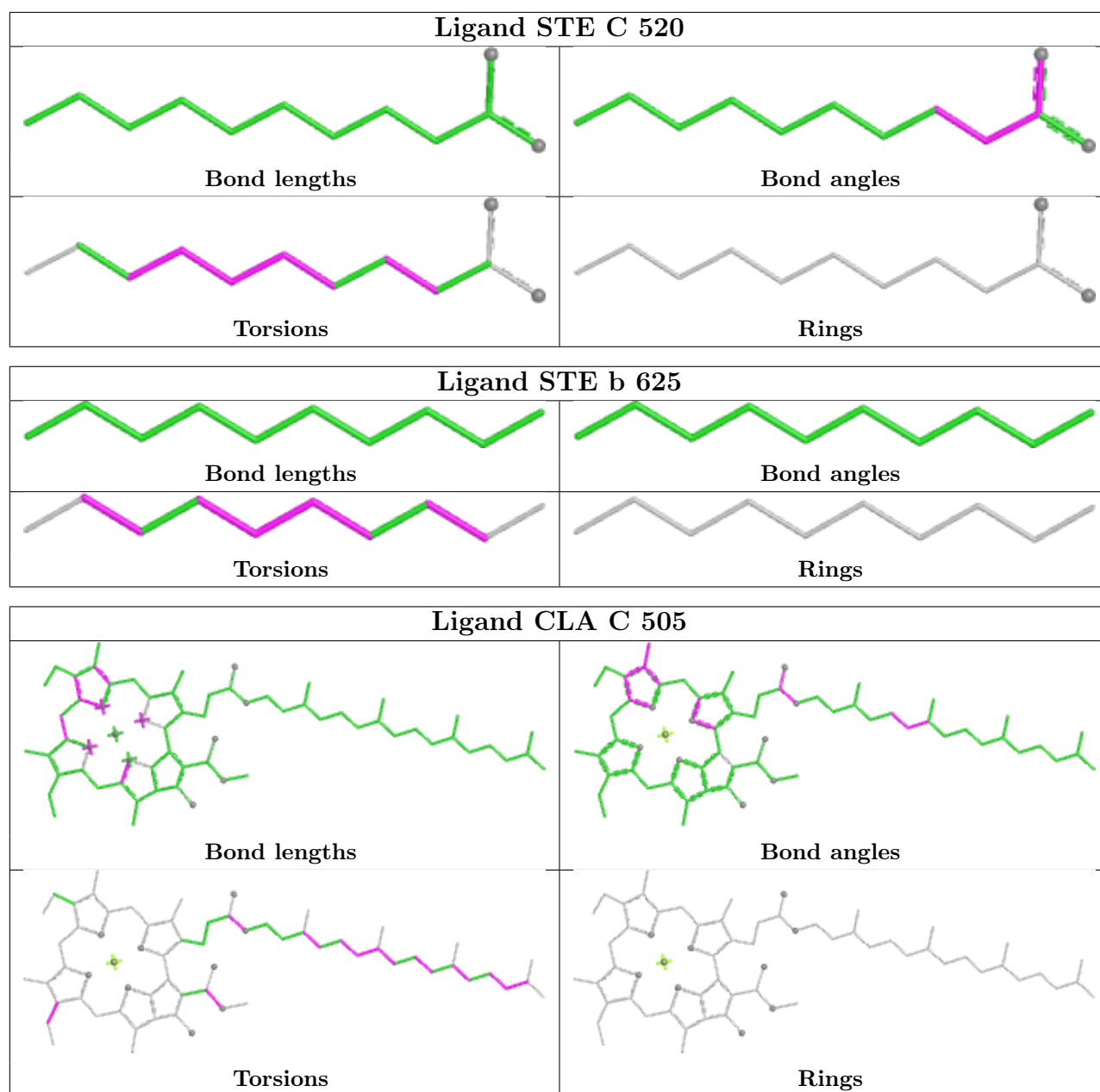


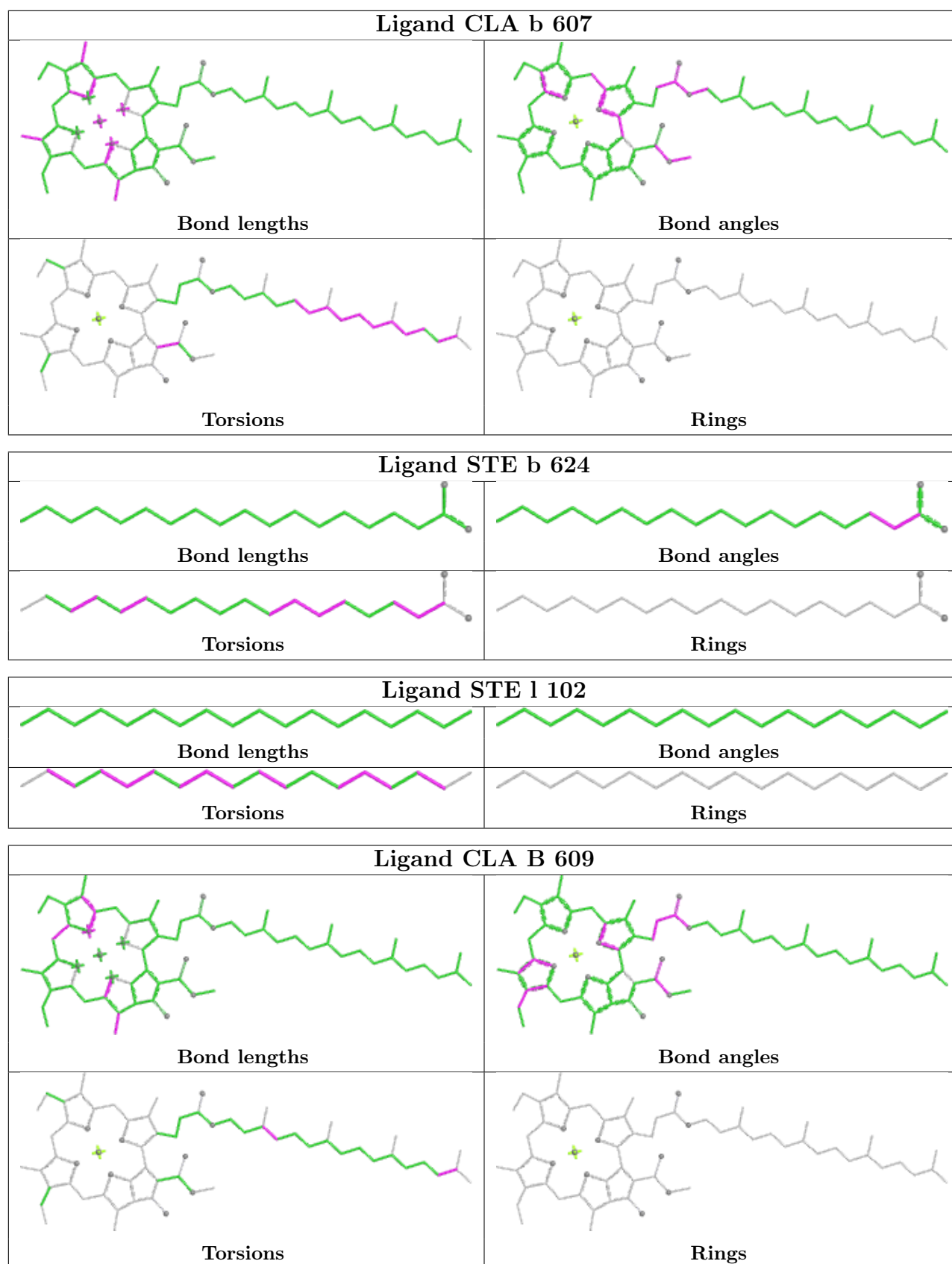


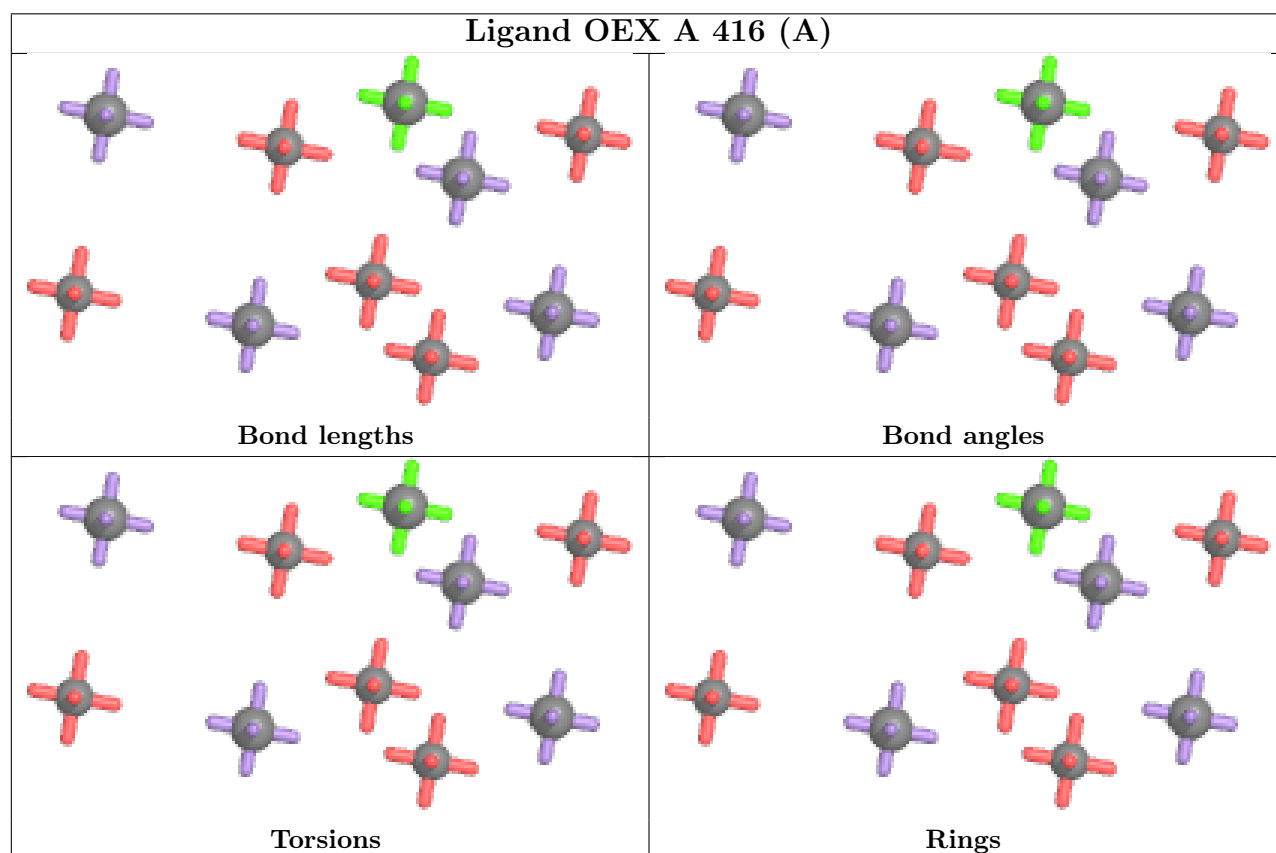
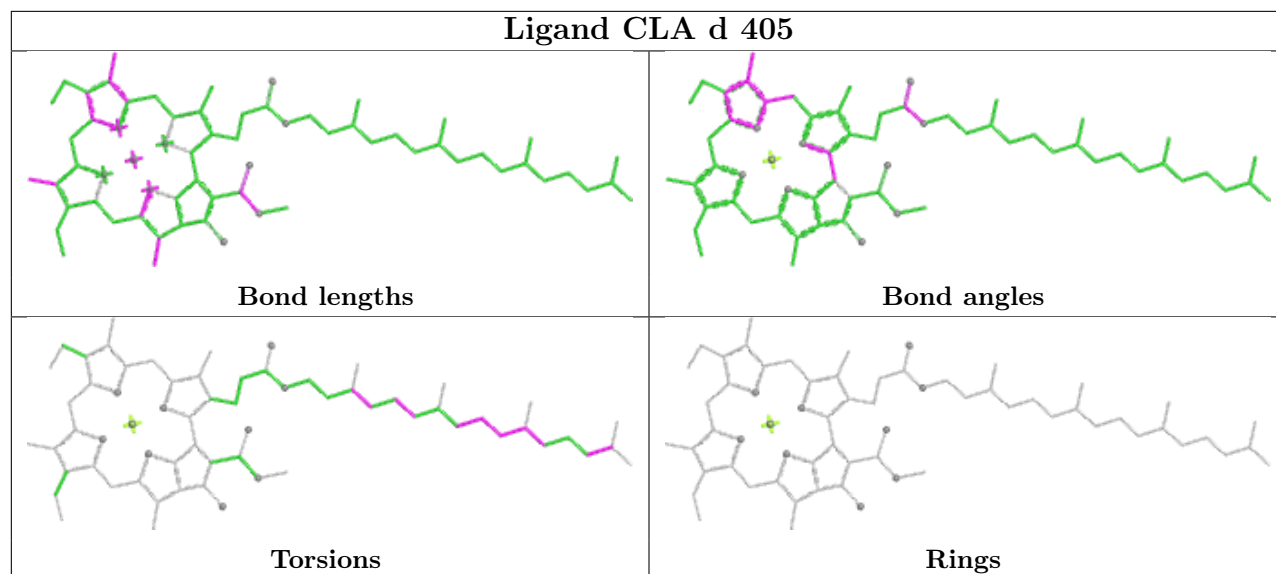


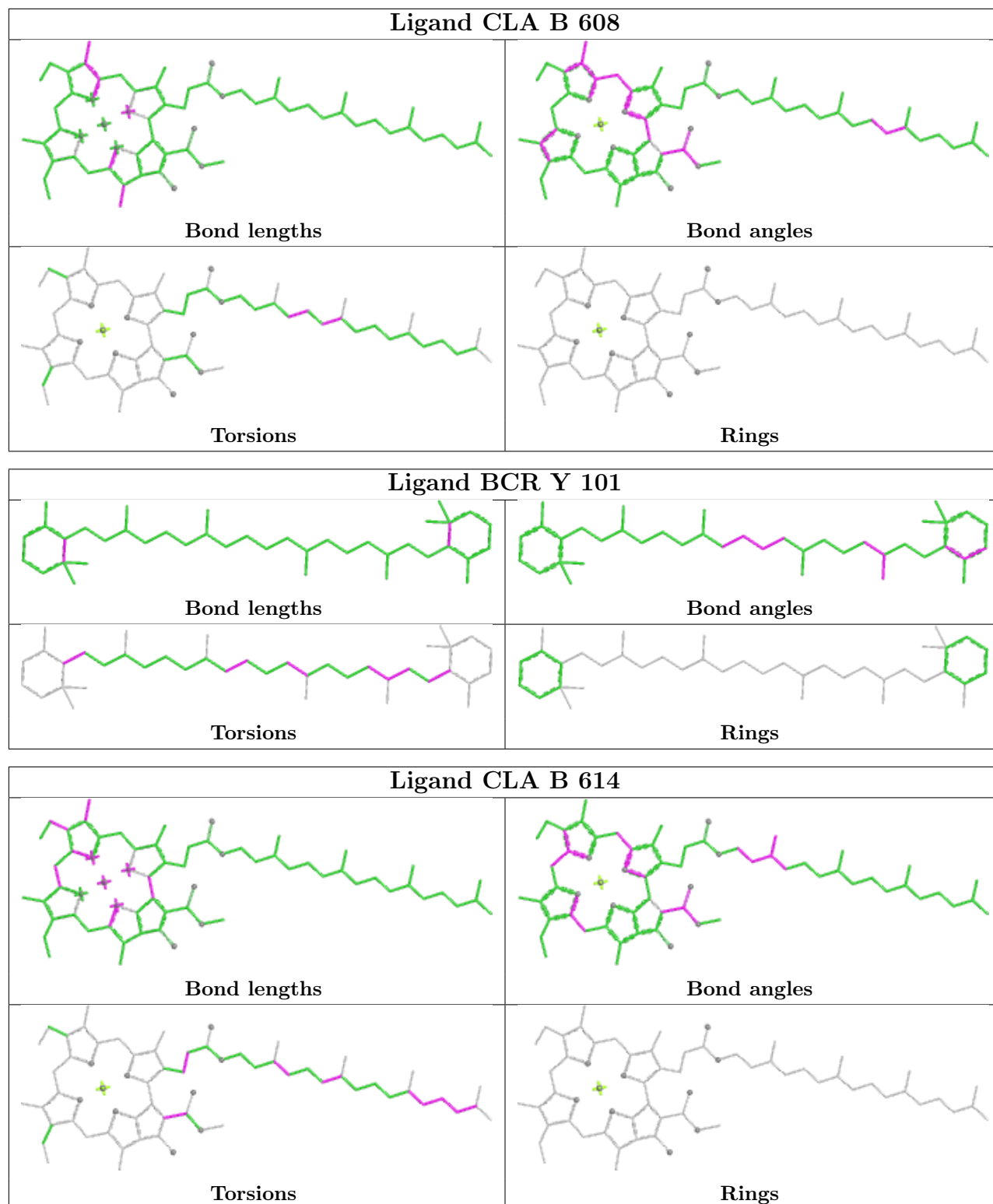


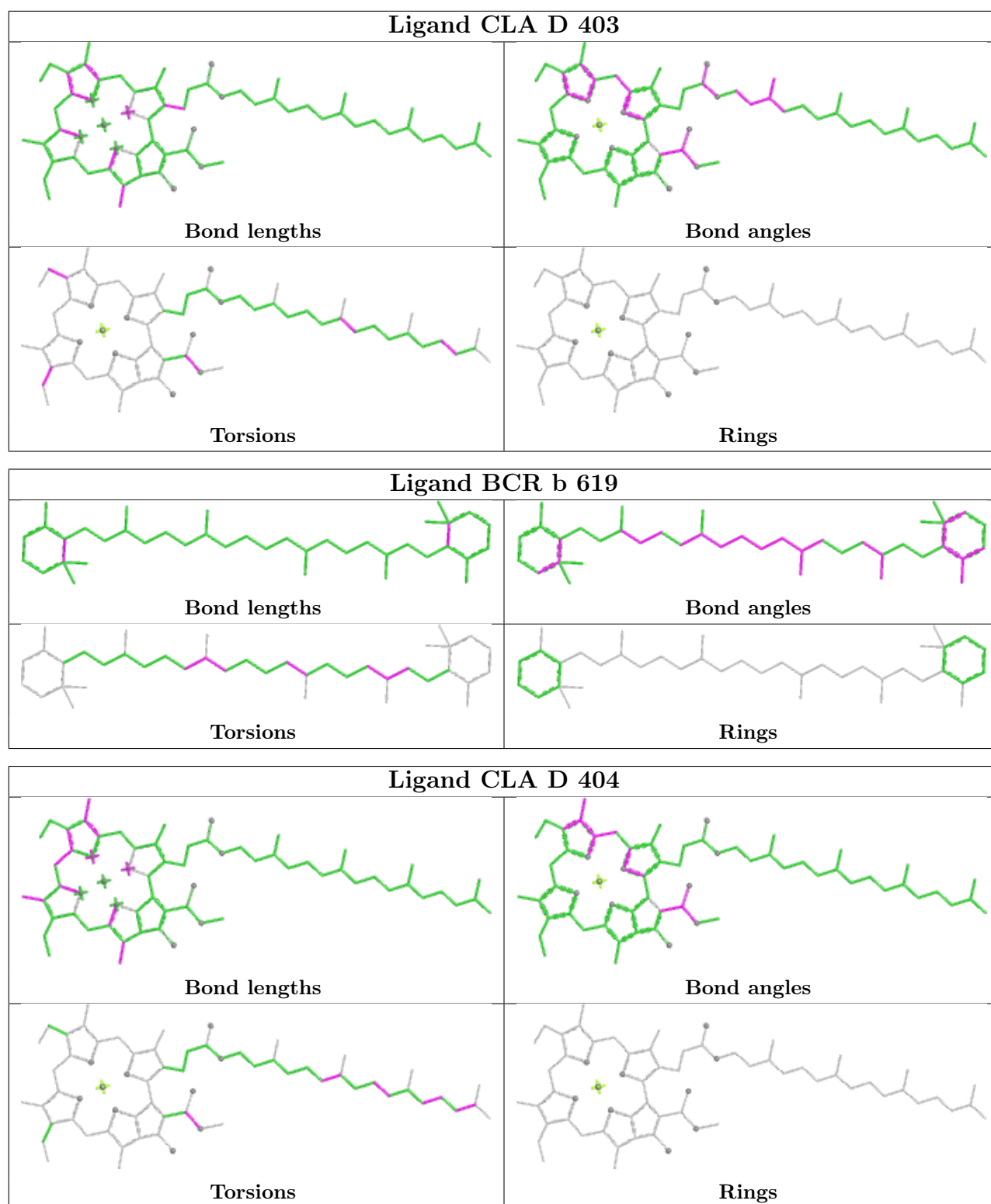


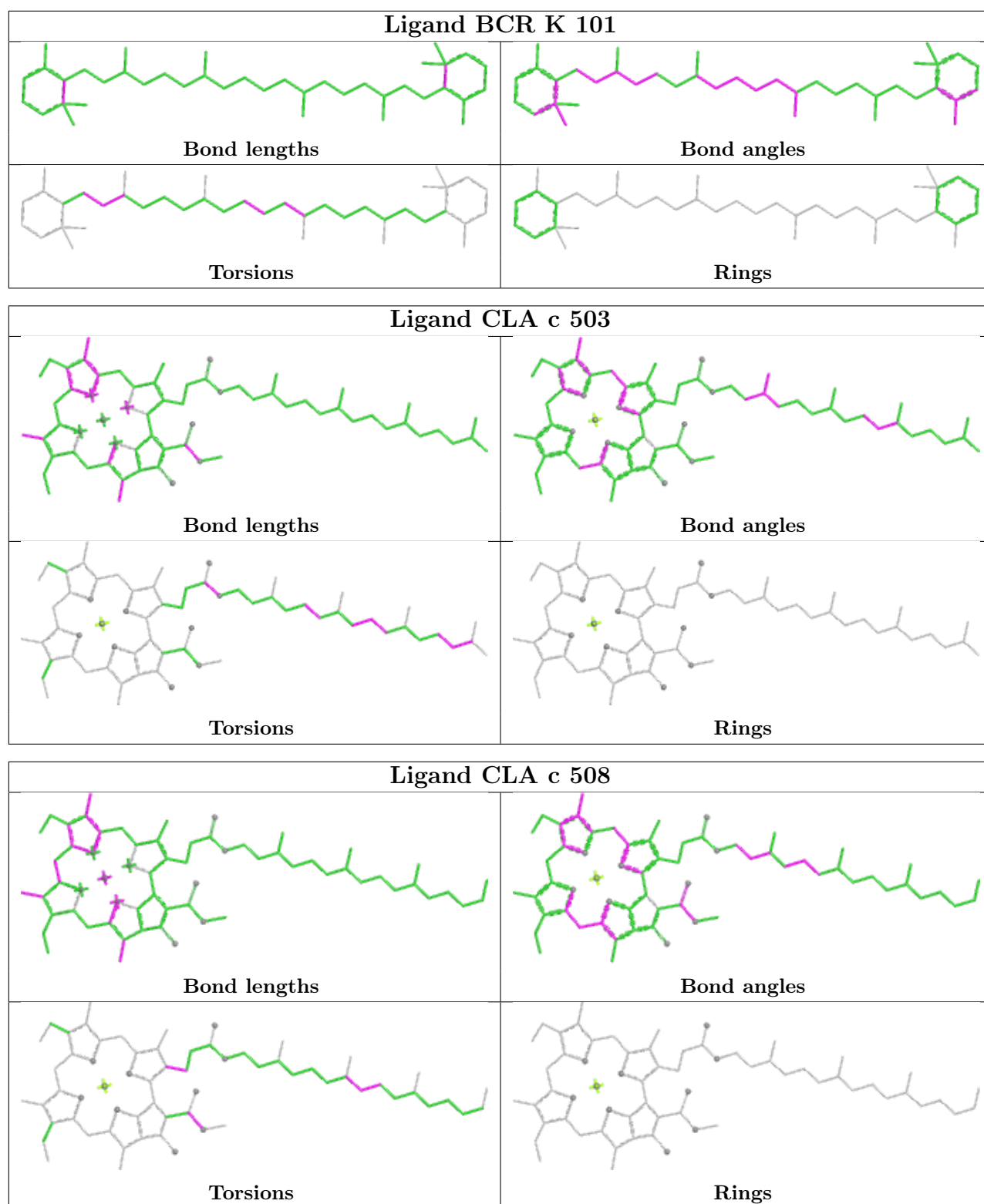


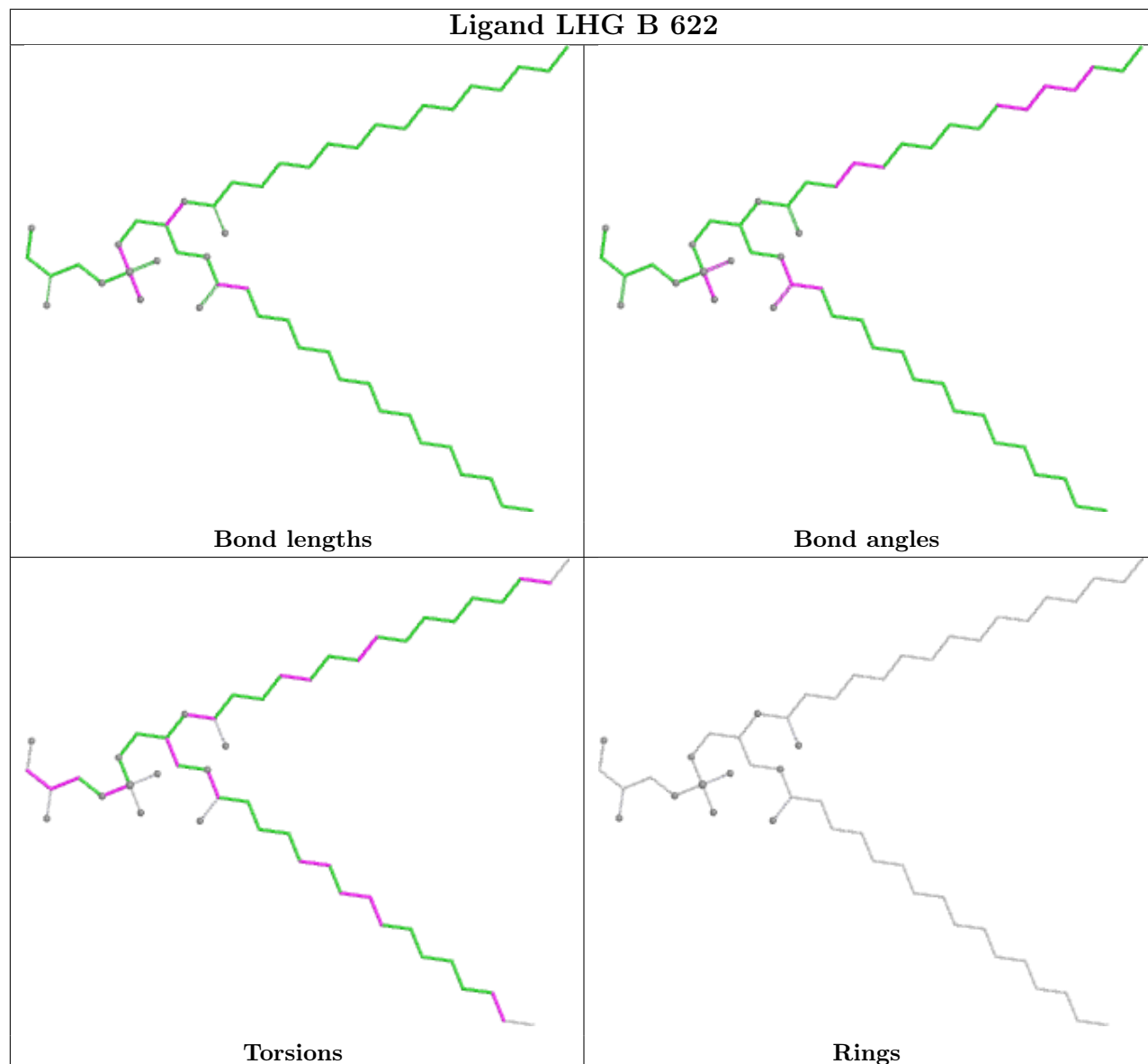
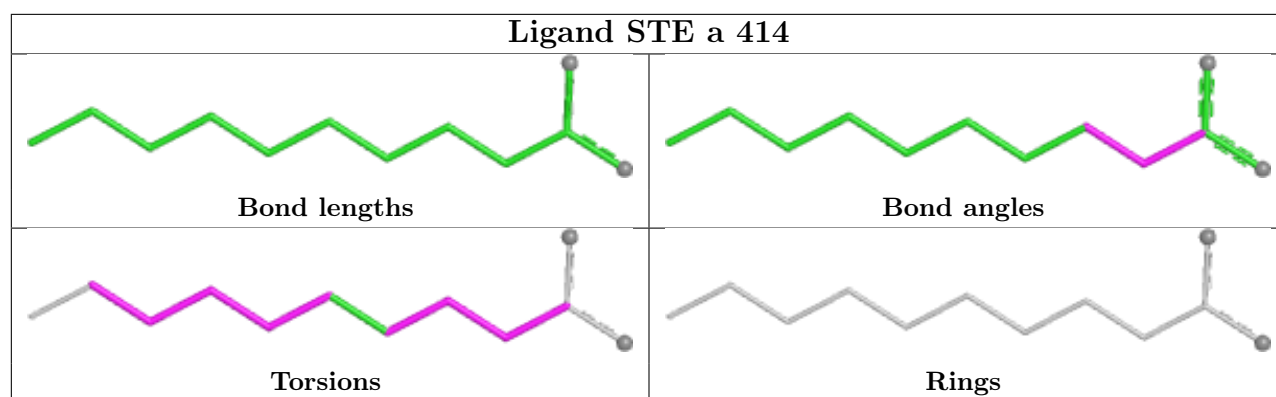


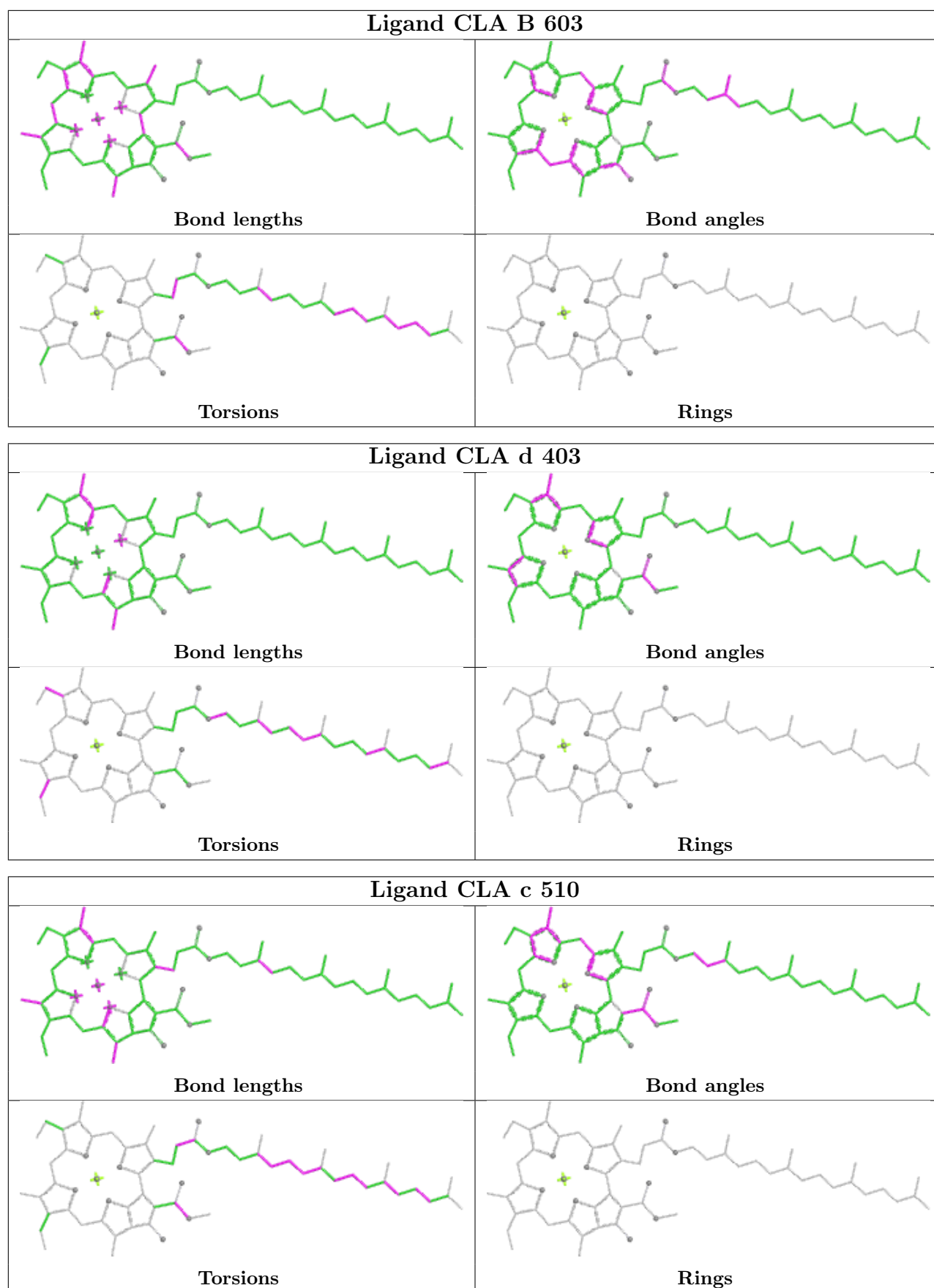


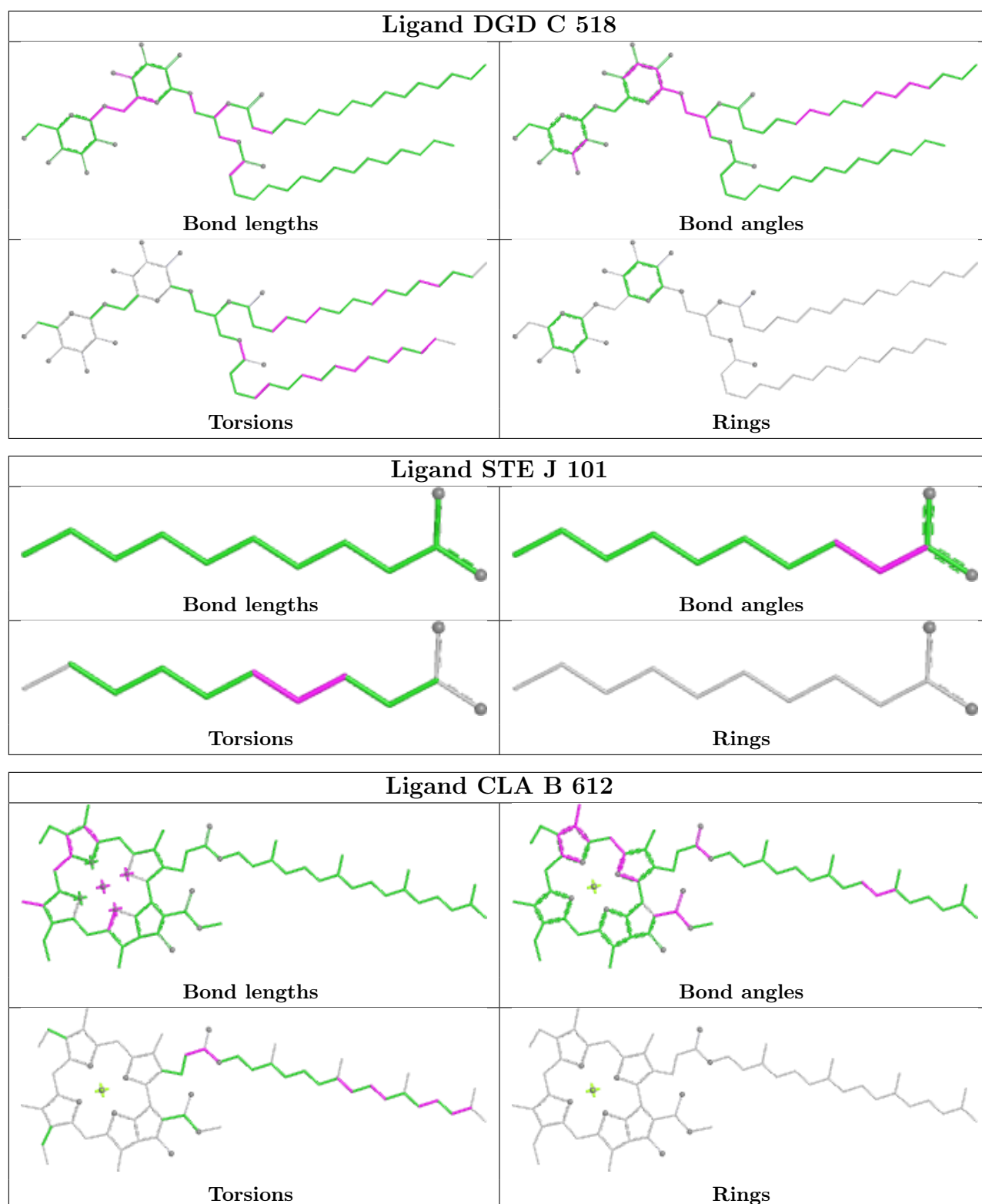


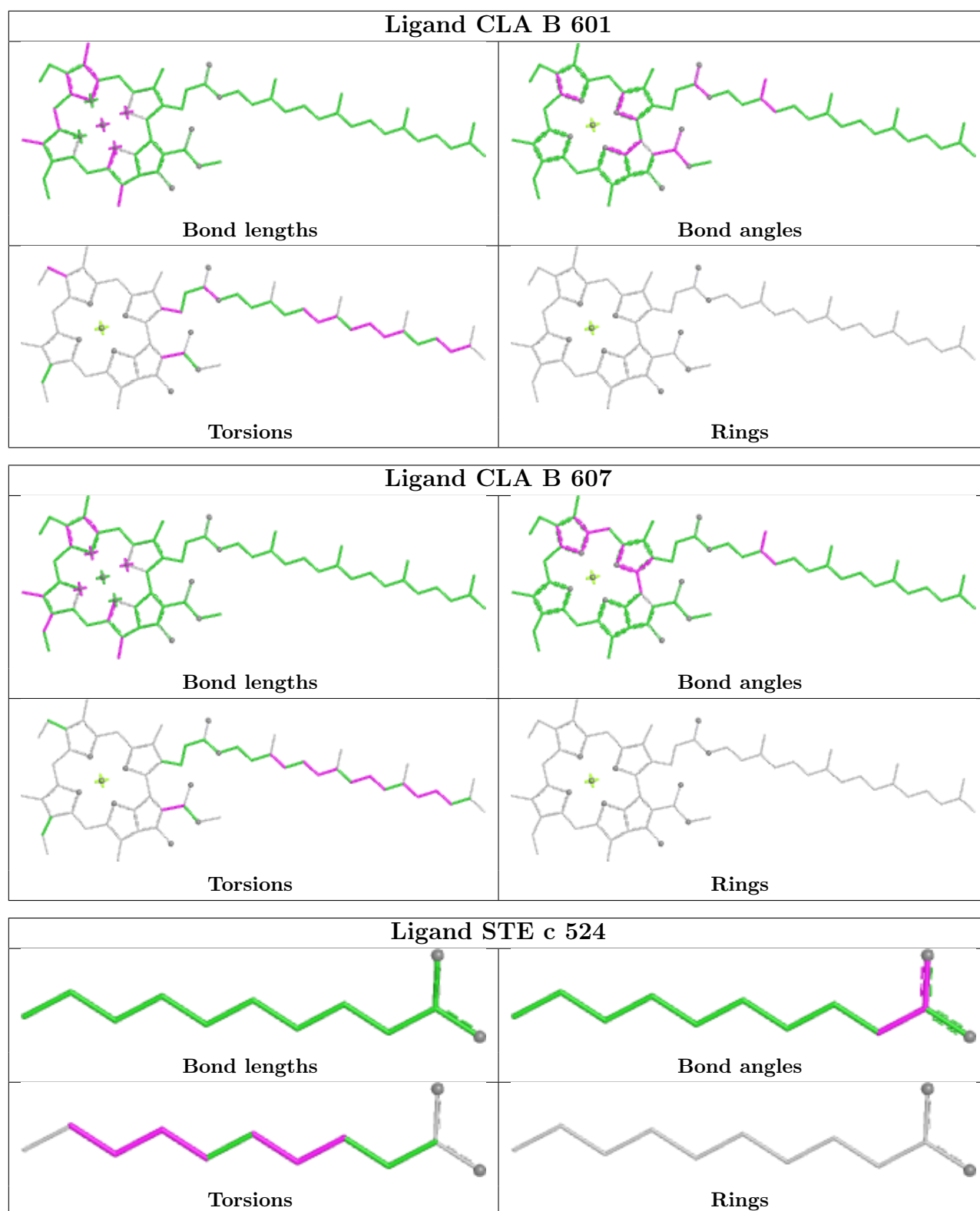


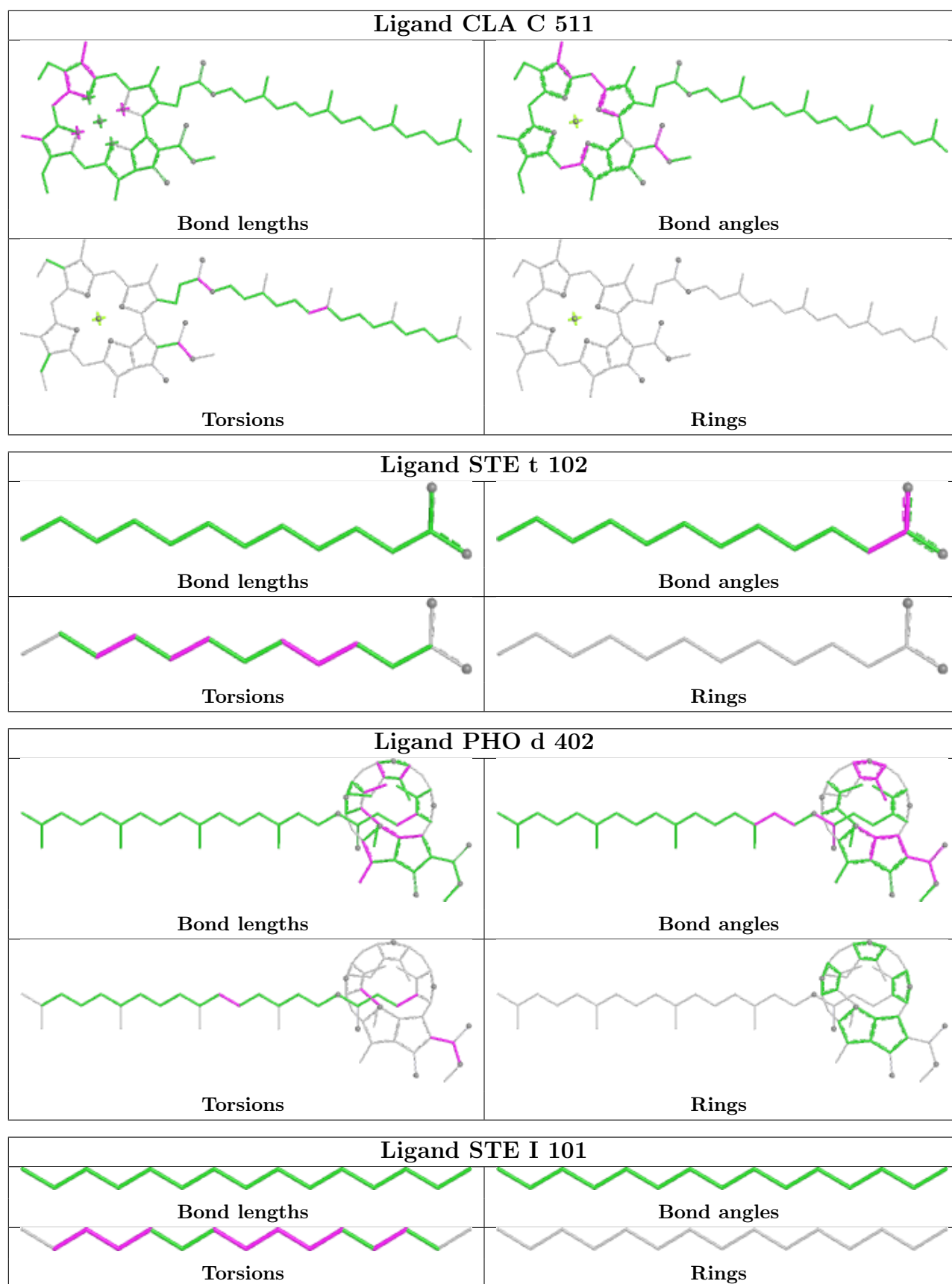


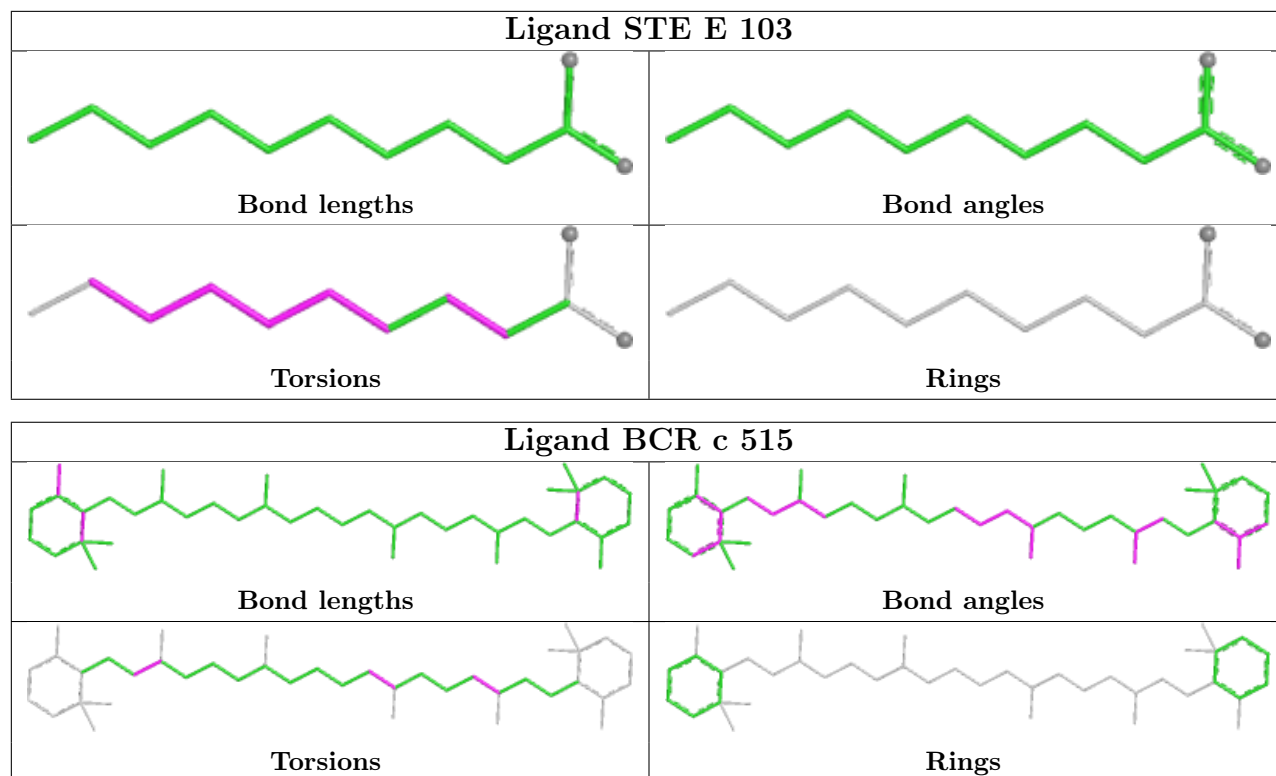


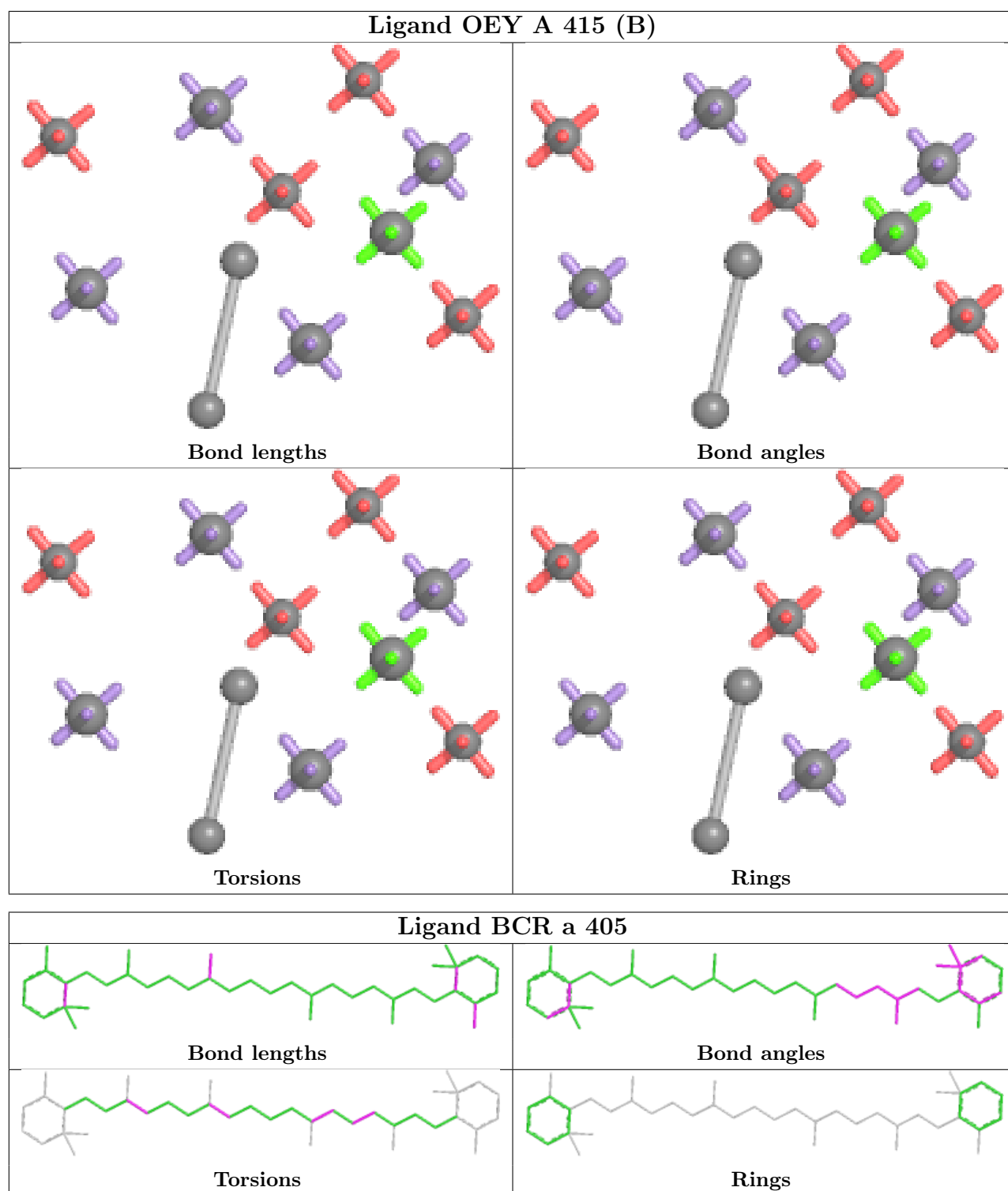


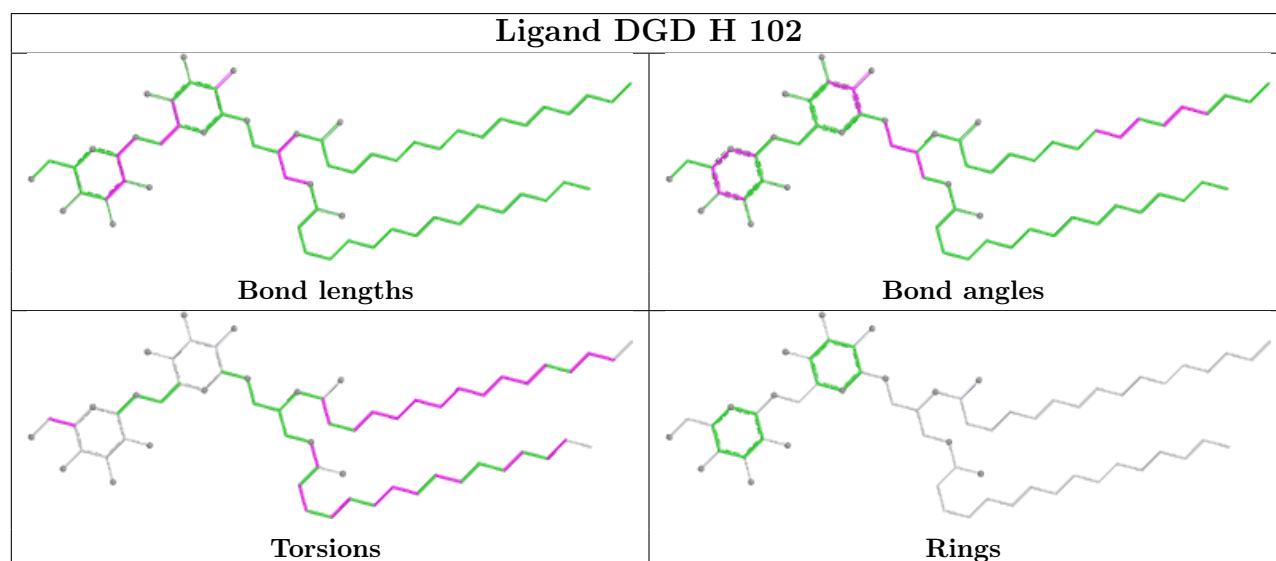
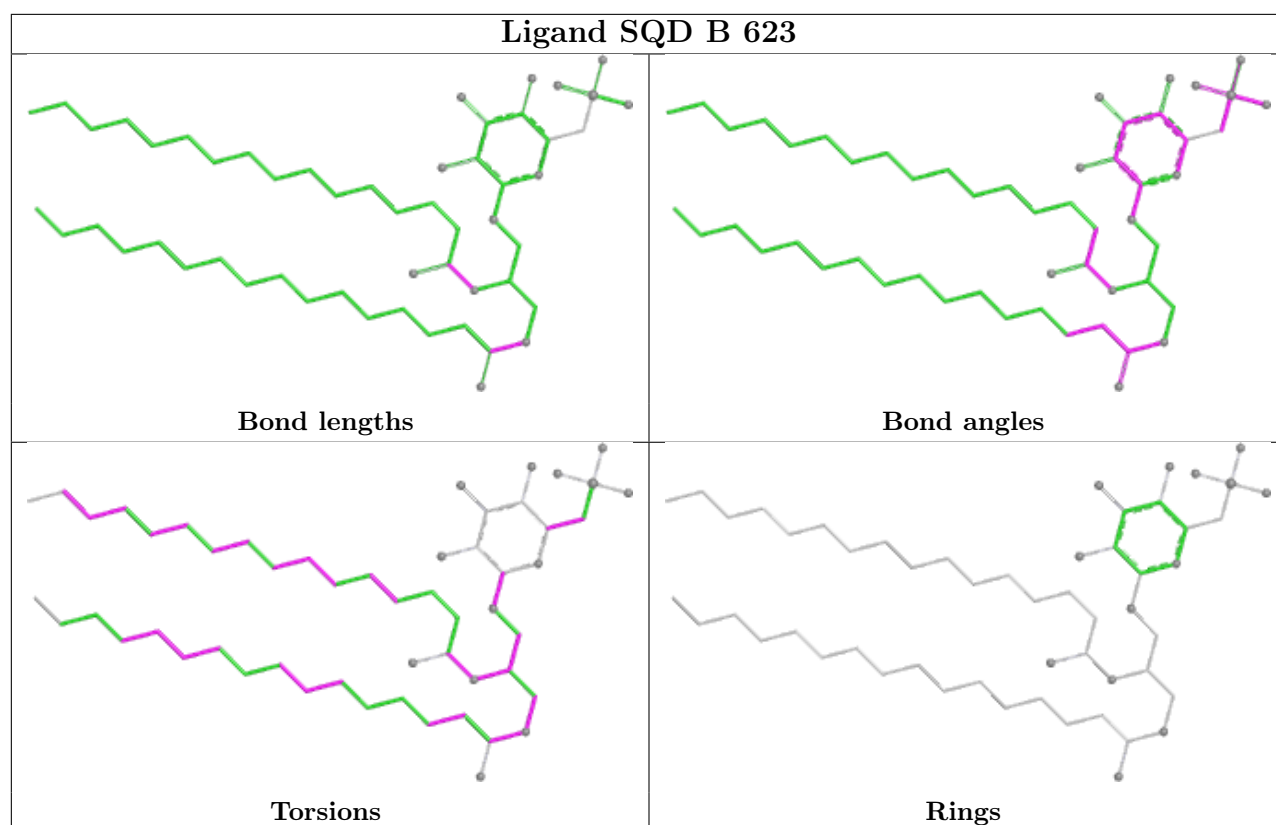


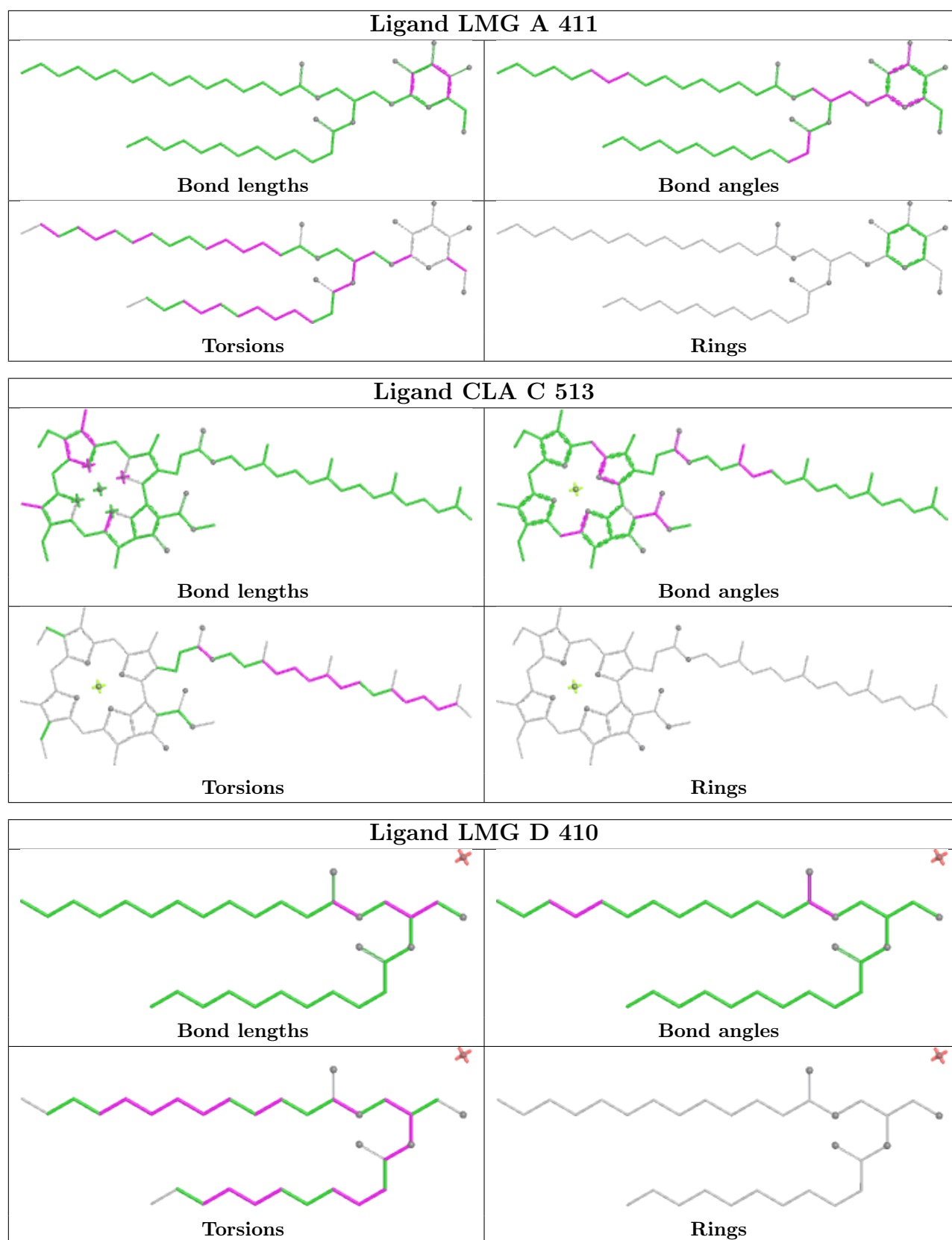


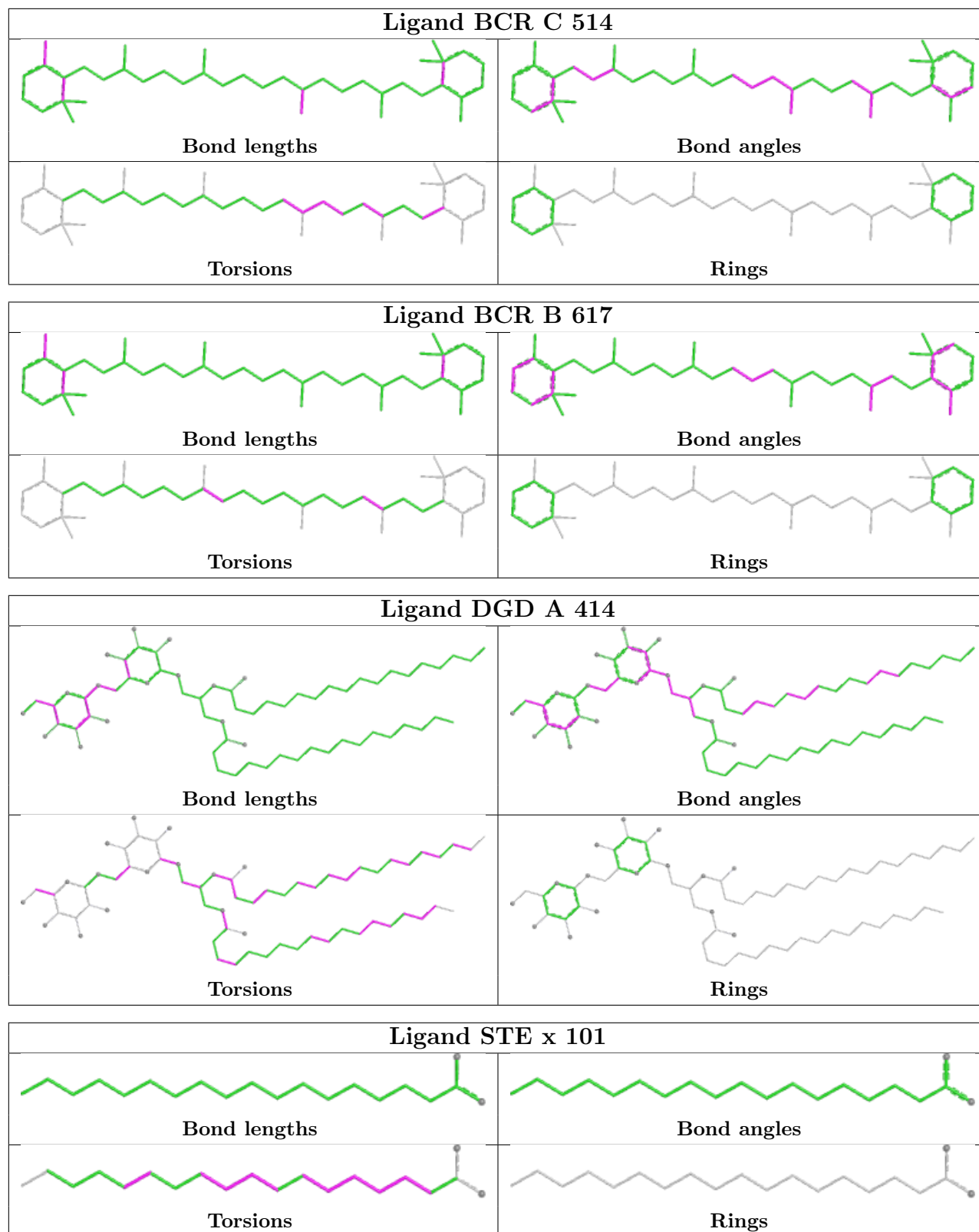


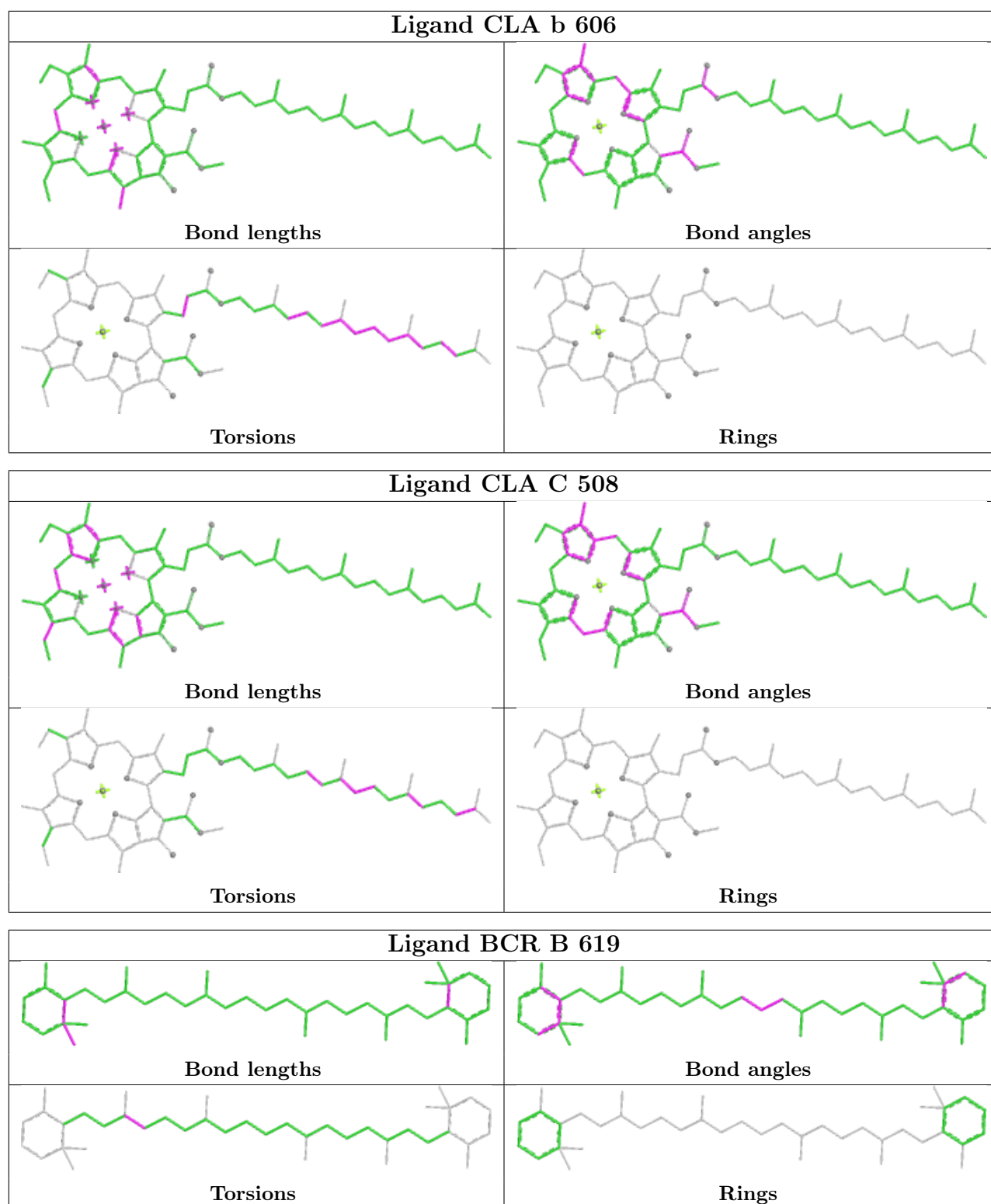


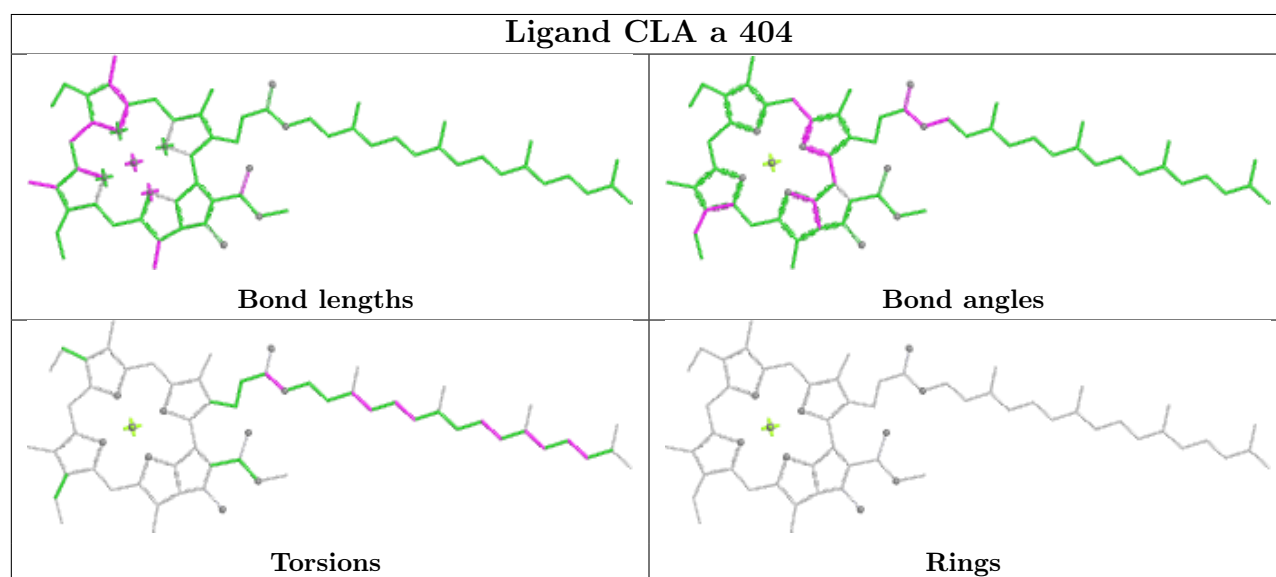
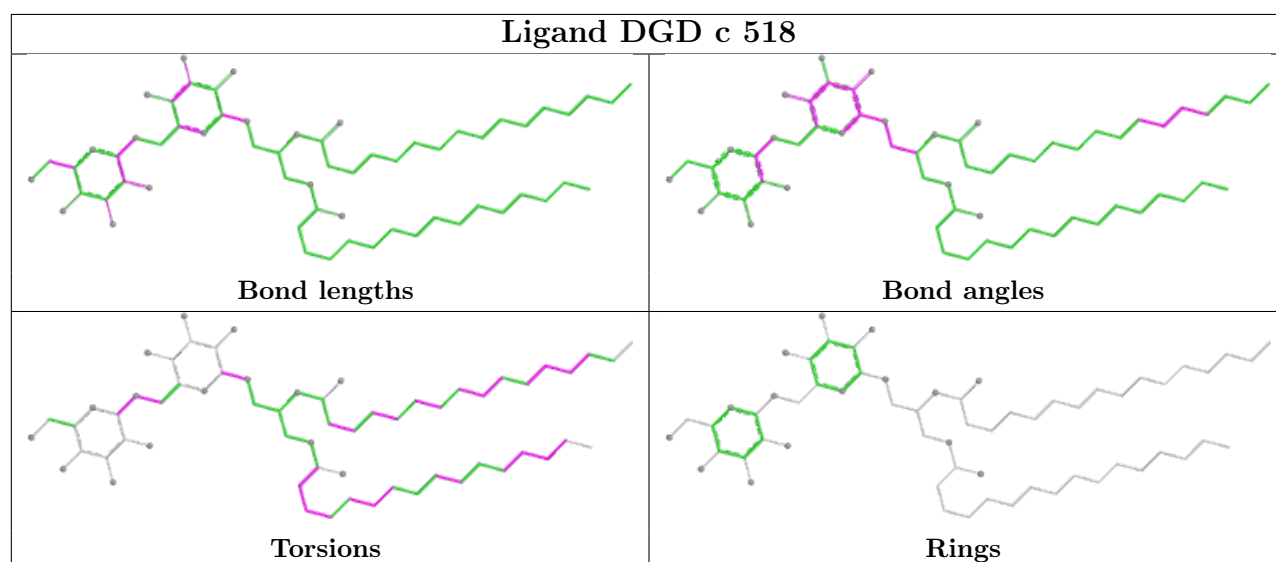
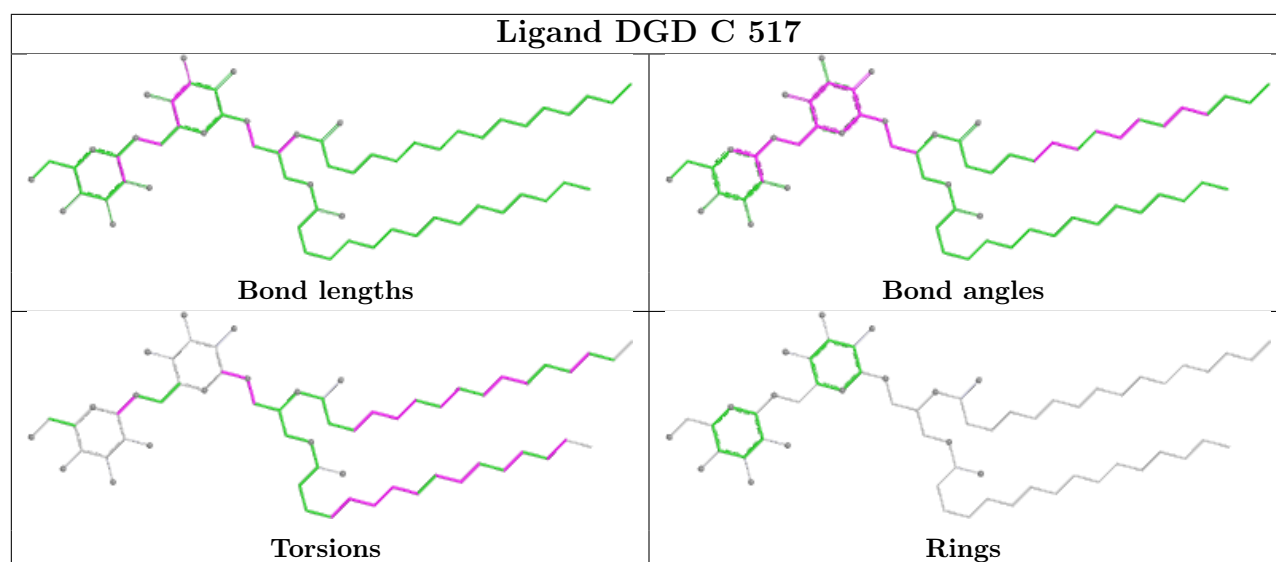


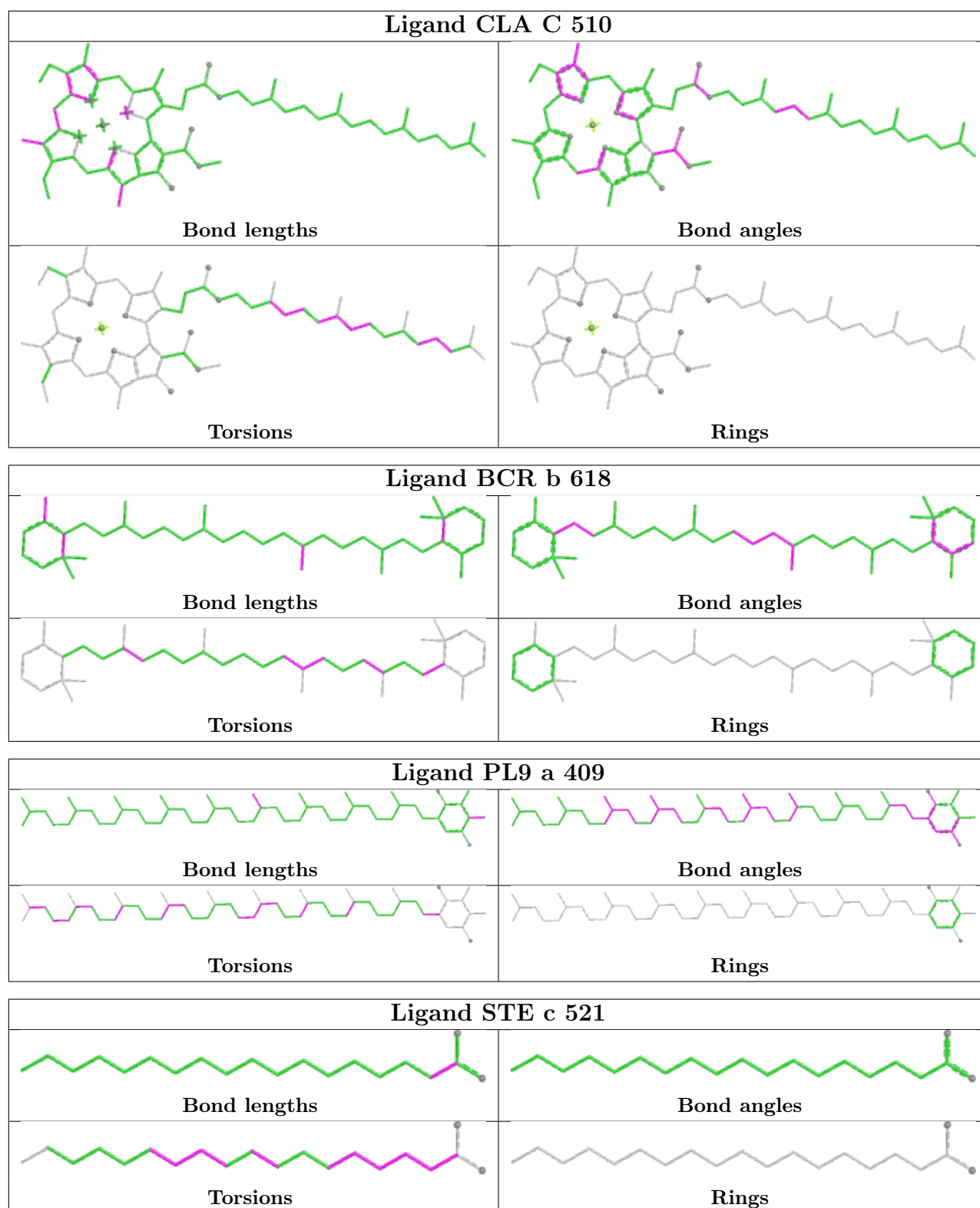


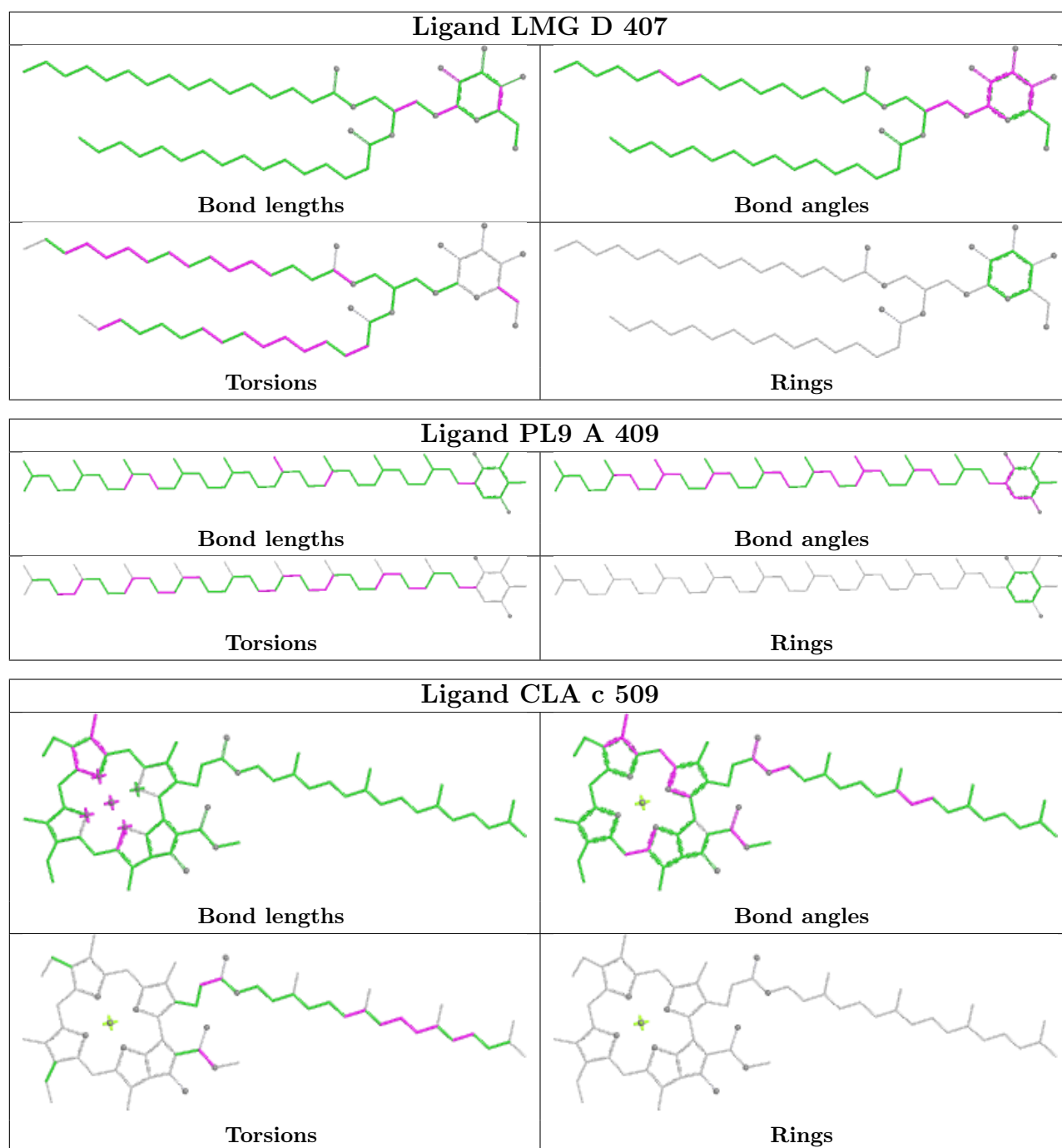


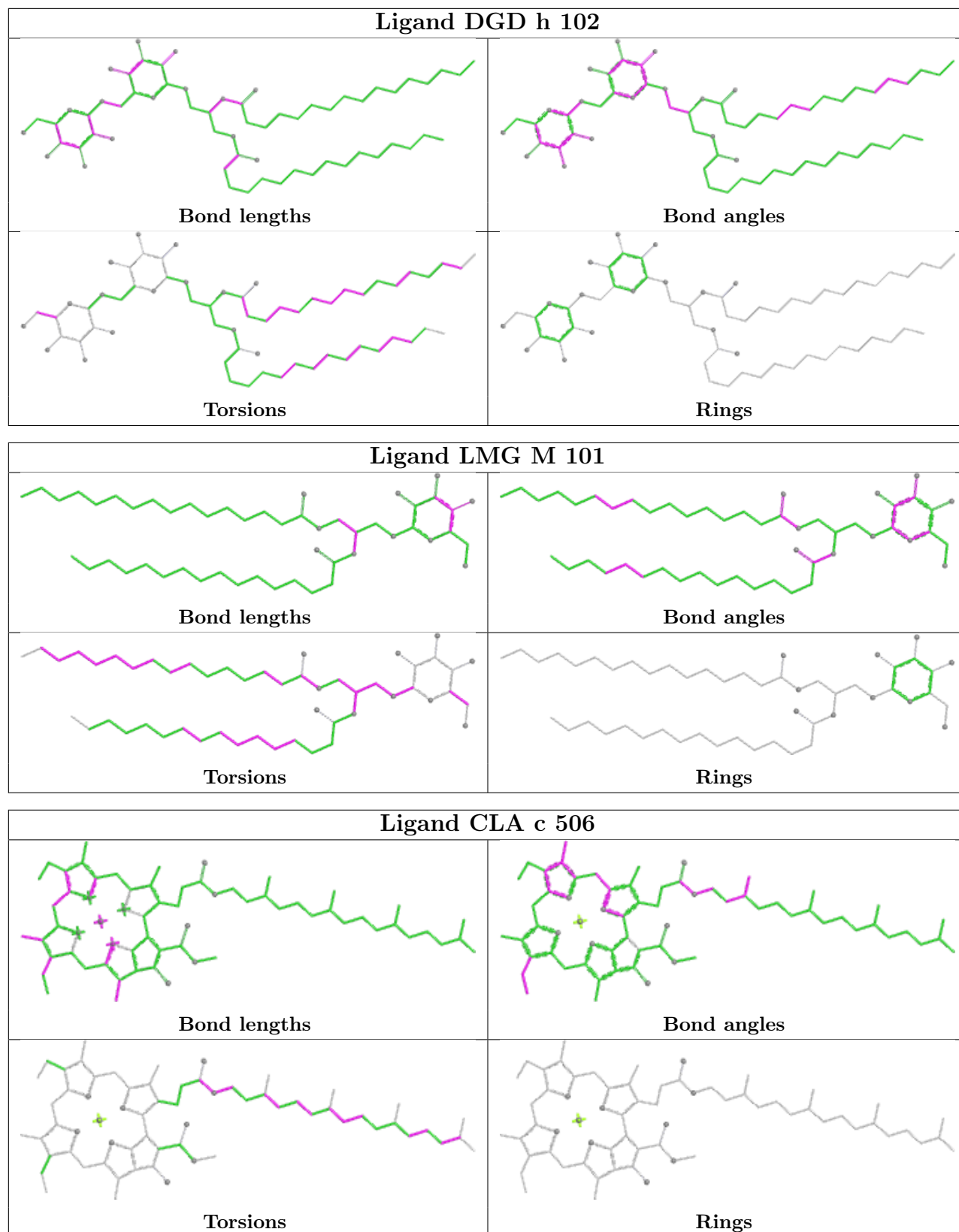


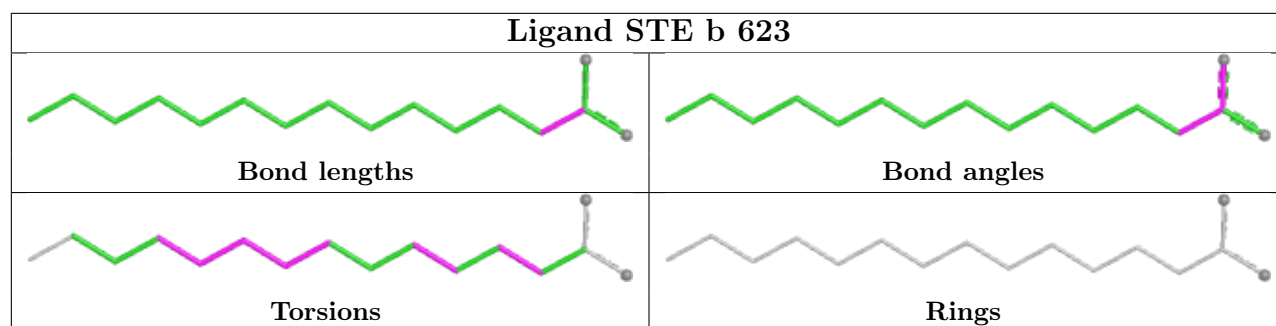
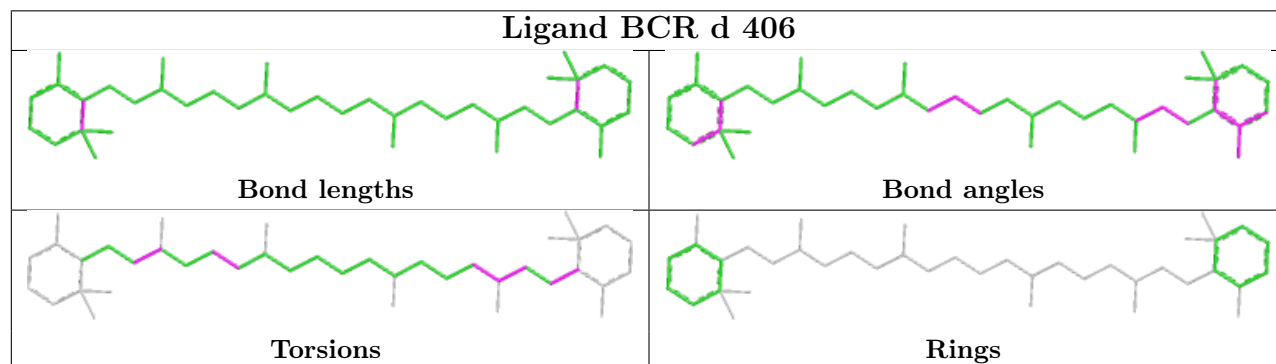
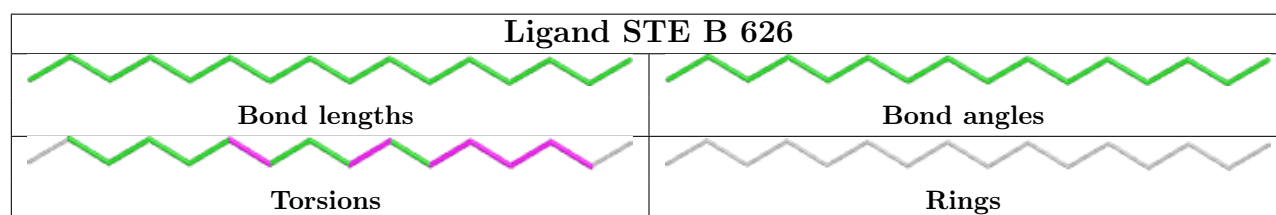
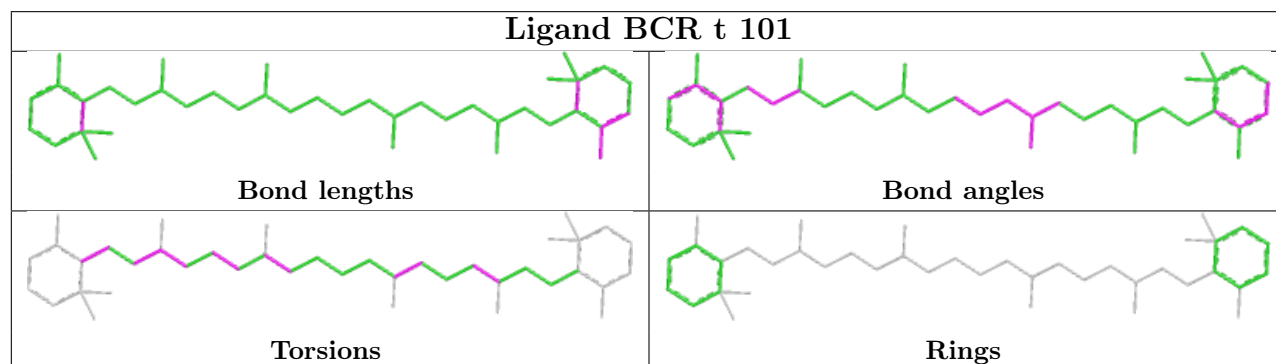
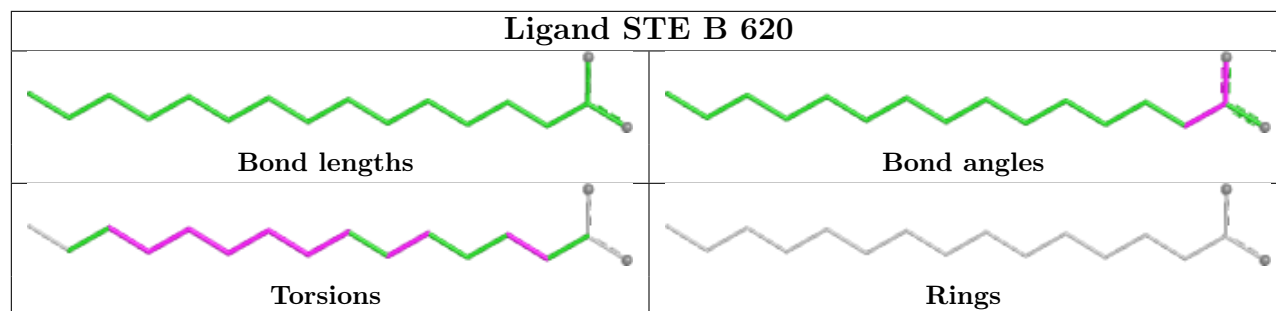


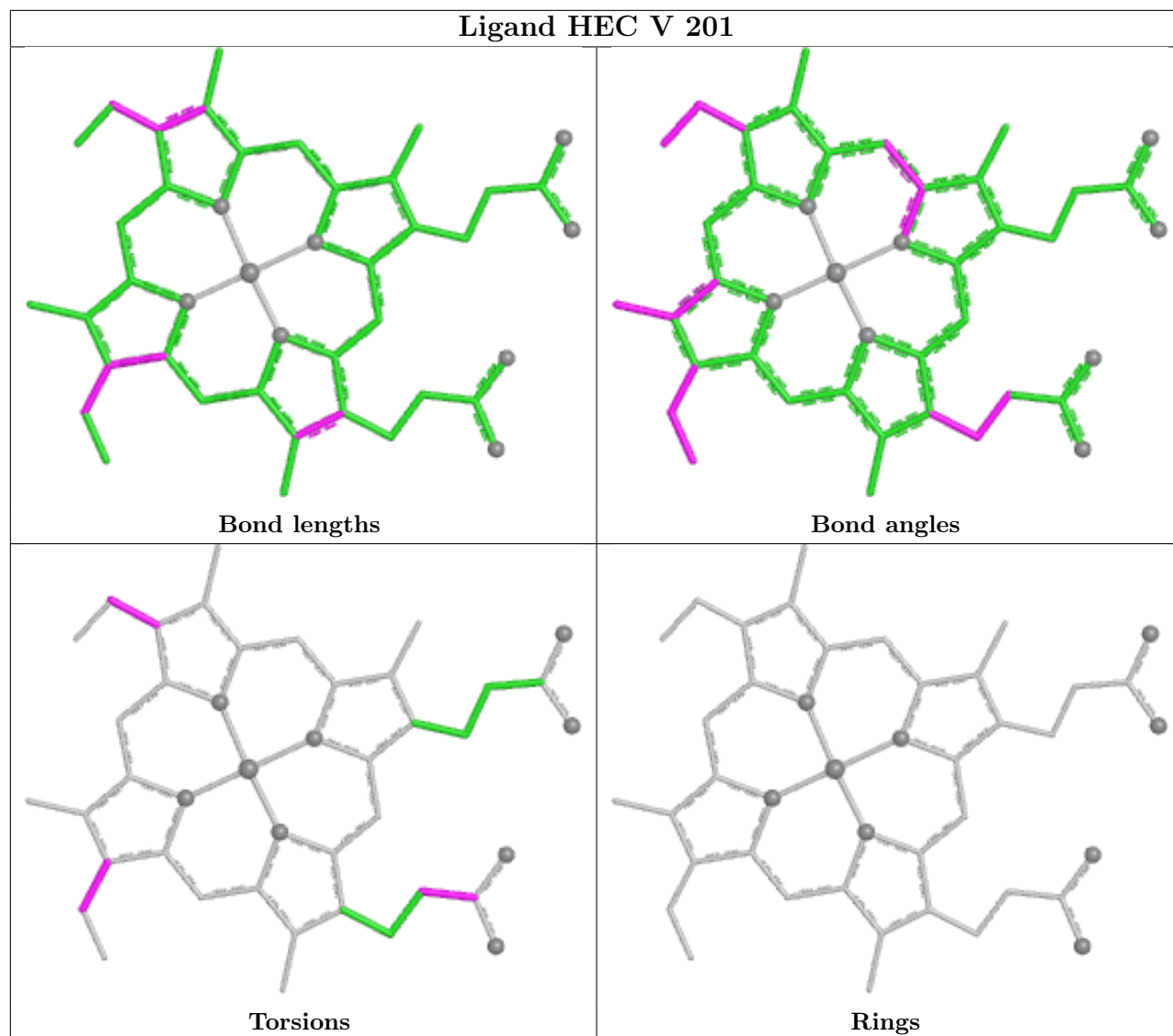


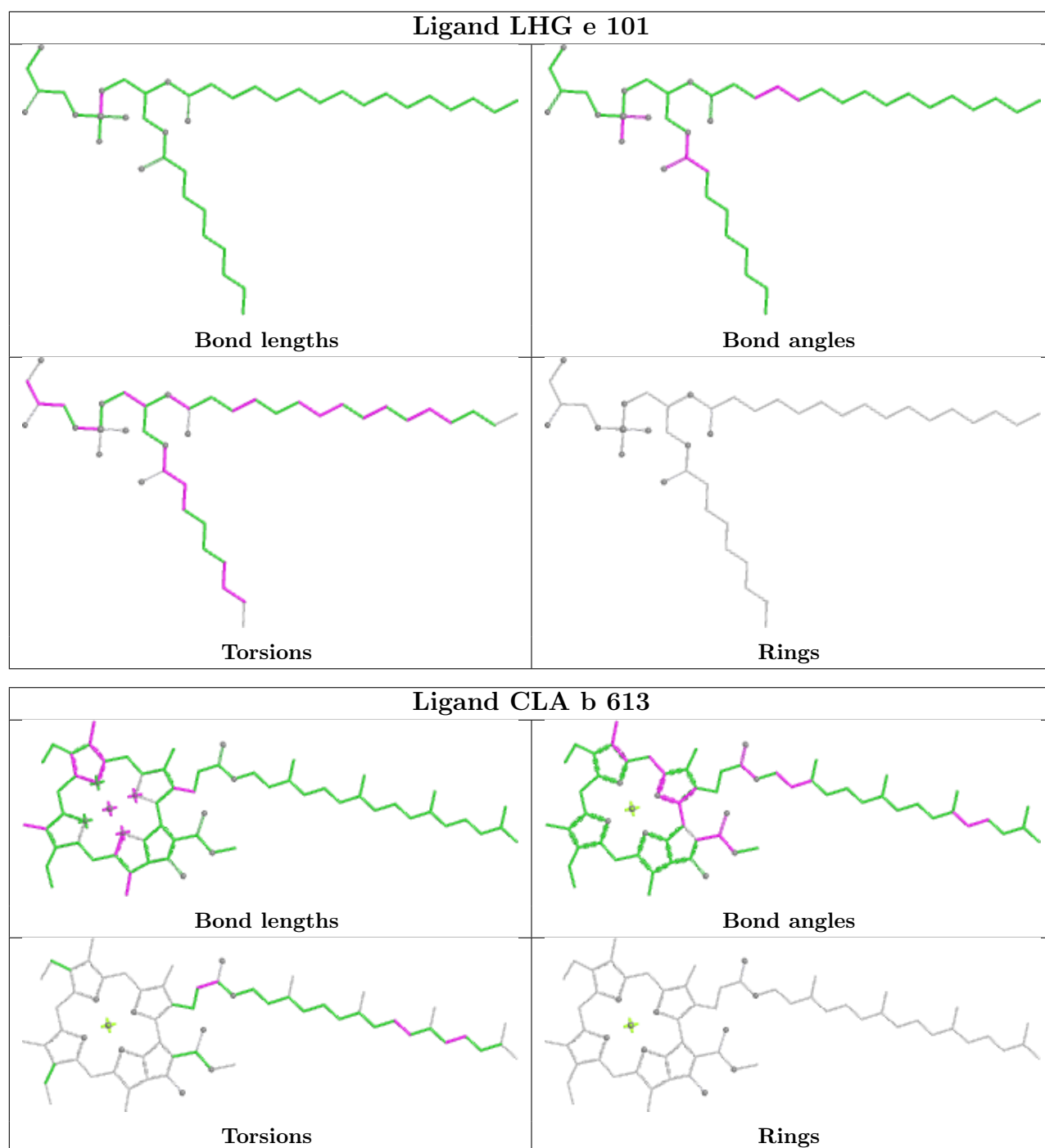


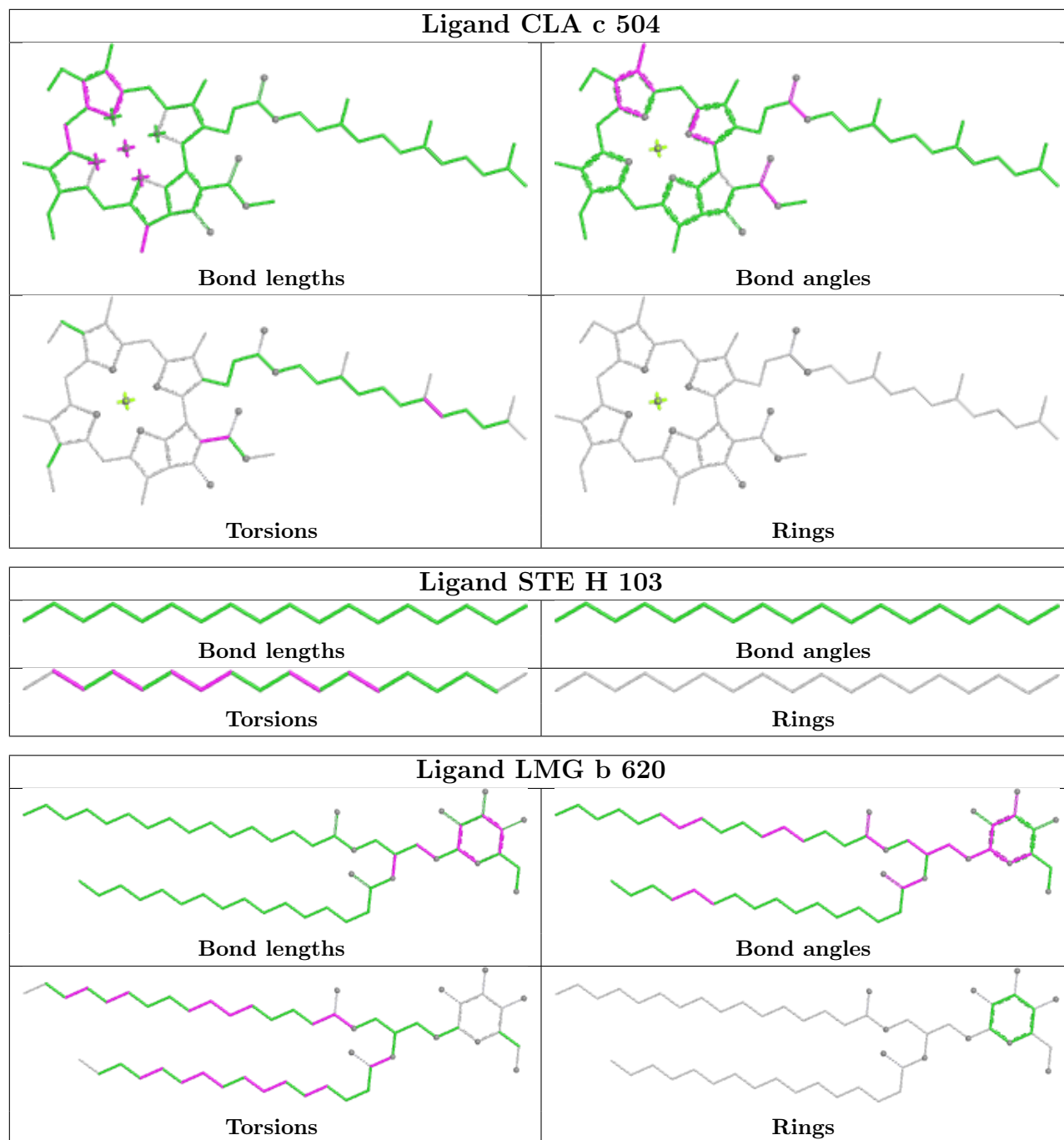


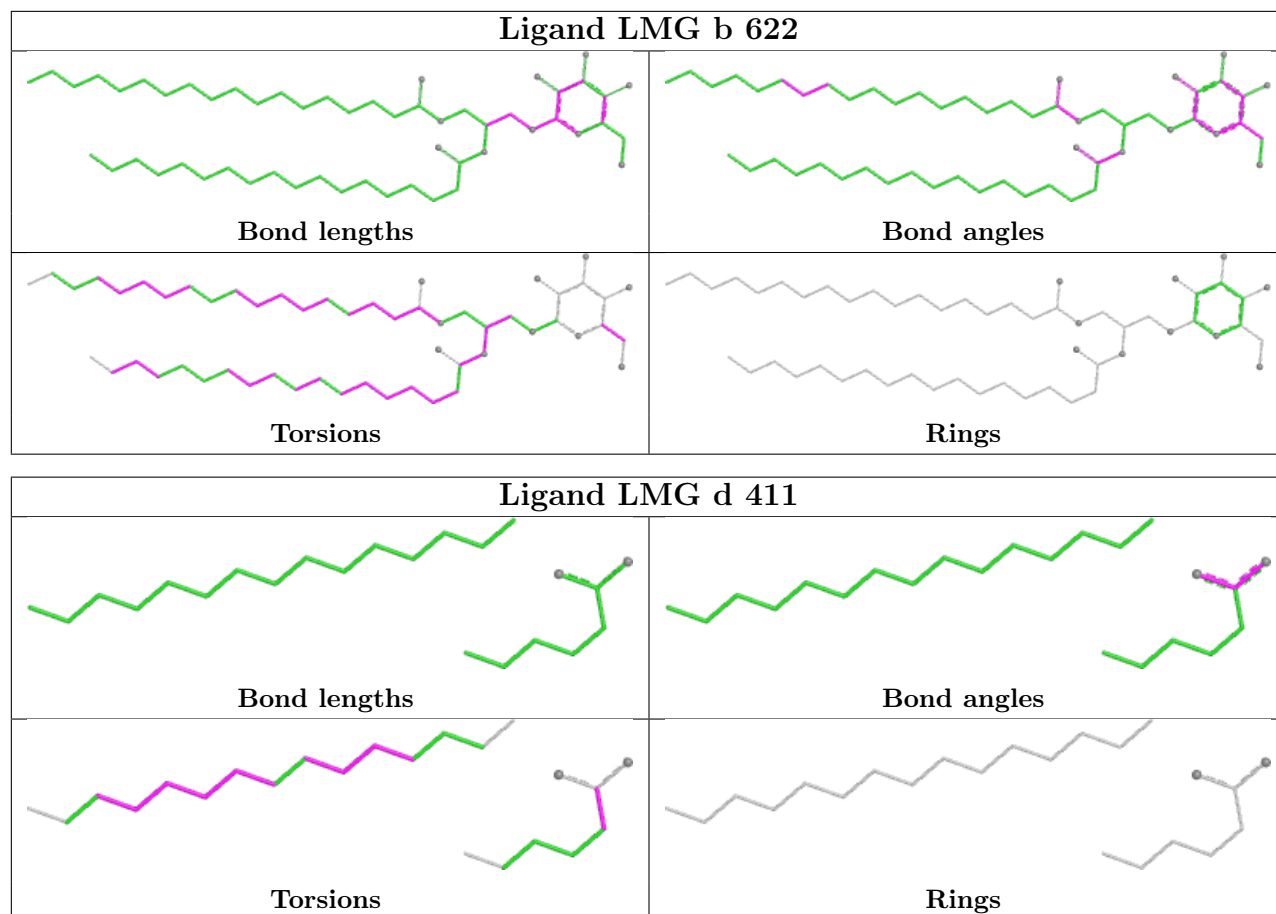


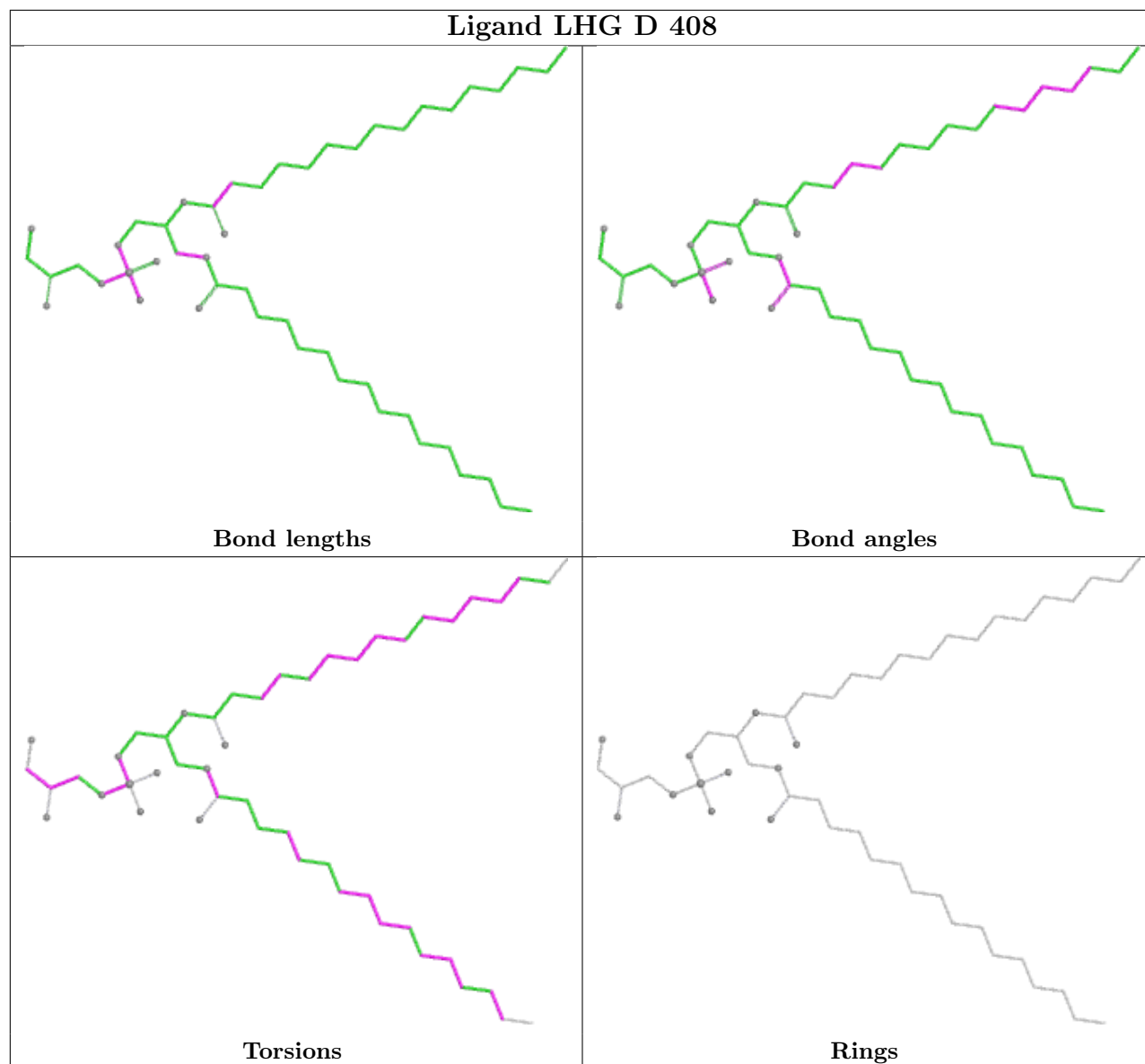


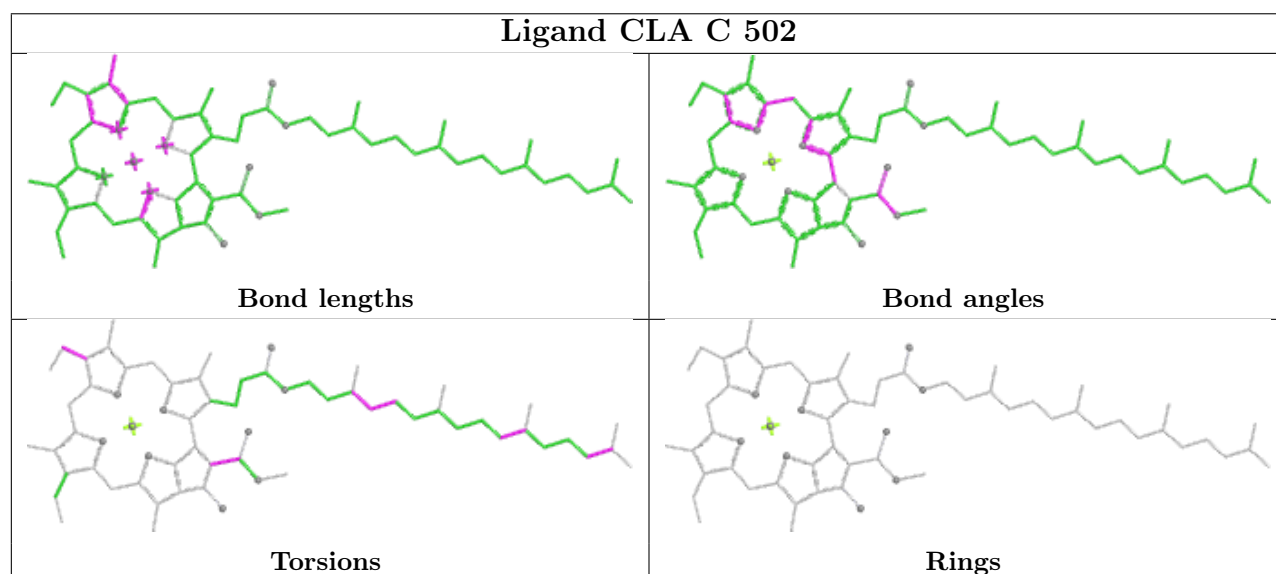
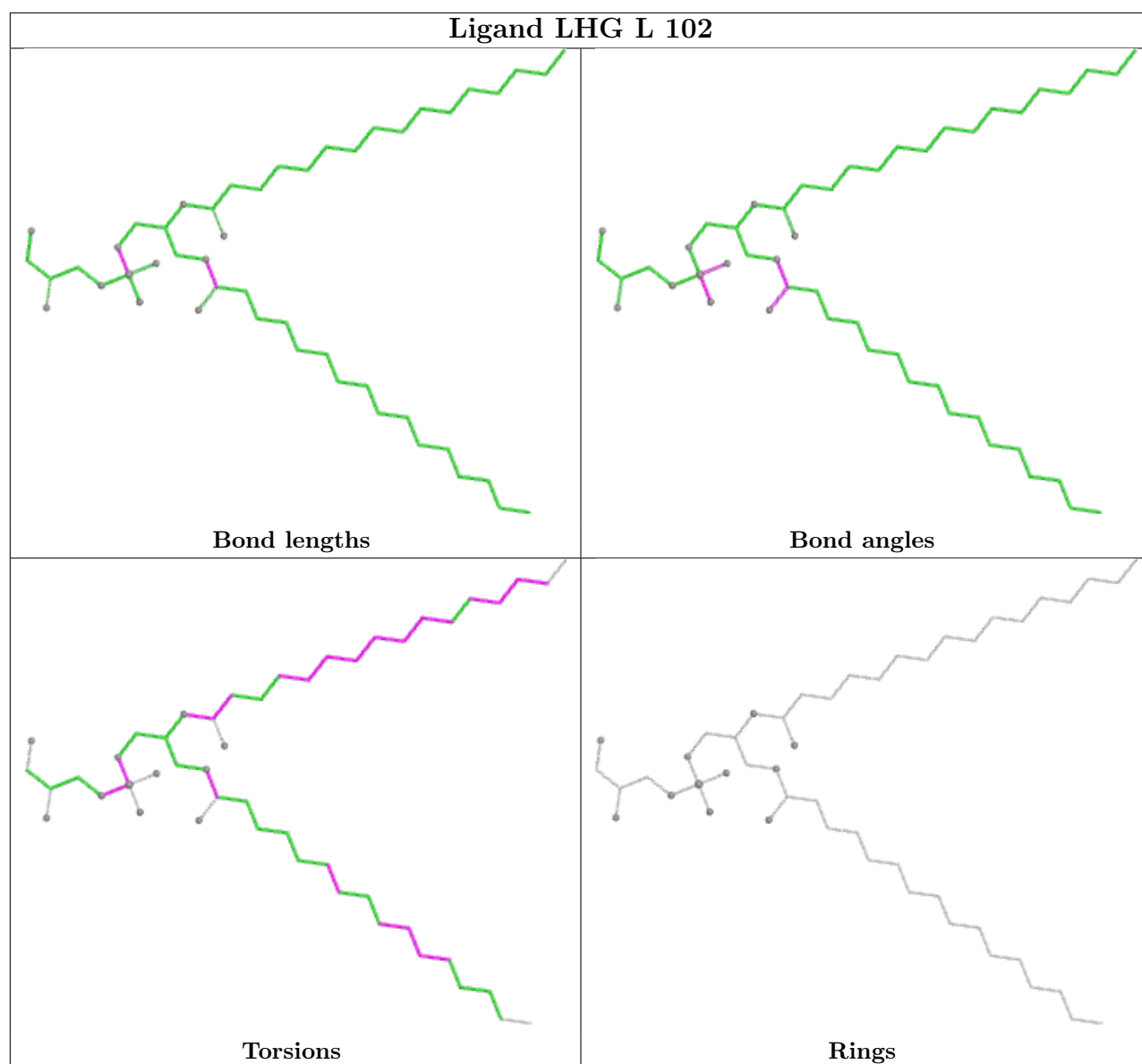


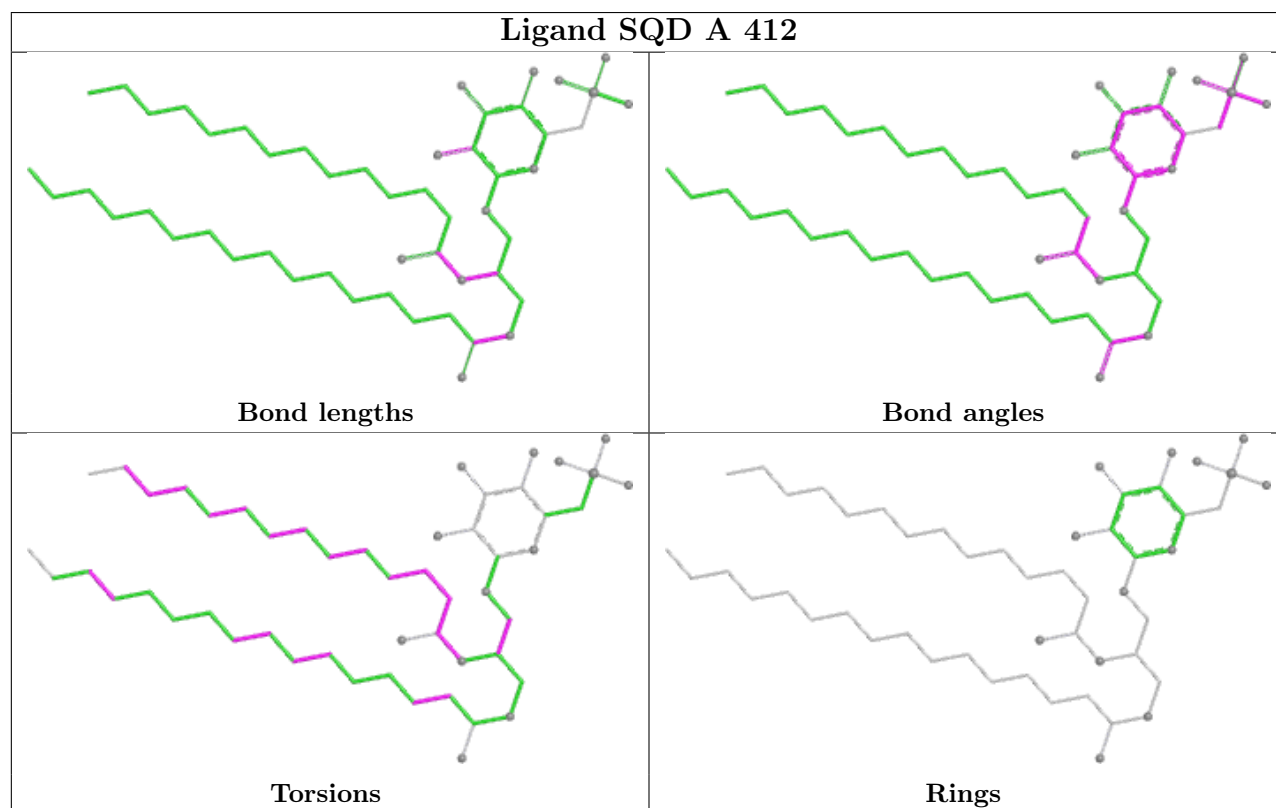
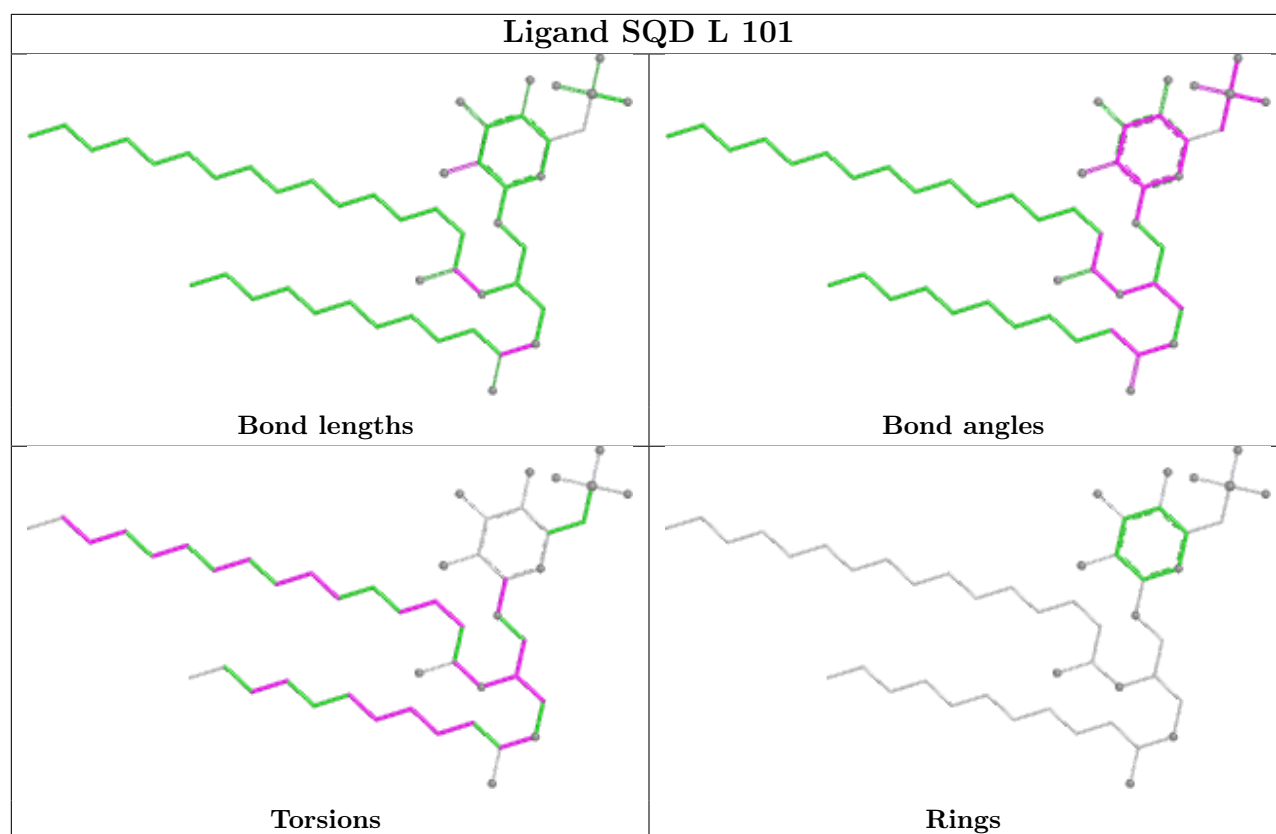


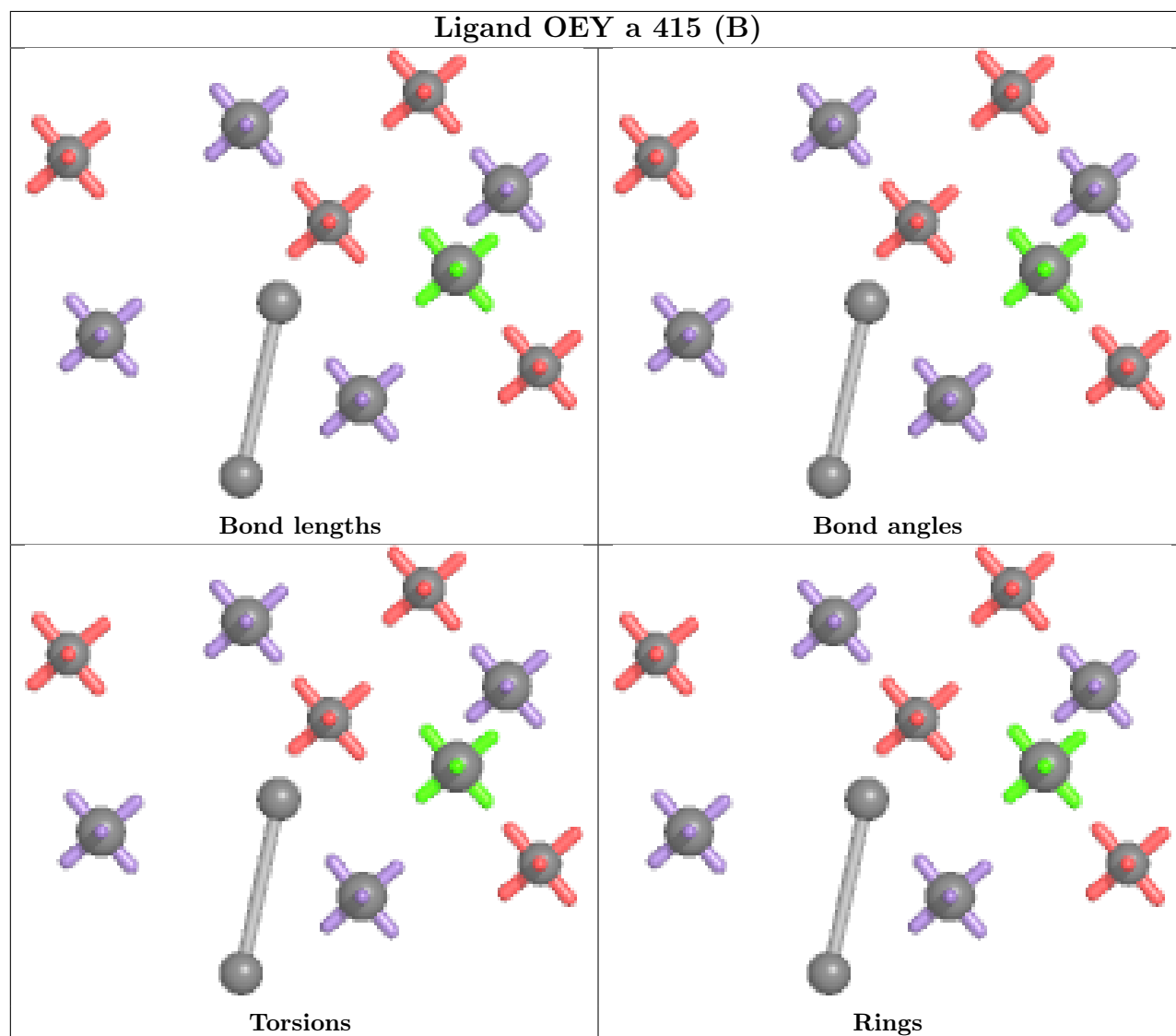
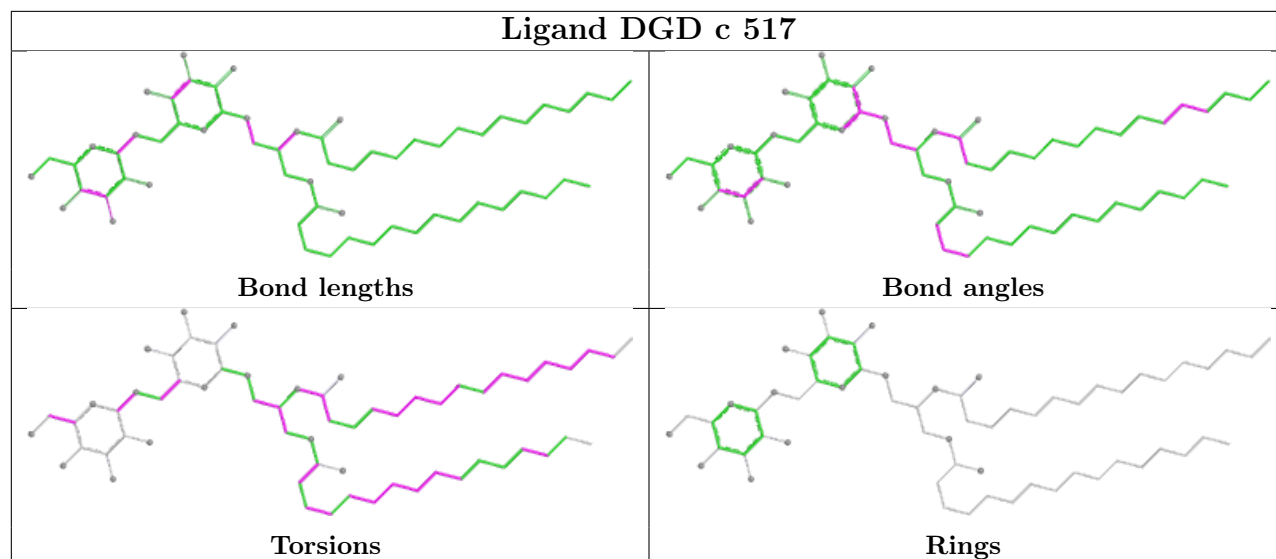


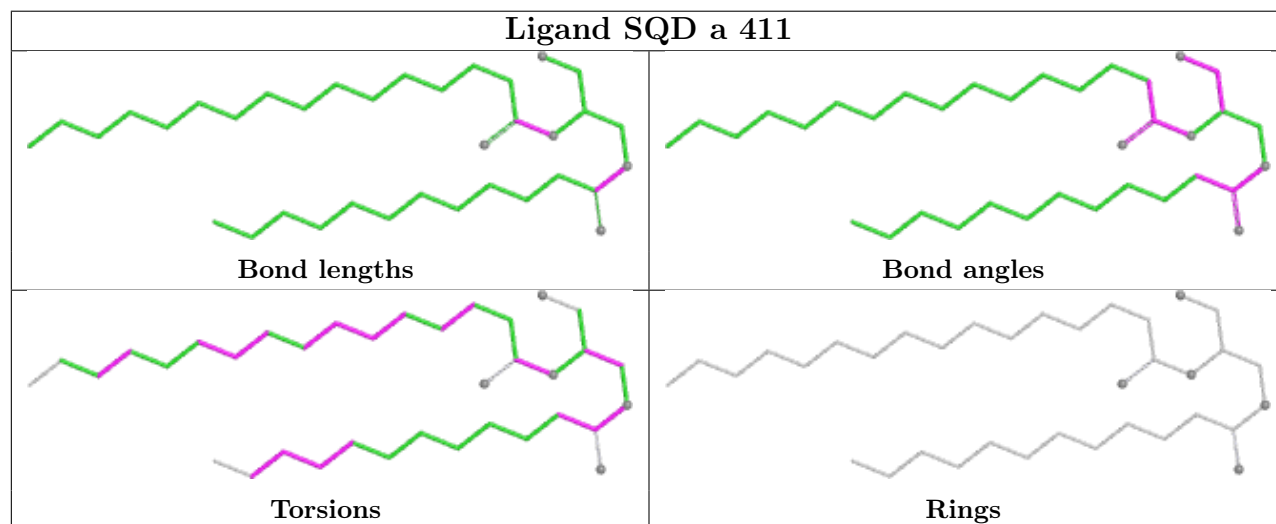
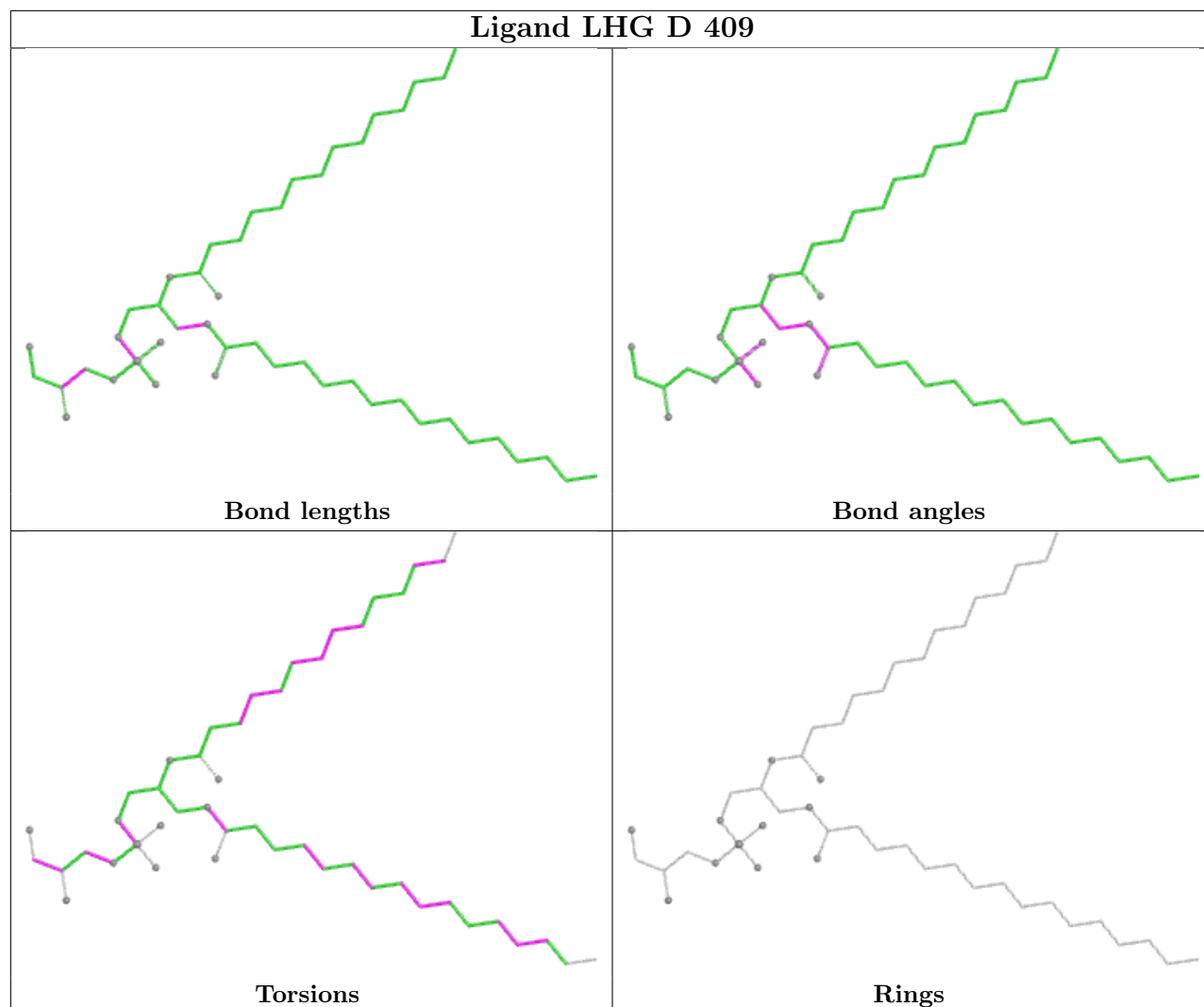


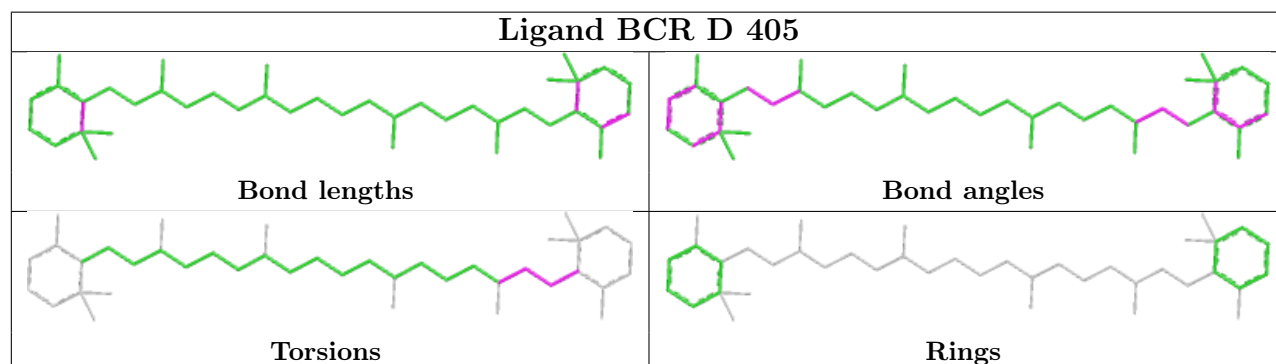
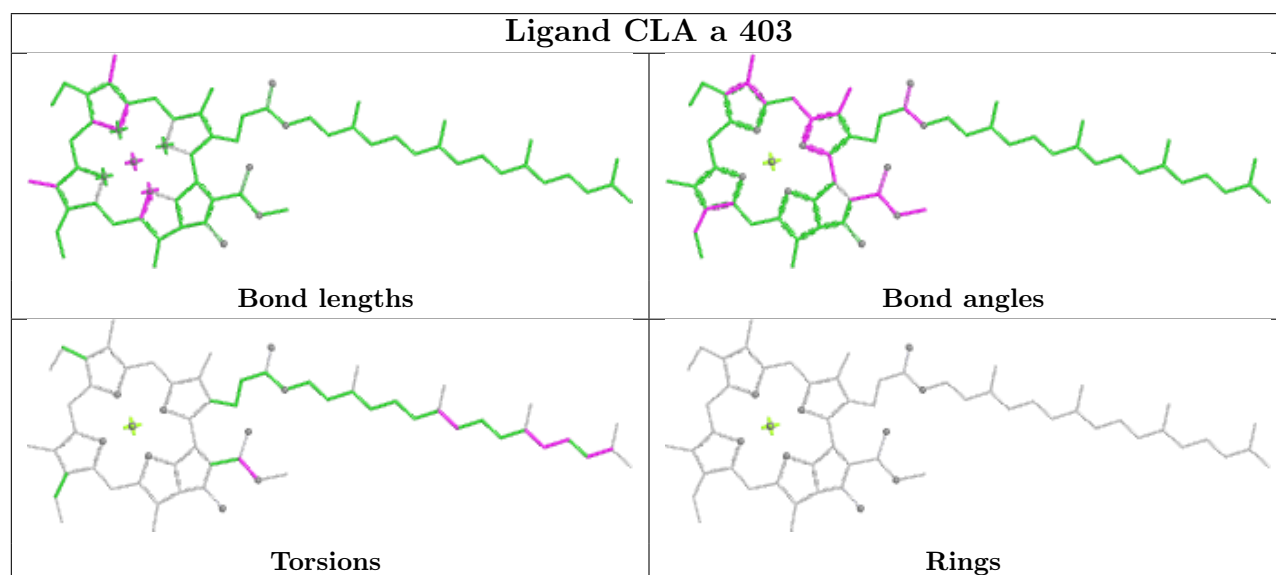
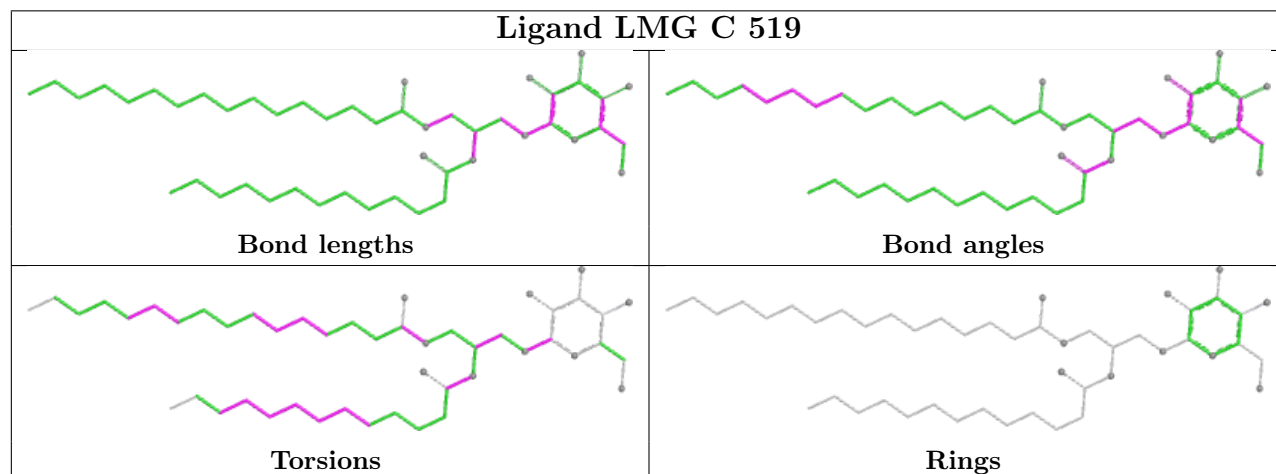
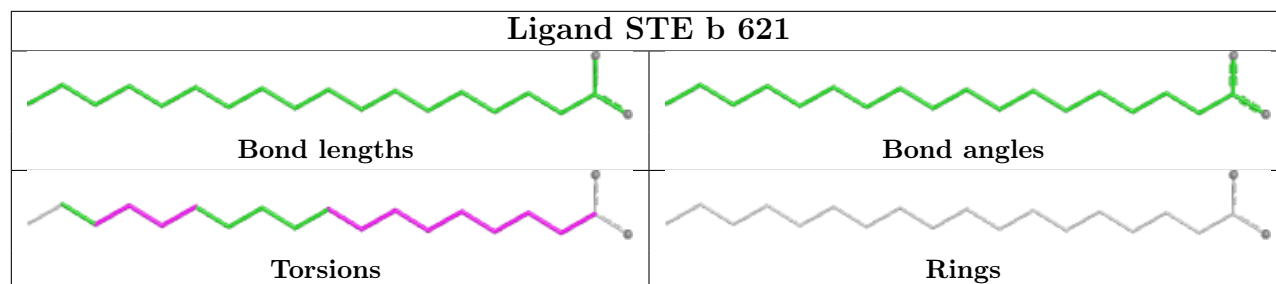


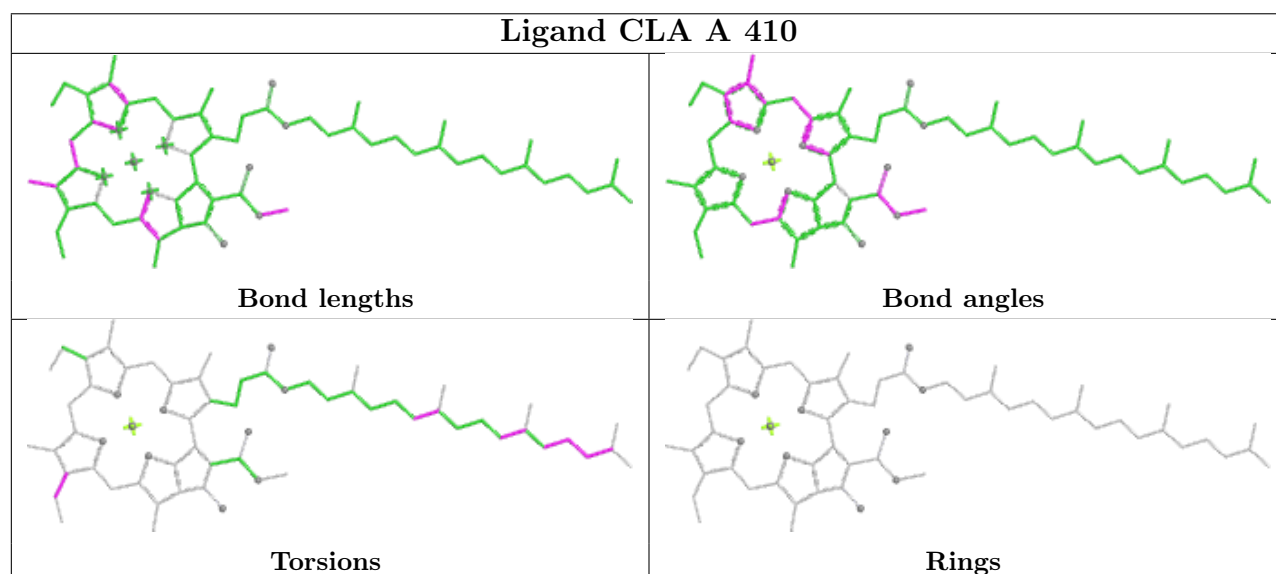
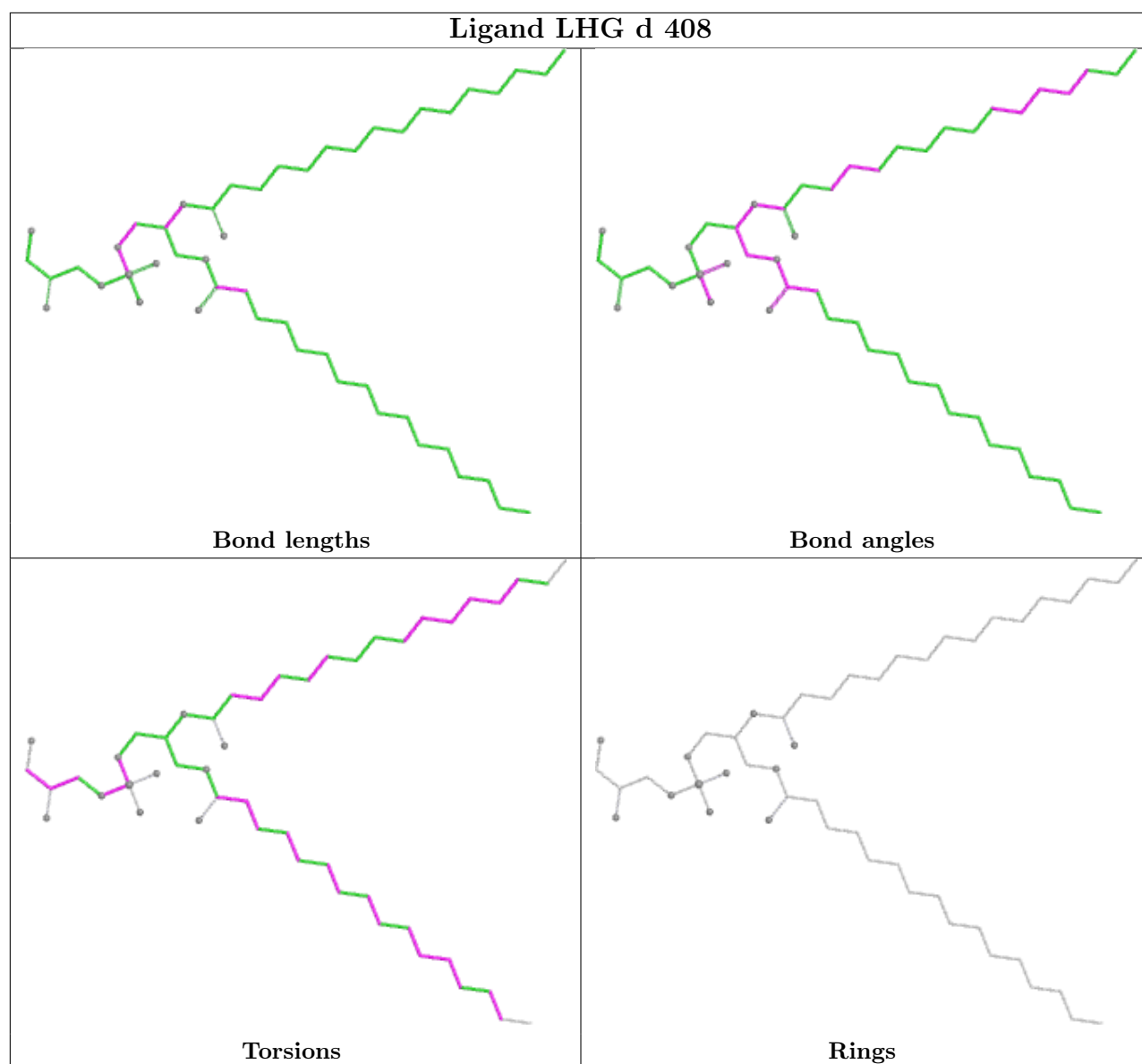


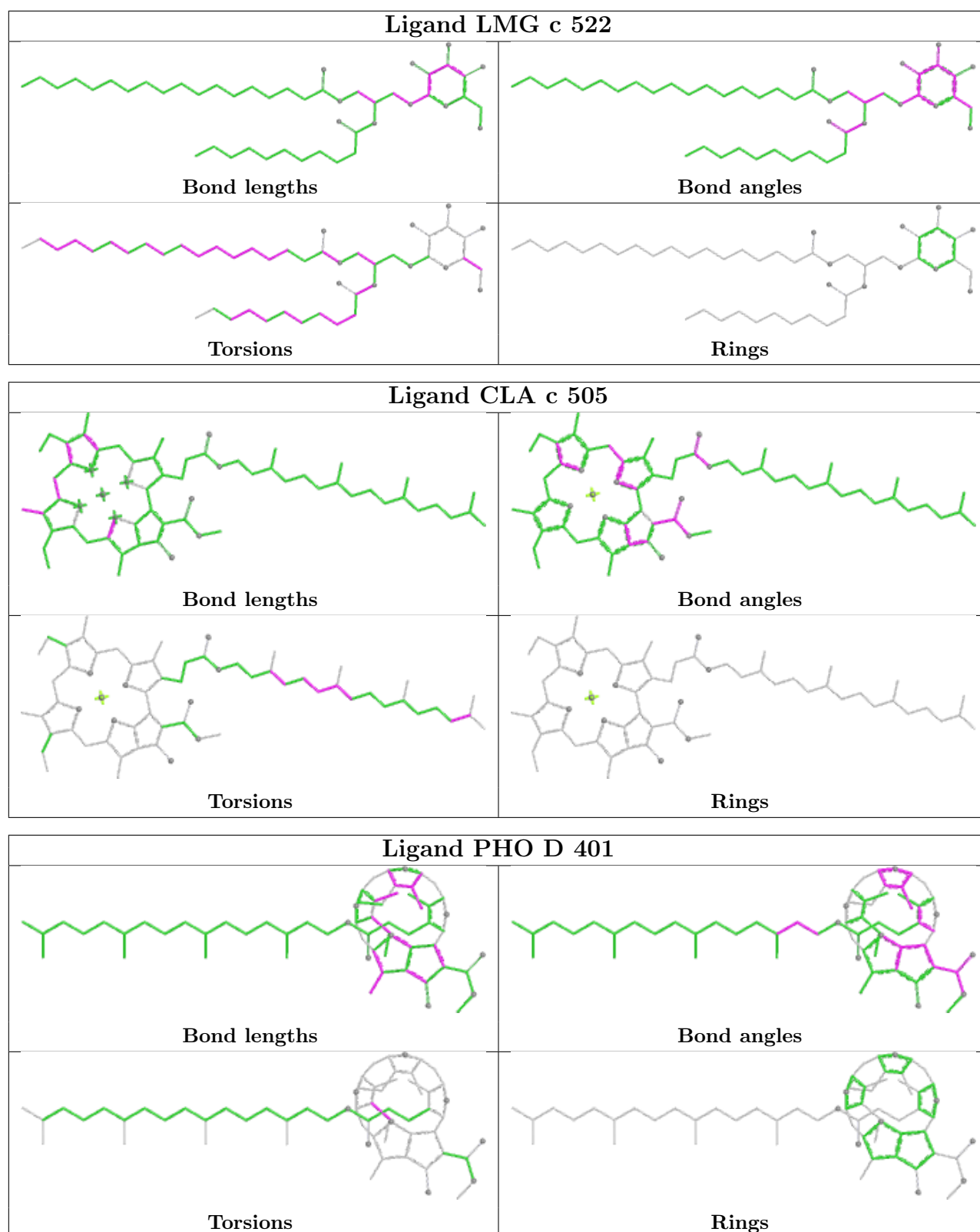


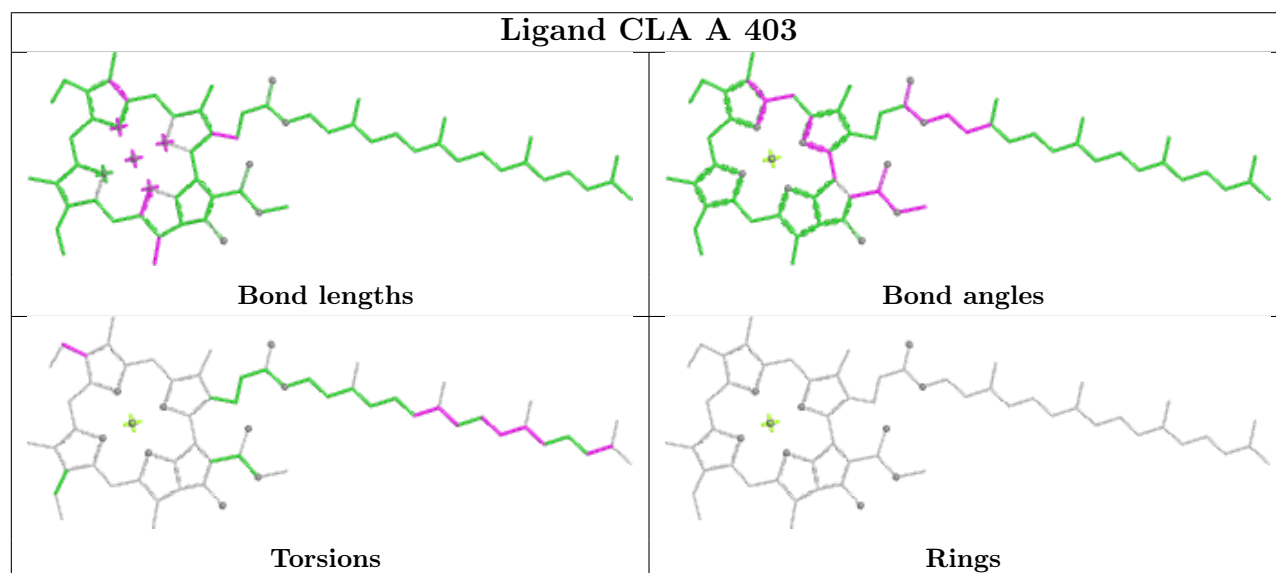
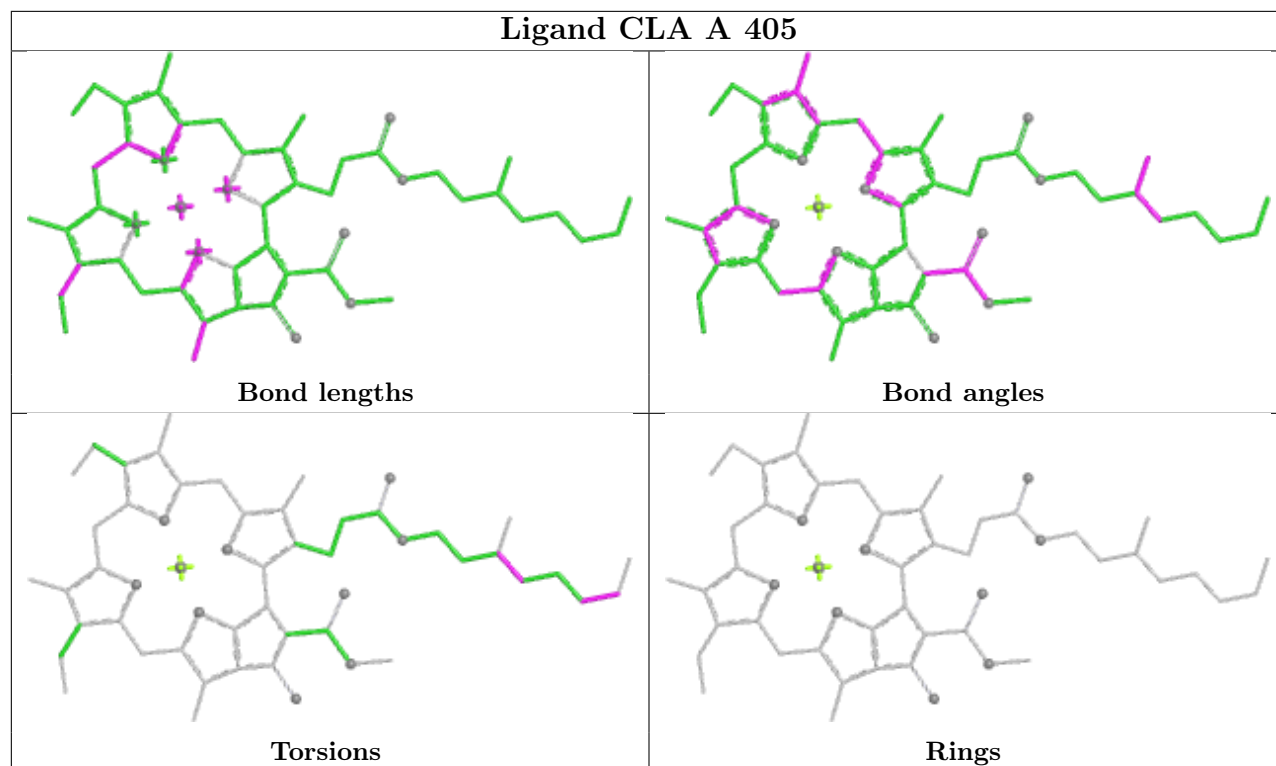


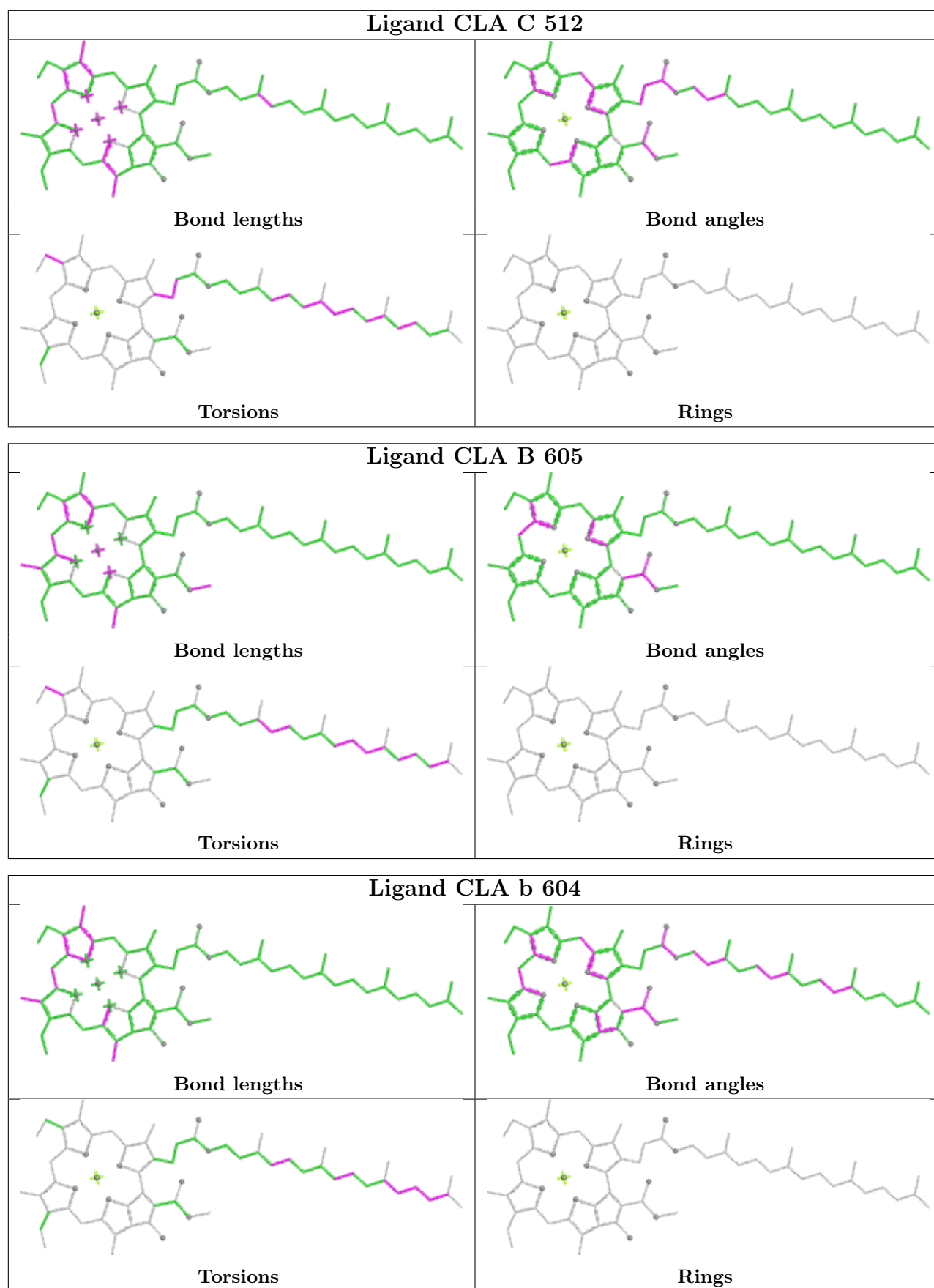


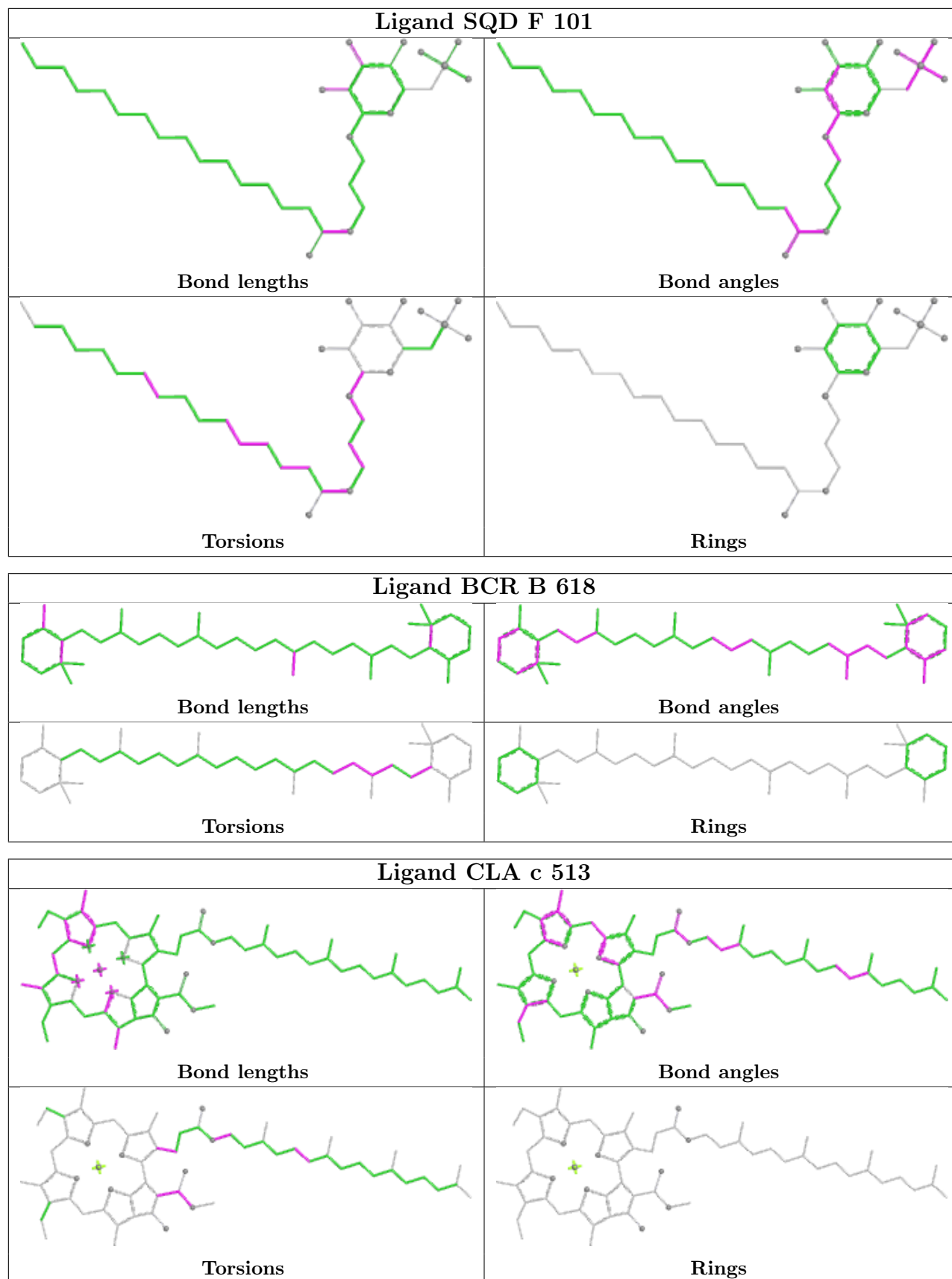


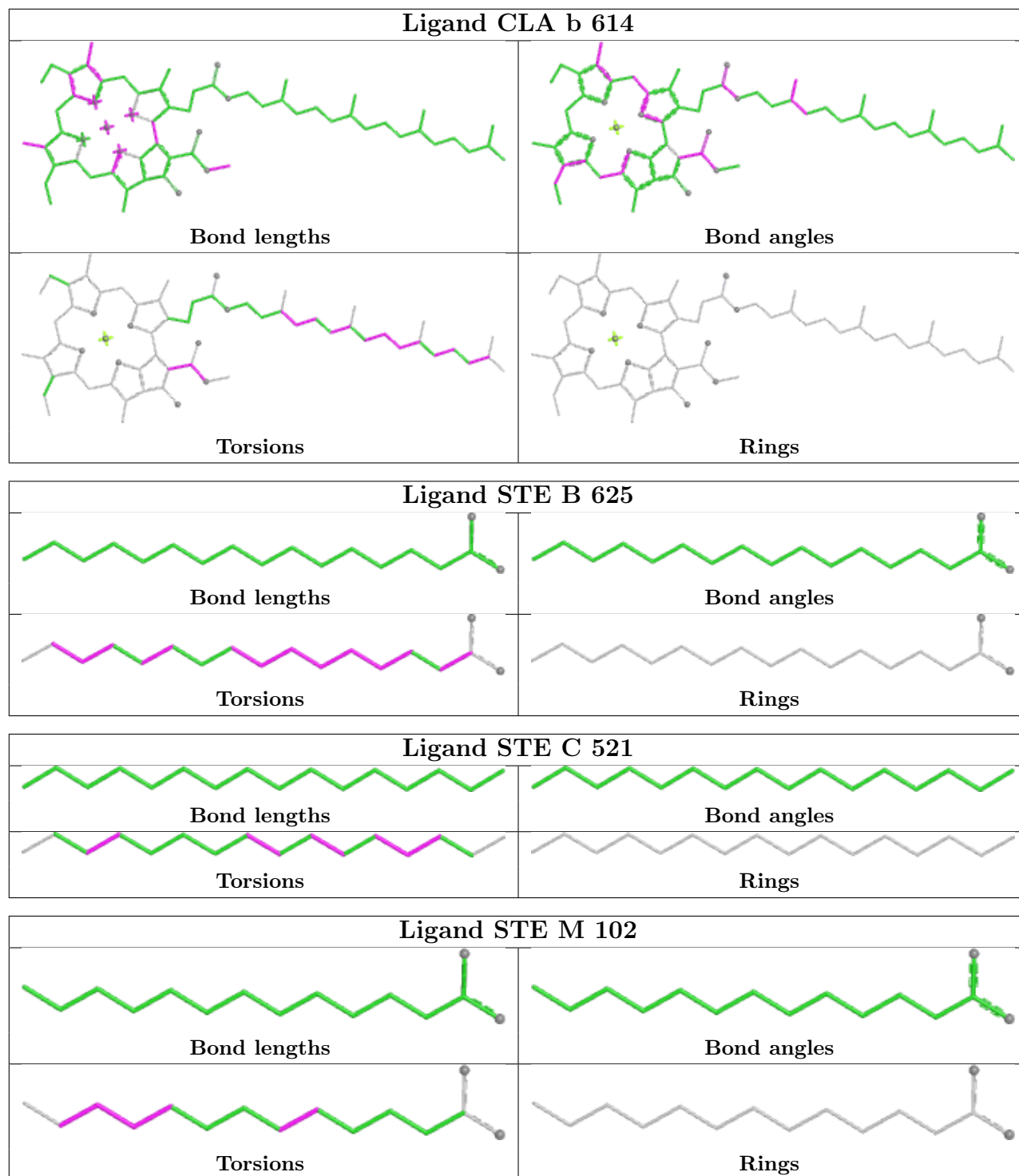


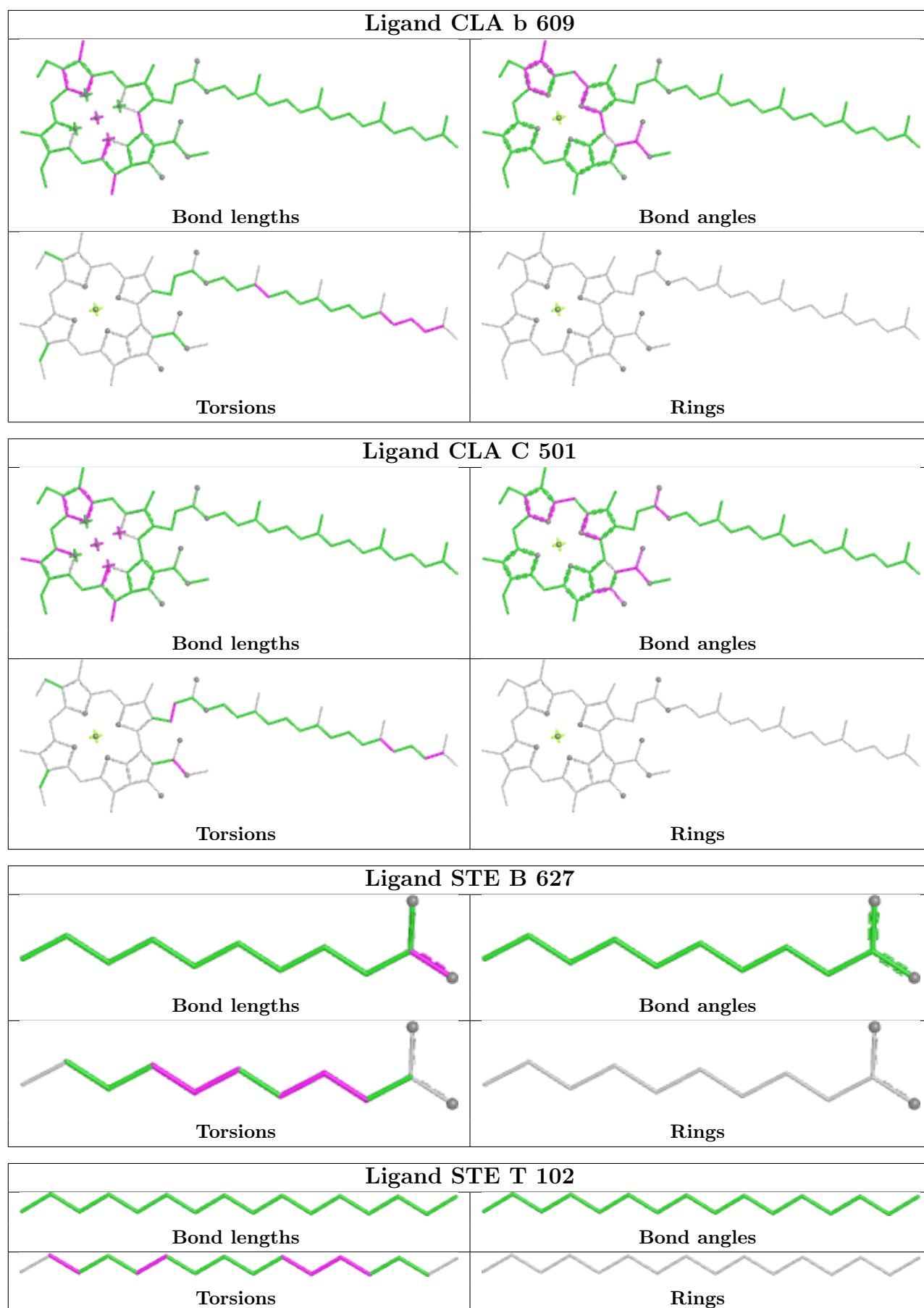


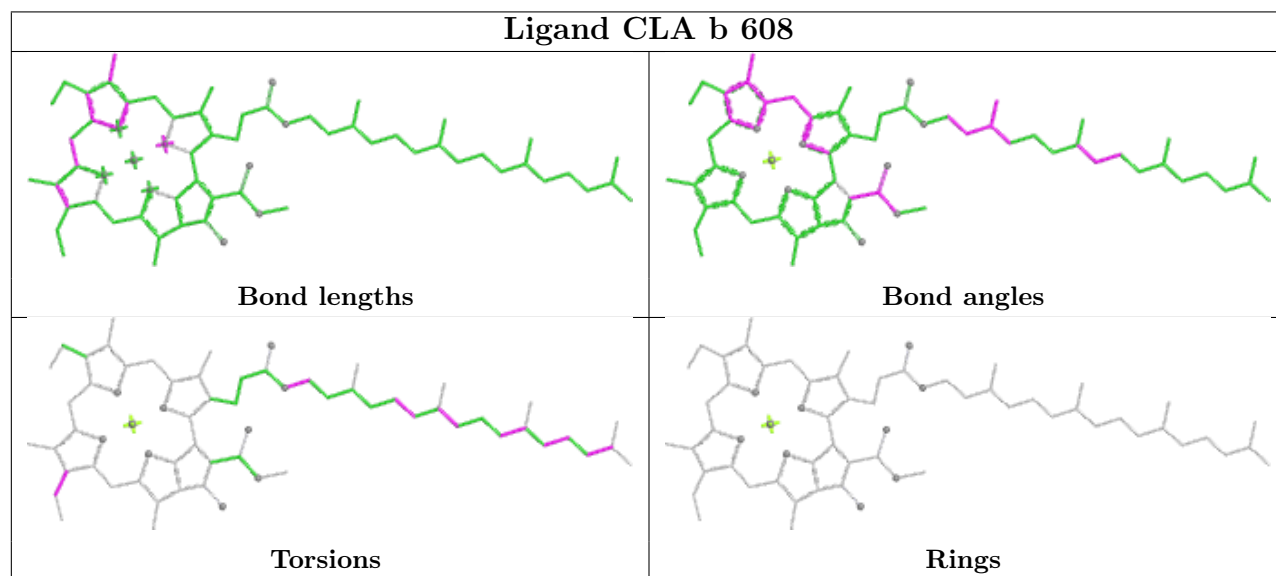
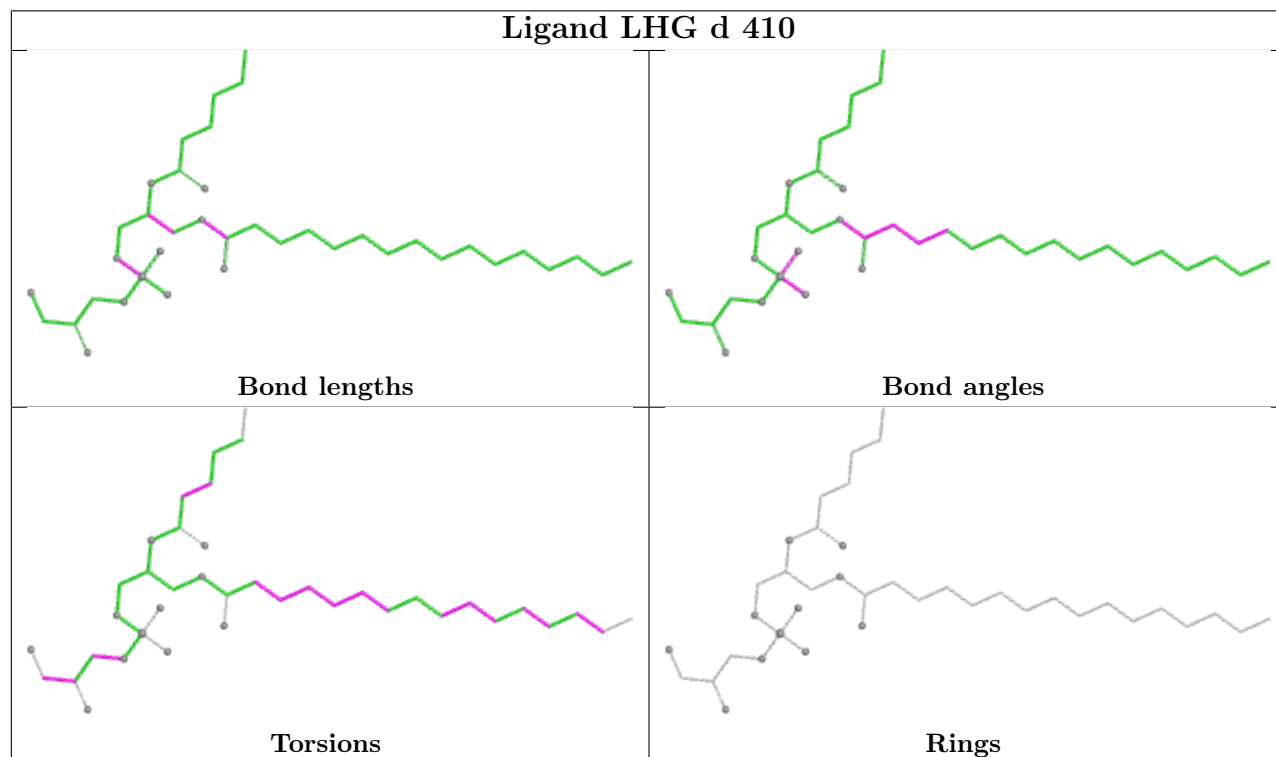
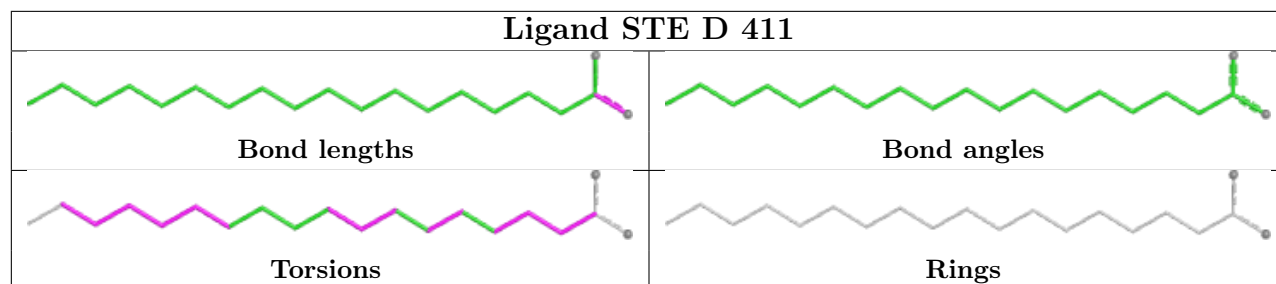


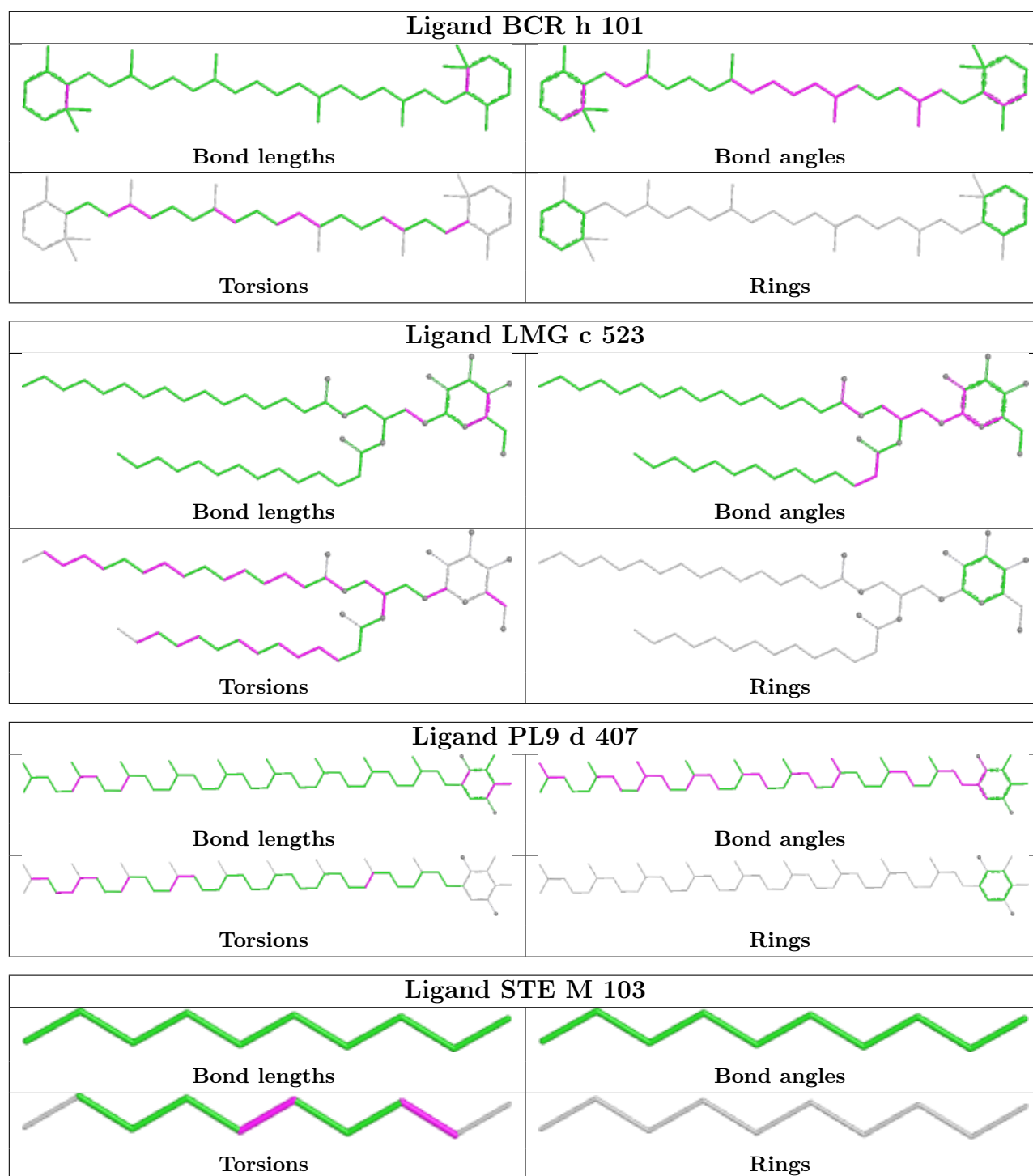


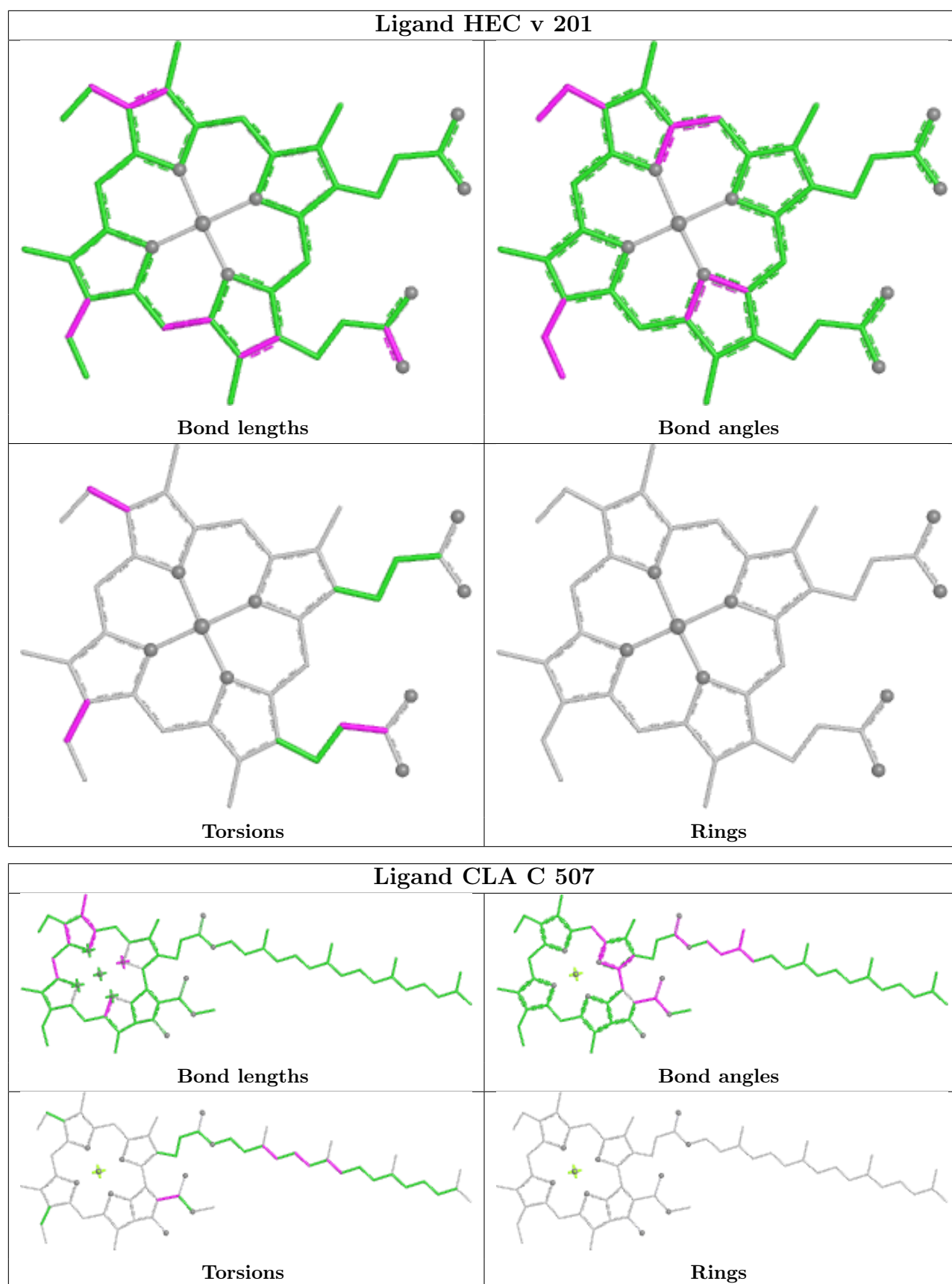


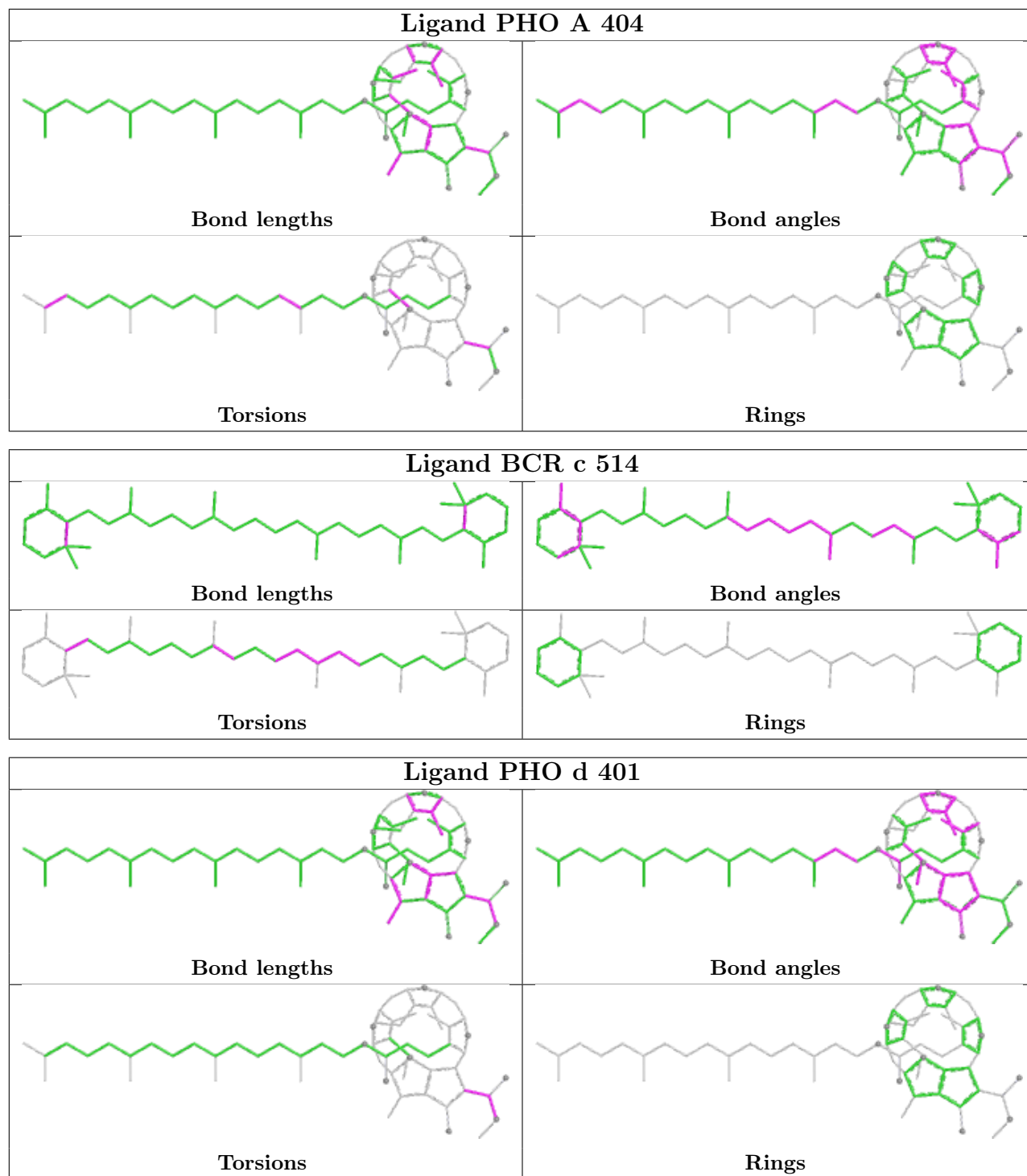


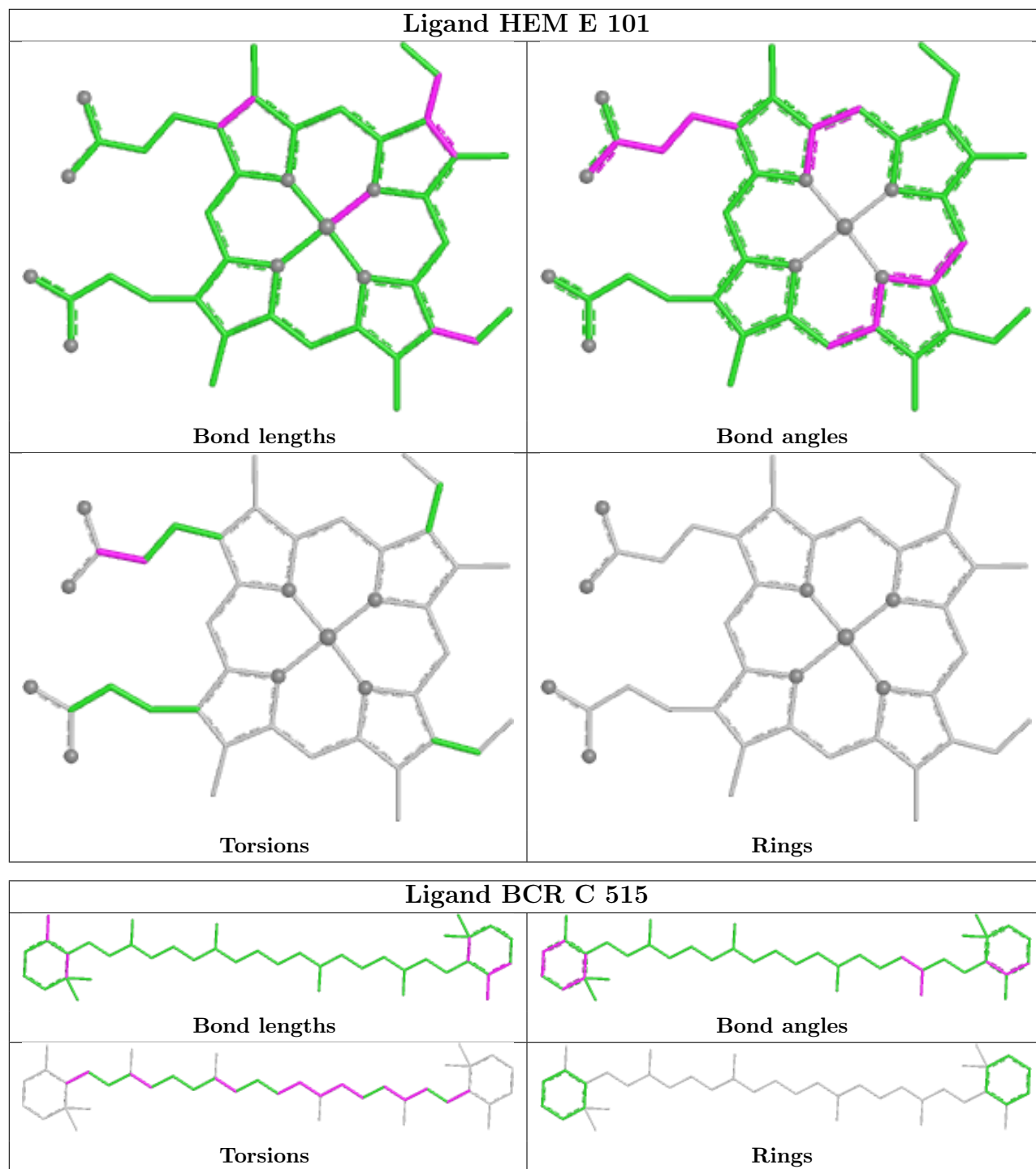


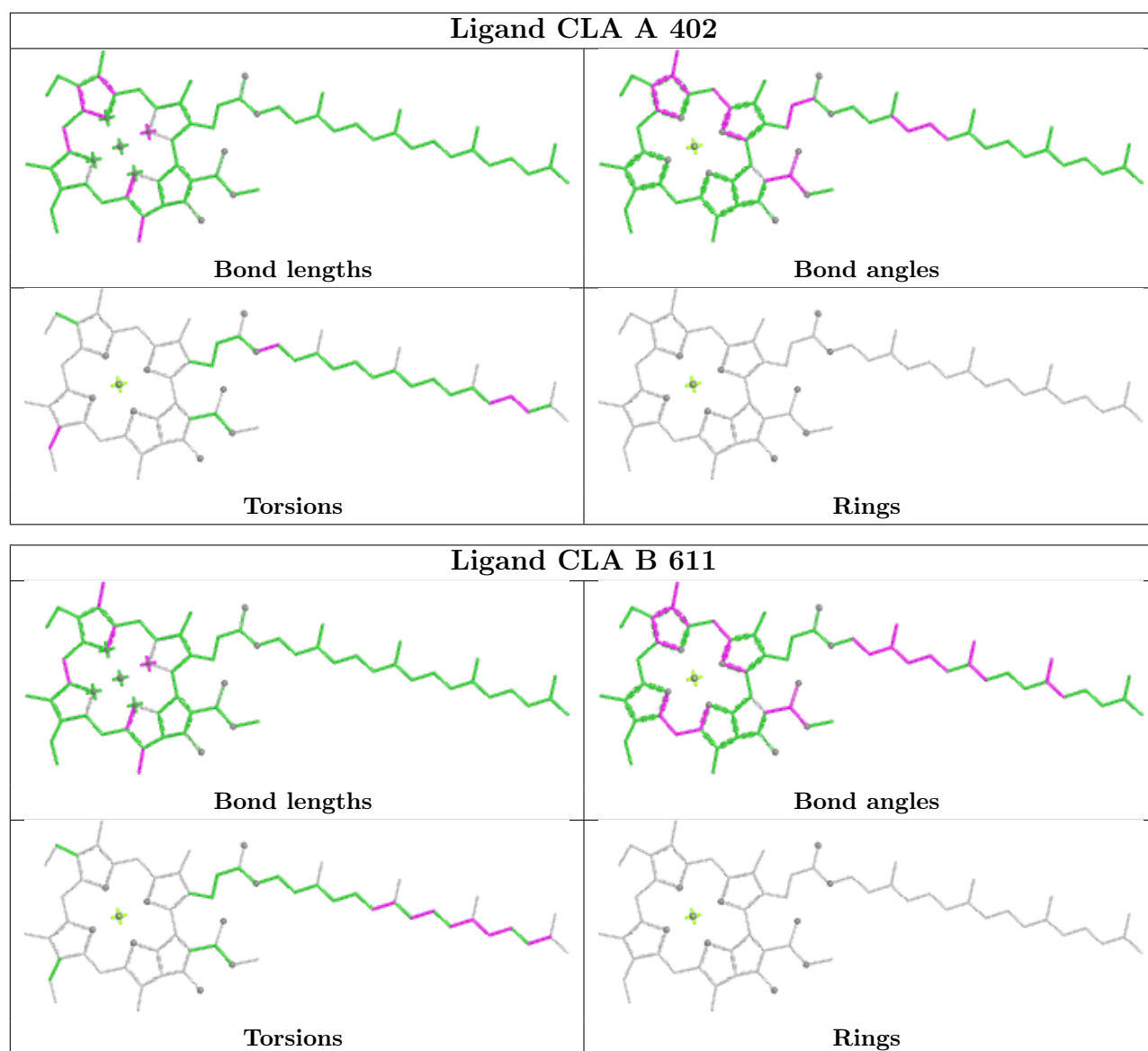


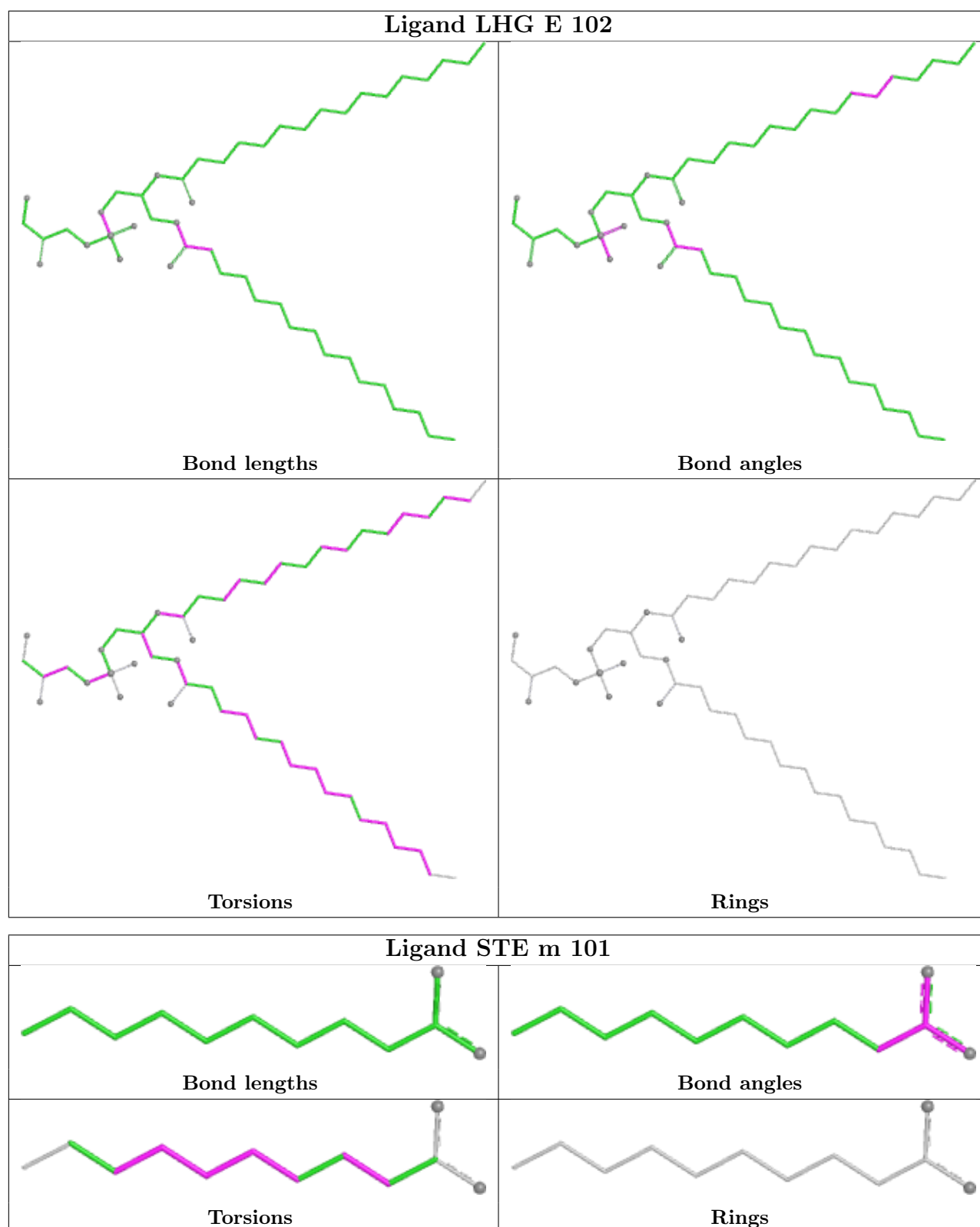


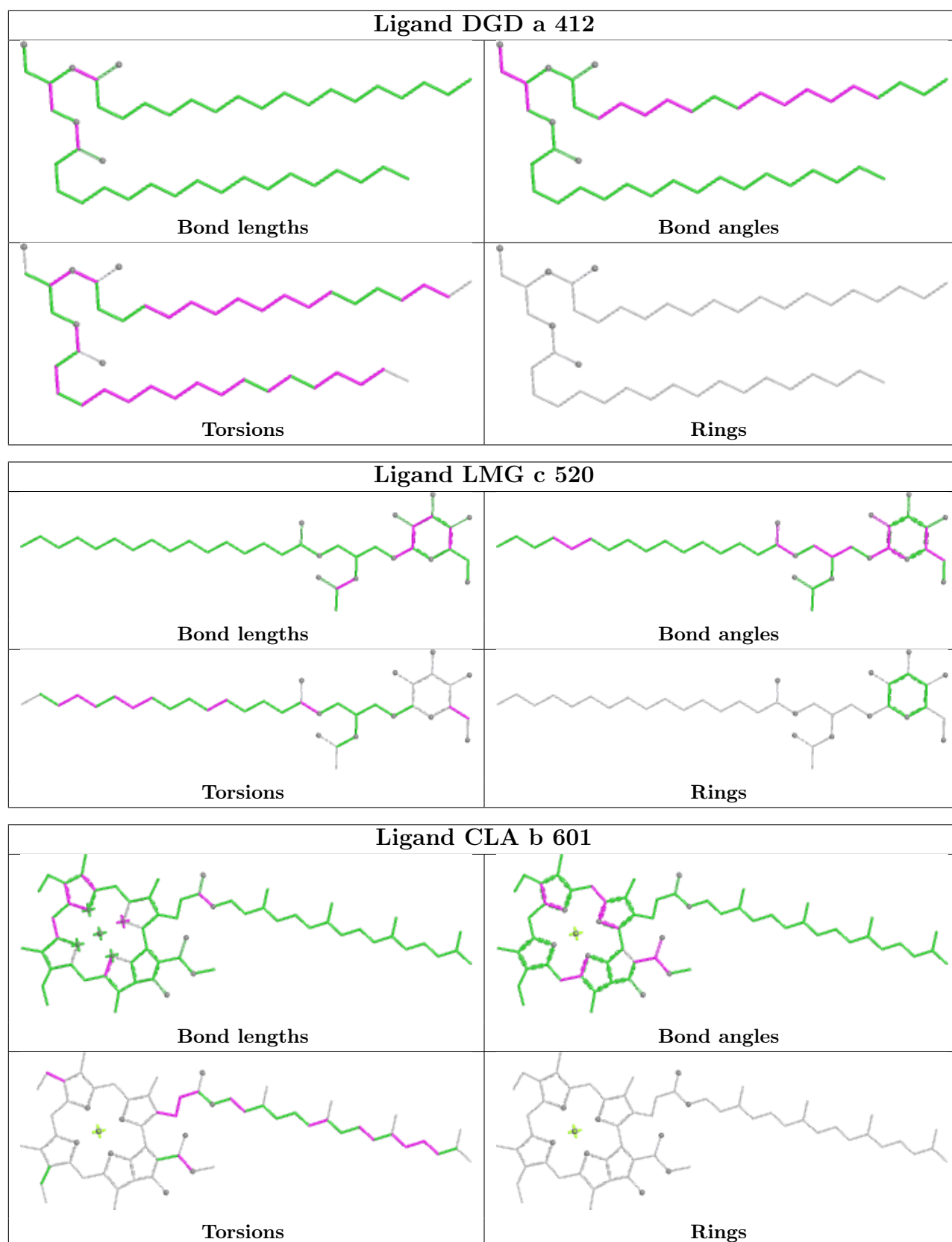


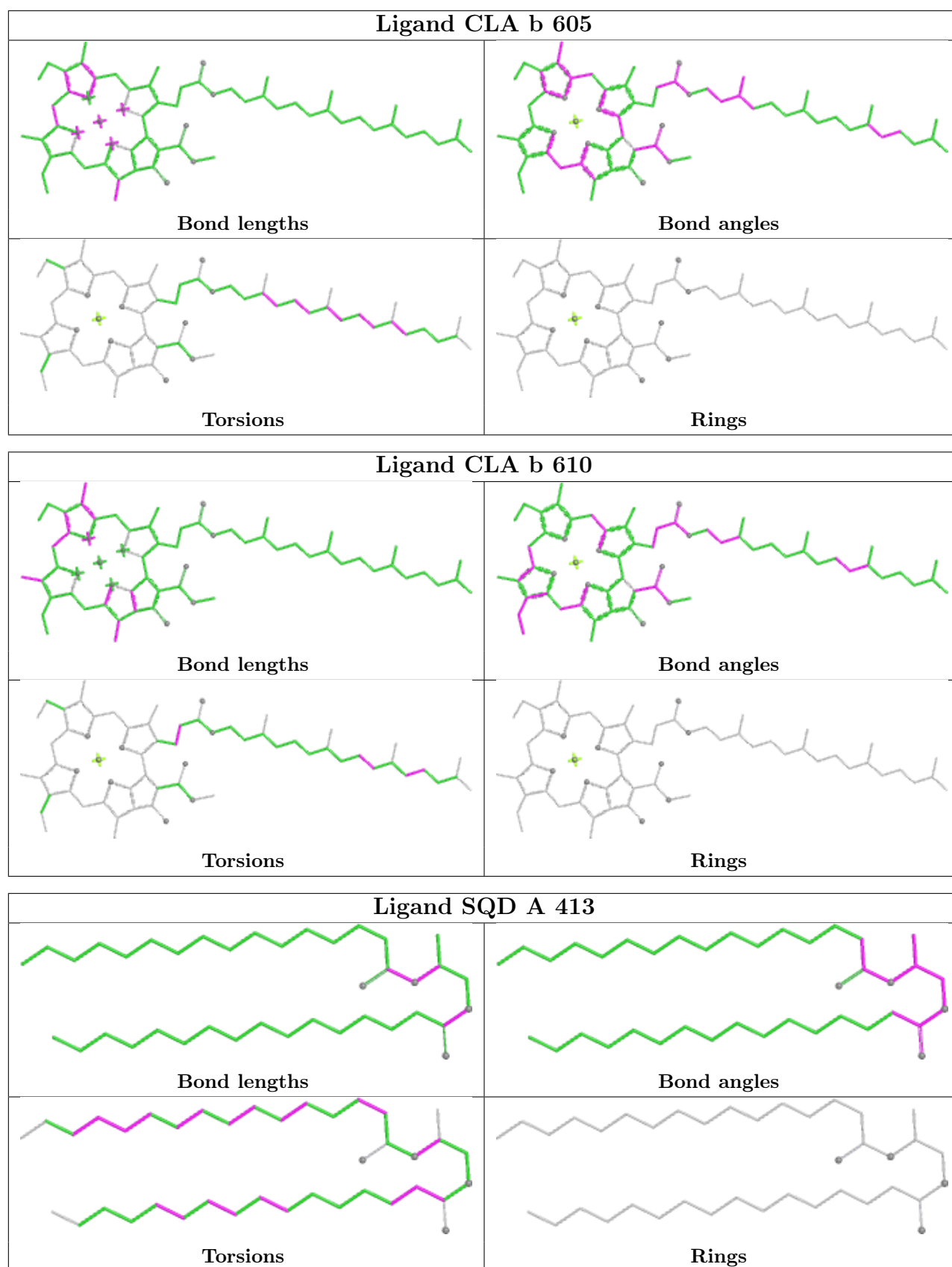


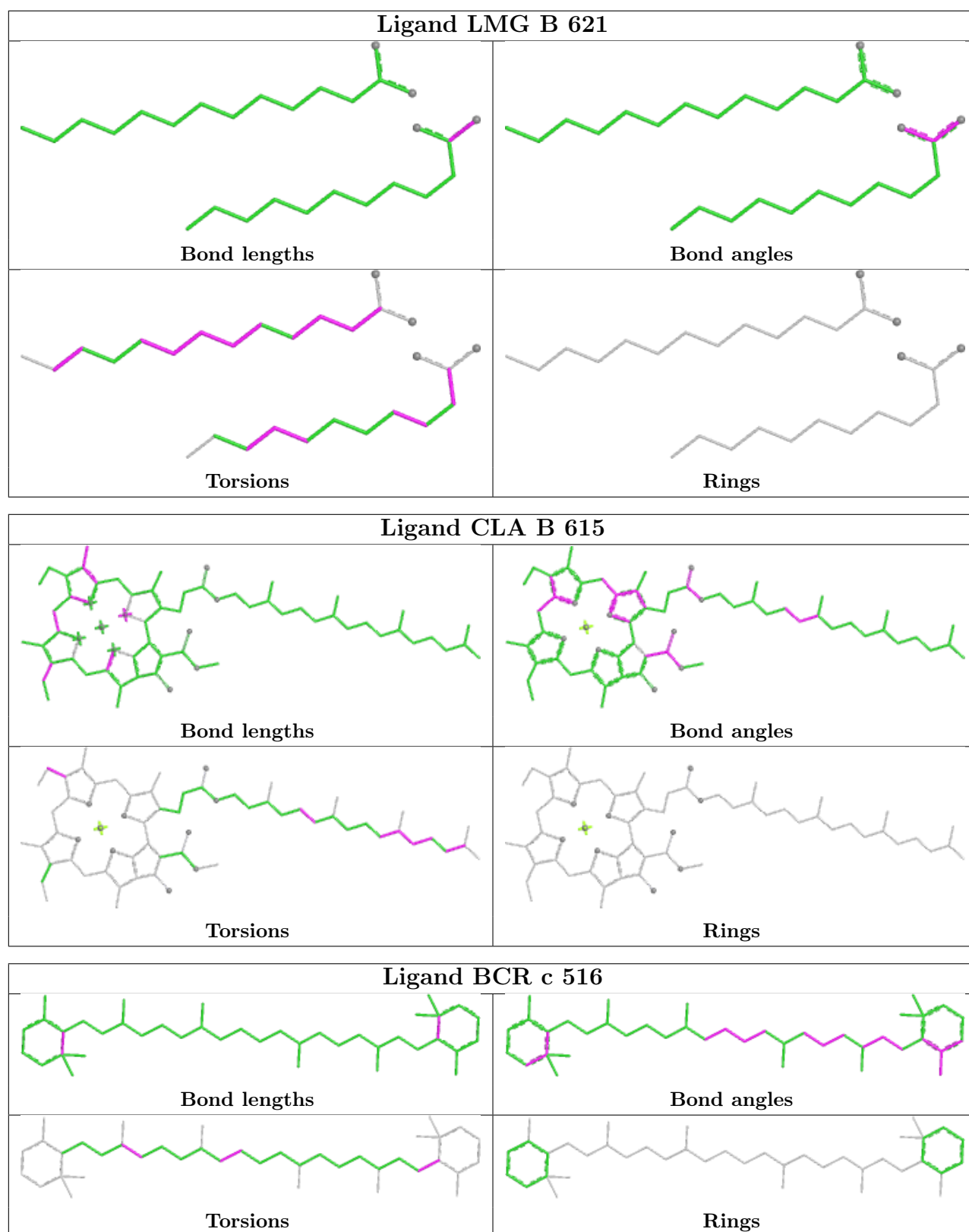


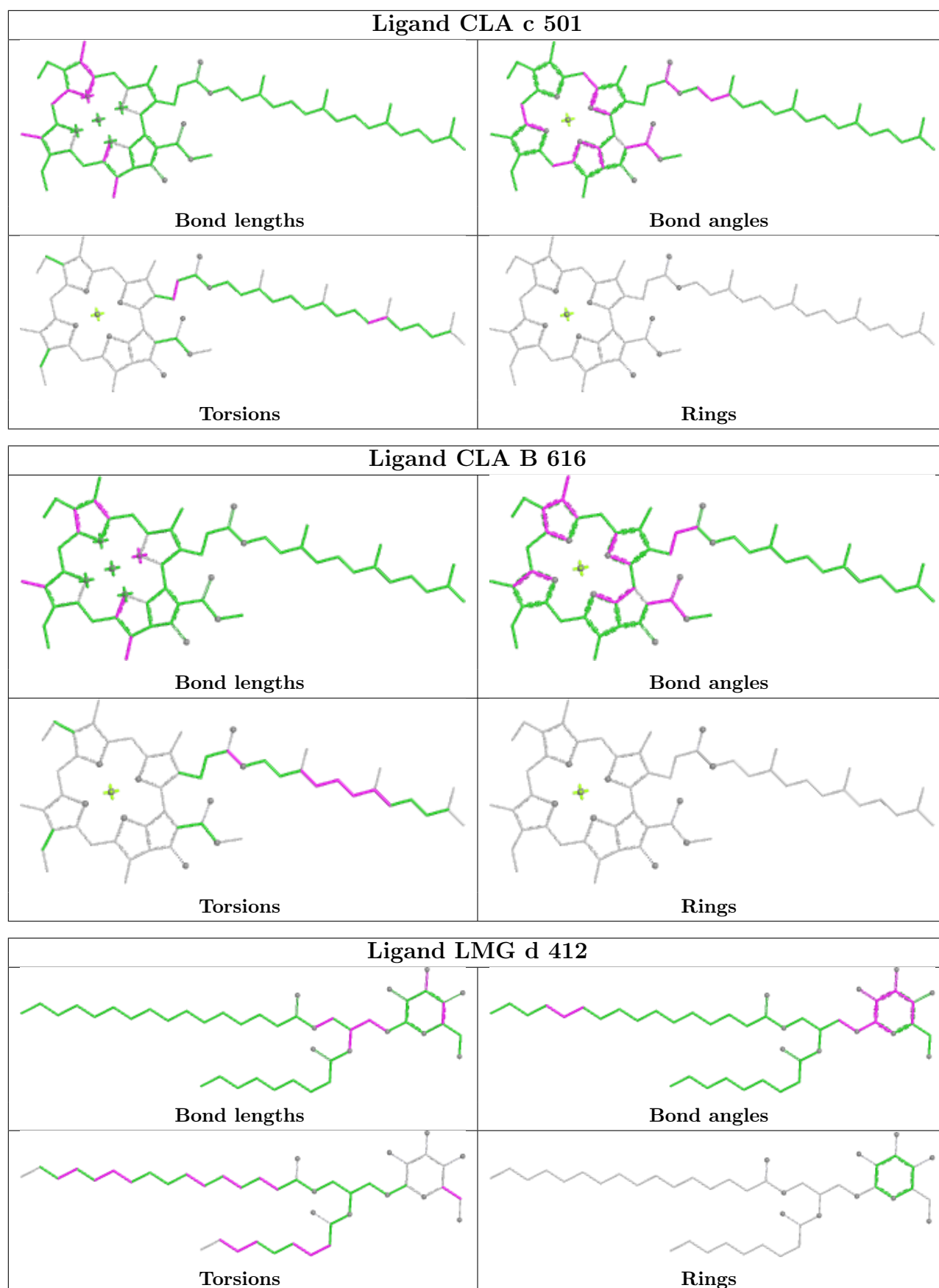




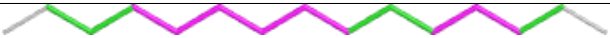

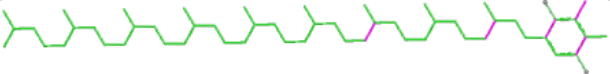

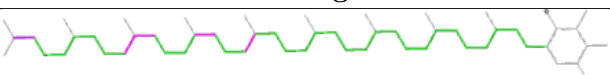
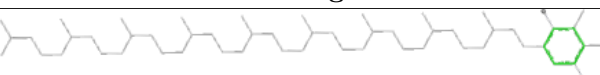
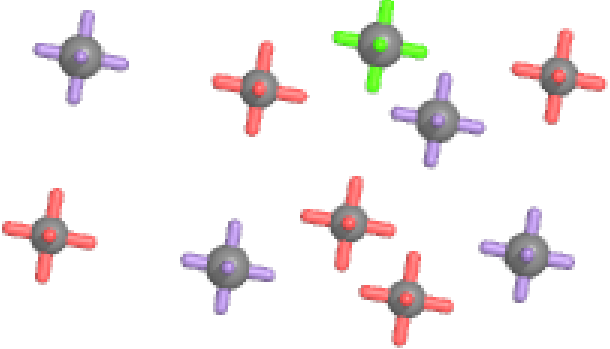
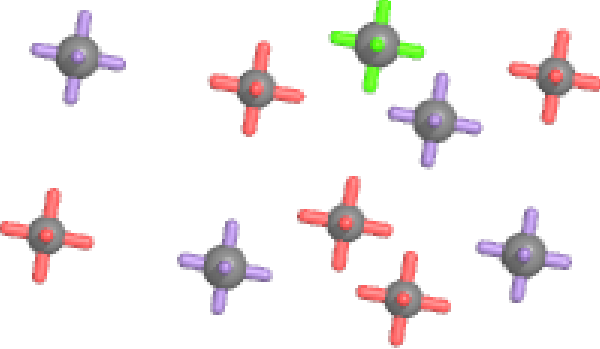
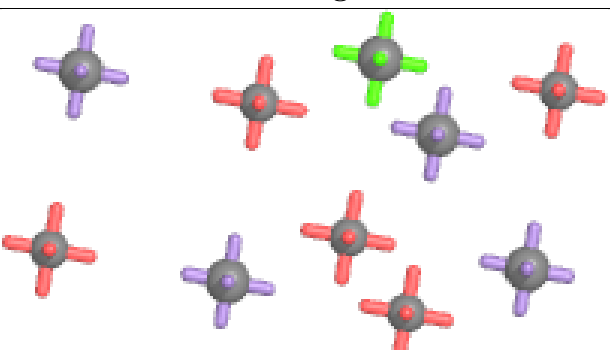
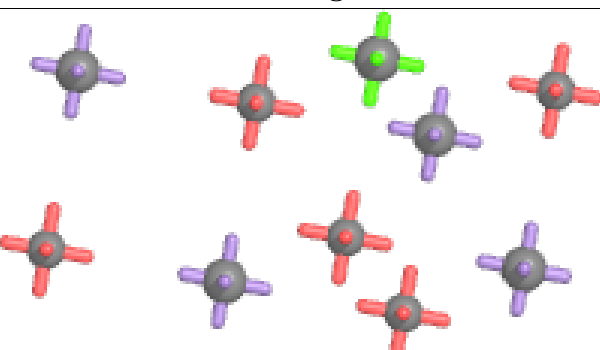


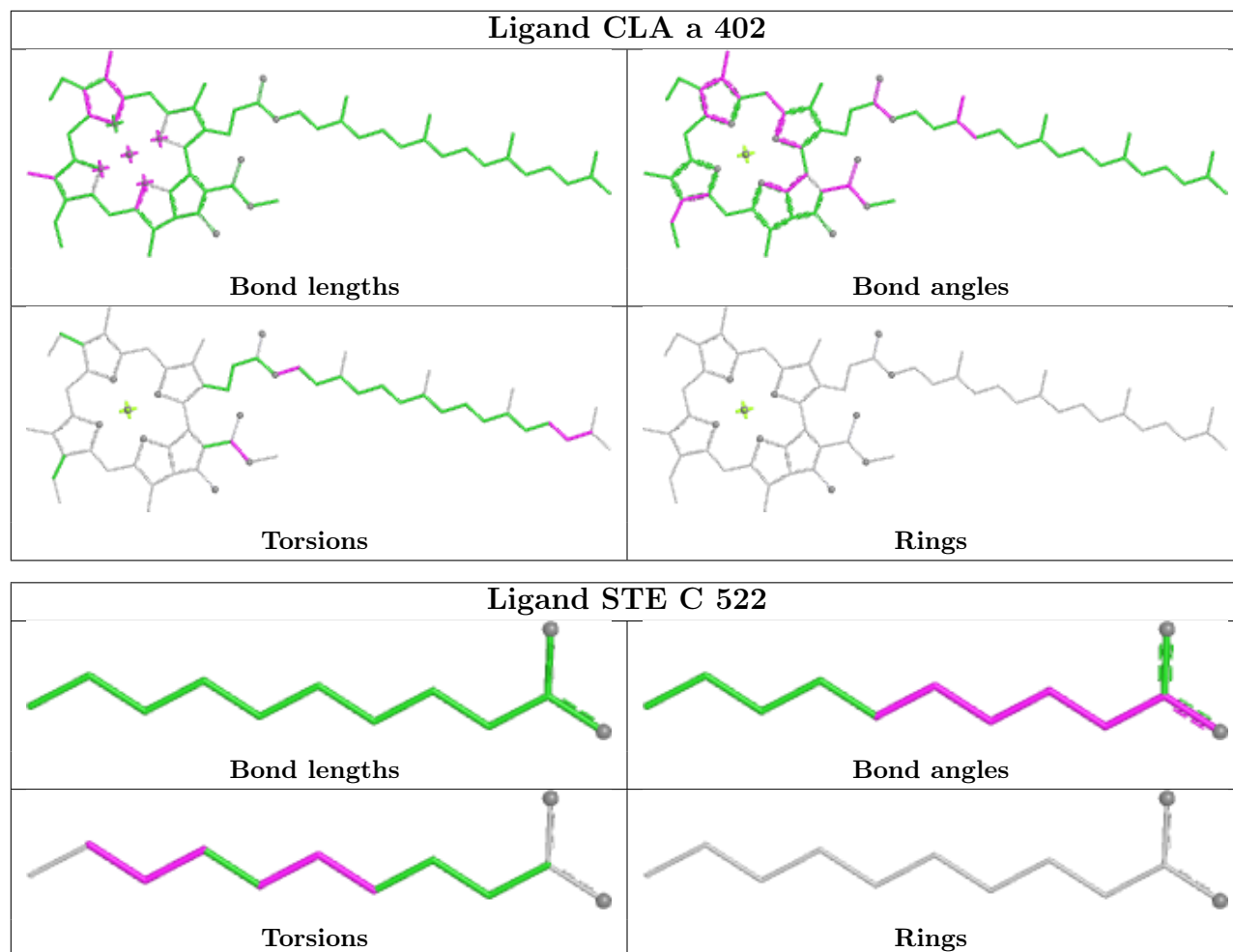


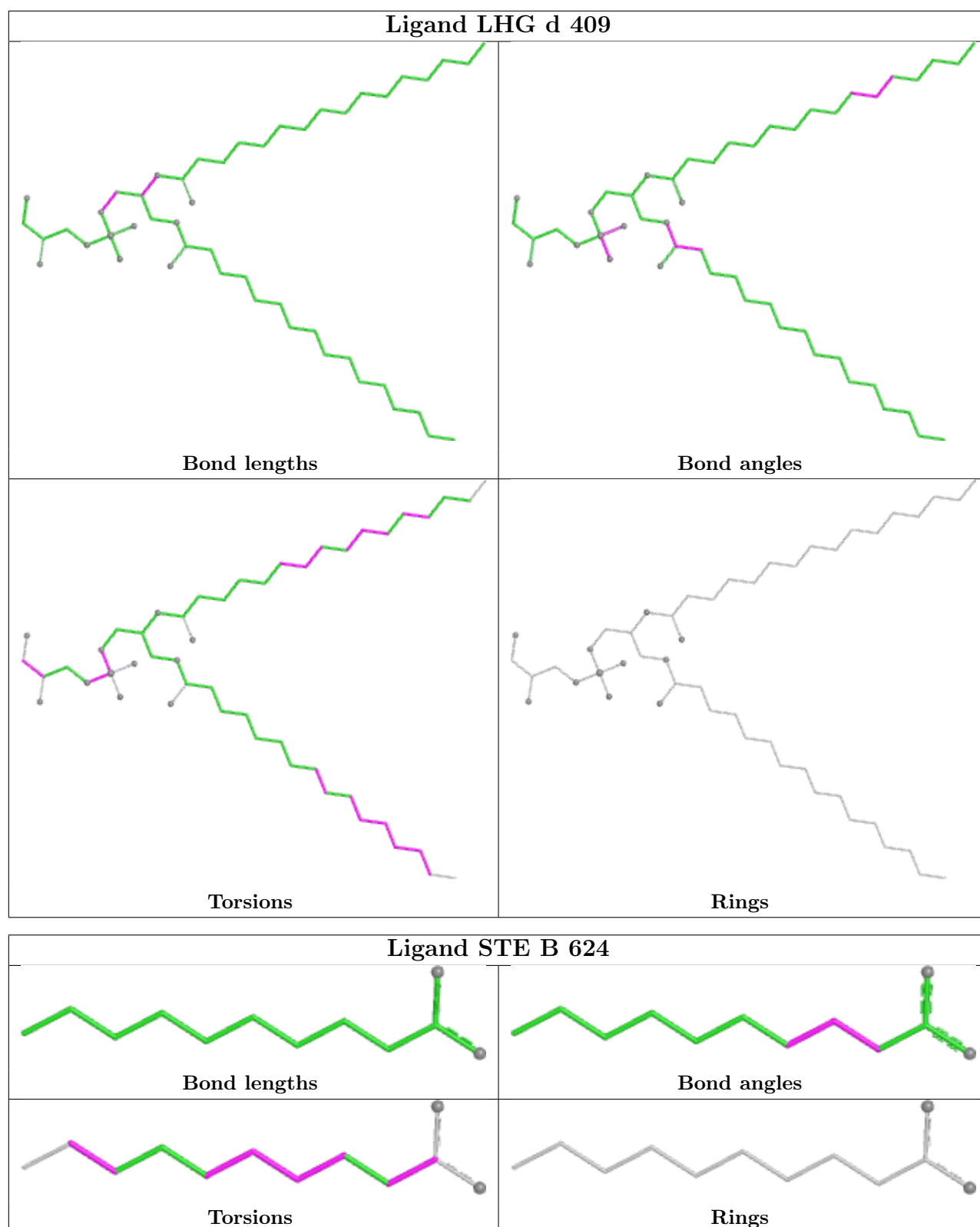


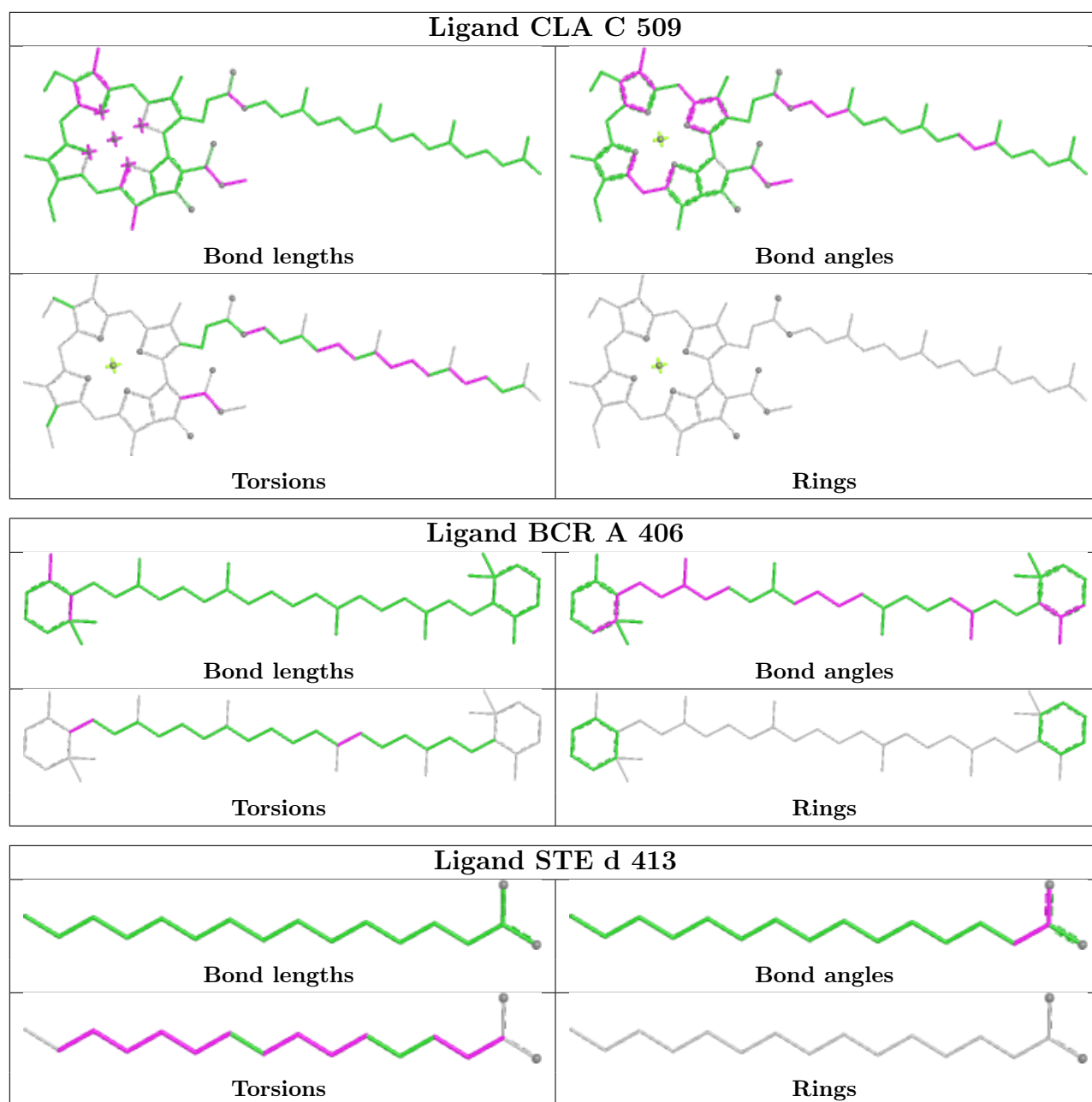


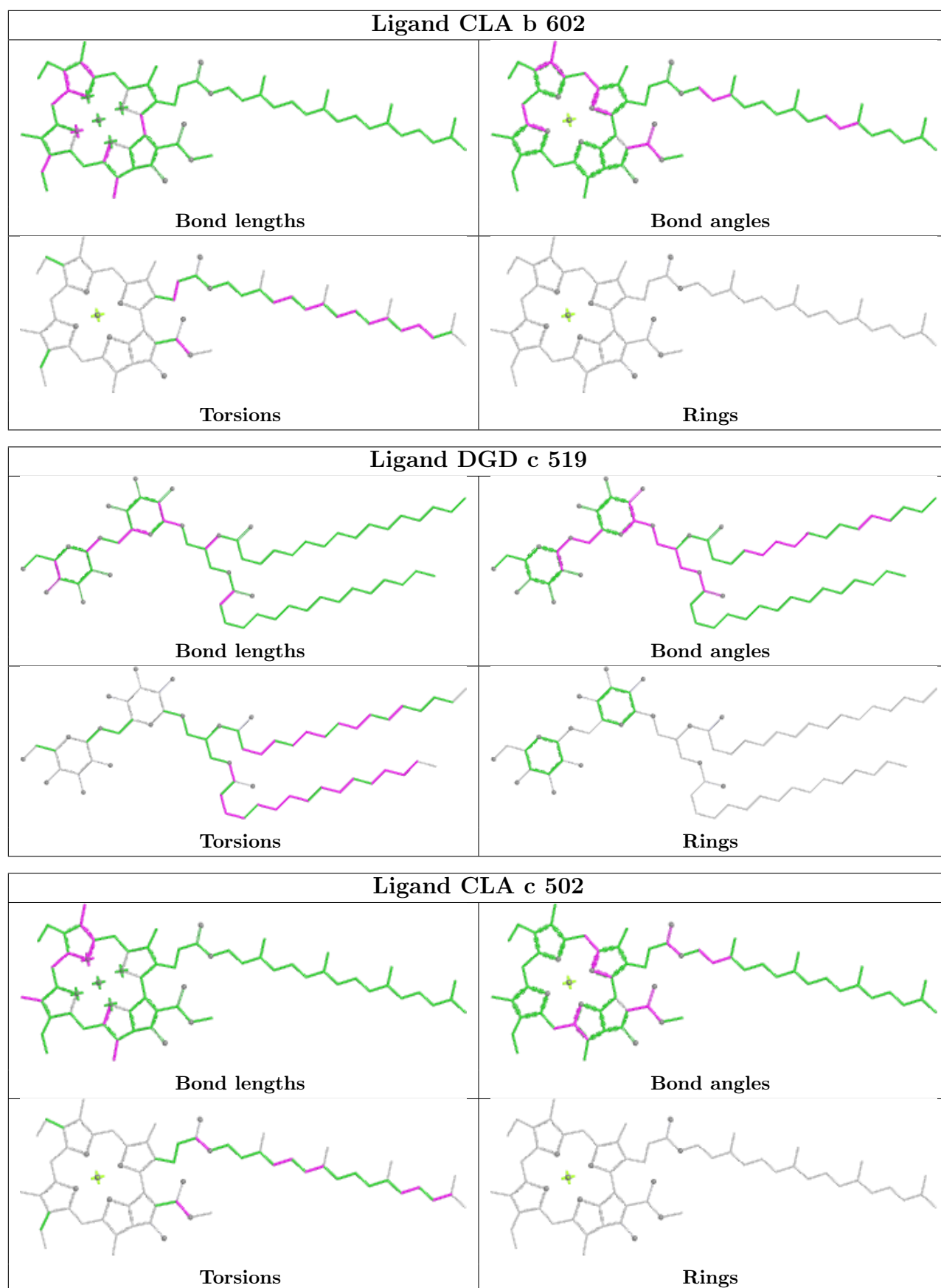


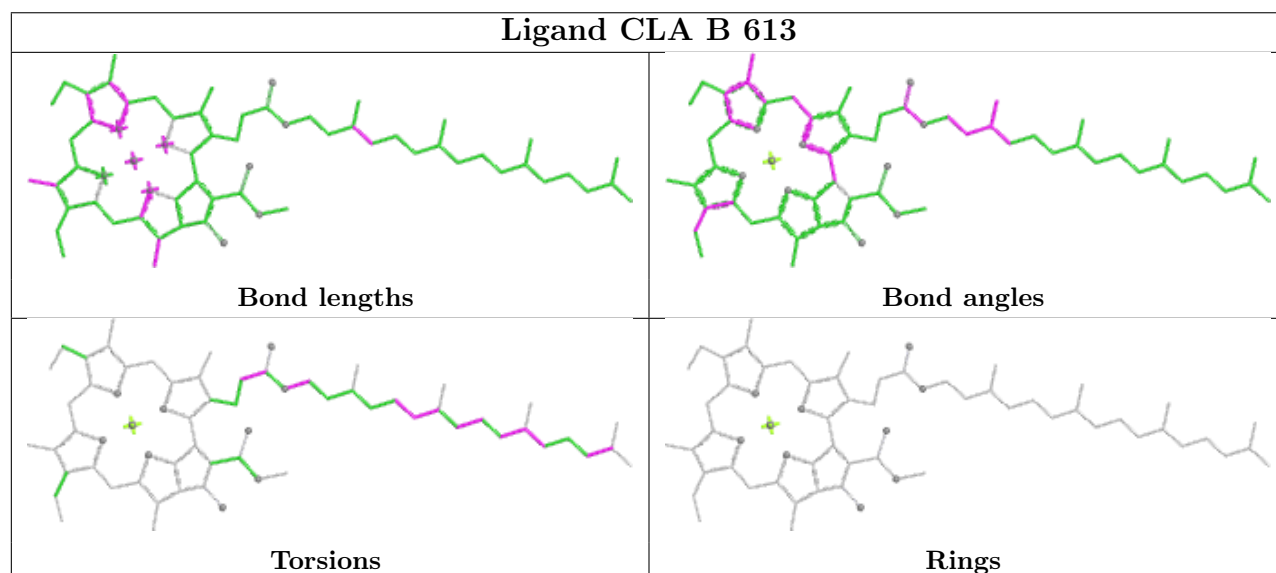
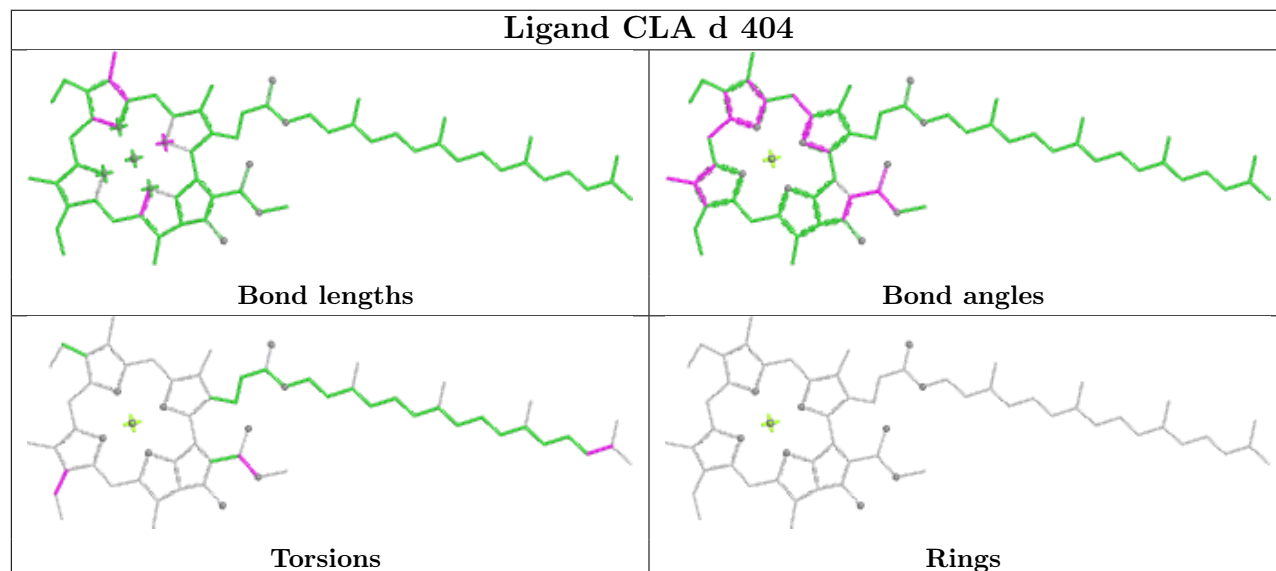
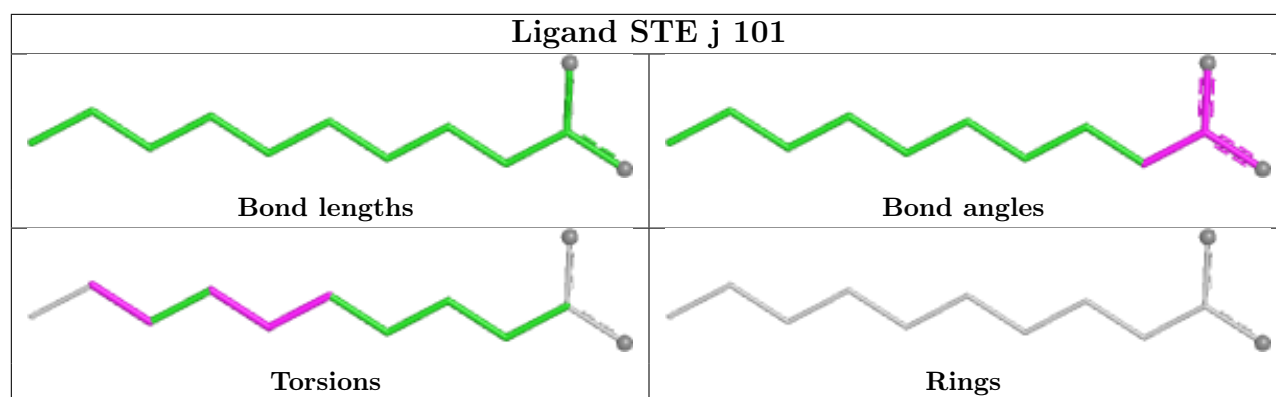
Ligand STE T 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand OEX a 416 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

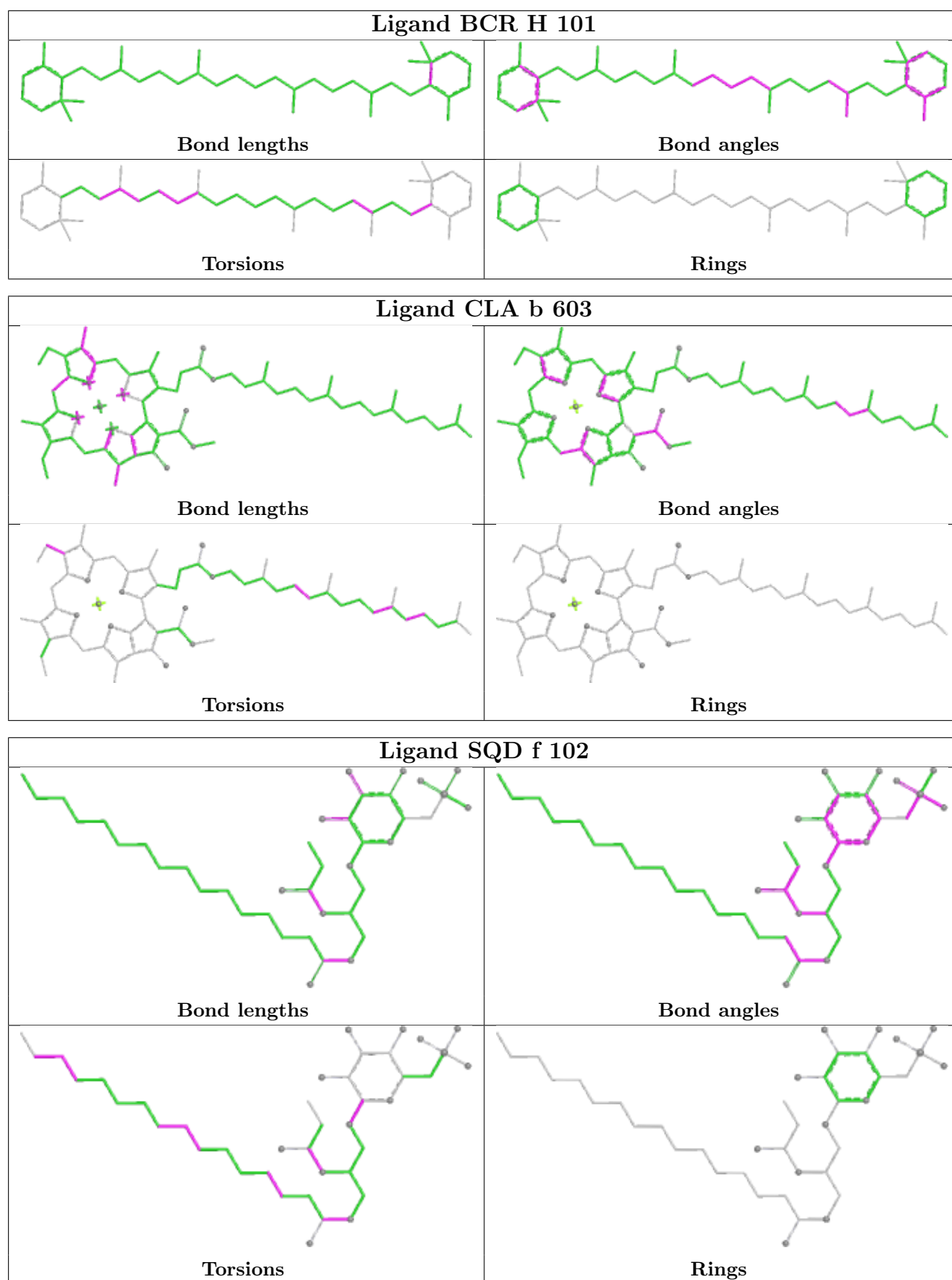


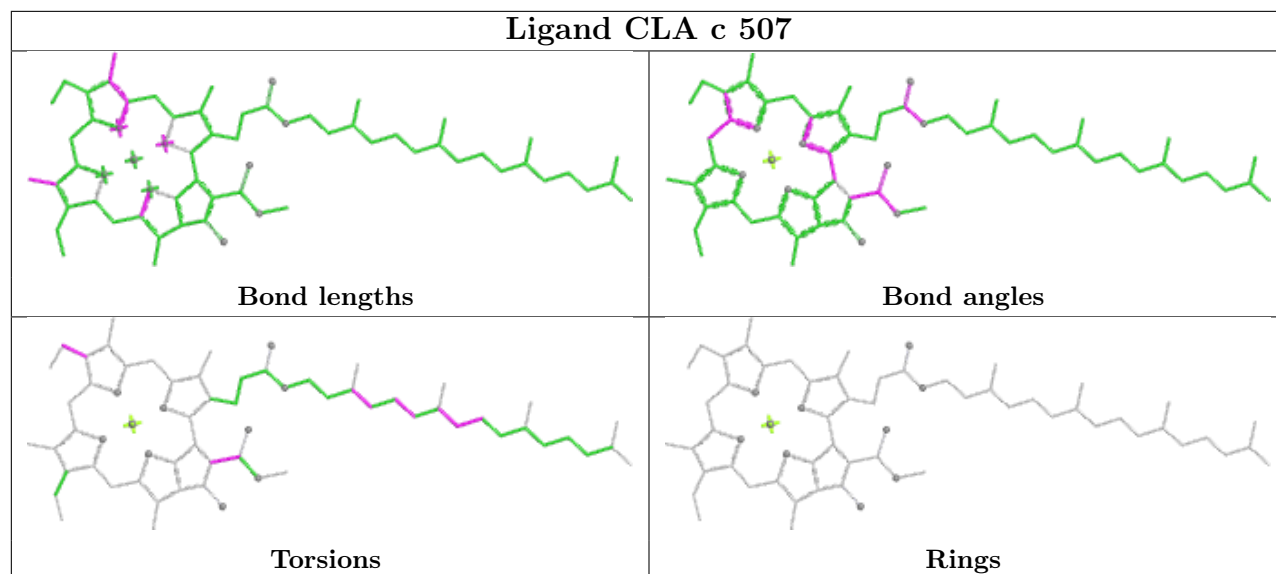












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.44	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	15, 35, 57, 92	64 (19%)
1	a	334/344 (97%)	-0.31	4 (1%) <span style="border: 1px solid black; padding: 0 2px;">76</span> <span style="border: 1px solid black; padding: 0 2px;">78</span>	15, 37, 69, 86	64 (19%)
2	B	505/510 (99%)	-0.39	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">91</span> <span style="border: 1px solid black; padding: 0 2px;">92</span>	20, 40, 69, 101	4 (0%)
2	b	505/510 (99%)	-0.24	5 (0%) <span style="border: 1px solid black; padding: 0 2px;">79</span> <span style="border: 1px solid black; padding: 0 2px;">81</span>	31, 43, 80, 129	0
3	C	442/461 (95%)	-0.33	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	17, 43, 61, 93	11 (2%)
3	c	451/461 (97%)	-0.21	3 (0%) <span style="border: 1px solid black; padding: 0 2px;">84</span> <span style="border: 1px solid black; padding: 0 2px;">86</span>	17, 47, 70, 107	12 (2%)
4	D	341/352 (96%)	-0.51	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	17, 37, 56, 88	2 (0%)
4	d	341/352 (96%)	-0.34	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">90</span> <span style="border: 1px solid black; padding: 0 2px;">91</span>	18, 41, 67, 94	3 (0%)
5	E	82/84 (97%)	0.24	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	38, 61, 78, 93	1 (1%)
5	e	82/84 (97%)	0.31	1 (1%) <span style="border: 1px solid black; padding: 0 2px;">76</span> <span style="border: 1px solid black; padding: 0 2px;">78</span>	45, 69, 89, 94	0
6	F	34/45 (75%)	-0.10	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	46, 53, 77, 98	0
6	f	34/45 (75%)	0.14	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	48, 57, 88, 102	0
7	H	65/66 (98%)	-0.19	2 (3%) <span style="border: 1px solid black; padding: 0 2px;">51</span> <span style="border: 1px solid black; padding: 0 2px;">54</span>	40, 49, 65, 83	0
7	h	63/66 (95%)	0.15	1 (1%) <span style="border: 1px solid black; padding: 0 2px;">70</span> <span style="border: 1px solid black; padding: 0 2px;">73</span>	47, 59, 71, 79	0
8	I	35/38 (92%)	-0.35	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	38, 45, 79, 89	0
8	i	35/38 (92%)	-0.21	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	37, 47, 85, 91	0
9	J	36/40 (90%)	-0.10	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	41, 57, 83, 101	0
9	j	36/40 (90%)	0.24	1 (2%) <span style="border: 1px solid black; padding: 0 2px;">55</span> <span style="border: 1px solid black; padding: 0 2px;">57</span>	46, 59, 95, 114	0
10	K	37/46 (80%)	0.06	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	52, 61, 84, 88	0
10	k	37/46 (80%)	0.23	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	51, 65, 80, 88	0
11	L	37/37 (100%)	-0.54	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	30, 37, 74, 77	0
11	l	36/37 (97%)	-0.55	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	28, 37, 79, 97	0
12	M	32/36 (88%)	-0.42	1 (3%) <span style="border: 1px solid black; padding: 0 2px;">51</span> <span style="border: 1px solid black; padding: 0 2px;">54</span>	31, 40, 68, 79	0
12	m	31/36 (86%)	-0.52	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	31, 41, 55, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.17	2 (0%) 82 84	31, 49, 89, 147	1 (0%)
13	o	244/272 (89%)	-0.19	1 (0%) 88 90	31, 48, 93, 137	0
14	R	28/41 (68%)	0.84	0 100 100	68, 85, 99, 113	0
14	r	28/41 (68%)	1.33	6 (21%) 2 2	82, 110, 127, 139	0
15	T	29/32 (90%)	-0.56	0 100 100	31, 37, 72, 80	0
15	t	29/32 (90%)	-0.40	1 (3%) 48 50	31, 38, 87, 95	0
16	U	97/134 (72%)	-0.17	0 100 100	36, 51, 77, 100	0
16	u	97/134 (72%)	-0.25	0 100 100	37, 47, 66, 89	0
17	V	137/163 (84%)	-0.32	0 100 100	34, 47, 63, 88	0
17	v	137/163 (84%)	-0.15	0 100 100	38, 54, 78, 93	0
18	X	38/41 (92%)	-0.05	0 100 100	47, 59, 84, 91	0
18	x	39/41 (95%)	0.24	1 (2%) 57 60	58, 69, 100, 115	0
19	Y	27/46 (58%)	0.88	2 (7%) 20 22	61, 83, 99, 111	0
19	y	30/46 (65%)	0.65	0 100 100	70, 85, 101, 108	0
20	Z	62/62 (100%)	0.72	2 (3%) 50 53	62, 79, 123, 138	0
20	z	62/62 (100%)	0.71	4 (6%) 25 26	67, 83, 125, 138	0
All	All	5293/5700 (92%)	-0.22	39 (0%) 84 86	15, 45, 84, 147	162 (3%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	t	30	THR	4.0
13	O	60	ARG	3.8
13	o	58	ASN	3.6
3	c	23	ALA	3.5
18	x	40	SER	3.2

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
15	FME	t	1	10/11	0.94	0.08	33,48,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FME	M	1	10/11	0.95	0.09	44,54,68,76	0
8	FME	I	1	10/11	0.95	0.08	40,52,64,70	0
15	FME	T	1	10/11	0.96	0.07	29,52,69,69	0
8	FME	i	1	10/11	0.96	0.08	41,51,64,67	0
12	FME	m	1	10/11	0.97	0.08	33,50,72,82	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
32	STE	H	103	18/20	0.74	0.18	43,78,89,95	0
32	STE	I	101	15/20	0.77	0.18	38,59,77,81	0
32	STE	b	624	20/20	0.78	0.15	51,69,78,93	0
32	STE	a	413	10/20	0.79	0.16	37,66,75,80	0
32	STE	b	625	10/20	0.79	0.14	40,53,63,74	0
32	STE	B	626	16/20	0.80	0.15	39,72,94,94	0
27	LMG	b	622	55/55	0.80	0.16	53,80,98,112	0
33	LHG	E	102	49/49	0.80	0.14	55,87,113,120	0
26	PL9	A	409	55/55	0.81	0.16	44,72,93,105	0
27	LMG	c	522	48/55	0.82	0.14	39,82,115,118	0
27	LMG	d	411	23/55	0.82	0.17	42,72,88,92	0
32	STE	m	101	12/20	0.82	0.16	48,64,76,82	0
32	STE	x	101	20/20	0.82	0.13	49,67,79,79	0
32	STE	b	623	16/20	0.82	0.16	50,68,83,94	0
32	STE	c	524	12/20	0.83	0.11	57,73,82,84	0
29	DGD	a	412	44/66	0.83	0.13	35,58,82,91	0
26	PL9	a	409	55/55	0.83	0.16	42,76,96,107	0
32	STE	E	103	12/20	0.83	0.16	63,80,88,95	0
32	STE	c	521	20/20	0.84	0.12	44,63,94,107	0
32	STE	T	102	16/20	0.84	0.14	41,53,78,79	0
32	STE	j	101	12/20	0.84	0.12	48,62,70,79	0
33	LHG	e	101	42/49	0.84	0.13	56,93,112,132	0
29	DGD	A	414	66/66	0.85	0.11	47,67,82,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	SQD	A	413	39/54	0.85	0.13	43,66,94,100	0
28	SQD	a	411	36/54	0.85	0.13	32,65,86,91	0
32	STE	J	101	12/20	0.86	0.12	49,62,72,73	0
32	STE	B	627	12/20	0.86	0.14	53,66,83,86	0
32	STE	C	521	16/20	0.86	0.13	38,58,85,88	0
32	STE	a	414	12/20	0.86	0.12	54,67,77,79	0
27	LMG	D	410	33/55	0.86	0.13	41,58,86,90	0
22	CLA	b	601	65/65	0.86	0.11	53,72,92,96	0
27	LMG	A	411	48/55	0.86	0.11	43,65,84,101	0
32	STE	B	625	18/20	0.87	0.12	41,59,81,88	0
27	LMG	B	621	28/55	0.87	0.14	37,53,66,72	0
32	STE	B	620	17/20	0.87	0.11	39,59,71,80	0
32	STE	T	103	15/20	0.87	0.14	44,60,81,84	0
32	STE	d	413	17/20	0.88	0.14	48,62,75,82	0
32	STE	M	103	10/20	0.88	0.11	36,54,57,61	0
28	SQD	F	101	36/54	0.88	0.12	43,77,93,98	0
27	LMG	c	520	37/55	0.88	0.12	43,72,92,96	0
28	SQD	f	102	41/54	0.88	0.12	63,89,107,109	0
32	STE	B	624	12/20	0.88	0.10	37,56,70,74	0
32	STE	l	102	18/20	0.89	0.12	37,54,88,89	0
28	SQD	B	623	54/54	0.89	0.10	43,66,97,109	0
27	LMG	b	620	51/55	0.89	0.10	38,57,76,91	0
32	STE	C	520	12/20	0.89	0.12	43,57,68,70	0
27	LMG	C	519	48/55	0.89	0.12	49,74,93,98	0
27	LMG	M	101	51/55	0.90	0.09	33,53,76,92	0
32	STE	b	621	20/20	0.90	0.10	39,58,79,80	0
28	SQD	L	101	49/54	0.90	0.09	40,61,93,97	0
22	CLA	B	601	65/65	0.90	0.10	35,64,90,100	0
32	STE	C	522	12/20	0.90	0.10	34,45,58,64	0
24	BCR	c	514	40/40	0.90	0.10	47,64,79,81	0
24	BCR	d	406	40/40	0.90	0.11	40,57,98,114	0
22	CLA	C	513	65/65	0.91	0.10	45,68,103,112	0
32	STE	D	411	20/20	0.91	0.09	38,55,79,84	0
24	BCR	K	101	40/40	0.91	0.11	51,65,74,78	0
32	STE	t	102	14/20	0.91	0.10	35,55,65,68	0
24	BCR	h	101	40/40	0.91	0.10	43,60,79,91	0
27	LMG	c	523	49/55	0.91	0.10	35,62,83,99	0
24	BCR	k	101	40/40	0.91	0.10	45,67,78,80	0
28	SQD	a	410	54/54	0.92	0.10	44,67,96,99	0
22	CLA	c	512	65/65	0.92	0.10	47,64,99,104	0
24	BCR	Y	101	40/40	0.92	0.09	43,58,76,83	0
24	BCR	b	618	40/40	0.92	0.08	30,44,56,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
29	DGD	C	517	62/66	0.92	0.09	41,56,102,121	0
29	DGD	H	102	62/66	0.92	0.09	33,48,61,66	0
24	BCR	B	618	40/40	0.92	0.08	28,41,58,61	0
29	DGD	h	102	62/66	0.92	0.09	33,53,64,71	0
24	BCR	D	405	40/40	0.92	0.10	35,49,85,89	0
24	BCR	H	101	40/40	0.92	0.09	38,53,64,74	0
22	CLA	c	513	65/65	0.93	0.10	49,74,106,110	0
24	BCR	c	515	40/40	0.93	0.08	35,47,58,72	0
32	STE	M	102	15/20	0.93	0.09	37,50,66,69	0
22	CLA	c	508	64/65	0.93	0.09	37,50,94,112	0
27	LMG	D	407	51/55	0.93	0.10	31,60,86,92	0
28	SQD	A	412	52/54	0.93	0.09	33,66,94,99	0
24	BCR	B	619	40/40	0.93	0.08	33,45,59,61	0
24	BCR	C	514	40/40	0.93	0.09	32,43,56,61	0
29	DGD	c	518	62/66	0.93	0.09	35,58,94,103	0
24	BCR	C	515	40/40	0.93	0.11	45,60,78,81	0
24	BCR	b	619	40/40	0.93	0.08	35,52,70,70	0
34	BCT	a	408	4/4	0.93	0.10	35,40,48,58	0
27	LMG	d	412	44/55	0.94	0.09	37,58,89,92	0
22	CLA	c	509	65/65	0.94	0.09	37,53,70,75	0
22	CLA	c	510	65/65	0.94	0.08	36,53,67,73	0
29	DGD	c	519	62/66	0.94	0.08	31,57,86,101	0
24	BCR	c	516	40/40	0.94	0.11	45,60,71,79	0
22	CLA	C	503	65/65	0.94	0.07	36,47,59,62	0
22	CLA	C	511	65/65	0.94	0.09	36,57,71,76	0
24	BCR	A	406	40/40	0.94	0.07	28,38,49,52	0
24	BCR	T	101	40/40	0.94	0.07	29,44,58,62	0
24	BCR	B	617	40/40	0.94	0.07	30,45,60,65	0
22	CLA	c	506	65/65	0.94	0.09	36,53,94,101	0
33	LHG	d	408	49/49	0.94	0.10	30,55,77,83	0
33	LHG	d	410	39/49	0.94	0.08	34,50,72,74	0
29	DGD	C	516	62/66	0.94	0.09	25,48,84,91	0
22	CLA	C	512	65/65	0.94	0.09	35,61,88,97	0
22	CLA	c	502	65/65	0.95	0.07	34,49,69,75	0
22	CLA	c	503	65/65	0.95	0.08	35,48,61,64	0
24	BCR	a	405	40/40	0.95	0.06	25,36,52,56	0
24	BCR	b	617	40/40	0.95	0.07	29,43,52,56	0
22	CLA	c	504	60/65	0.95	0.07	35,50,87,88	0
22	CLA	c	505	65/65	0.95	0.08	28,45,71,75	0
22	CLA	C	505	65/65	0.95	0.08	22,44,72,75	0
22	CLA	c	507	65/65	0.95	0.08	30,49,61,66	0
22	CLA	C	506	65/65	0.95	0.09	29,49,89,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	C	508	65/65	0.95	0.08	32,46,104,115	0
22	CLA	C	509	65/65	0.95	0.09	32,50,65,74	0
22	CLA	c	511	65/65	0.95	0.09	43,60,78,82	0
24	BCR	t	101	40/40	0.95	0.06	27,39,55,58	0
22	CLA	C	510	65/65	0.95	0.07	34,49,66,74	0
29	DGD	C	518	62/66	0.95	0.08	33,54,82,91	0
26	PL9	D	406	55/55	0.95	0.07	24,38,49,50	0
22	CLA	B	609	65/65	0.95	0.08	29,42,56,59	0
26	PL9	d	407	55/55	0.95	0.07	27,38,45,52	0
22	CLA	d	405	65/65	0.95	0.09	32,53,93,101	0
22	CLA	B	615	65/65	0.95	0.07	29,42,67,77	0
22	CLA	C	502	65/65	0.95	0.07	35,47,60,68	0
22	CLA	a	403	65/65	0.95	0.09	30,45,99,107	0
22	CLA	B	606	65/65	0.95	0.07	28,41,71,77	0
33	LHG	B	622	49/49	0.95	0.09	28,48,68,77	0
33	LHG	D	409	47/49	0.95	0.09	29,53,82,99	0
22	CLA	b	606	65/65	0.95	0.08	29,45,77,78	0
33	LHG	L	102	49/49	0.95	0.07	30,44,59,74	0
22	CLA	b	608	65/65	0.95	0.07	34,48,64,68	0
22	CLA	b	614	65/65	0.95	0.08	25,44,78,85	0
22	CLA	b	615	65/65	0.95	0.07	31,45,61,65	0
33	LHG	l	101	49/49	0.95	0.07	34,48,59,67	0
22	CLA	b	616	60/65	0.95	0.09	34,48,89,91	0
22	CLA	a	402	65/65	0.96	0.06	24,35,48,62	0
22	CLA	B	602	65/65	0.96	0.07	27,40,62,65	0
22	CLA	a	404	65/65	0.96	0.08	21,40,80,85	0
22	CLA	d	403	65/65	0.96	0.07	23,40,60,68	0
22	CLA	d	404	65/65	0.96	0.06	24,35,46,50	0
22	CLA	B	616	60/65	0.96	0.09	28,45,84,100	0
23	PHO	A	404	64/64	0.96	0.05	20,31,40,48	0
23	PHO	D	401	64/64	0.96	0.06	25,37,45,53	0
23	PHO	d	401	64/64	0.96	0.06	23,35,43,48	0
23	PHO	d	402	64/64	0.96	0.06	32,43,54,63	0
22	CLA	b	602	65/65	0.96	0.08	31,46,65,71	0
22	CLA	b	603	65/65	0.96	0.07	24,40,71,79	0
22	CLA	b	604	65/65	0.96	0.07	24,39,80,93	0
22	CLA	b	605	65/65	0.96	0.07	24,39,54,60	0
22	CLA	C	501	65/65	0.96	0.07	26,41,54,58	0
22	CLA	b	607	65/65	0.96	0.07	21,40,65,77	0
22	CLA	B	604	65/65	0.96	0.07	26,38,75,80	0
22	CLA	b	609	65/65	0.96	0.08	32,50,71,77	0
22	CLA	b	610	65/65	0.96	0.08	28,42,53,58	0

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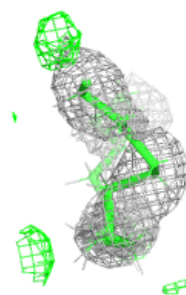
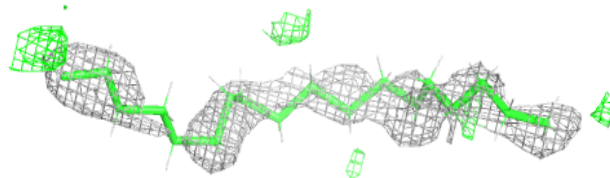
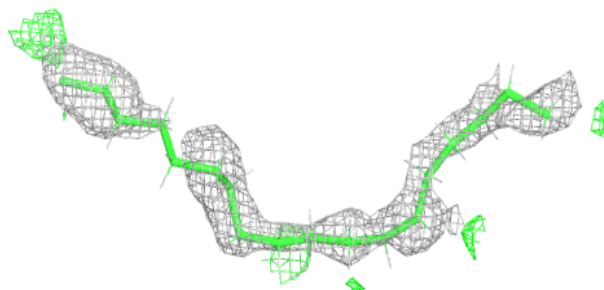
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	CLA	b	611	65/65	0.96	0.07	27,39,57,66	0
22	CLA	b	612	65/65	0.96	0.07	26,39,54,63	0
22	CLA	b	613	65/65	0.96	0.07	26,40,76,83	0
22	CLA	B	605	65/65	0.96	0.07	24,35,49,54	0
22	CLA	C	504	59/65	0.96	0.07	32,47,85,92	0
22	CLA	A	403	65/65	0.96	0.09	26,40,103,112	0
22	CLA	c	501	65/65	0.96	0.07	31,44,54,62	0
22	CLA	B	608	65/65	0.96	0.06	22,39,59,65	0
22	CLA	C	507	65/65	0.96	0.07	27,45,60,65	0
33	LHG	D	408	49/49	0.96	0.07	26,44,56,63	0
29	DGD	c	517	62/66	0.96	0.07	25,46,77,83	0
22	CLA	A	402	65/65	0.96	0.06	21,32,46,56	0
22	CLA	B	610	65/65	0.96	0.07	23,35,47,51	0
22	CLA	B	611	65/65	0.96	0.07	23,35,50,56	0
33	LHG	d	409	49/49	0.96	0.07	30,49,61,71	0
22	CLA	B	612	65/65	0.96	0.07	25,36,50,55	0
22	CLA	B	613	65/65	0.96	0.07	21,35,71,75	0
22	CLA	B	614	65/65	0.96	0.08	26,43,77,92	0
34	BCT	D	402	4/4	0.96	0.09	32,33,37,44	0
22	CLA	D	404	65/65	0.96	0.08	27,47,106,117	0
22	CLA	A	410	65/65	0.97	0.06	20,32,52,58	0
22	CLA	B	607	65/65	0.97	0.07	17,37,68,76	0
22	CLA	B	603	65/65	0.97	0.06	24,38,63,64	0
22	CLA	D	403	65/65	0.97	0.06	22,32,59,60	0
35	HEM	E	101	43/43	0.97	0.08	42,57,75,75	0
35	HEM	f	101	43/43	0.97	0.09	46,64,89,90	0
22	CLA	A	405	54/65	0.98	0.06	20,34,68,73	0
25	CL	a	406	1/1	0.98	0.05	30,30,30,30	0
36	HEC	V	201	43/43	0.98	0.07	24,37,49,51	0
36	HEC	v	201	43/43	0.98	0.06	32,41,52,55	0
31	OEX	a	416[A]	10/10	0.99	0.03	32,38,41,41	10
25	CL	a	407	1/1	0.99	0.08	33,33,33,33	0
25	CL	A	407	1/1	0.99	0.04	33,33,33,33	0
25	CL	A	408	1/1	0.99	0.07	32,32,32,32	0
21	FE2	a	401	1/1	0.99	0.02	37,37,37,37	0
31	OEX	A	416[A]	10/10	0.99	0.03	35,37,41,41	10
30	OEY	A	415[B]	11/11	1.00	0.03	21,26,30,34	11
30	OEY	a	415[B]	11/11	1.00	0.02	25,27,31,37	11
21	FE2	A	401	1/1	1.00	0.02	33,33,33,33	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.

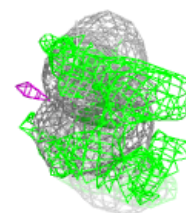
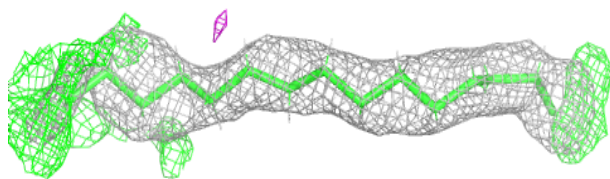
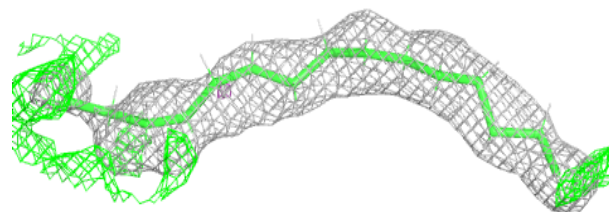
**Electron density around STE H 103:**

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



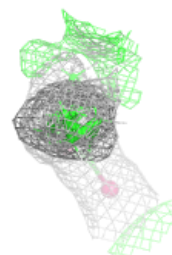
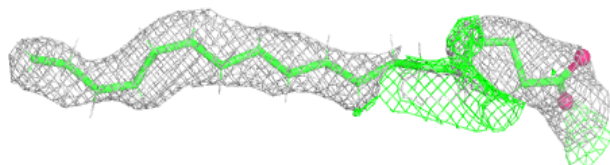
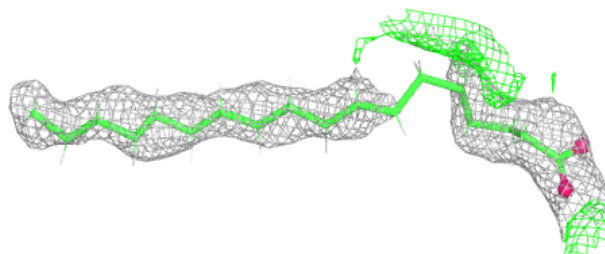
**Electron density around STE I 101:**

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

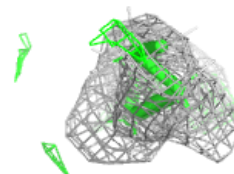
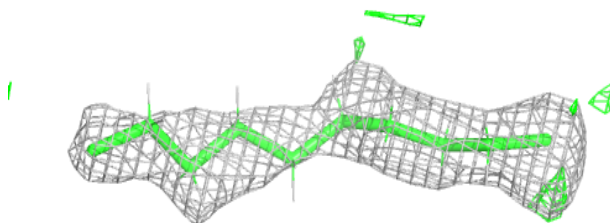
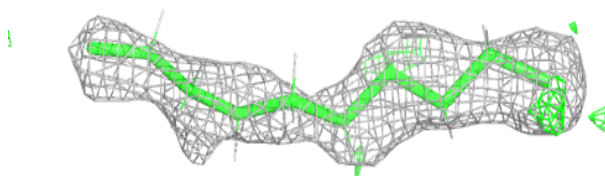


**Electron density around STE b 624:**

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

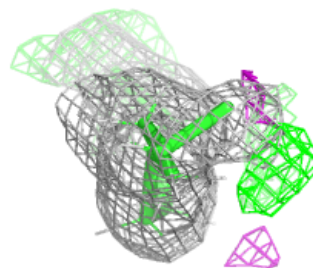
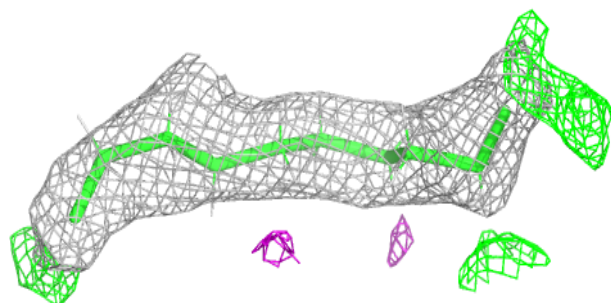
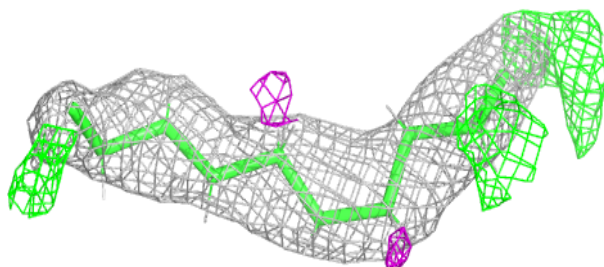
**Electron density around STE a 413:**

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

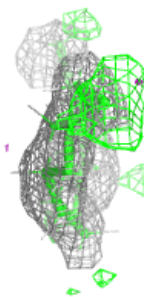
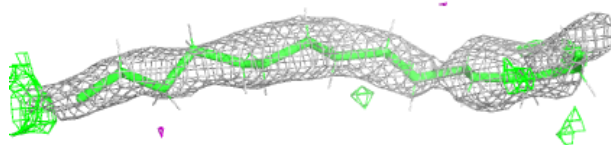


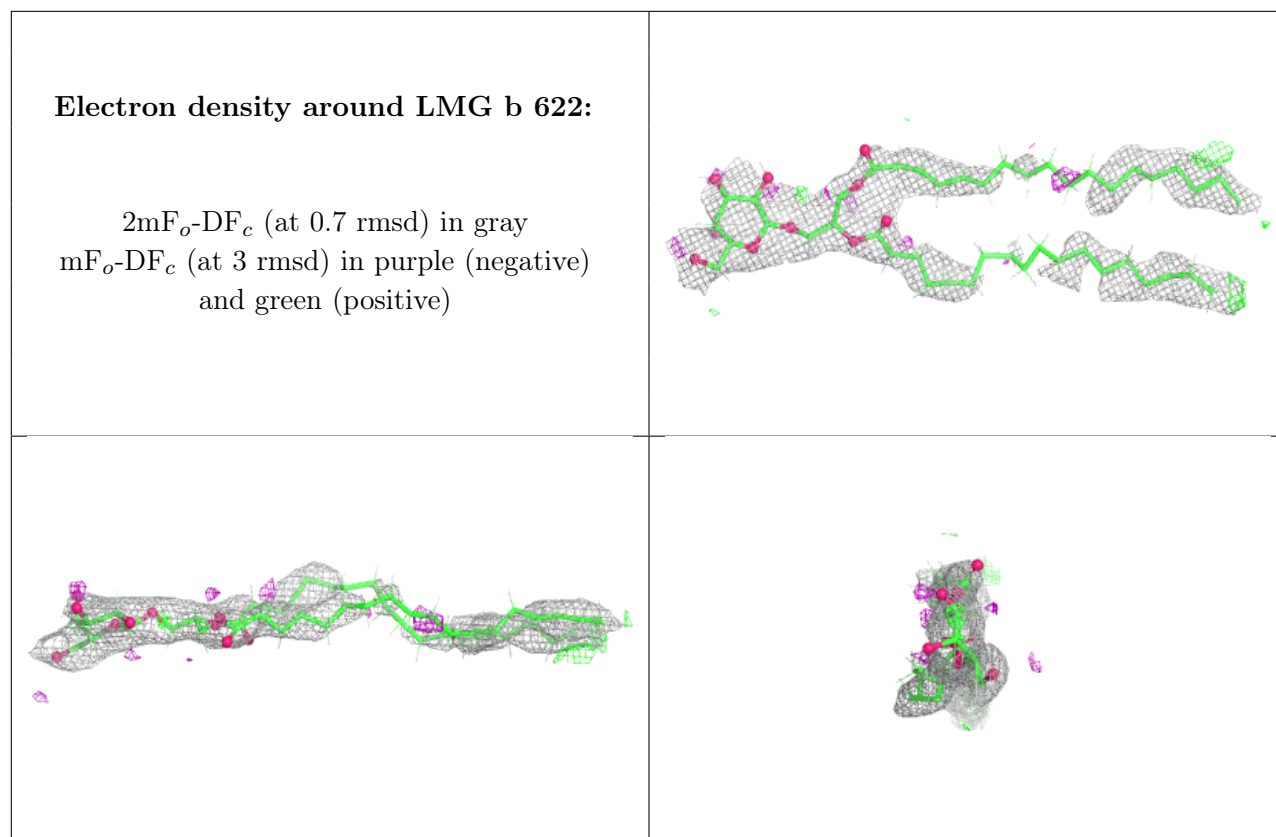
**Electron density around STE b 625:**

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

**Electron density around STE B 626:**

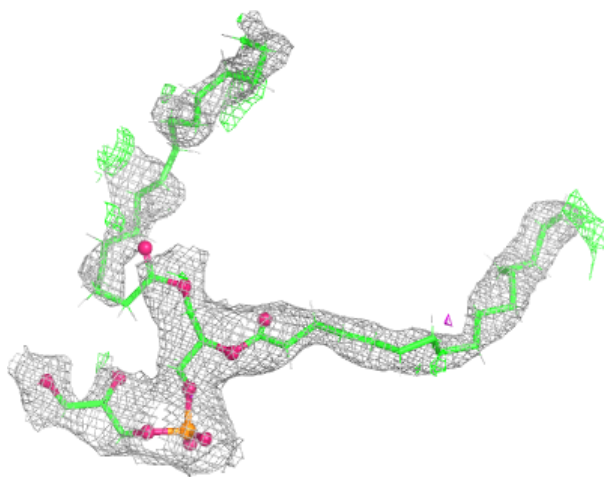
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





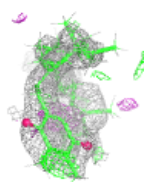
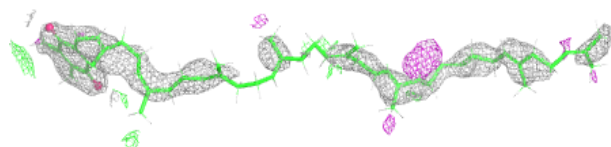
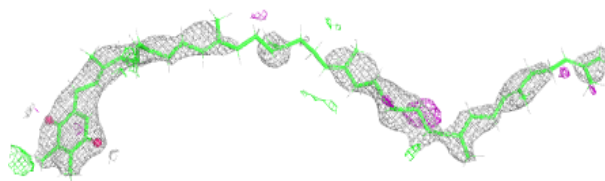
**Electron density around LHG E 102:**

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and green (positive)

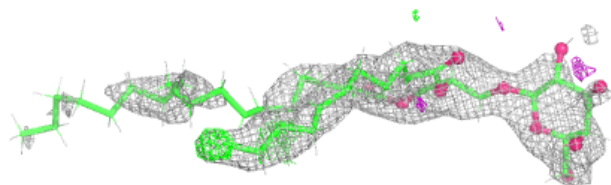


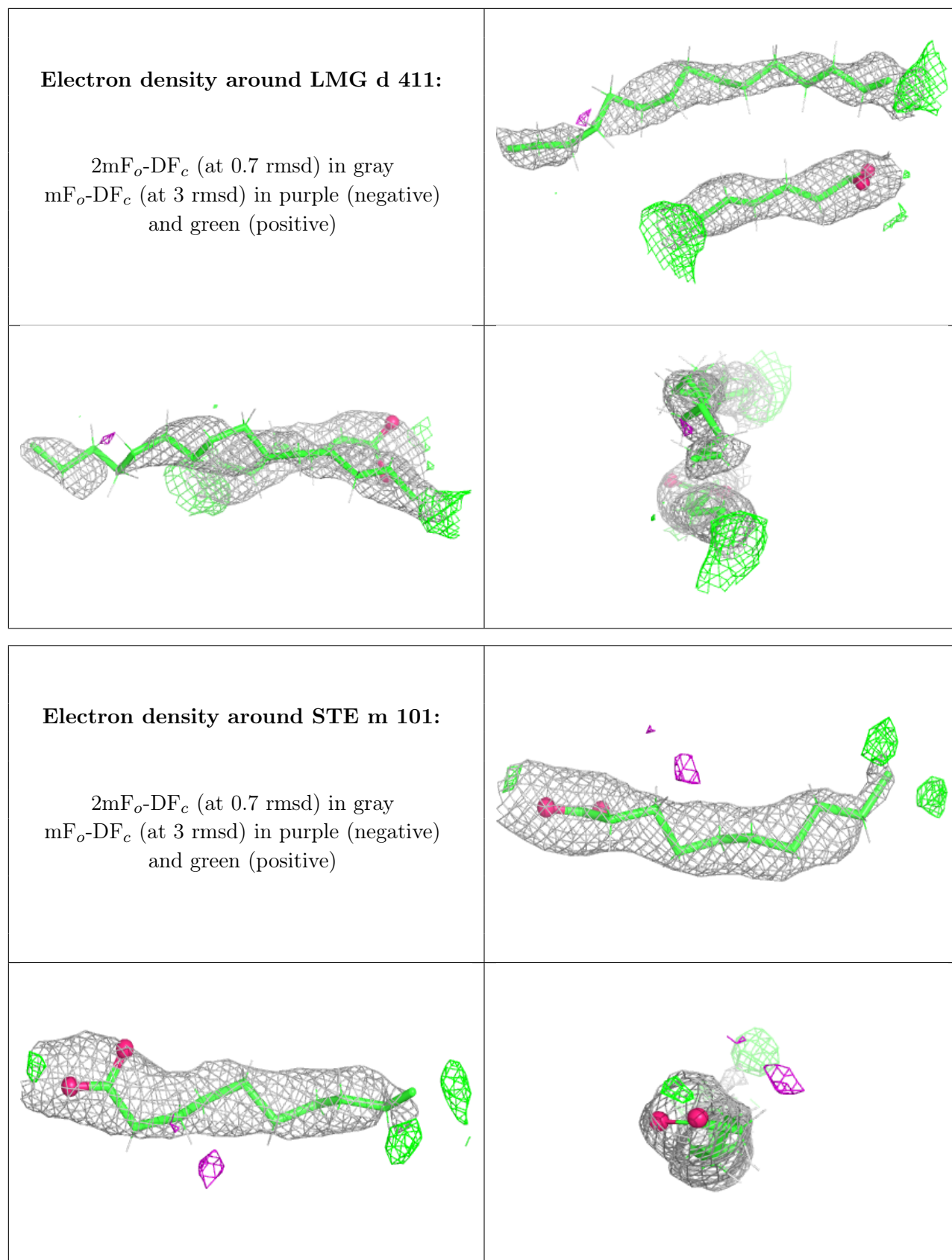
**Electron density around PL9 A 409:**

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

**Electron density around LMG c 522:**

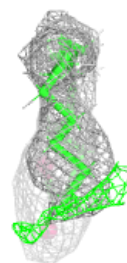
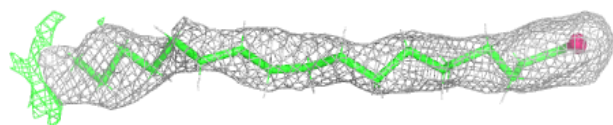
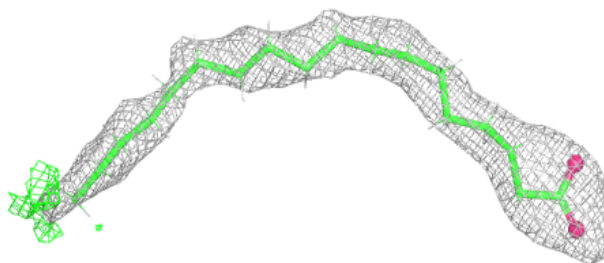
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



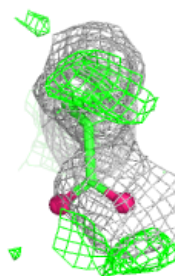
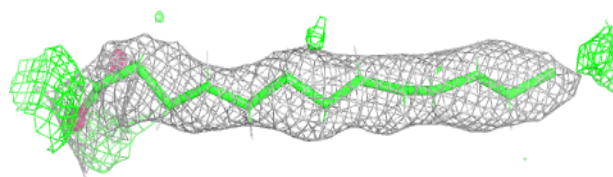
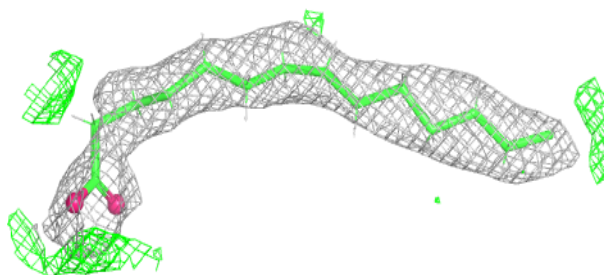


**Electron density around STE x 101:**

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

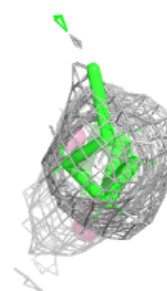
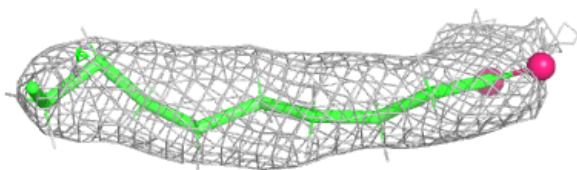
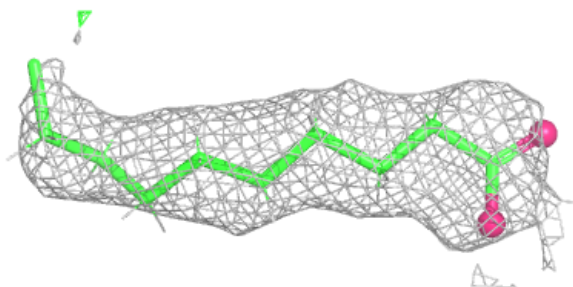
**Electron density around STE b 623:**

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

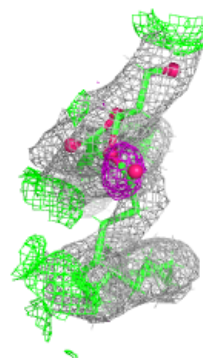
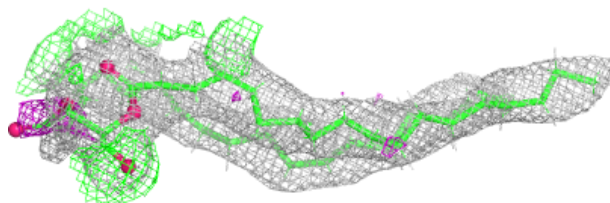
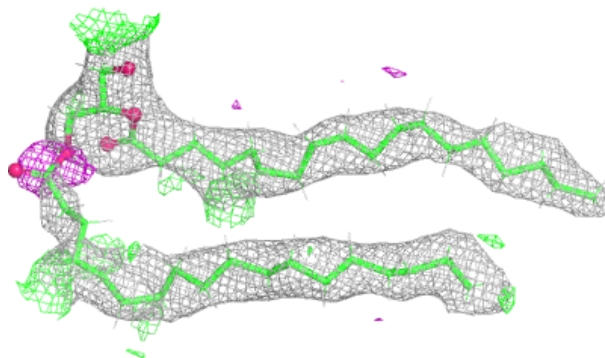


**Electron density around STE c 524:**

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

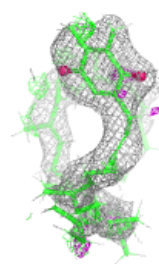
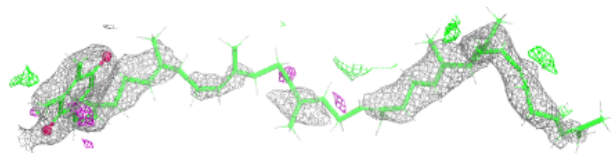
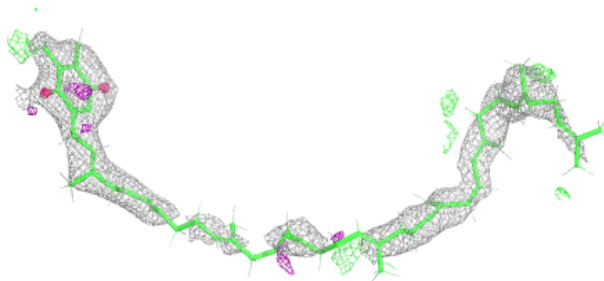
**Electron density around DGD a 412:**

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

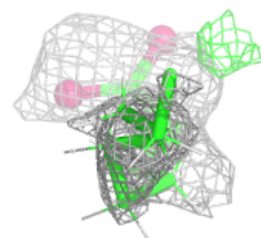
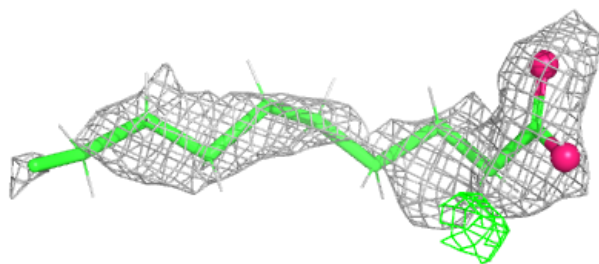
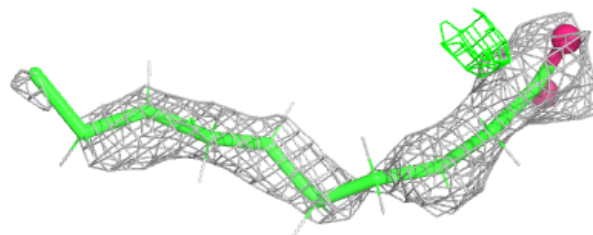


**Electron density around PL9 a 409:**

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

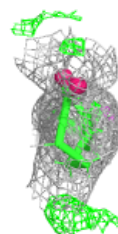
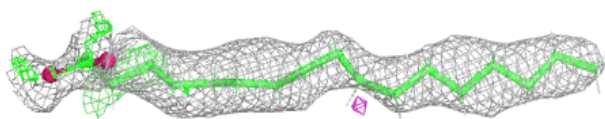
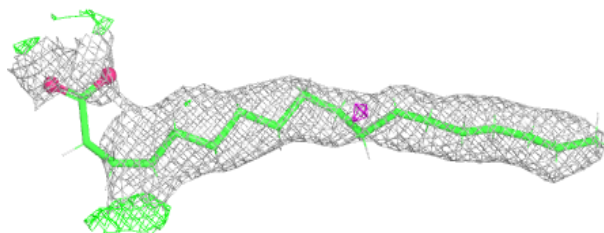
**Electron density around STE E 103:**

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

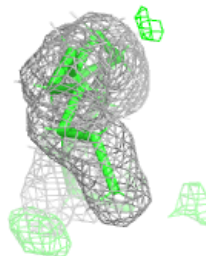
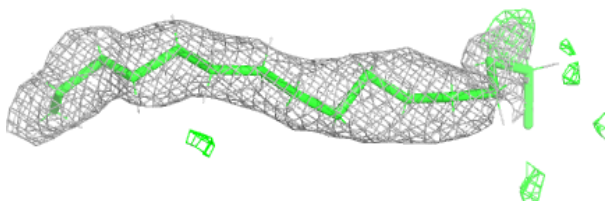
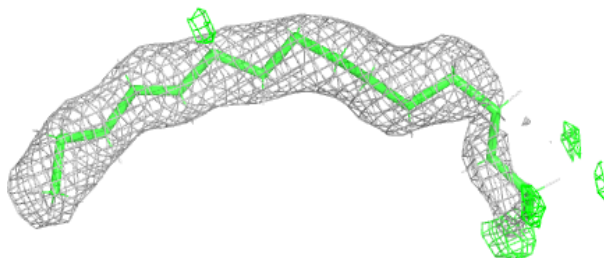


**Electron density around STE c 521:**

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

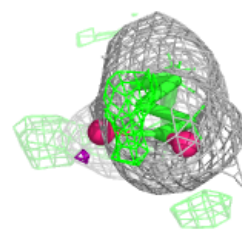
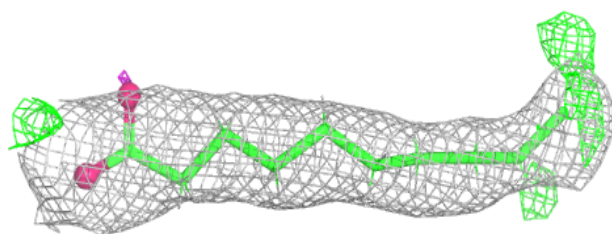
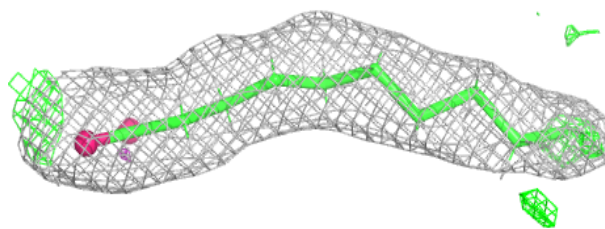
**Electron density around STE T 102:**

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

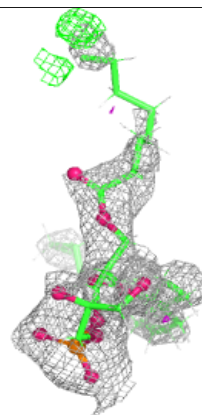
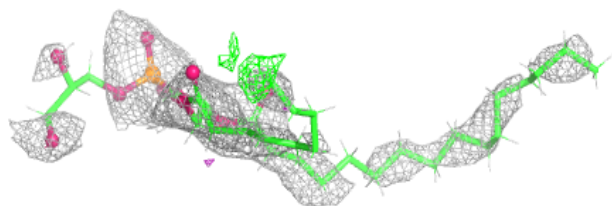
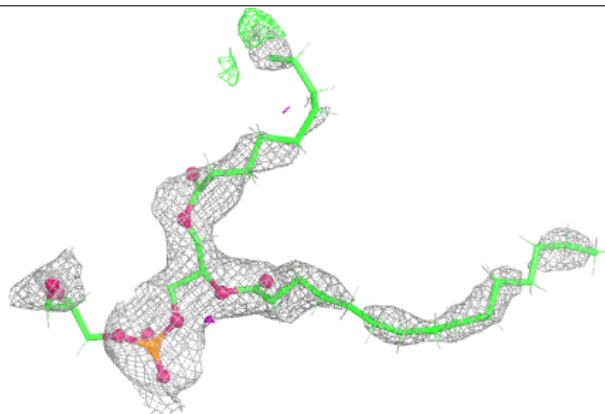


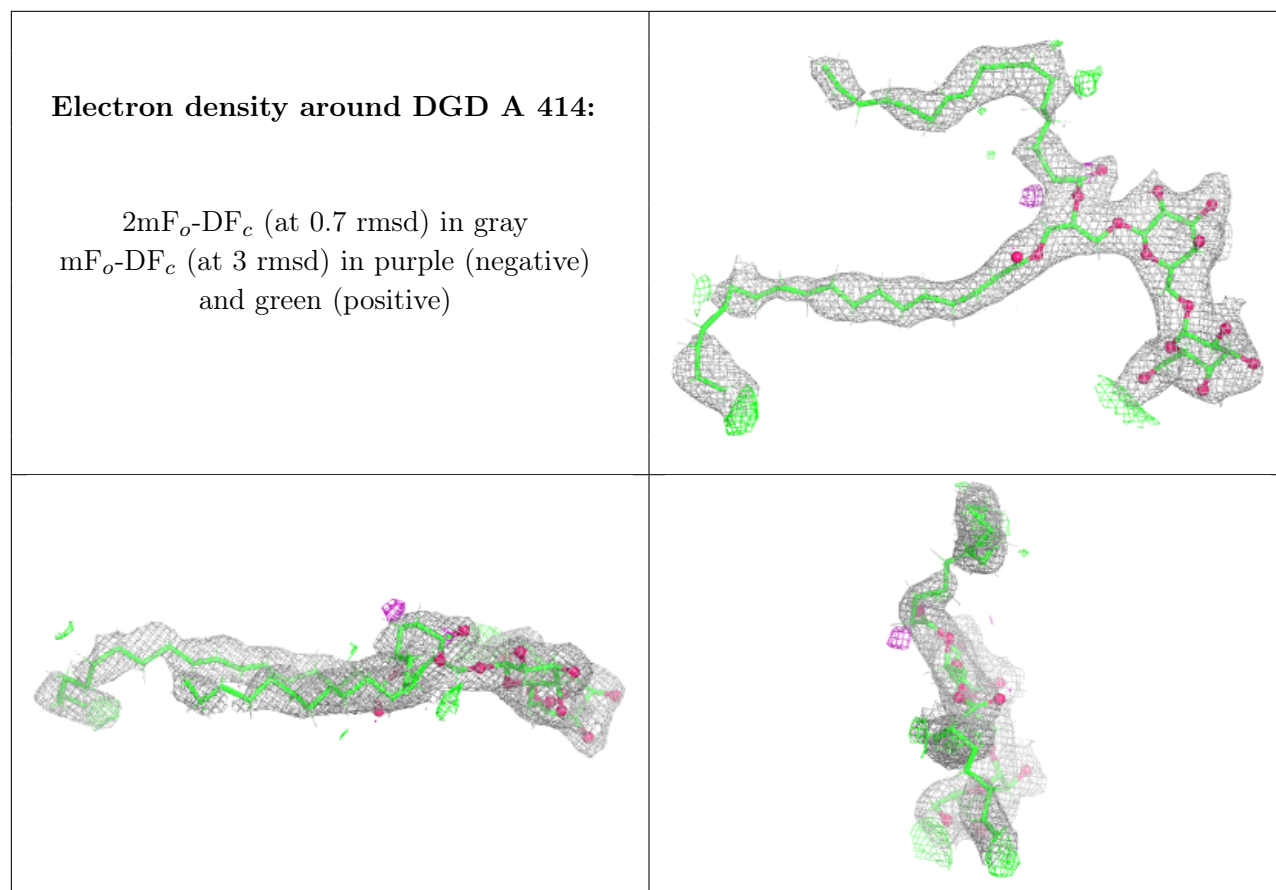
**Electron density around STE j 101:**

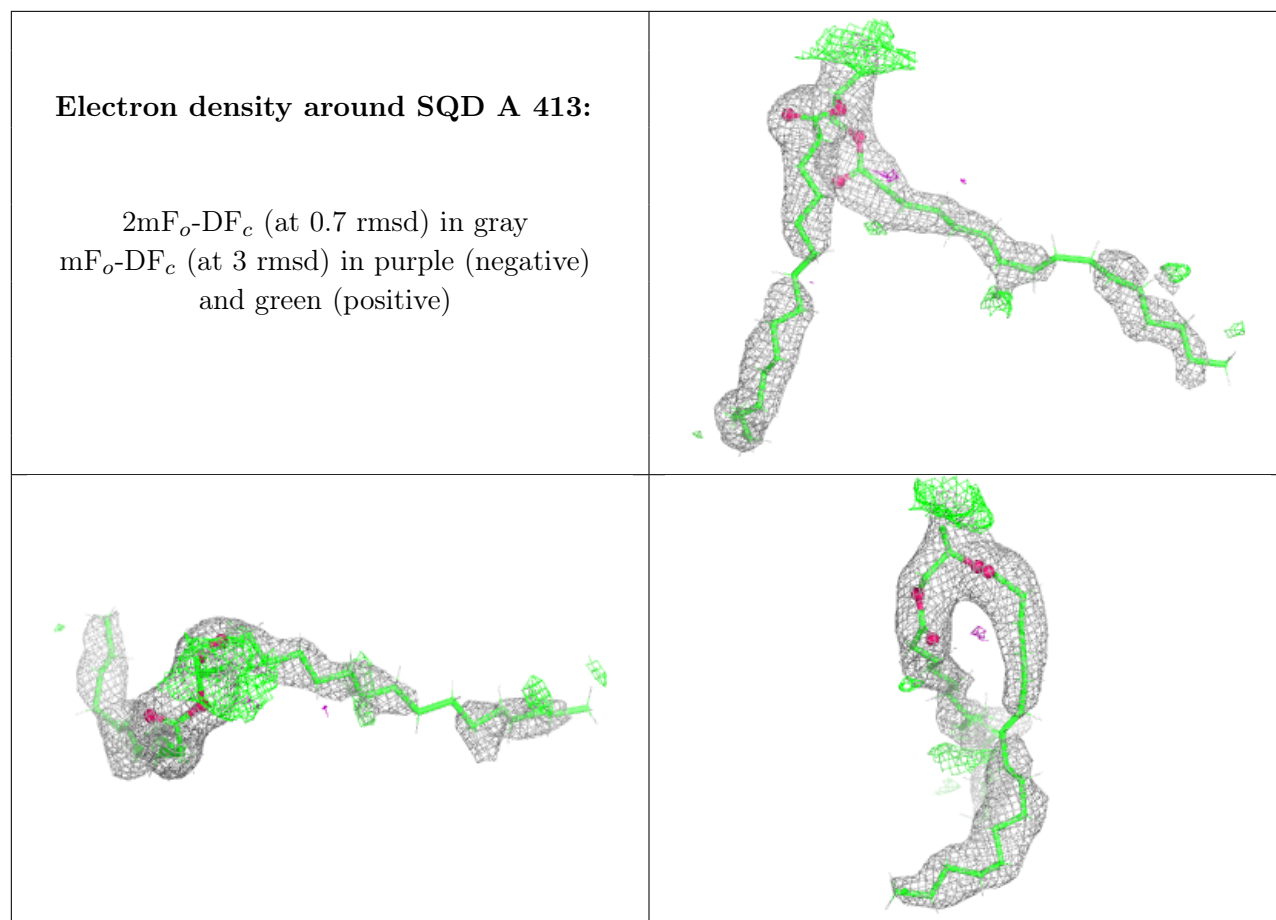
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LHG e 101:**

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

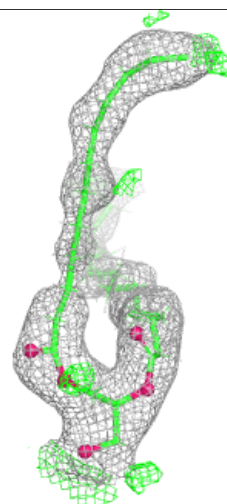
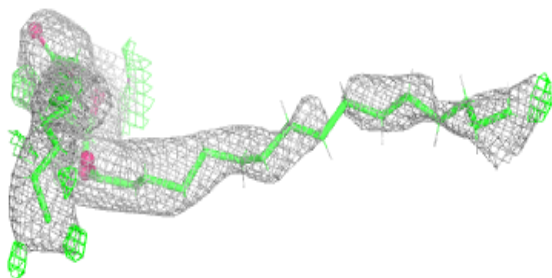






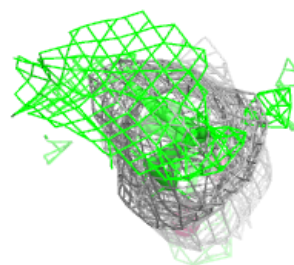
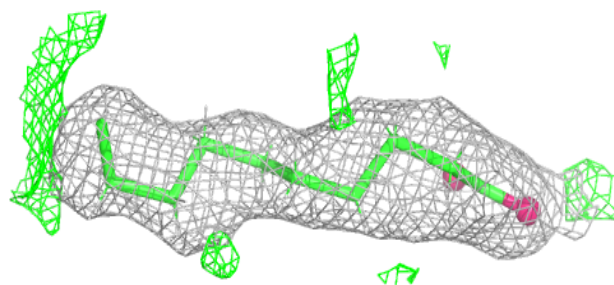
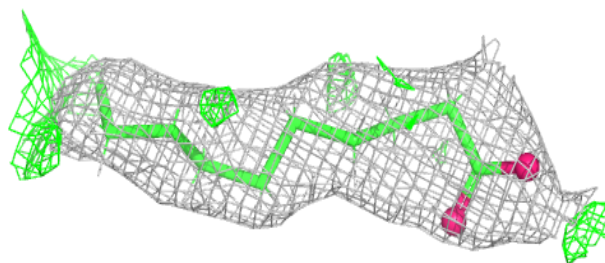
**Electron density around SQD a 411:**

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

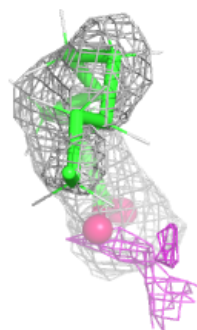
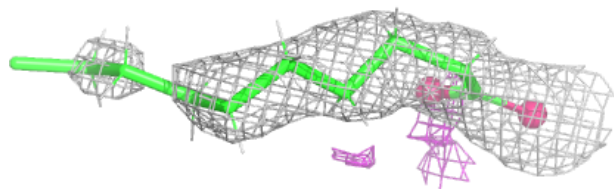
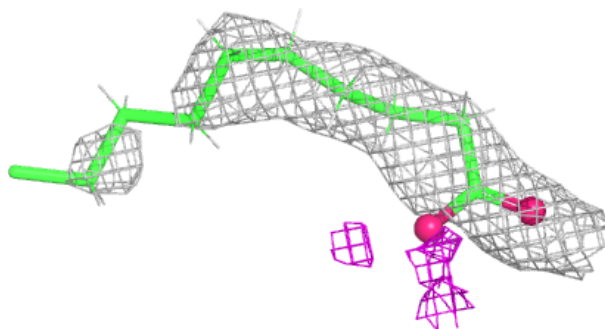


**Electron density around STE J 101:**

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

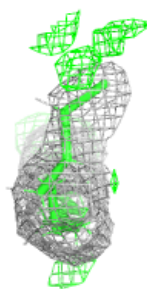
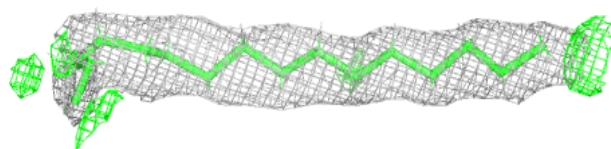
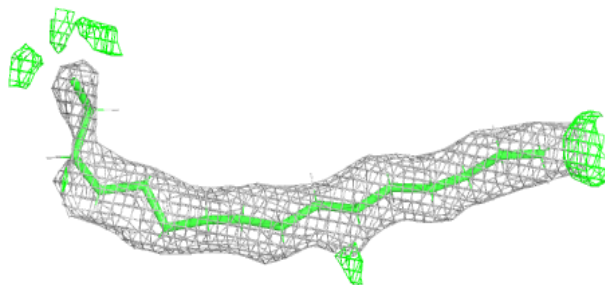
**Electron density around STE B 627:**

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

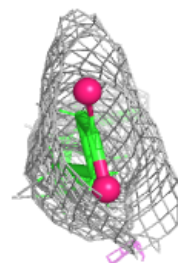
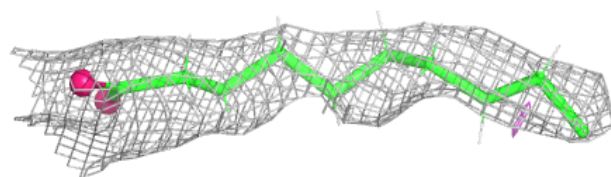
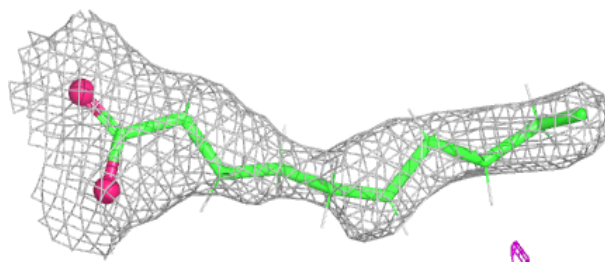


**Electron density around STE C 521:**

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

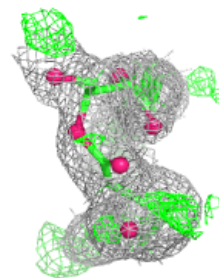
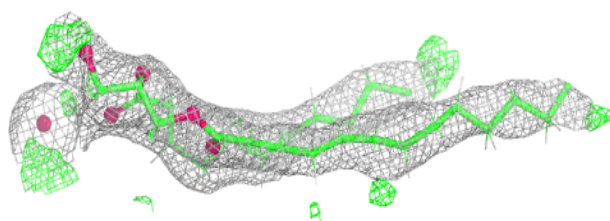
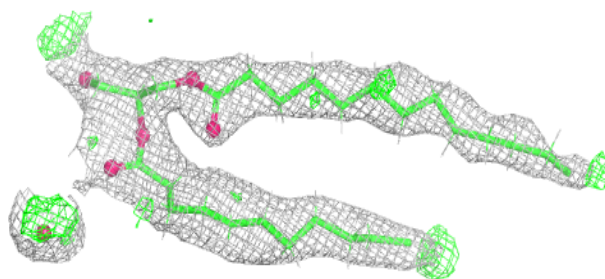
**Electron density around STE a 414:**

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

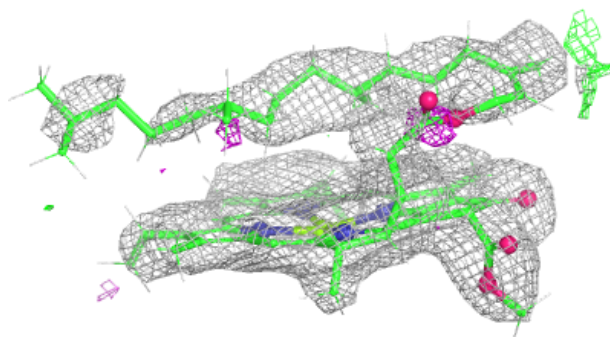
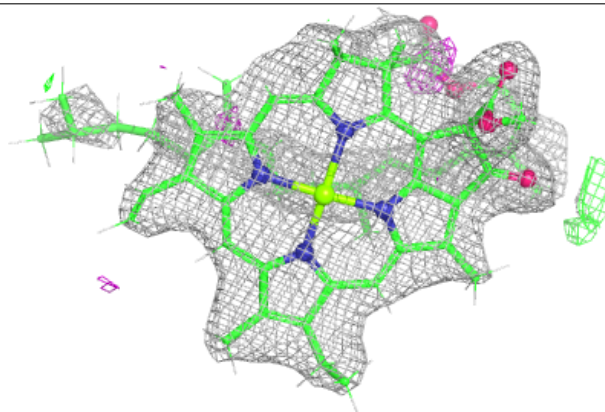


**Electron density around LMG D 410:**

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

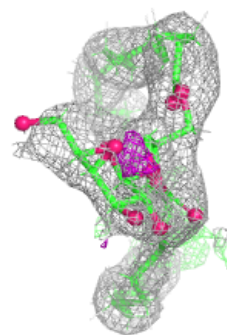
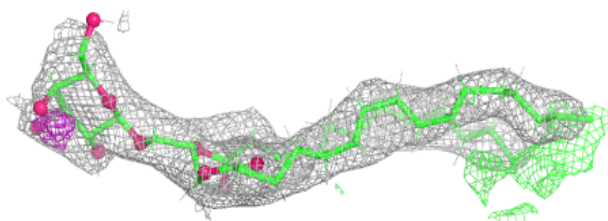
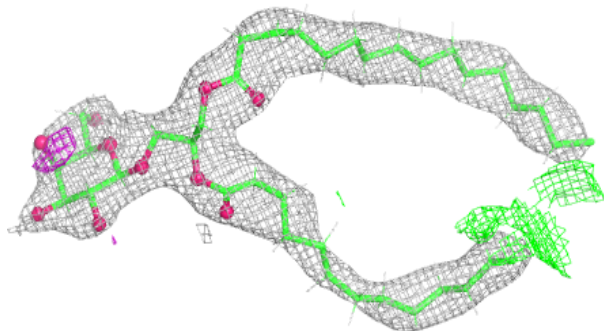
**Electron density around CLA b 601:**

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

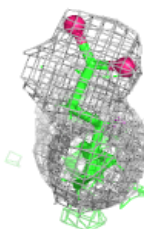
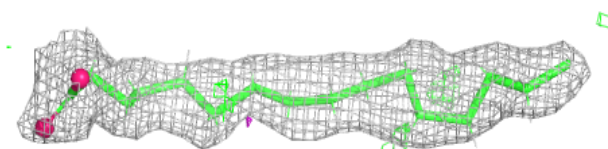
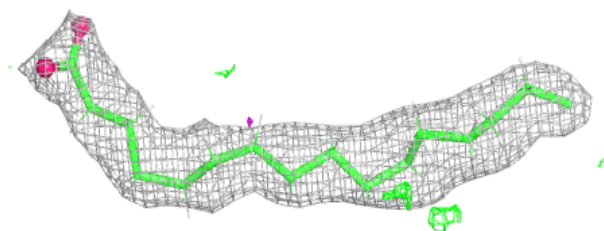


**Electron density around LMG A 411:**

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

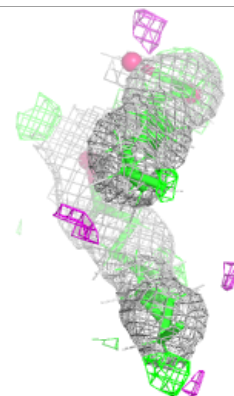
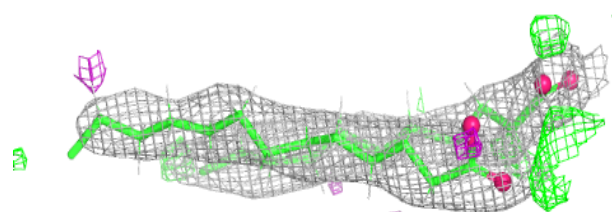
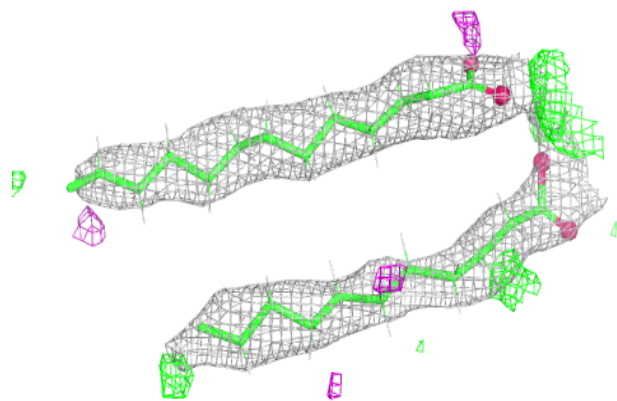
**Electron density around STE B 625:**

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

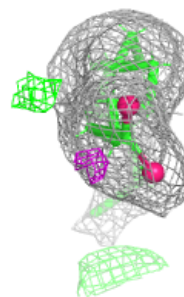
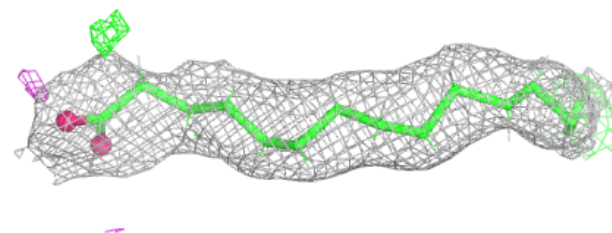
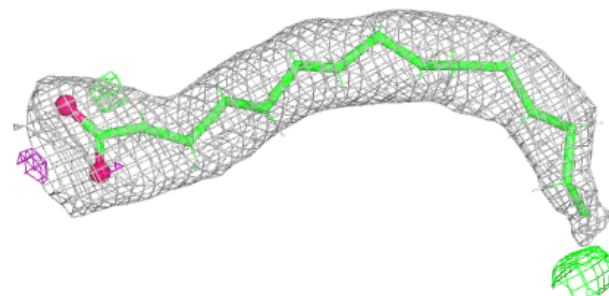


**Electron density around LMG B 621:**

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

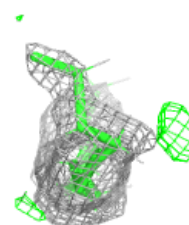
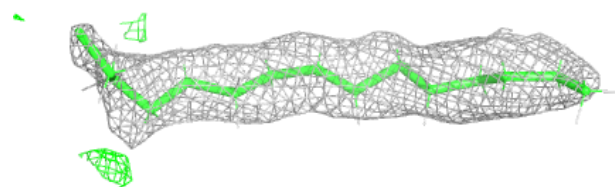
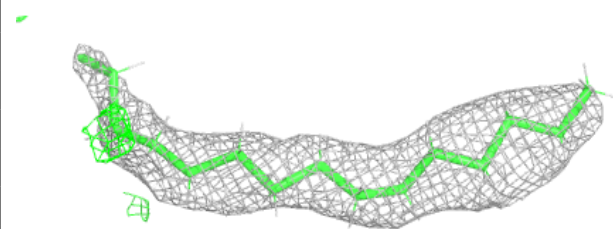
**Electron density around STE B 620:**

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

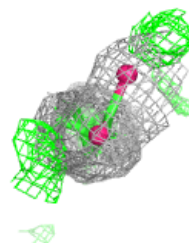
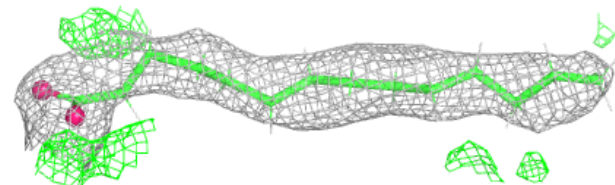
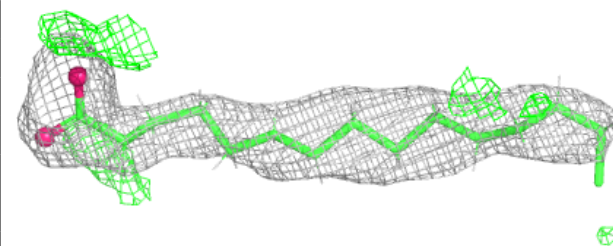


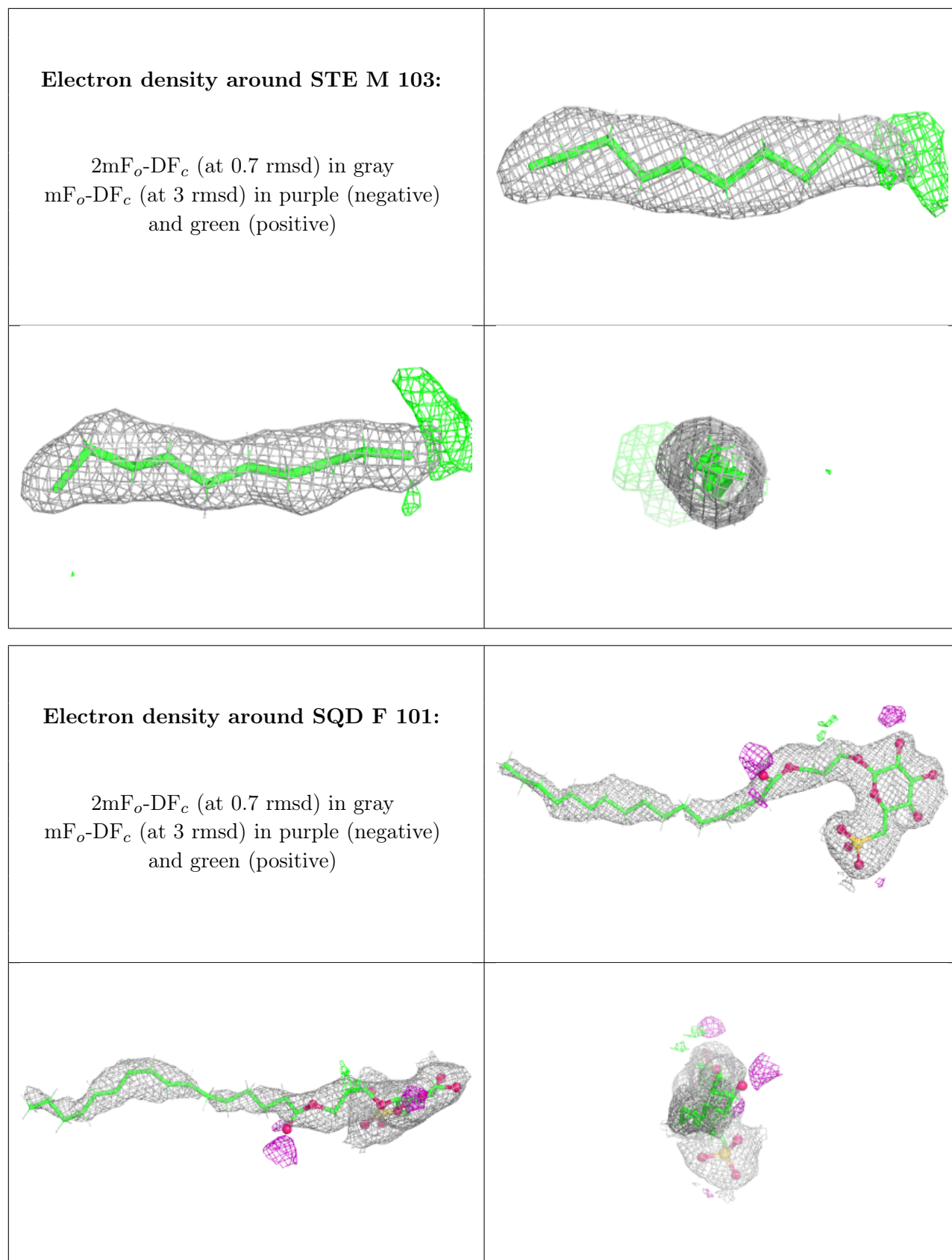
**Electron density around STE T 103:**

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

**Electron density around STE d 413:**

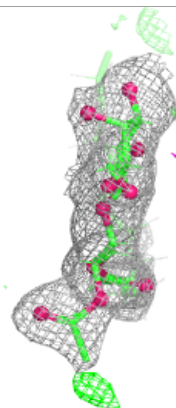
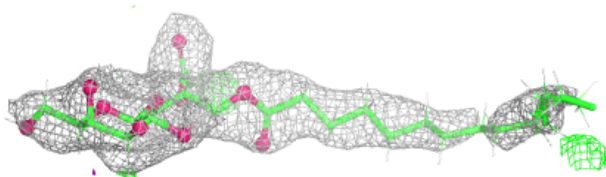
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



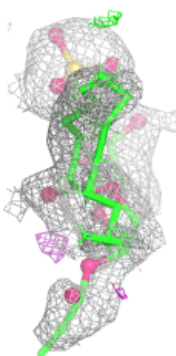
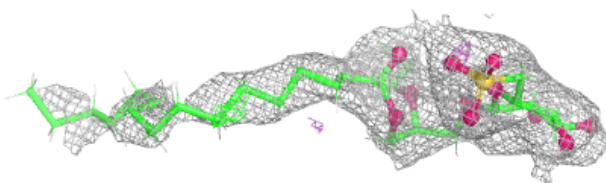
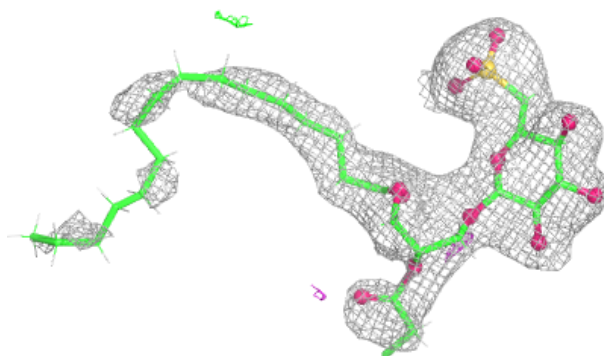


**Electron density around LMG c 520:**

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

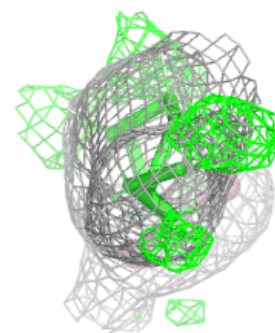
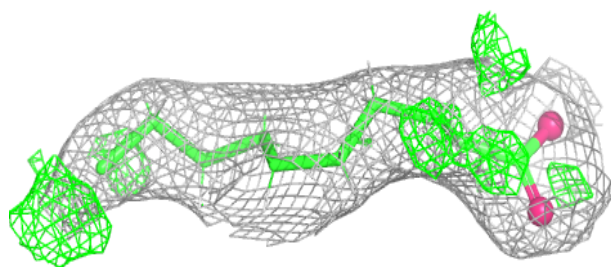
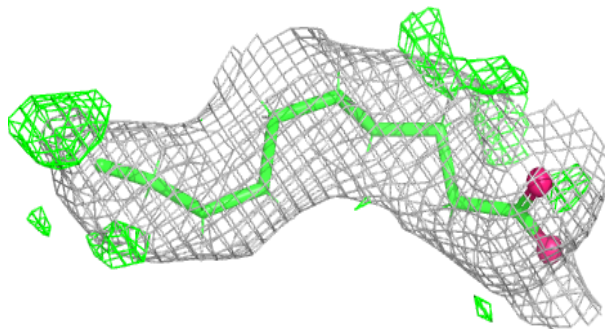
**Electron density around SQD f 102:**

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

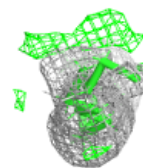
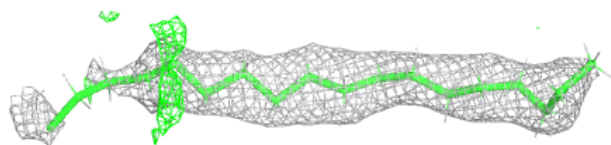
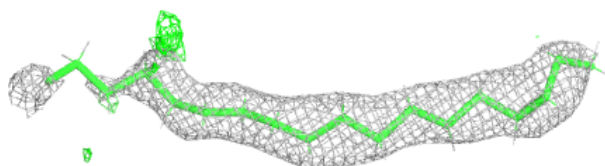


**Electron density around STE B 624:**

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

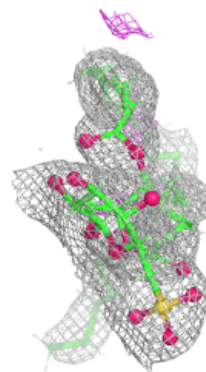
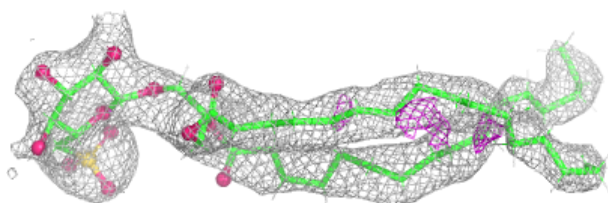
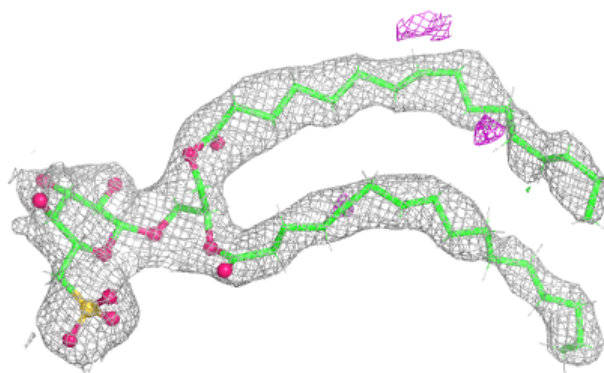
**Electron density around STE I 102:**

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

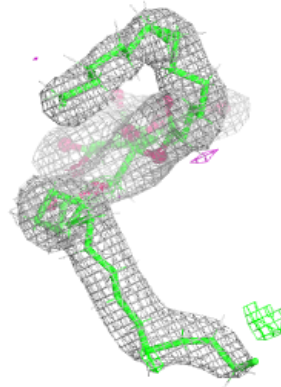
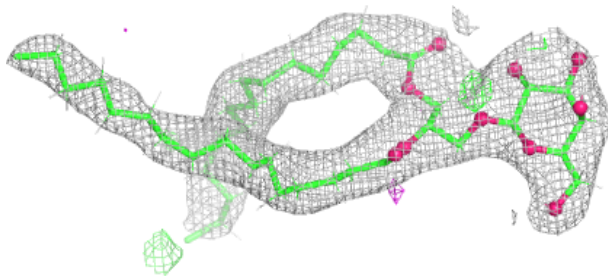
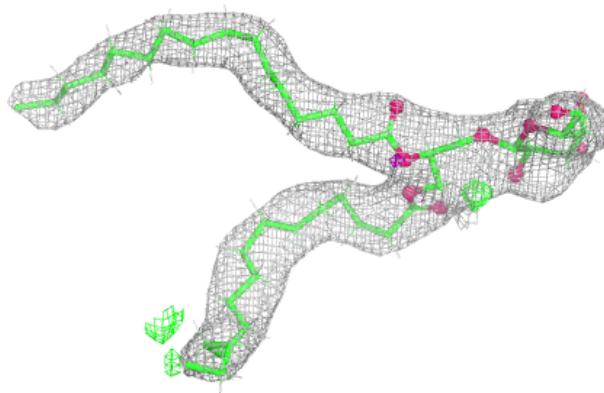


**Electron density around SQD B 623:**

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

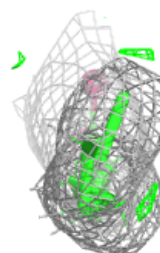
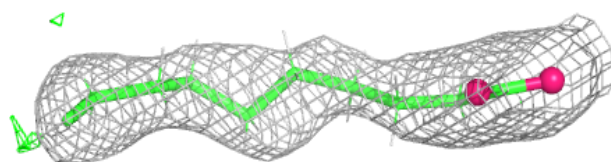
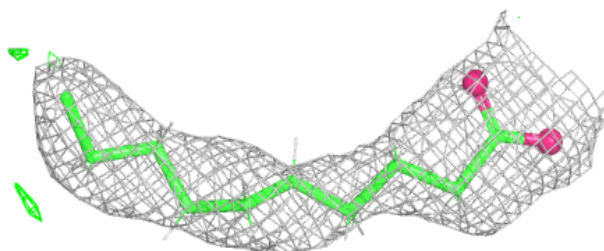
**Electron density around LMG b 620:**

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



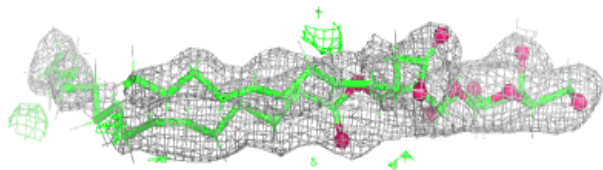
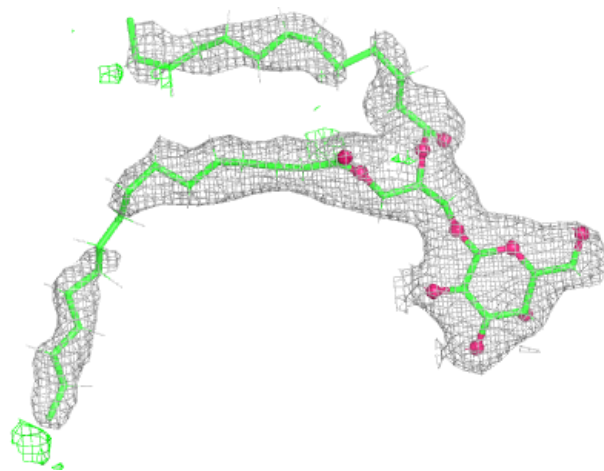
**Electron density around STE C 520:**

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



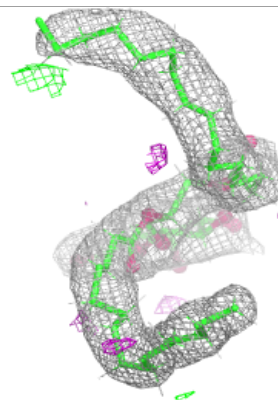
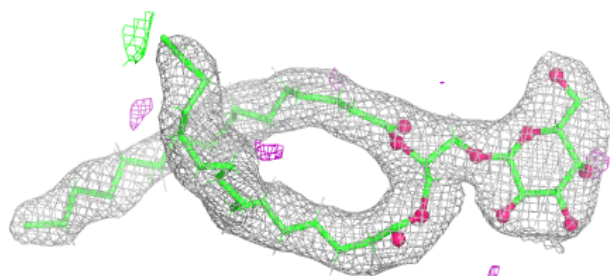
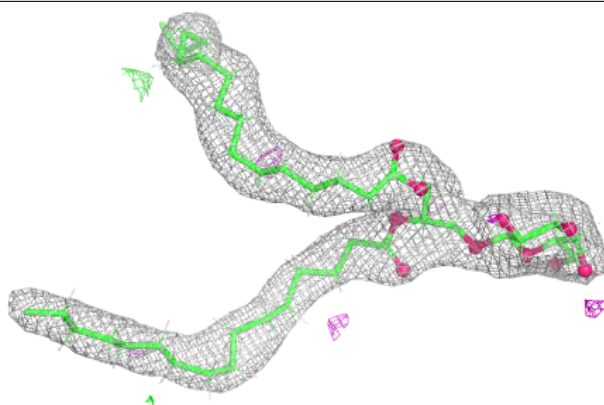
**Electron density around LMG C 519:**

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

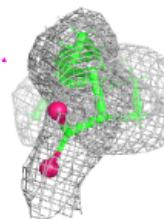
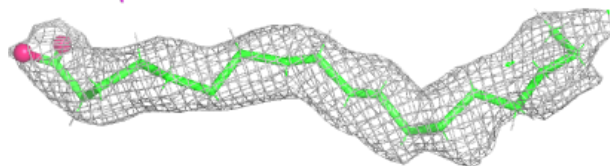
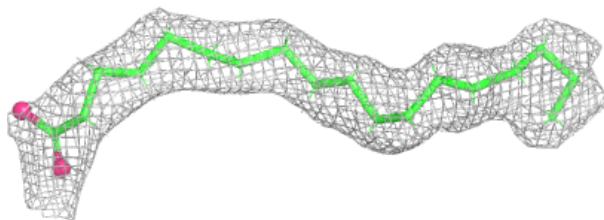


**Electron density around LMG M 101:**

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

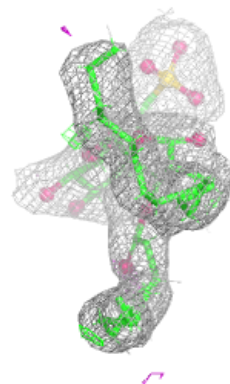
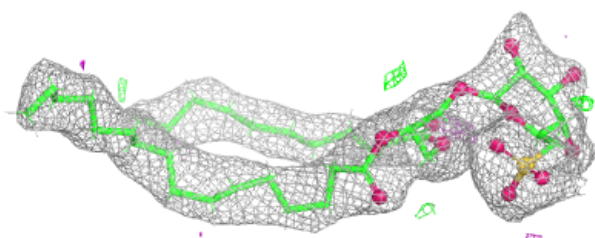
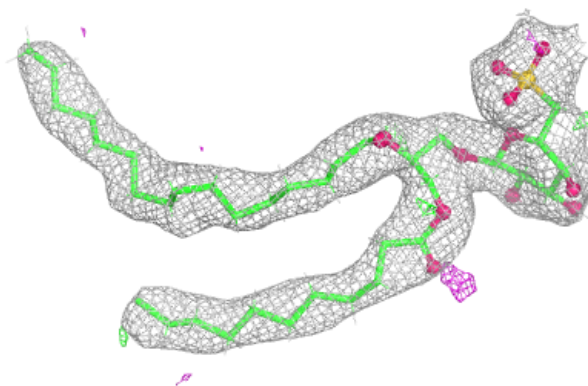
**Electron density around STE b 621:**

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

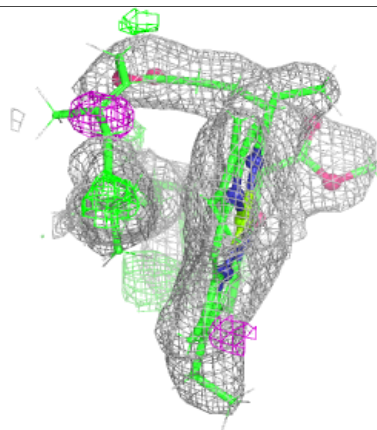
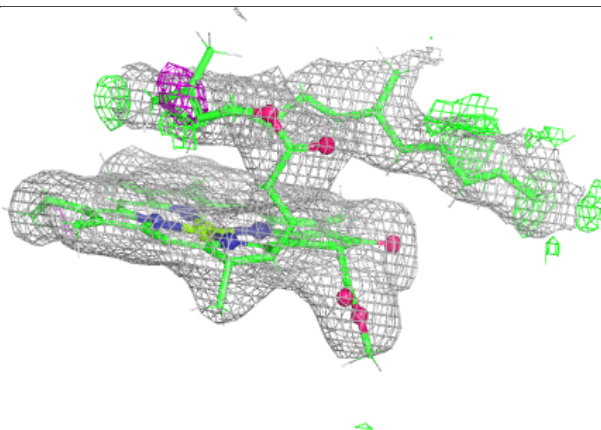
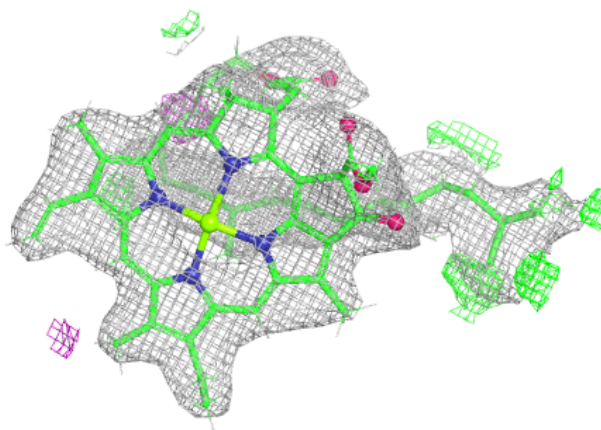


**Electron density around SQD L 101:**

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

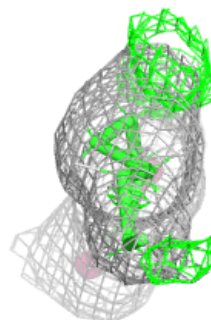
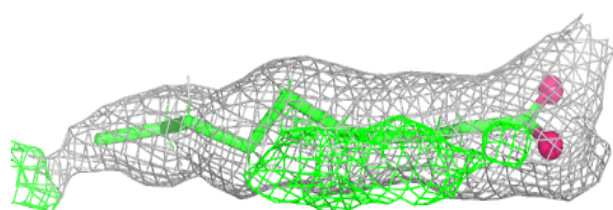
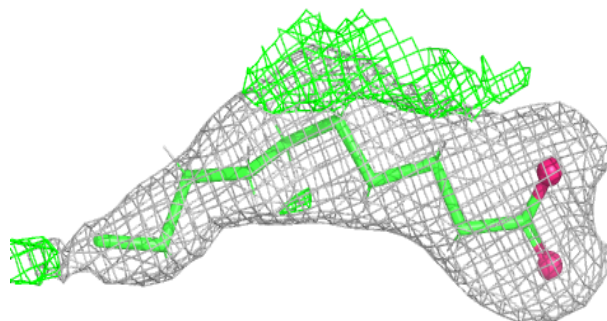
**Electron density around CLA B 601:**

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

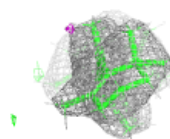
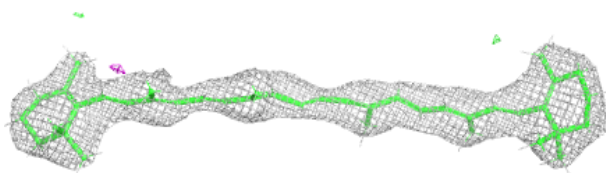
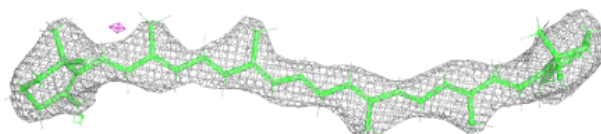


**Electron density around STE C 522:**

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

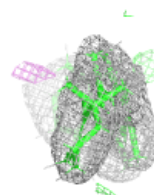
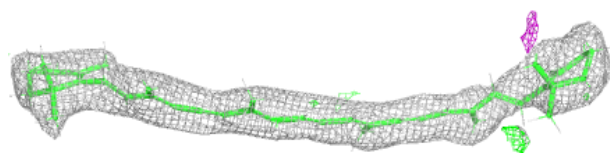
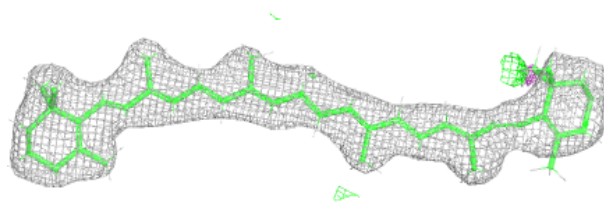
**Electron density around BCR c 514:**

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

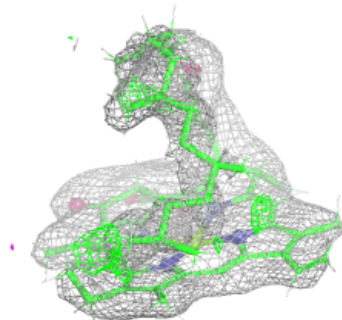
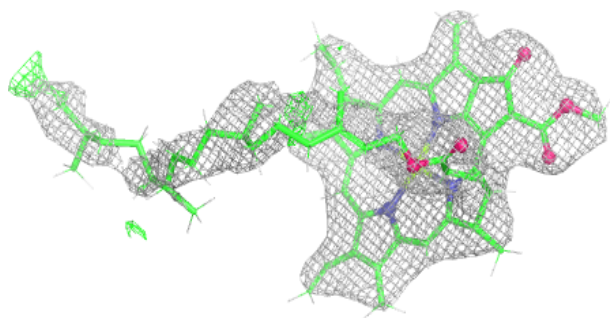
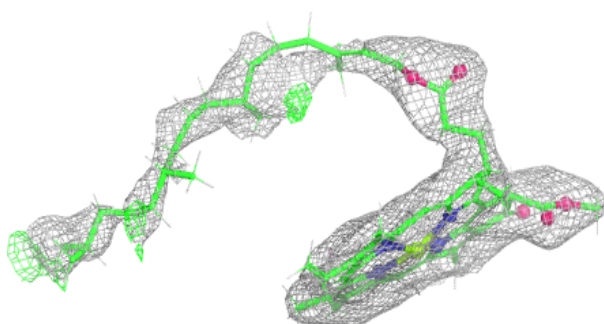


**Electron density around BCR d 406:**

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

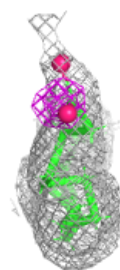
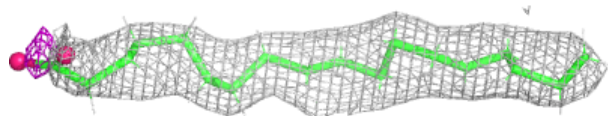
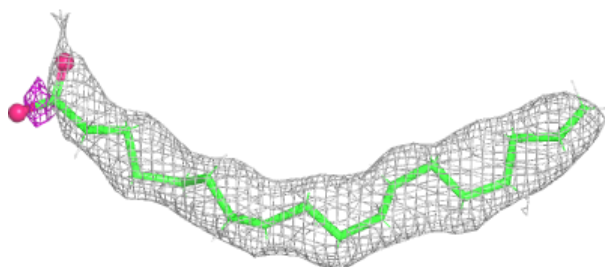
**Electron density around CLA C 513:**

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

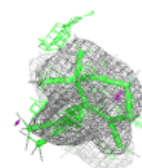
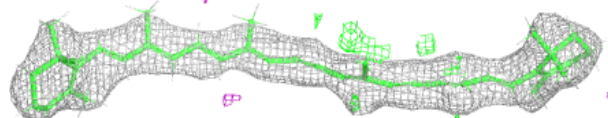
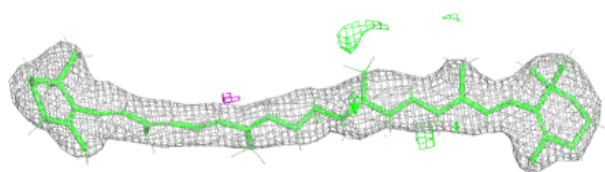


**Electron density around STE D 411:**

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

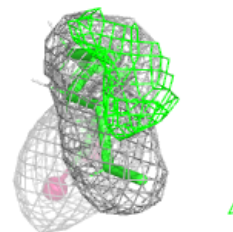
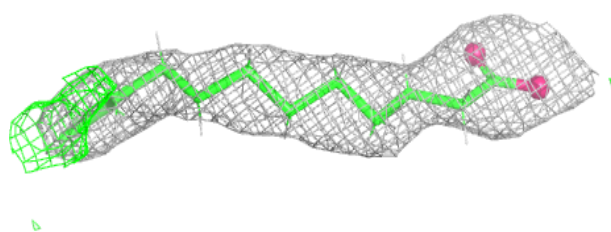
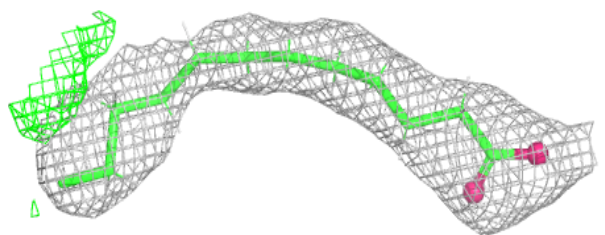
**Electron density around BCR K 101:**

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

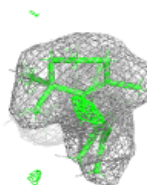
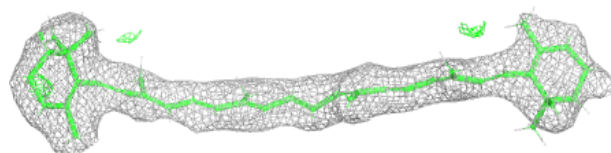
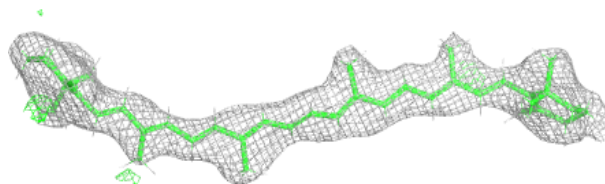


**Electron density around STE t 102:**

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

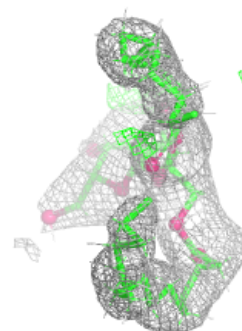
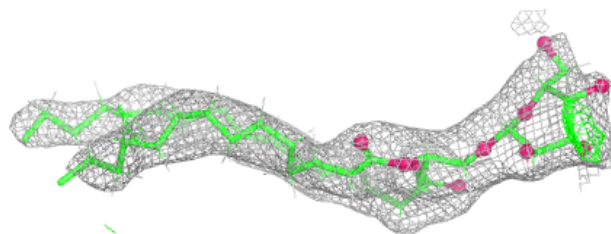
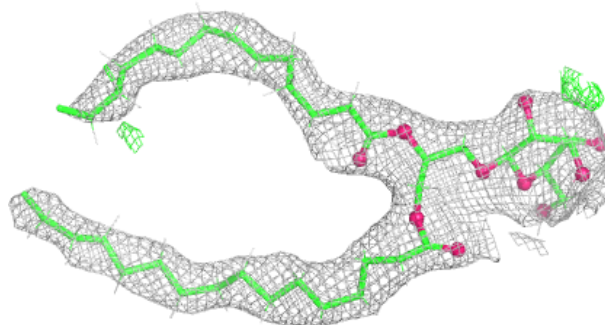
**Electron density around BCR h 101:**

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

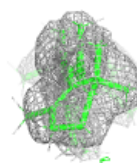
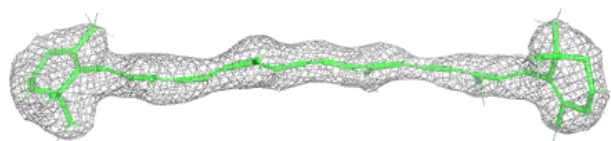


**Electron density around LMG c 523:**

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

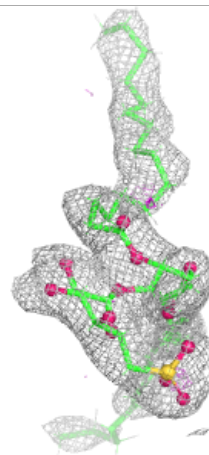
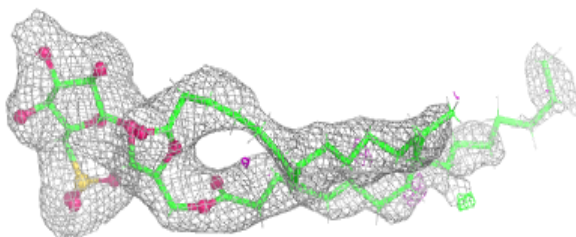
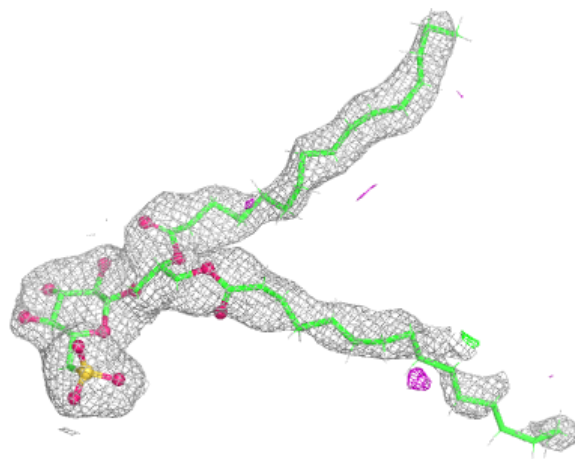
**Electron density around BCR k 101:**

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



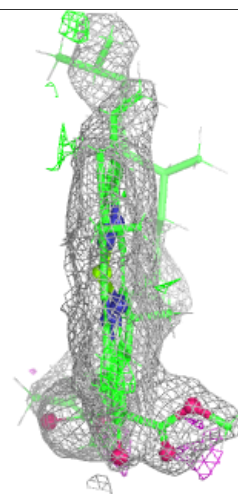
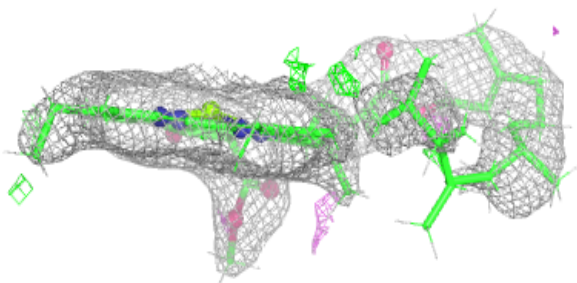
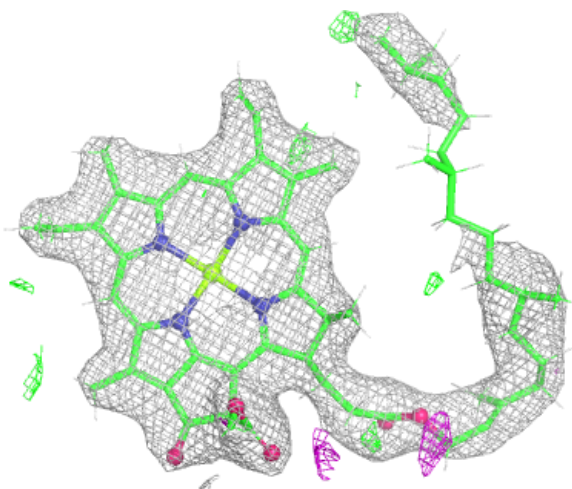
**Electron density around SQD a 410:**

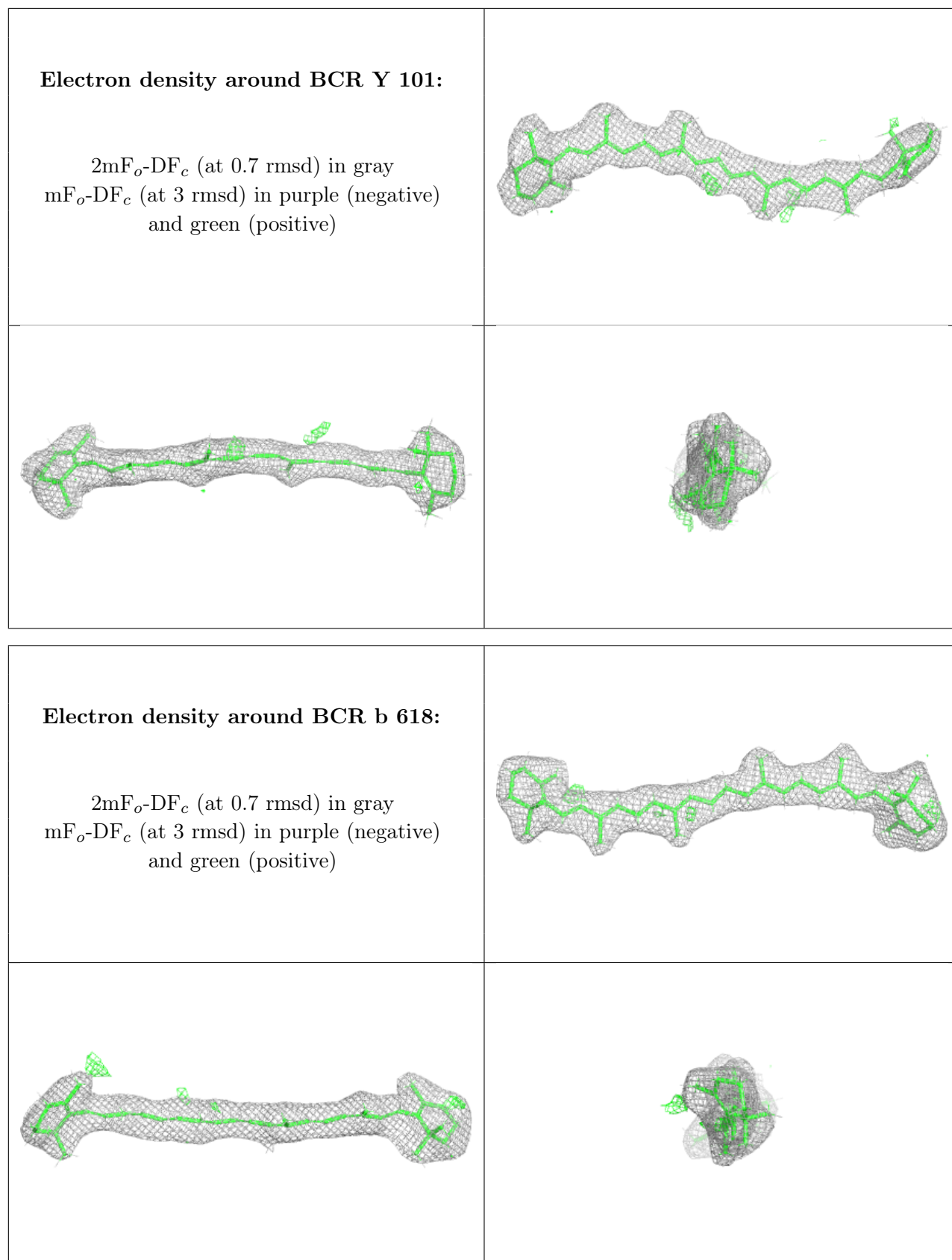
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA c 512:**

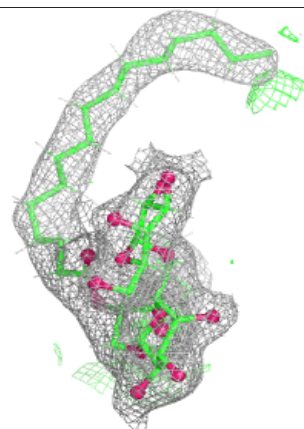
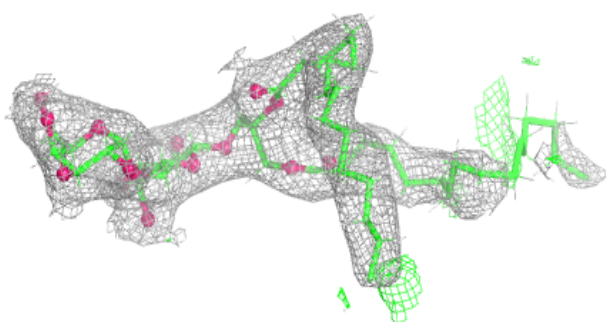
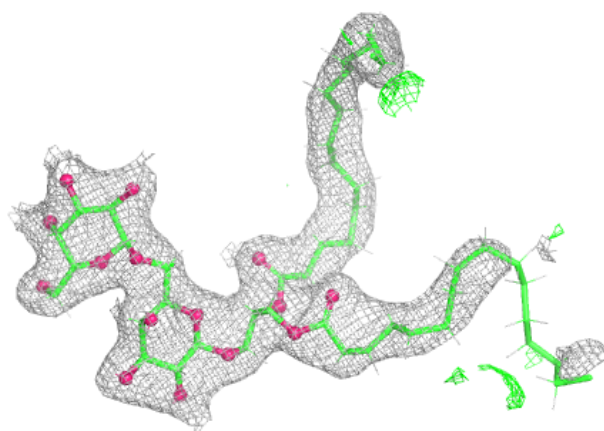
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



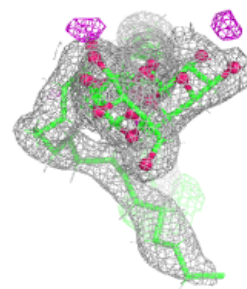
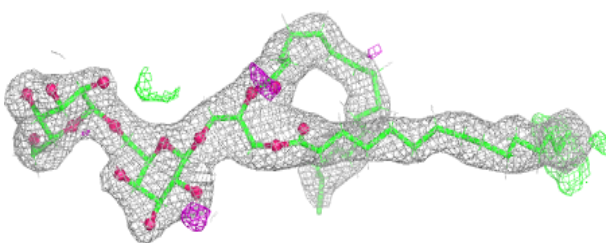
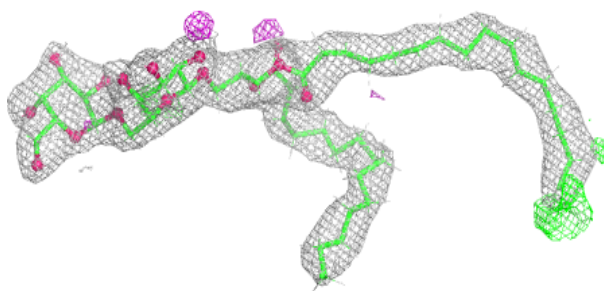


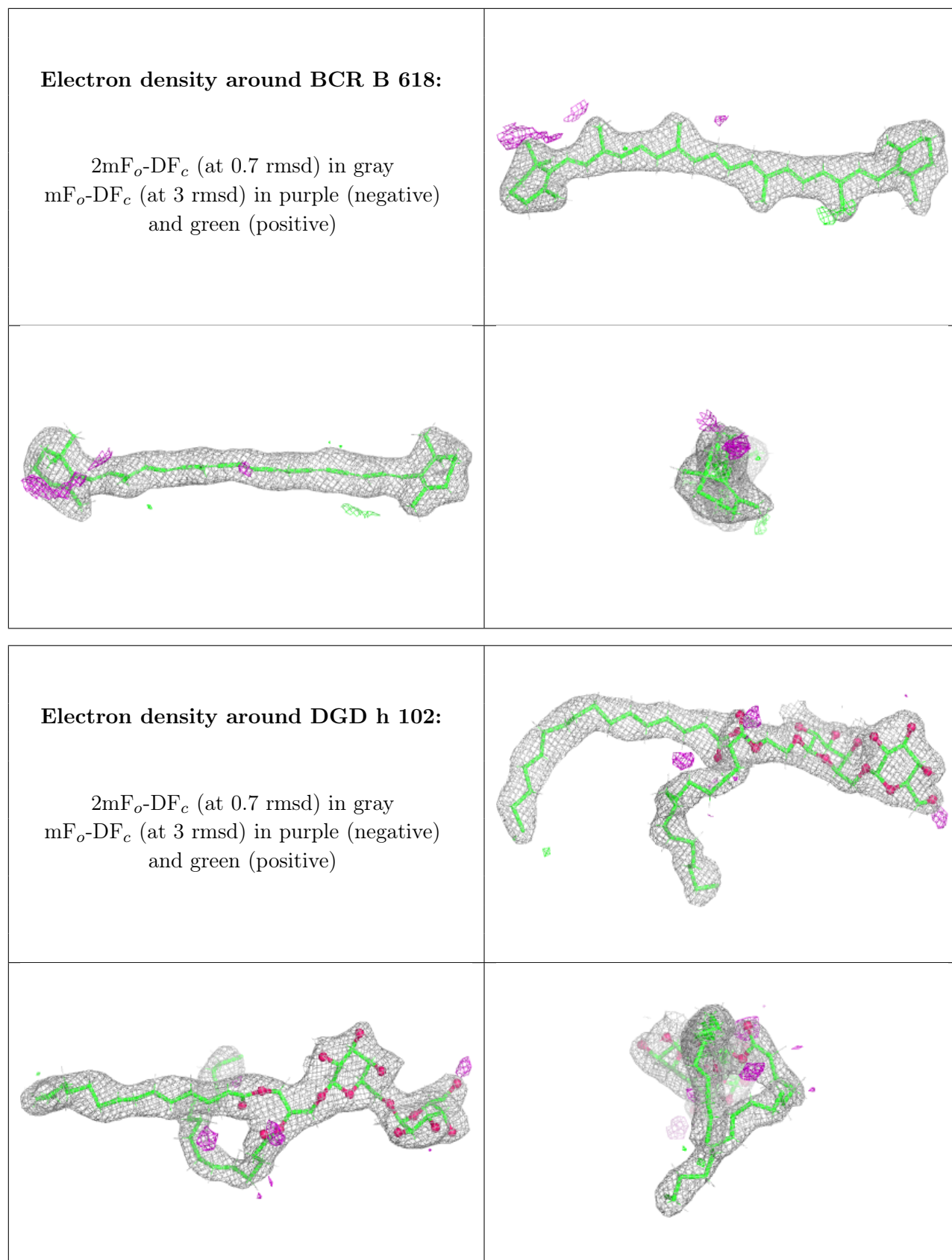
**Electron density around DGD C 517:**

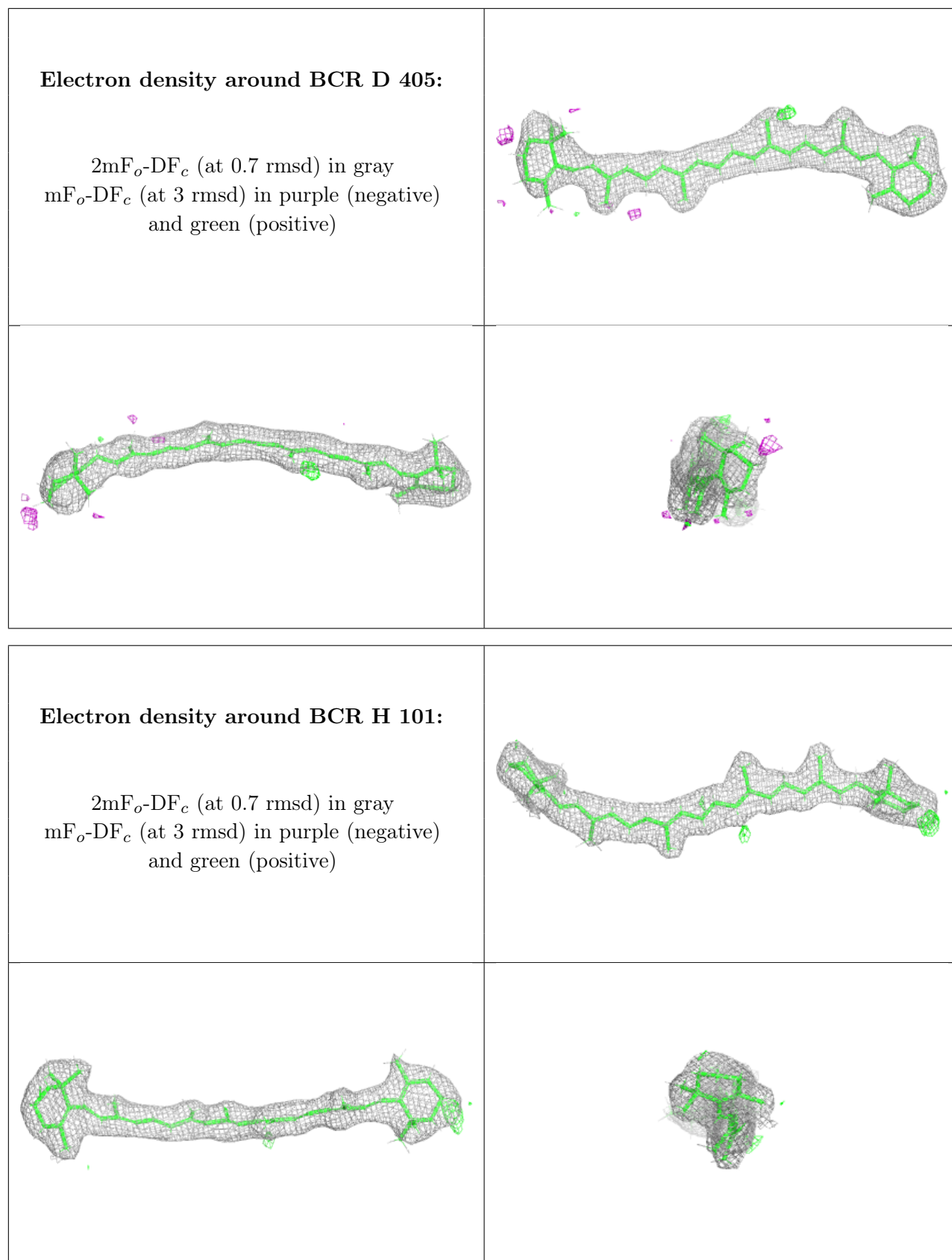
$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)

**Electron density around DGD H 102:**

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

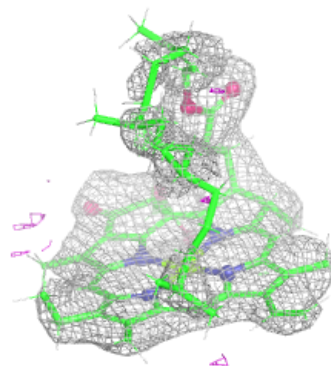
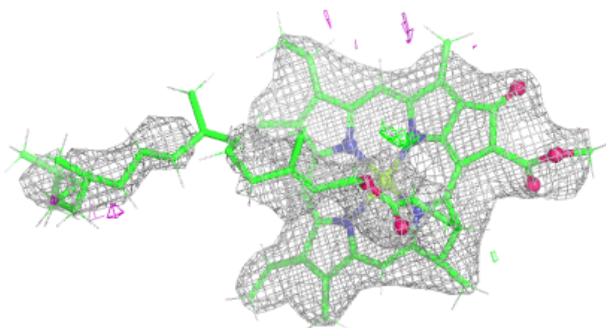
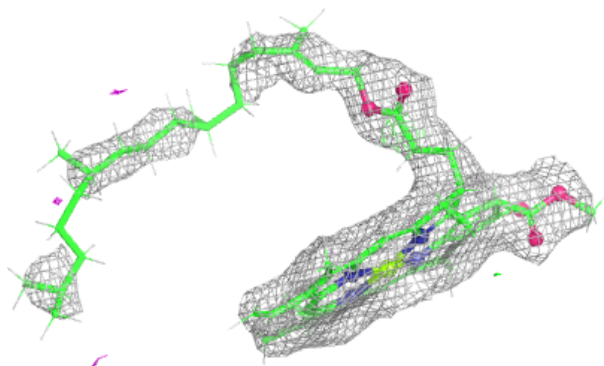




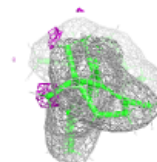
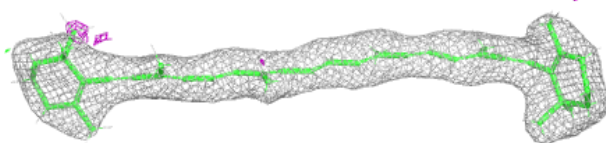
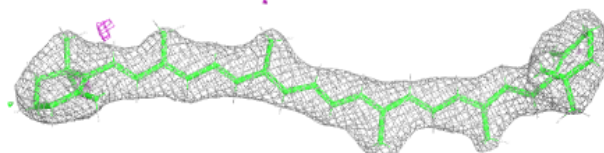


**Electron density around CLA c 513:**

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

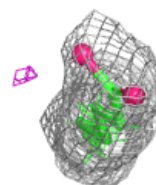
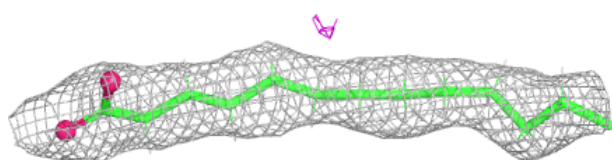
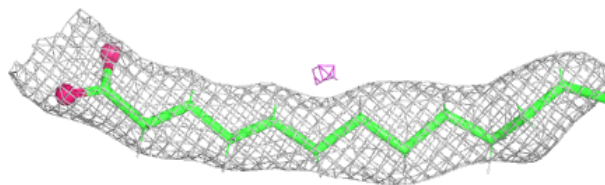
**Electron density around BCR c 515:**

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

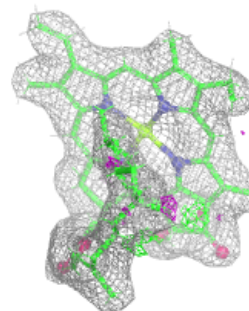
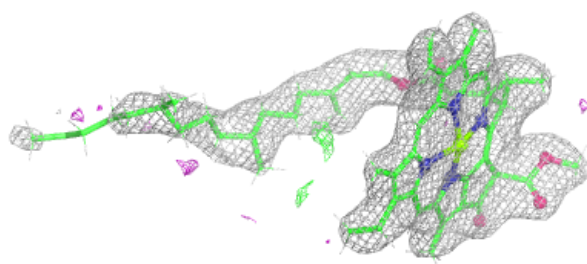
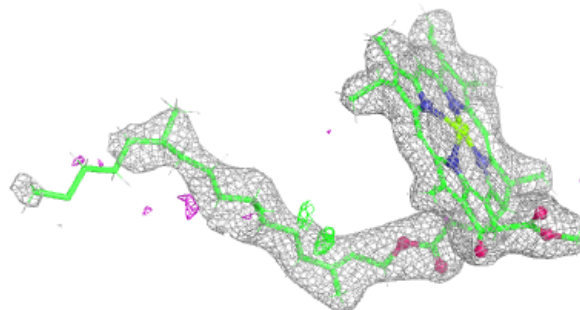


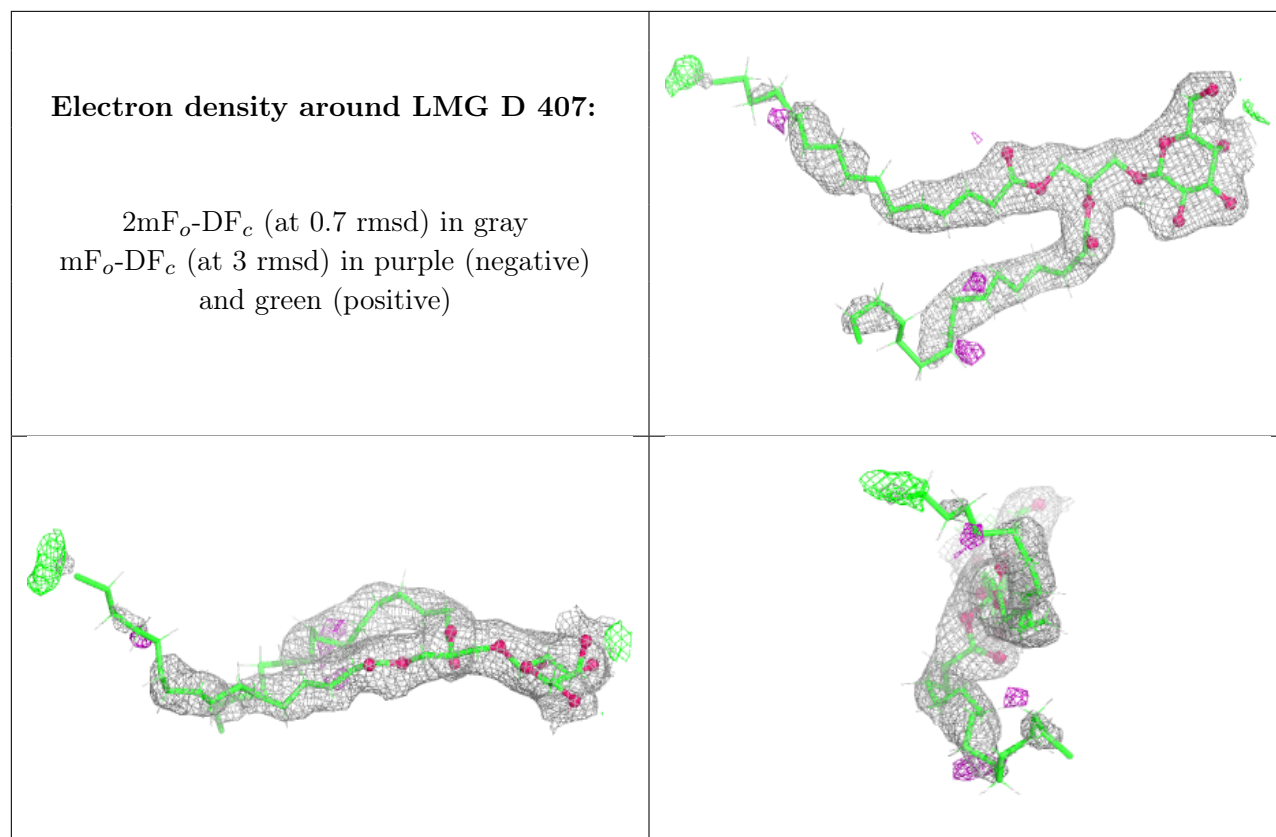
**Electron density around STE M 102:**

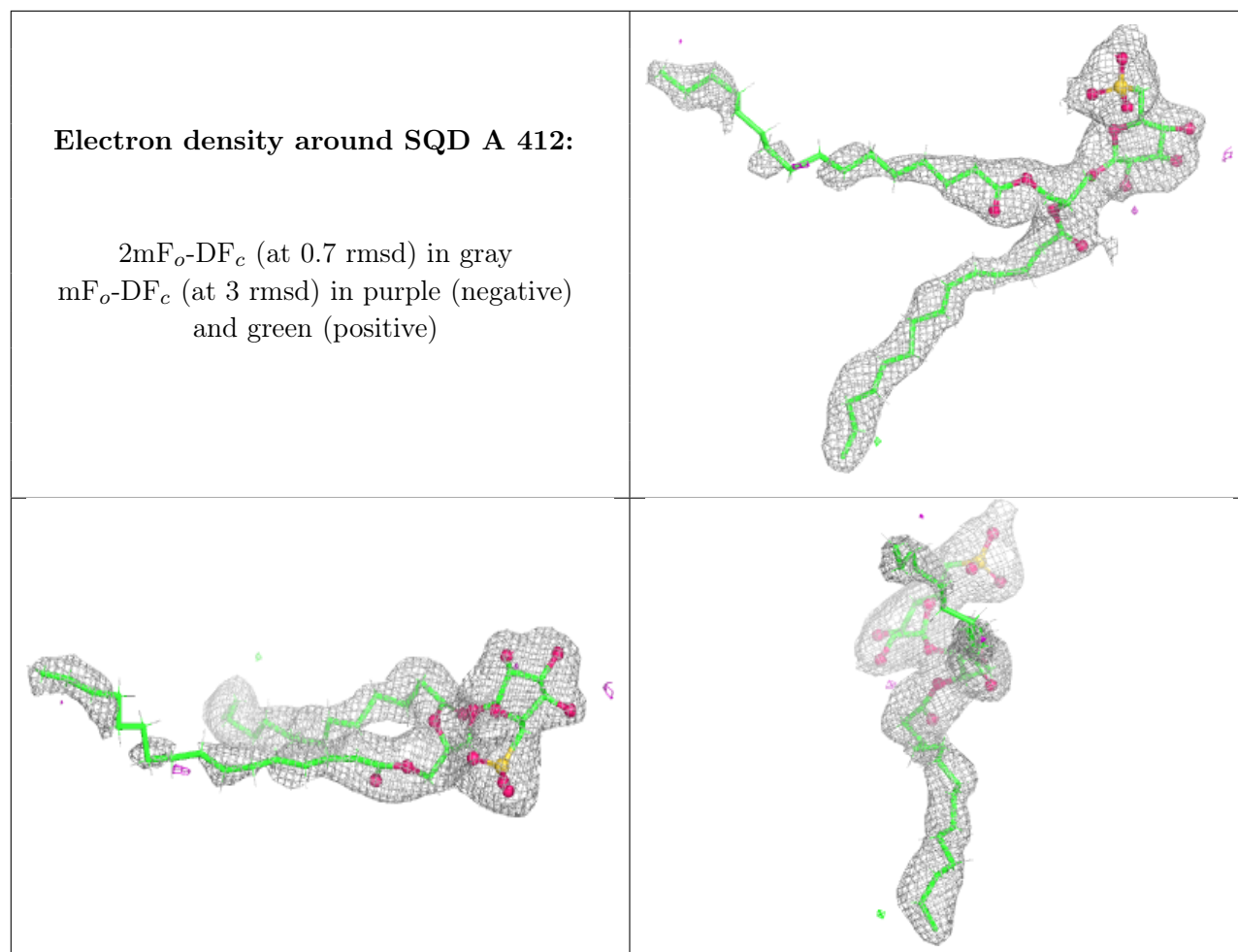
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

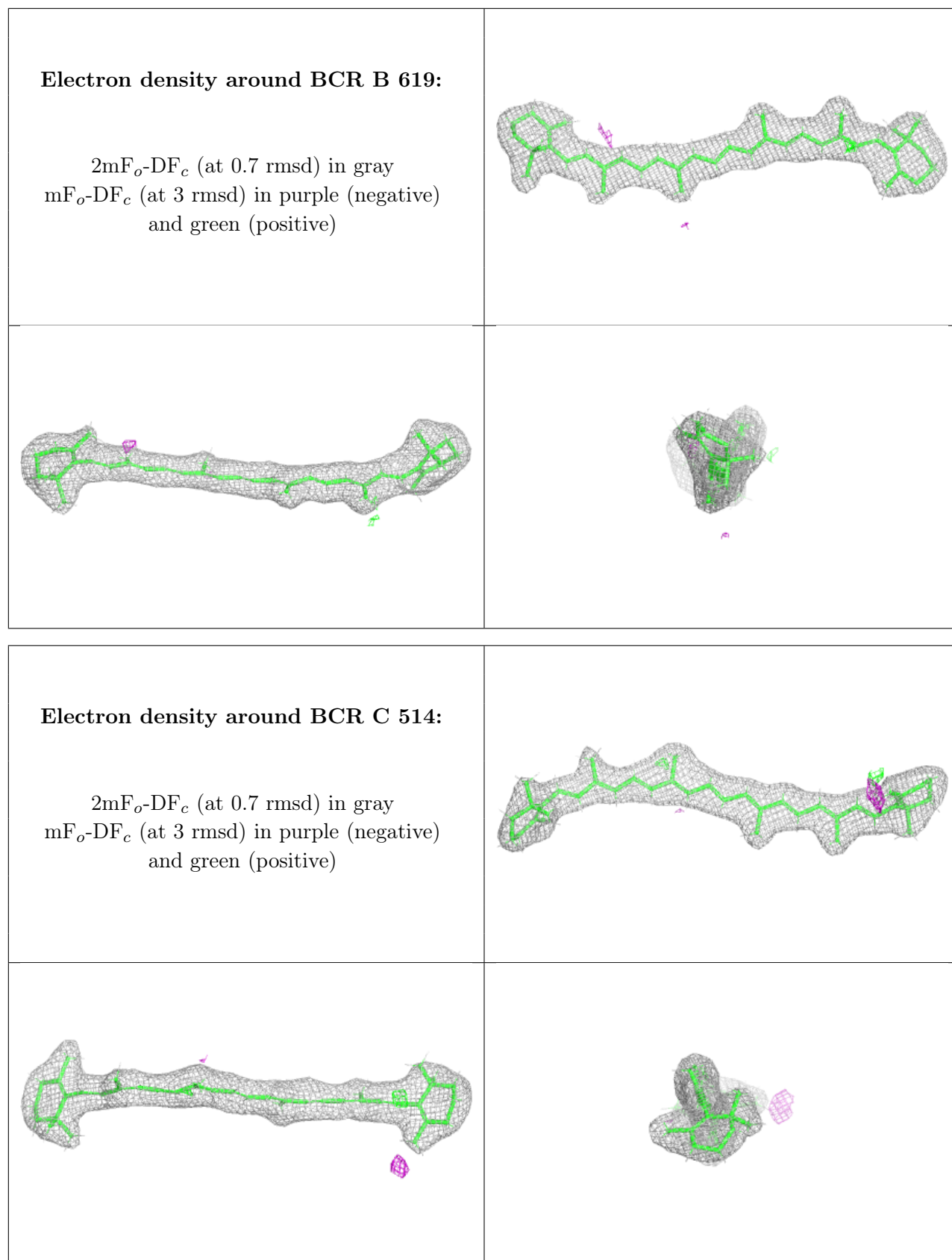
**Electron density around CLA c 508:**

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



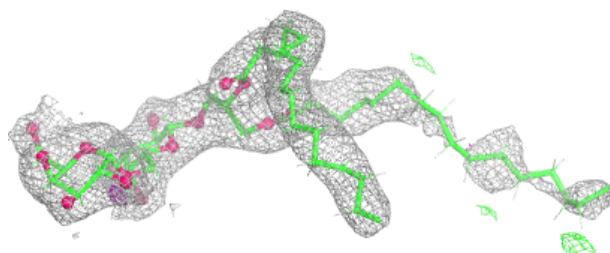




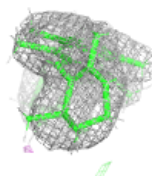
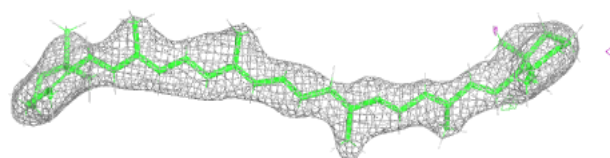
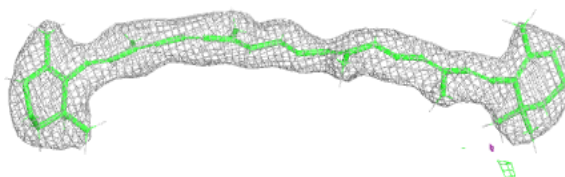


**Electron density around DGD c 518:**

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

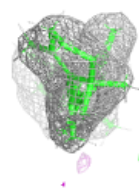
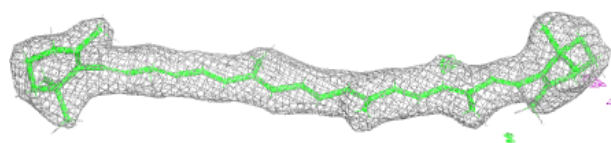
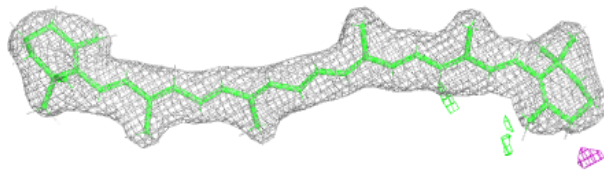
**Electron density around BCR C 515:**

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

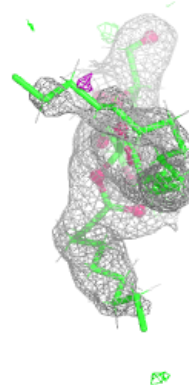
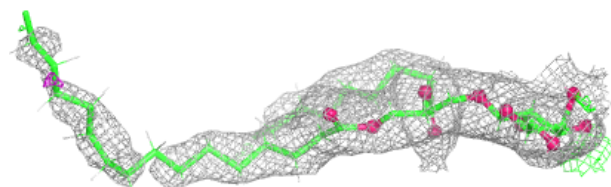
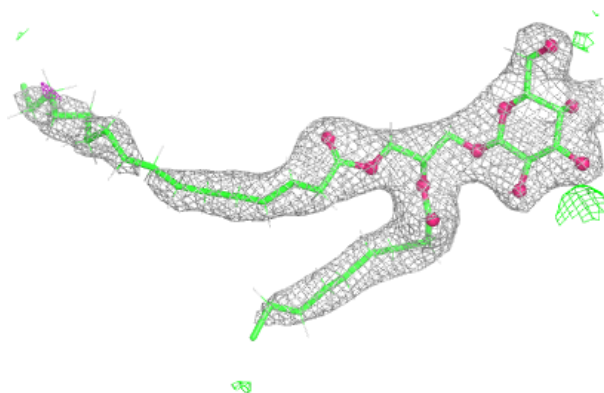


**Electron density around BCR b 619:**

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

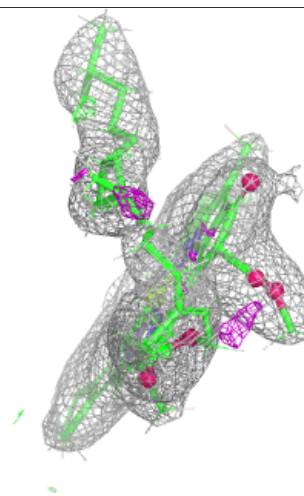
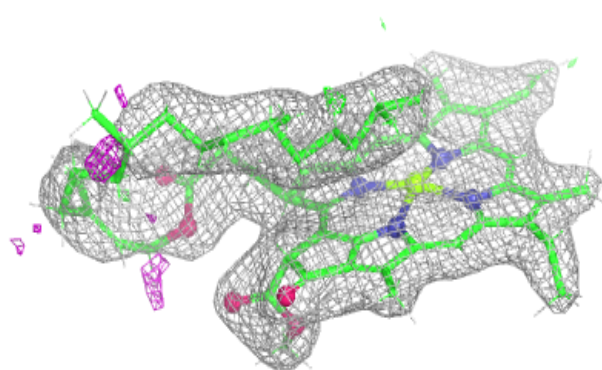
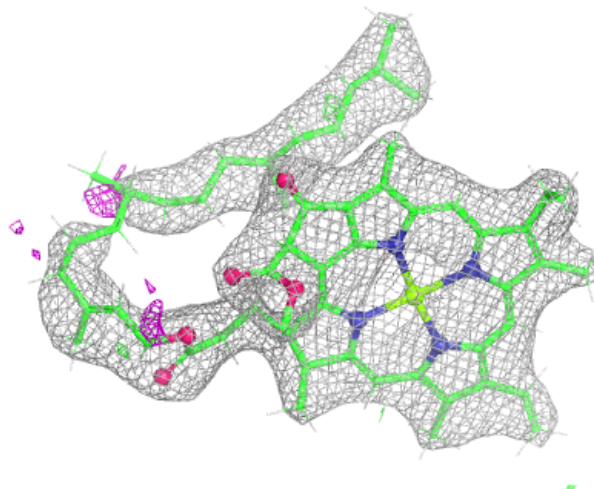
**Electron density around LMG d 412:**

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



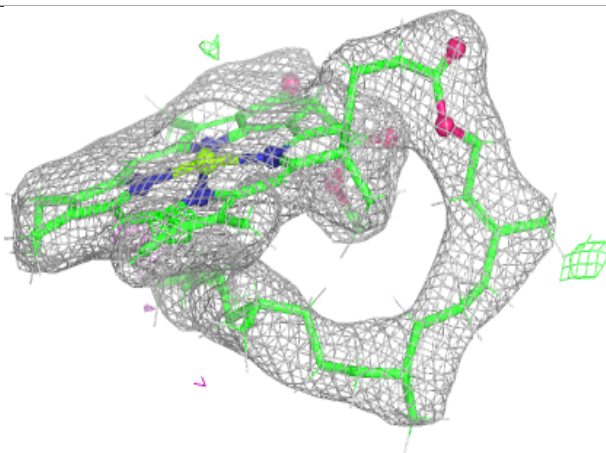
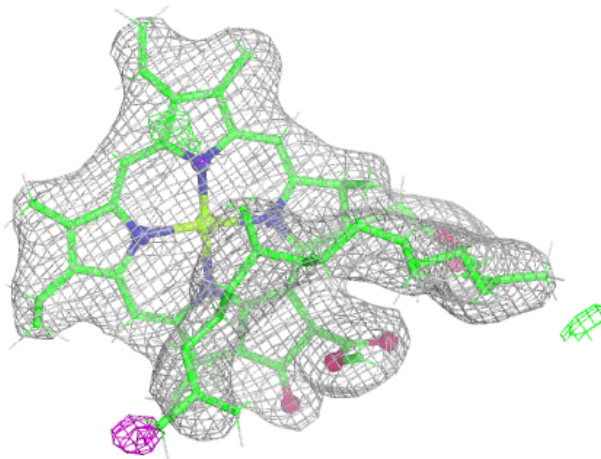
**Electron density around CLA c 509:**

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



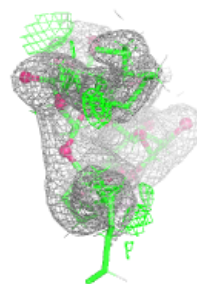
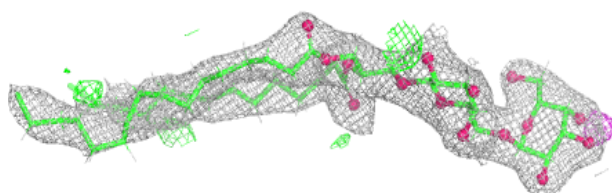
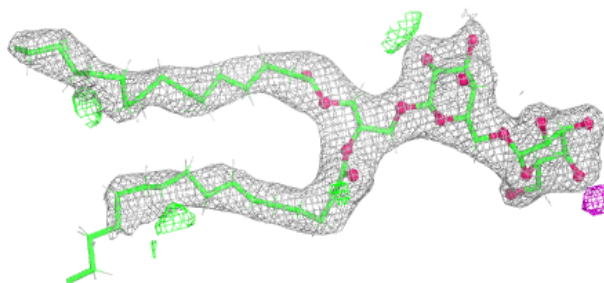
**Electron density around CLA c 510:**

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

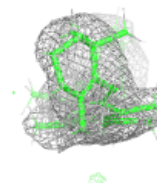
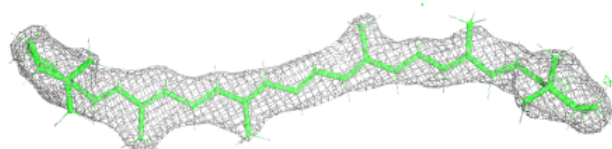
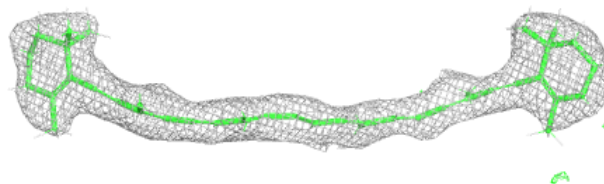


**Electron density around DGD c 519:**

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

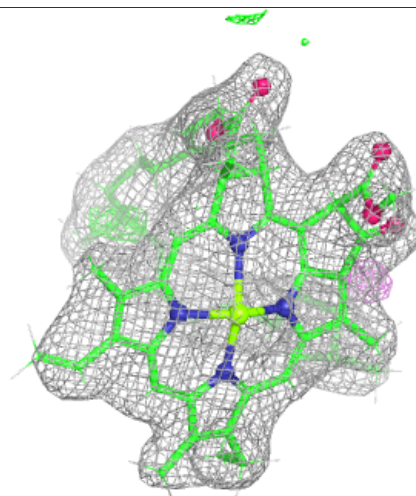
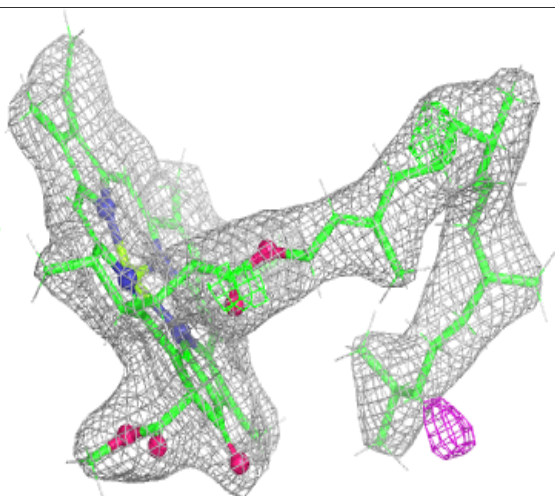
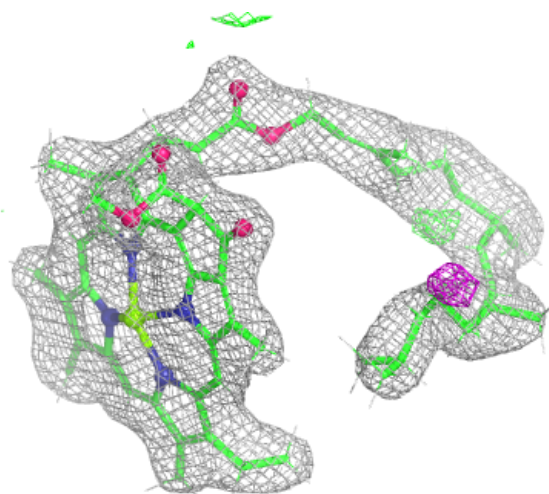
**Electron density around BCR c 516:**

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



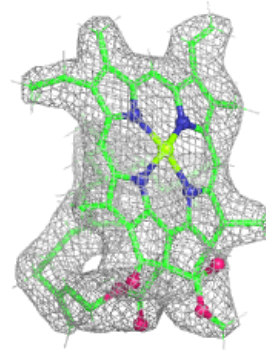
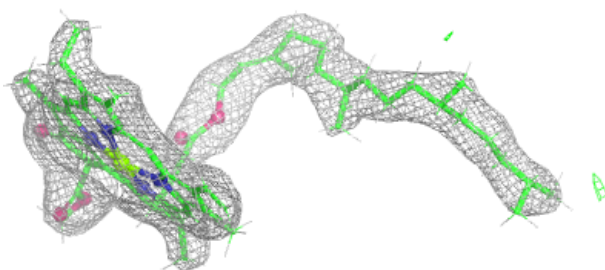
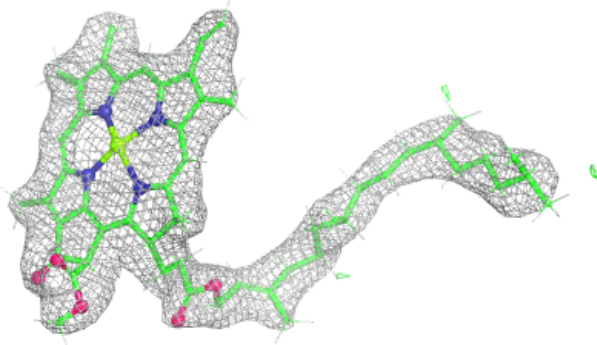
**Electron density around CLA C 503:**

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

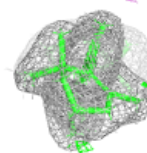
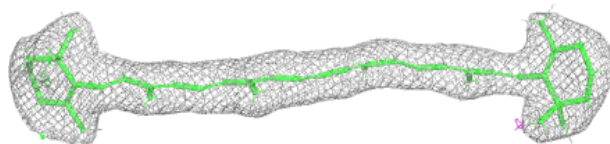
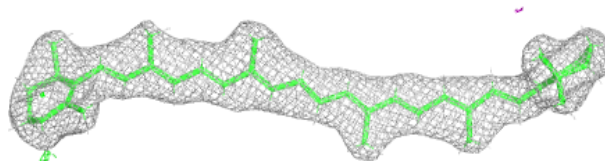


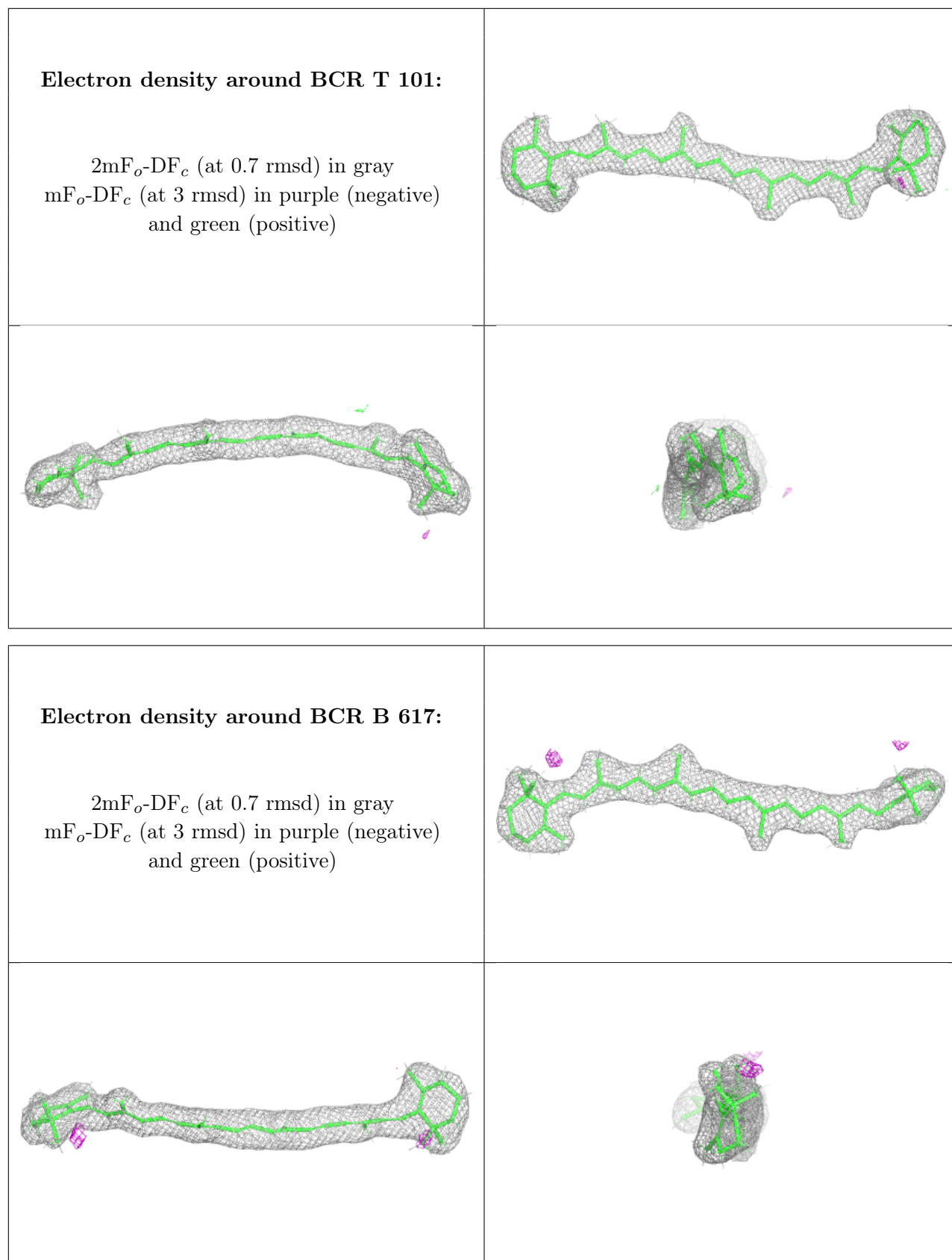
**Electron density around CLA C 511:**

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

**Electron density around BCR A 406:**

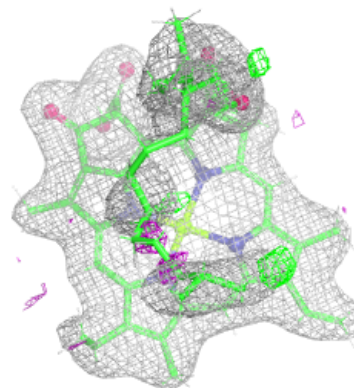
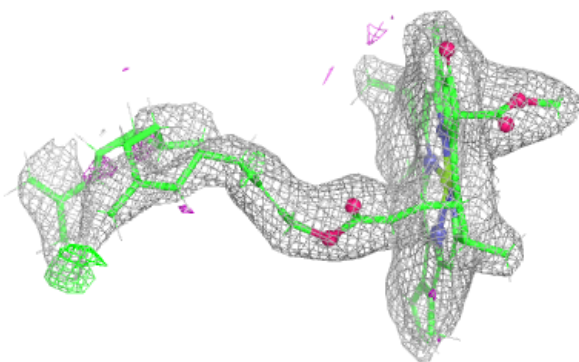
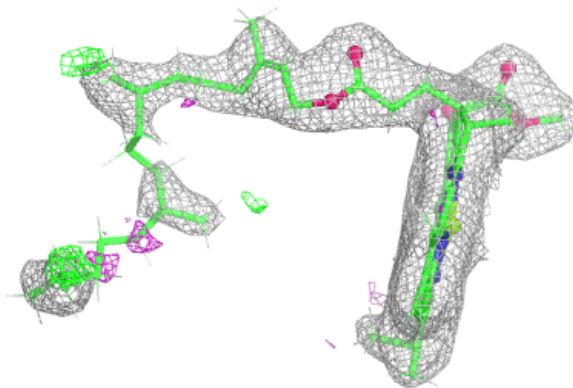
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



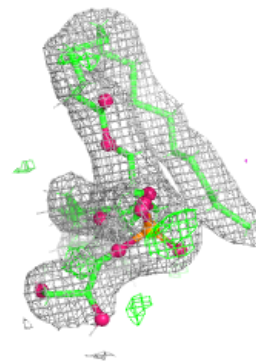
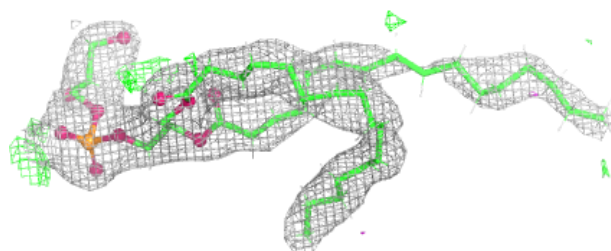
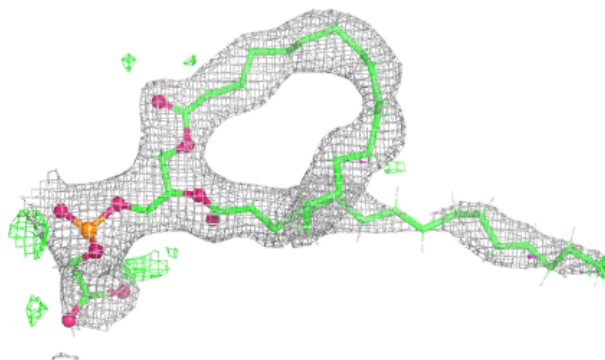


**Electron density around CLA c 506:**

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

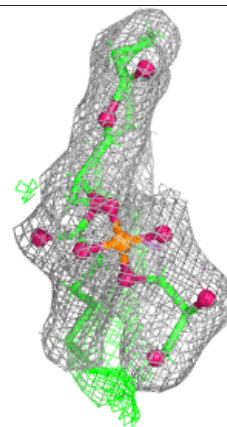
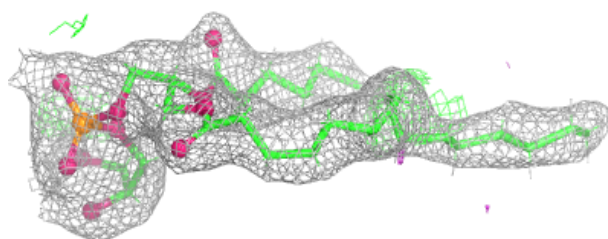
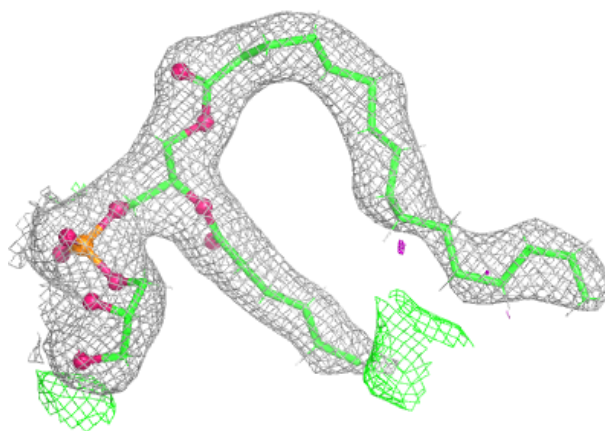
**Electron density around LHG d 408:**

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

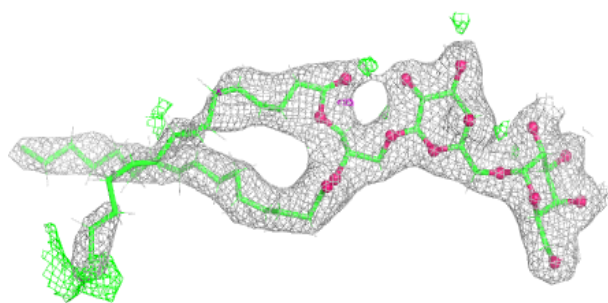
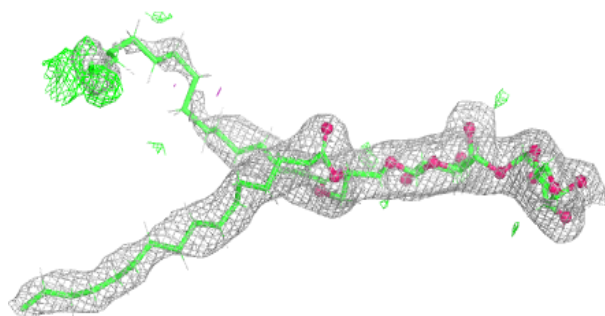


**Electron density around LHG d 410:**

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

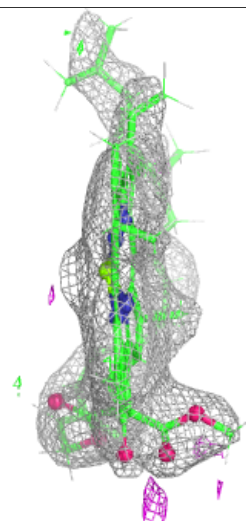
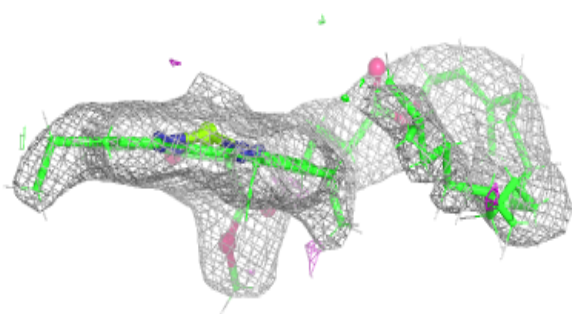
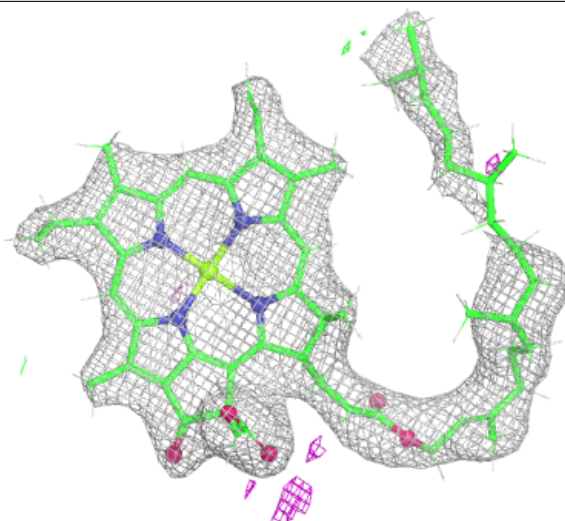
**Electron density around DGD C 516:**

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



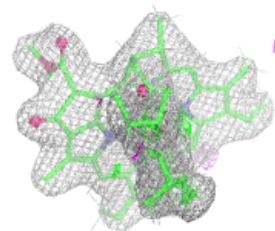
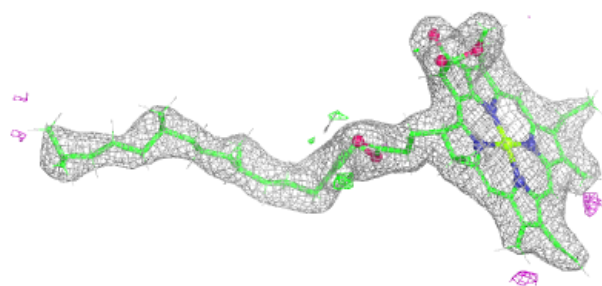
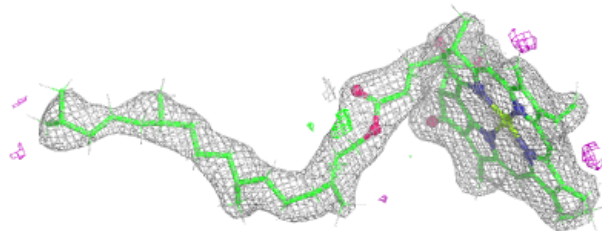
**Electron density around CLA C 512:**

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



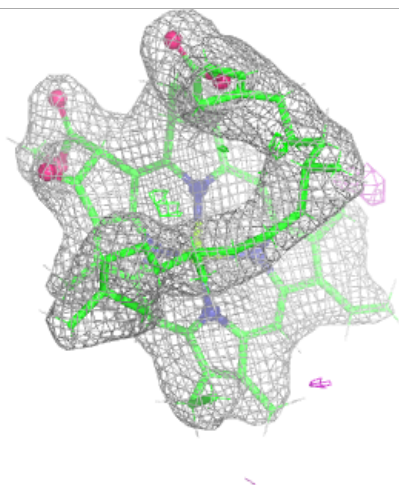
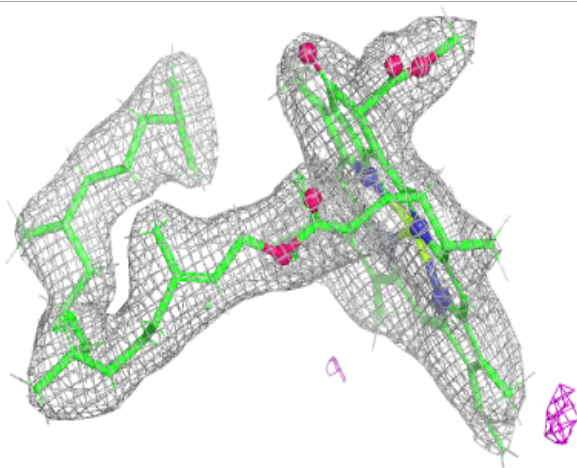
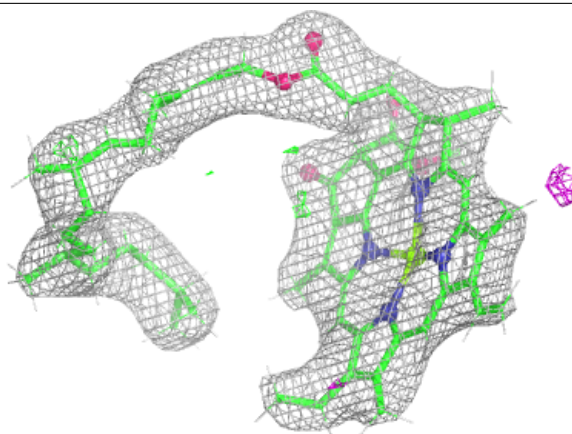
**Electron density around CLA c 502:**

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



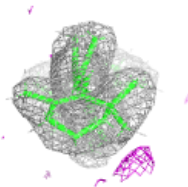
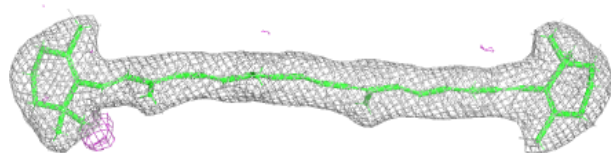
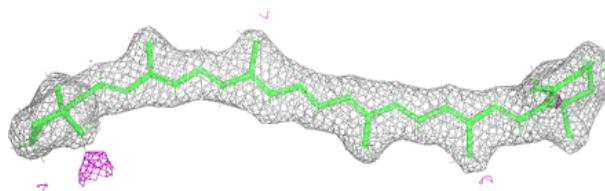
**Electron density around CLA c 503:**

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

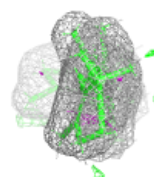
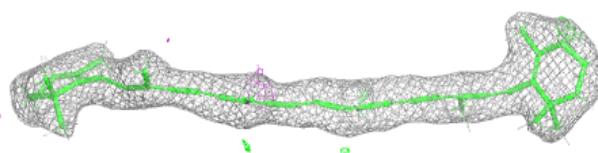
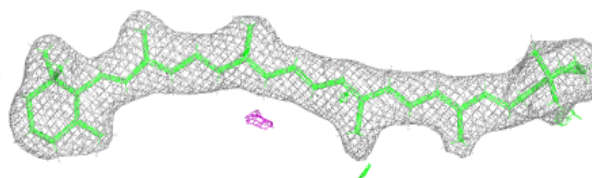


**Electron density around BCR a 405:**

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

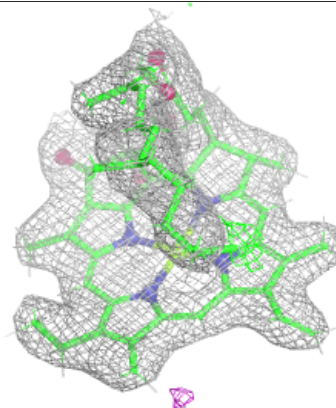
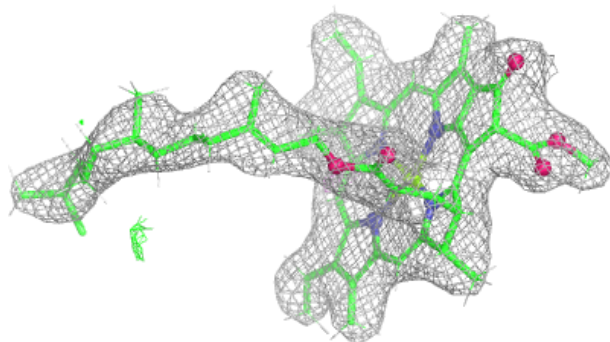
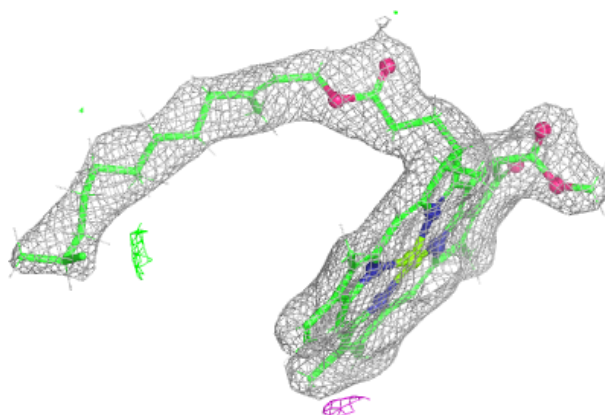
**Electron density around BCR b 617:**

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

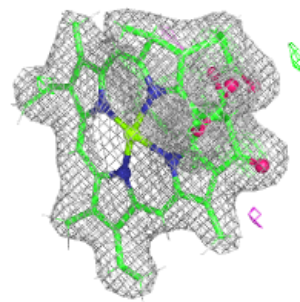
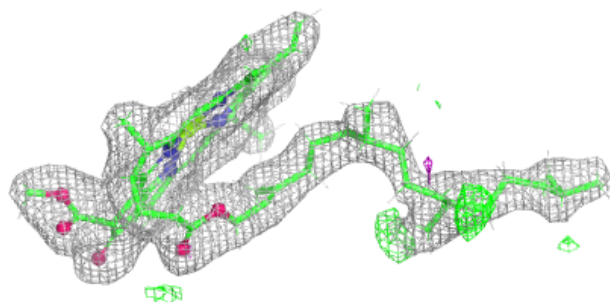
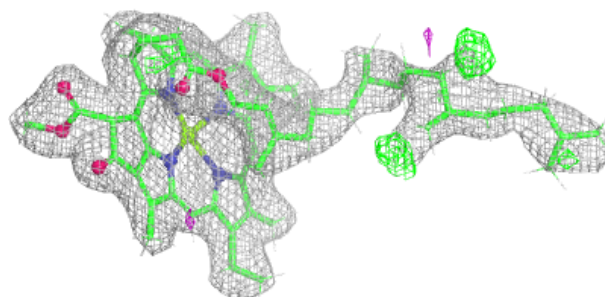


**Electron density around CLA c 504:**

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

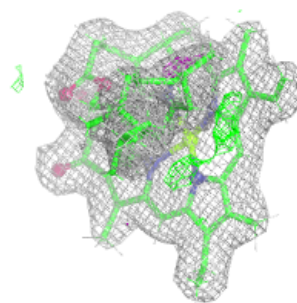
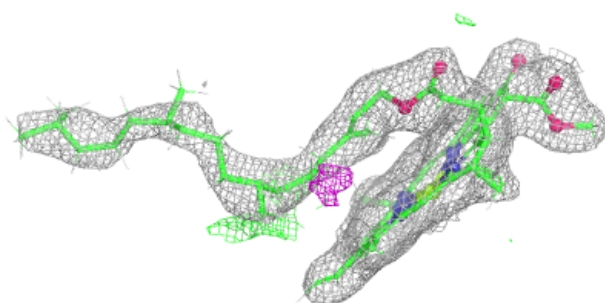
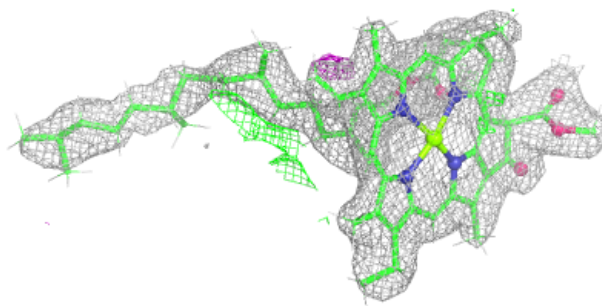
**Electron density around CLA c 505:**

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



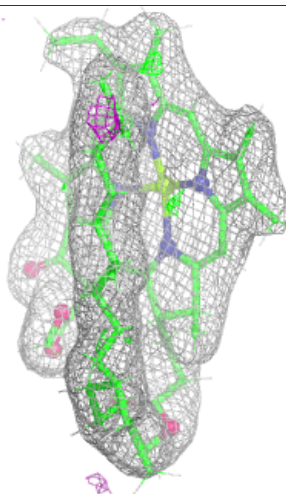
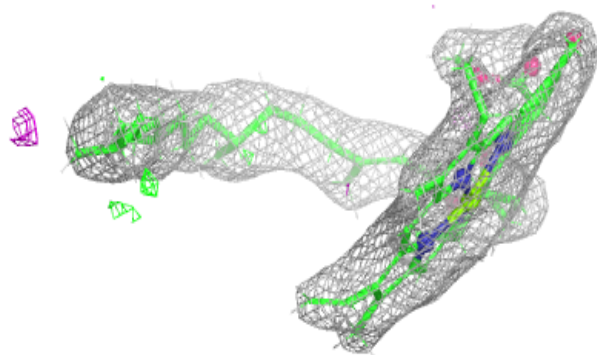
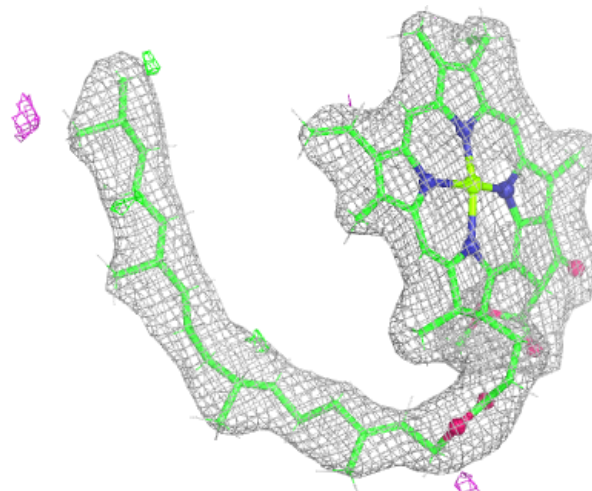
**Electron density around CLA C 505:**

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



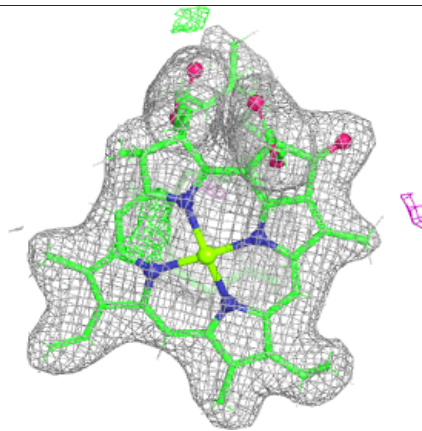
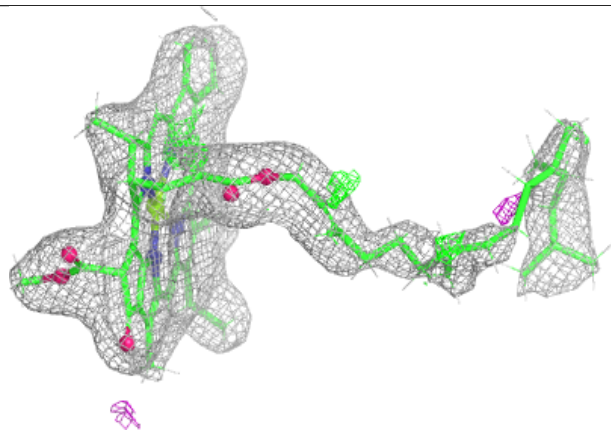
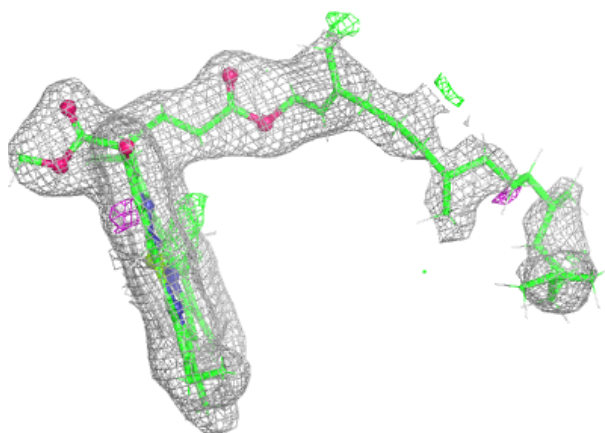
**Electron density around CLA c 507:**

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

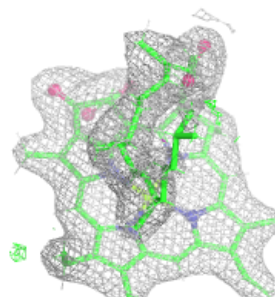
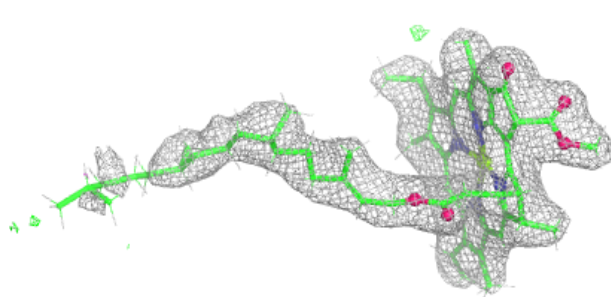
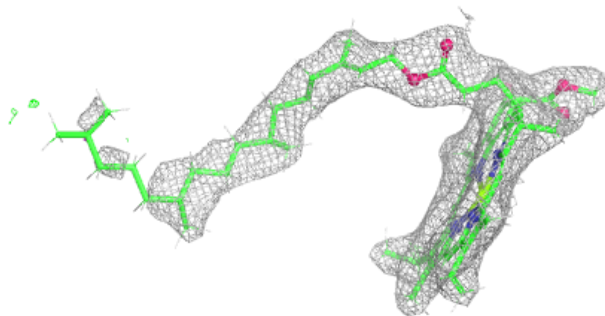


**Electron density around CLA C 506:**

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

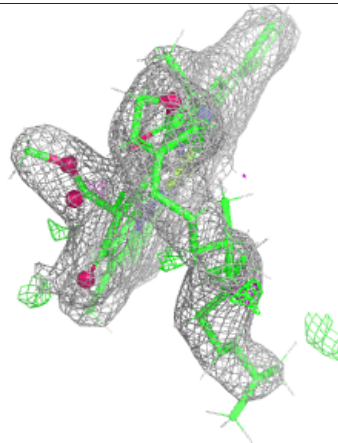
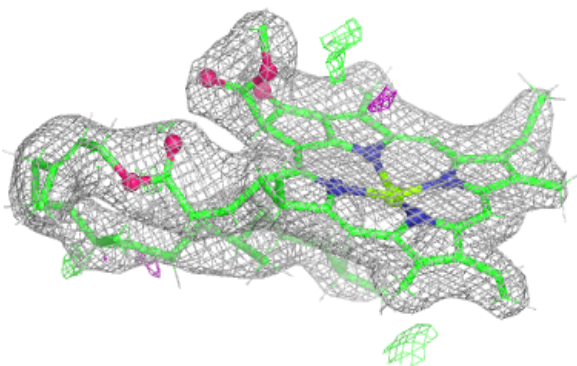
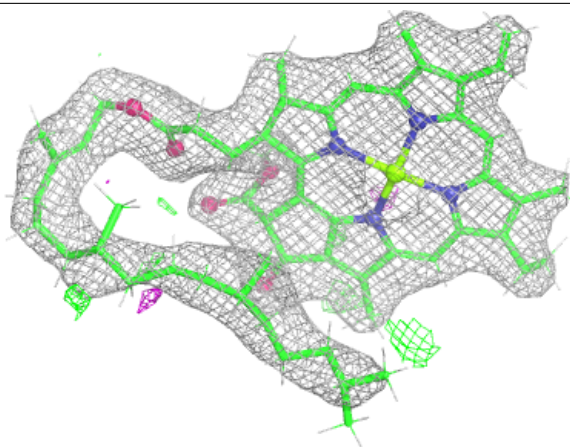
**Electron density around CLA C 508:**

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



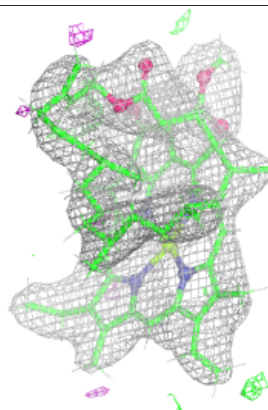
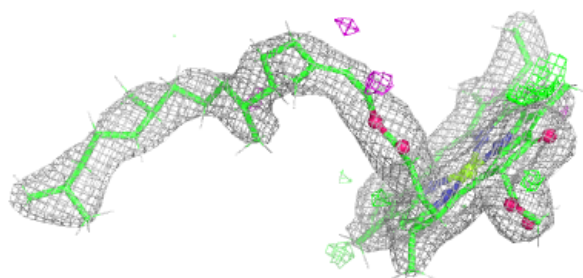
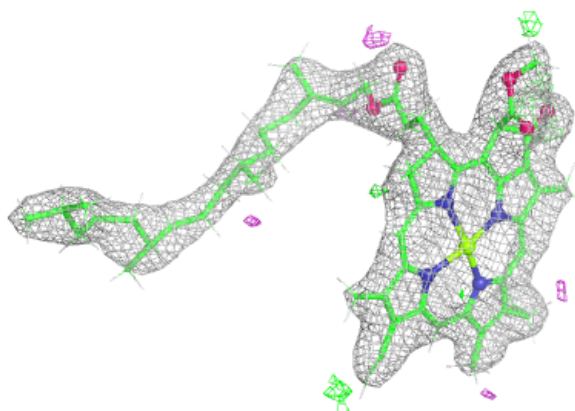
**Electron density around CLA C 509:**

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

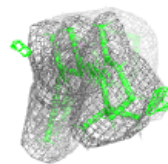
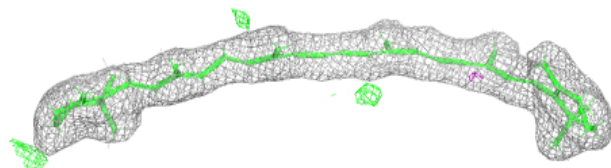
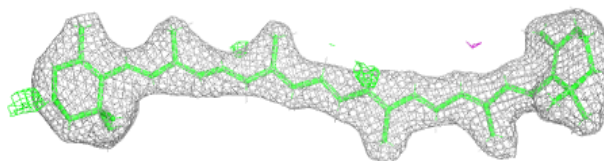


**Electron density around CLA c 511:**

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

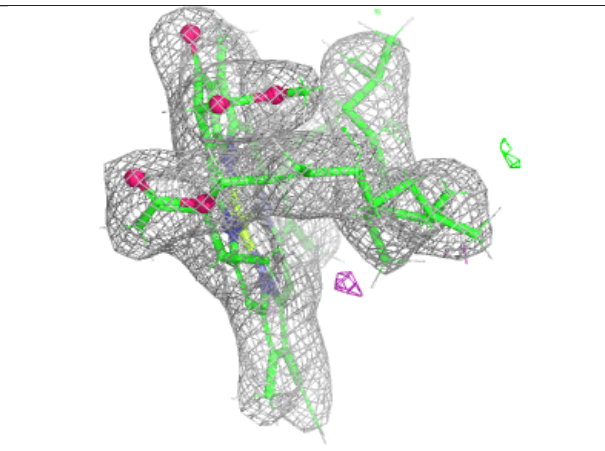
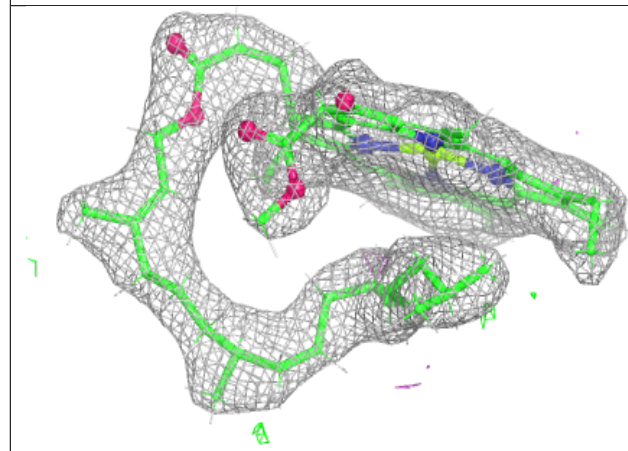
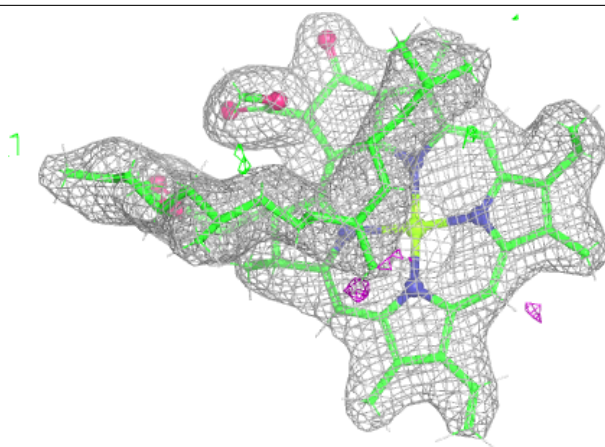
**Electron density around BCR t 101:**

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

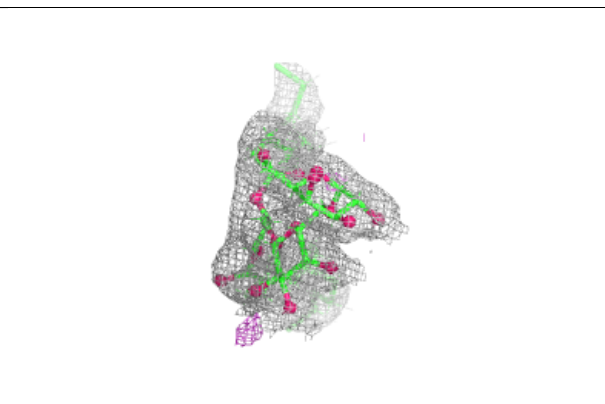
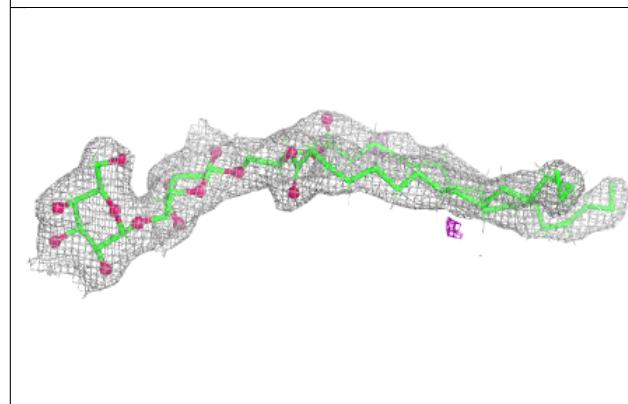
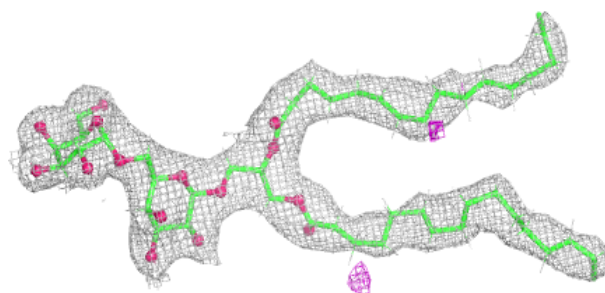


**Electron density around CLA C 510:**

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

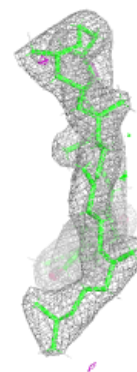
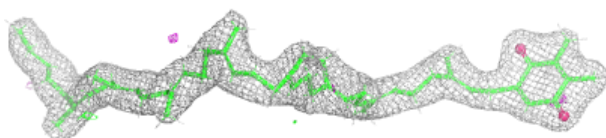
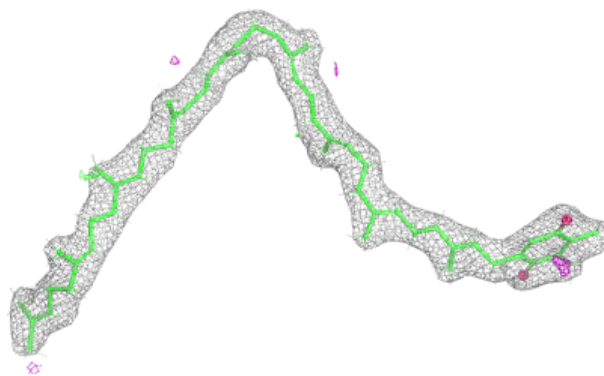
**Electron density around DGD C 518:**

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

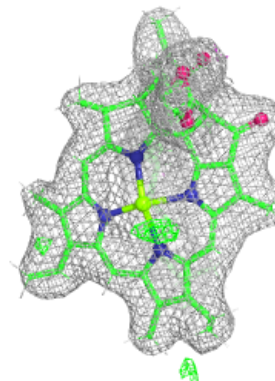
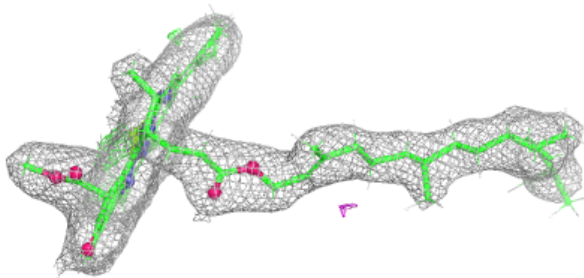
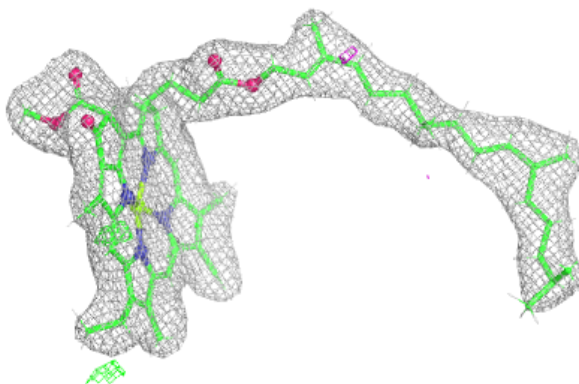


**Electron density around PL9 D 406:**

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

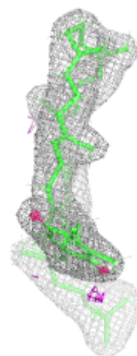
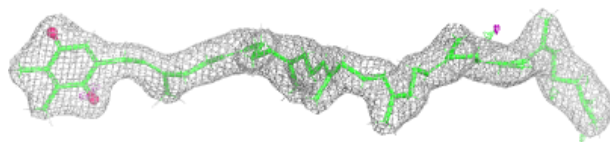
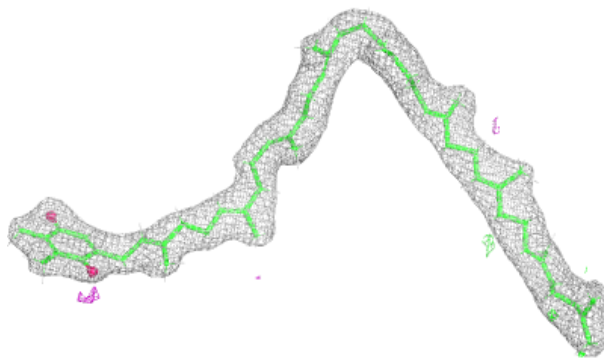
**Electron density around CLA B 609:**

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

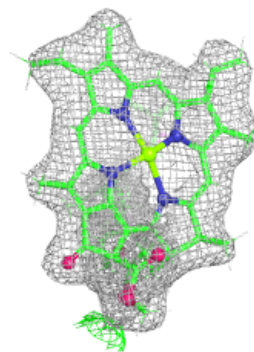
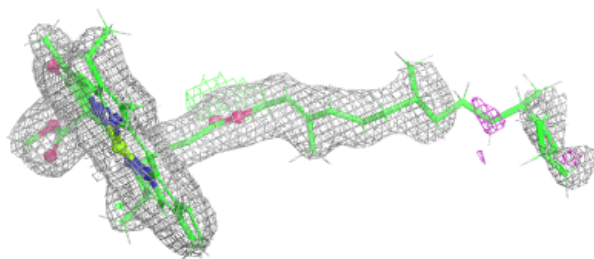
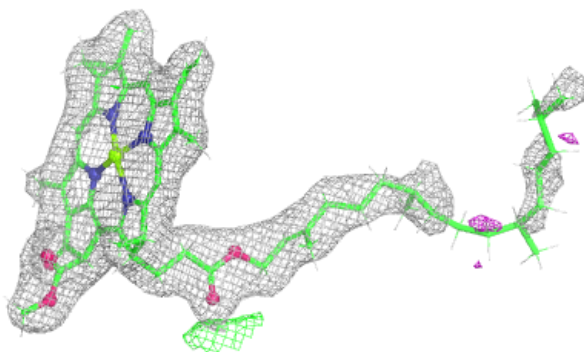


**Electron density around PL9 d 407:**

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

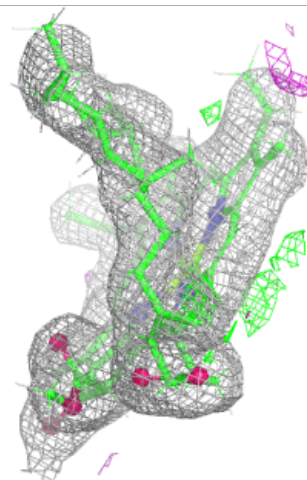
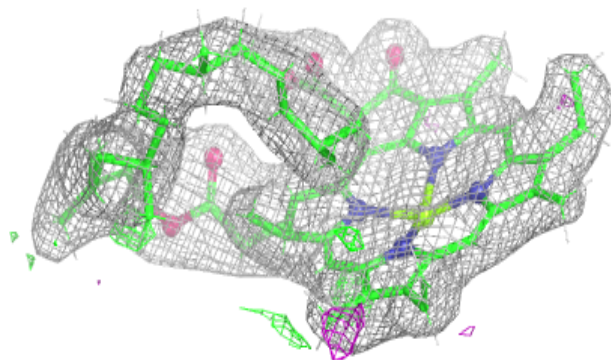
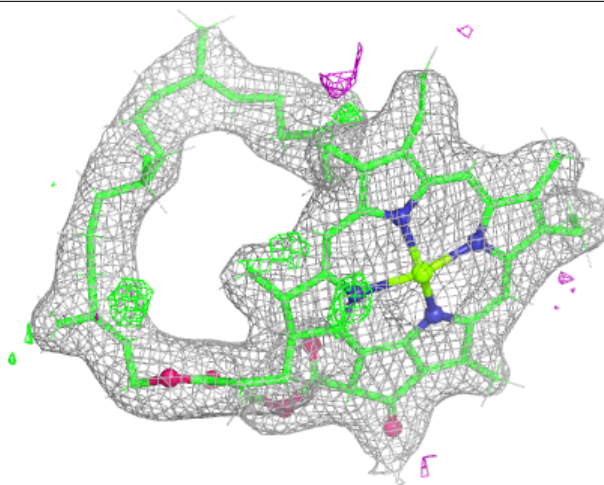
**Electron density around CLA d 405:**

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



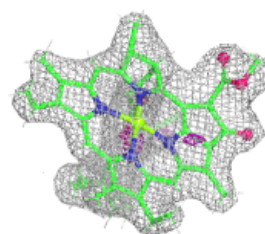
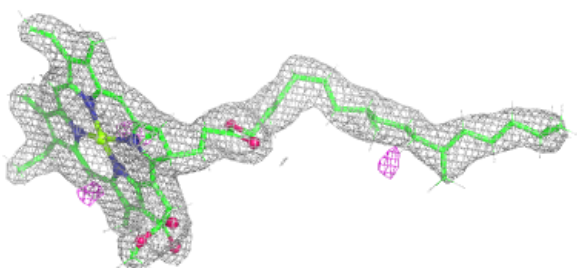
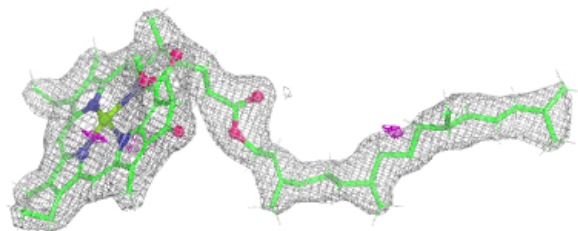
**Electron density around CLA B 615:**

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

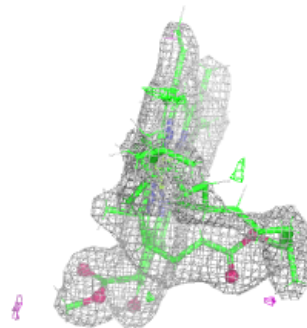
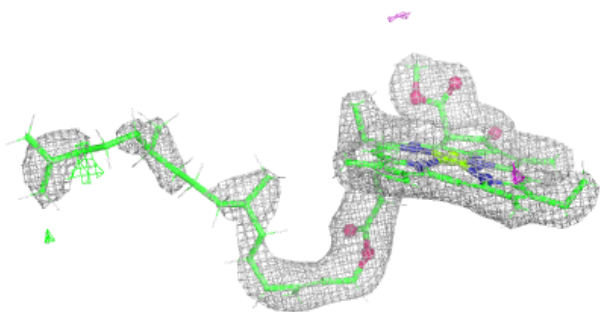
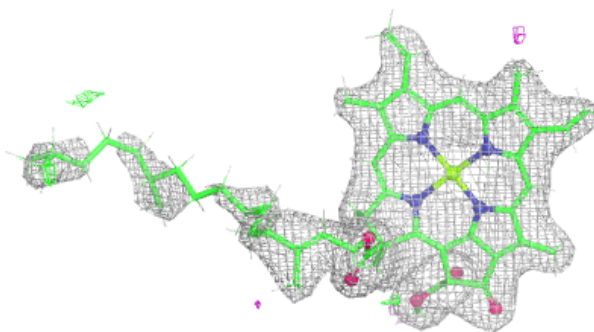


**Electron density around CLA C 502:**

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

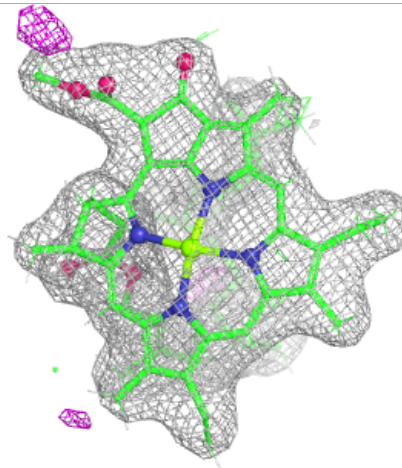
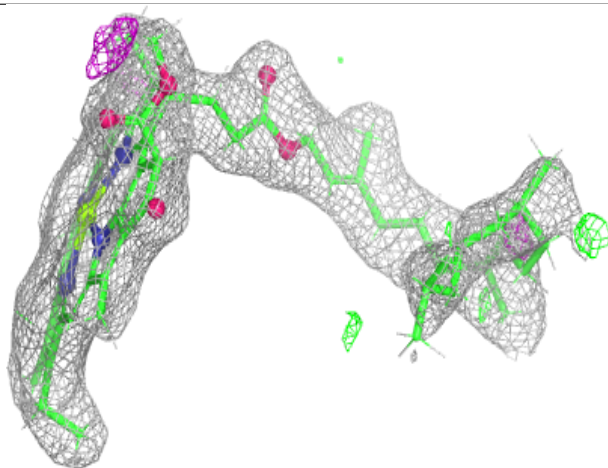
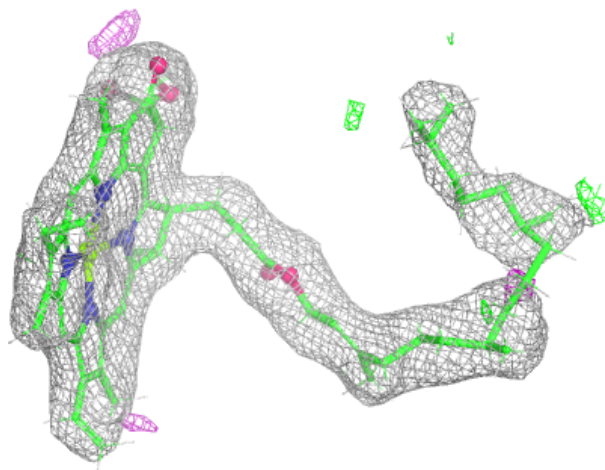
**Electron density around CLA a 403:**

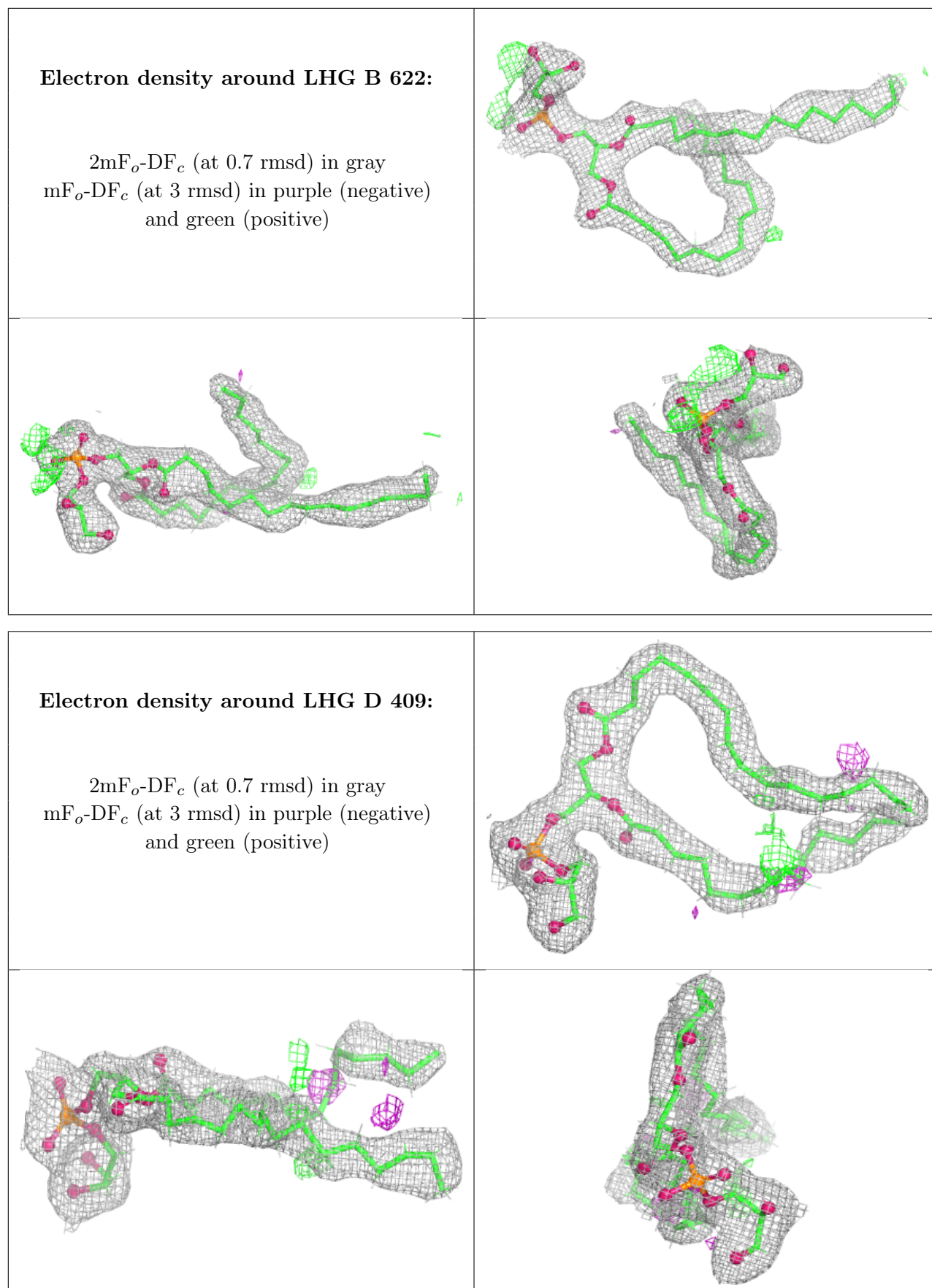
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 606:**

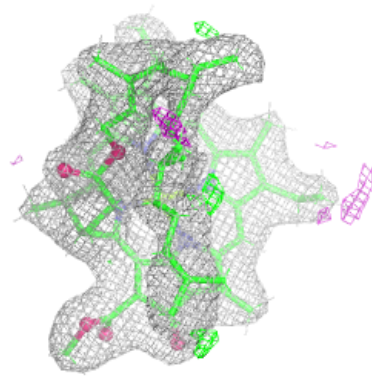
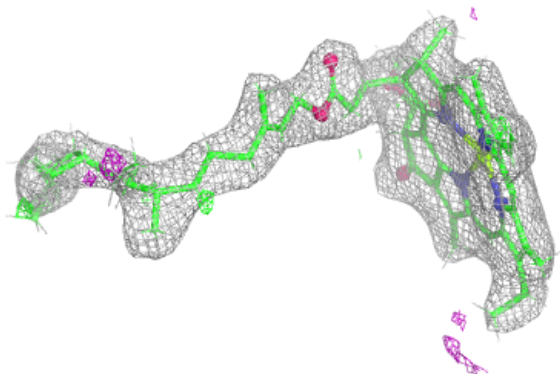
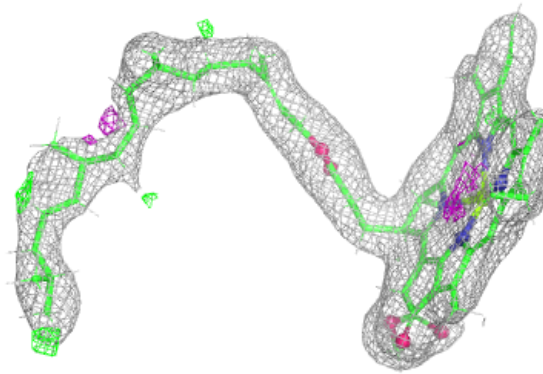
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





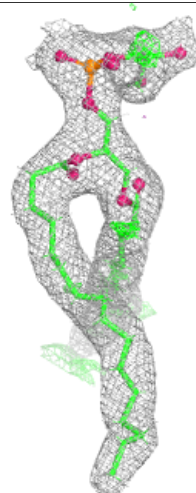
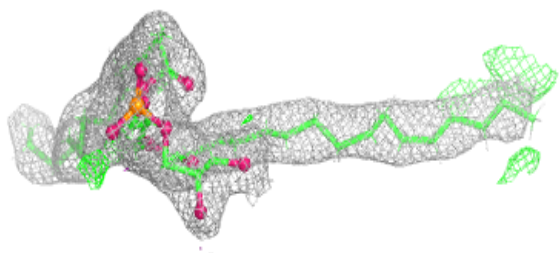
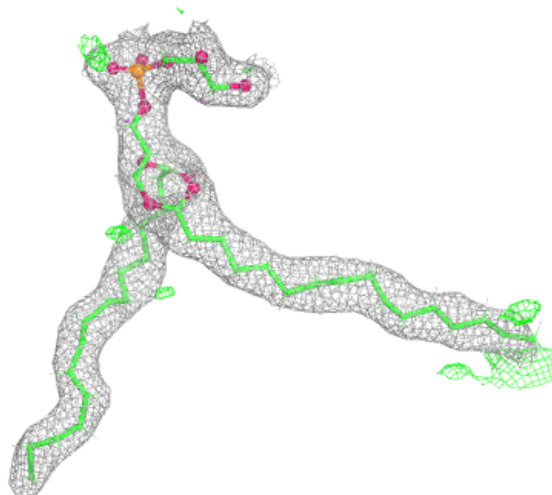
**Electron density around CLA b 606:**

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



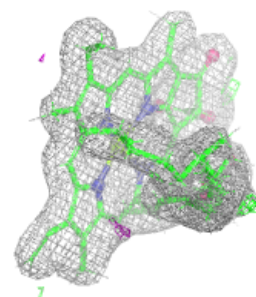
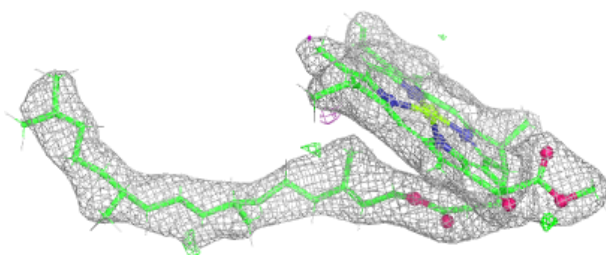
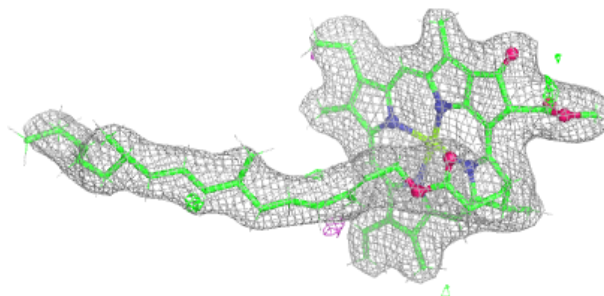
**Electron density around LHG L 102:**

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

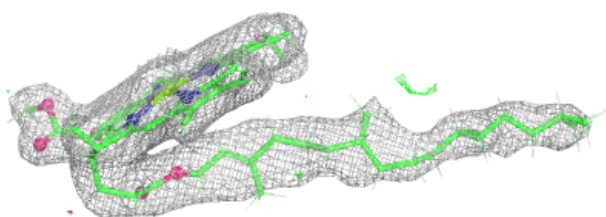
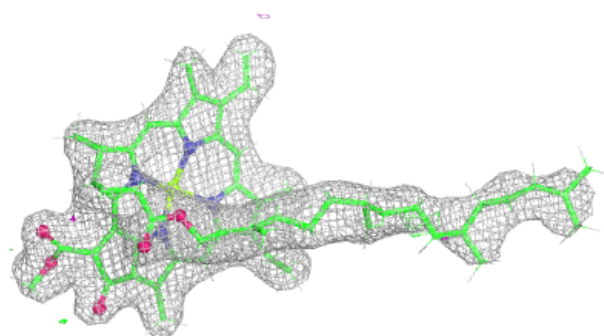


**Electron density around CLA b 608:**

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

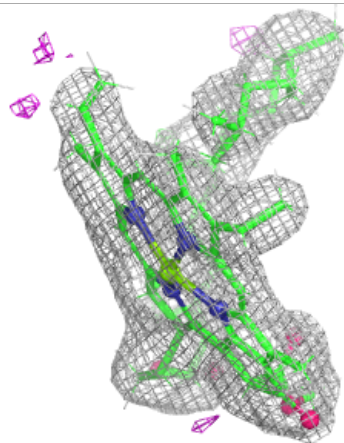
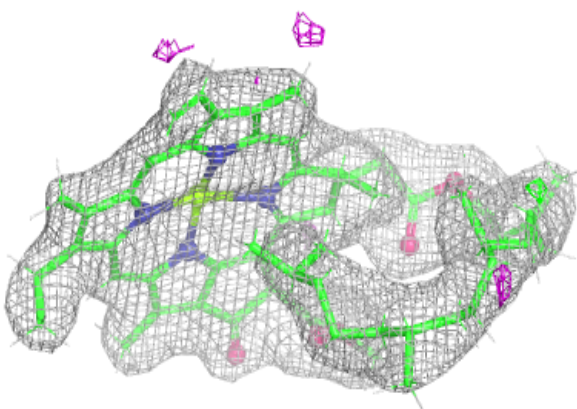
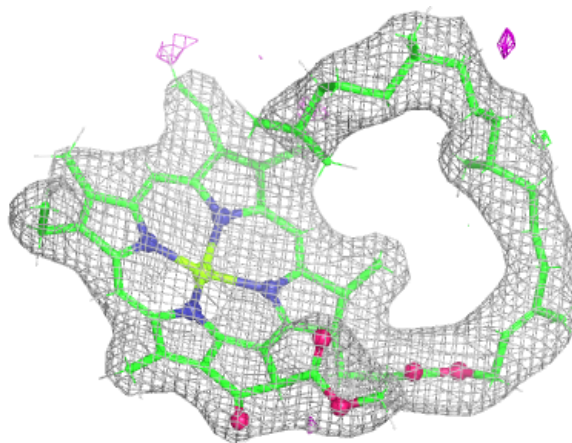
**Electron density around CLA b 614:**

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



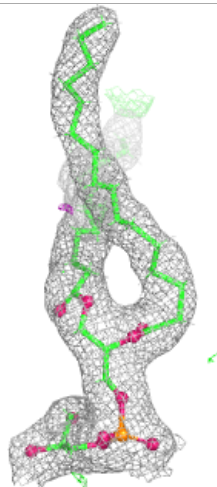
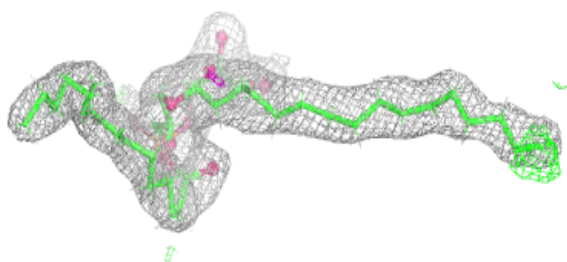
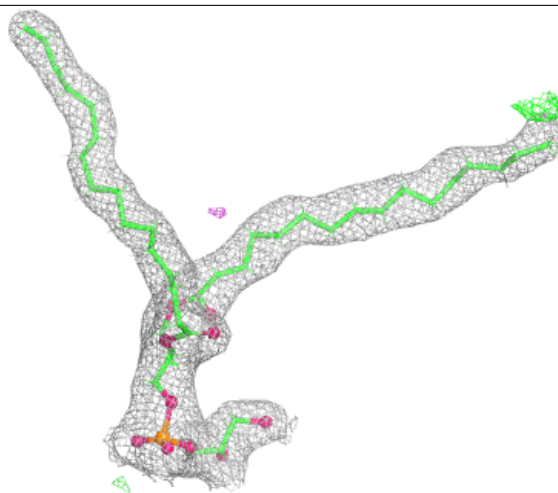
**Electron density around CLA b 615:**

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



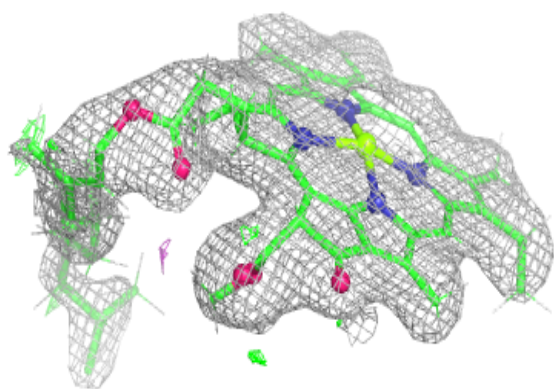
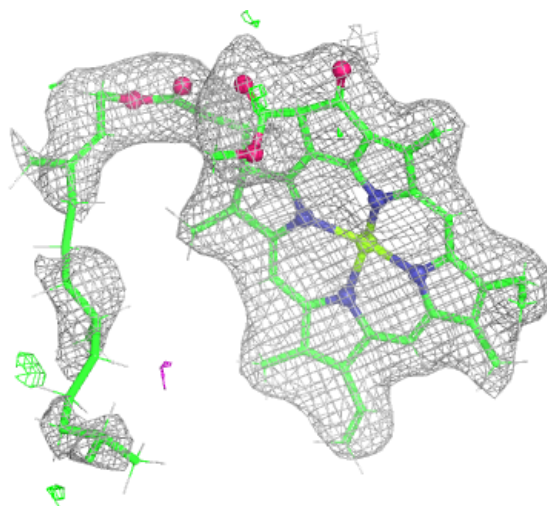
**Electron density around LHG 1 101:**

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



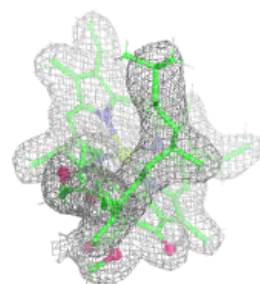
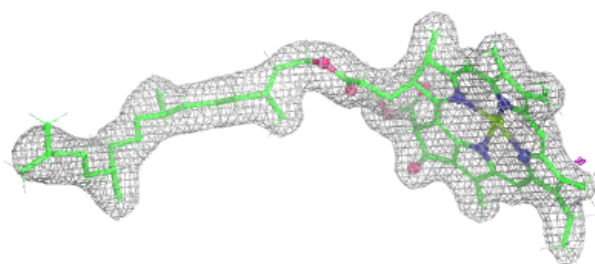
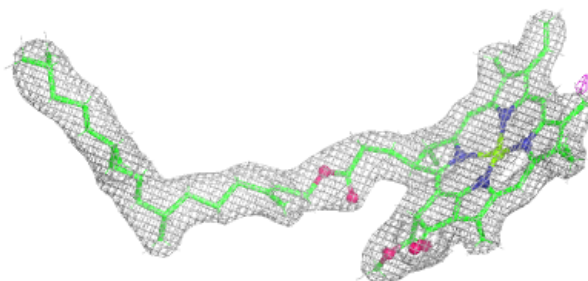
**Electron density around CLA b 616:**

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

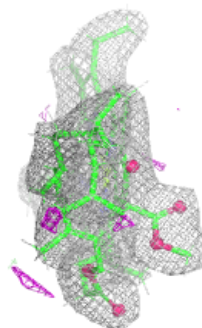
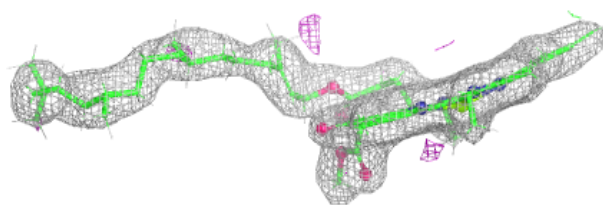
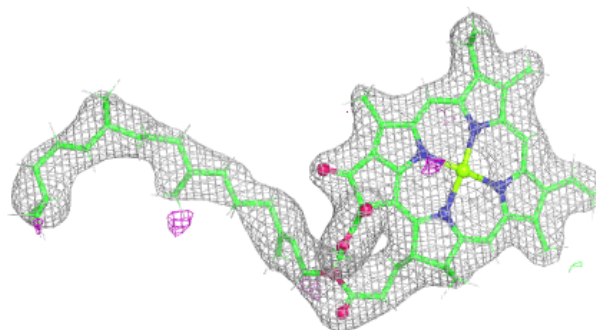


**Electron density around CLA a 402:**

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

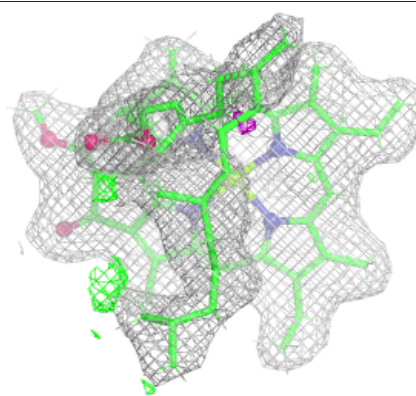
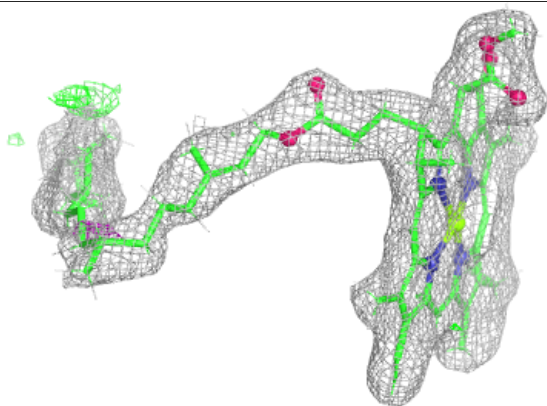
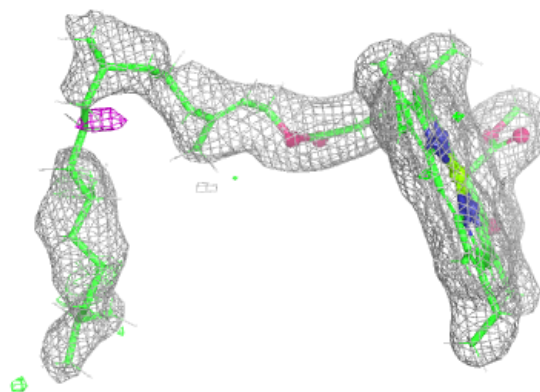
**Electron density around CLA B 602:**

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

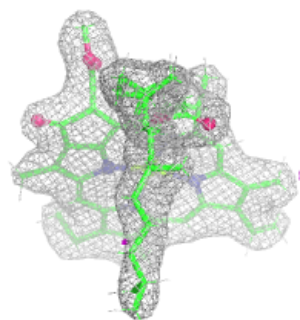
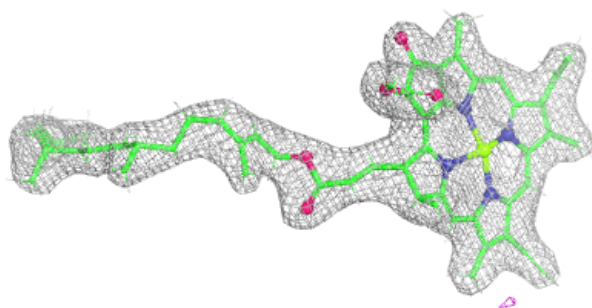
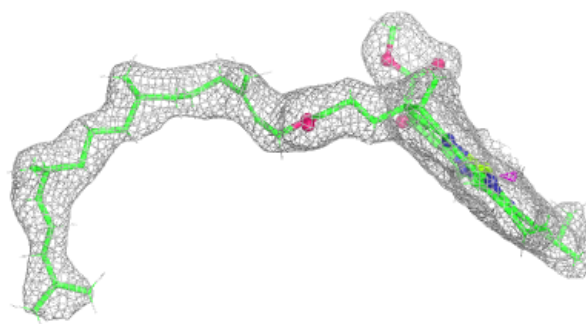


**Electron density around CLA a 404:**

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

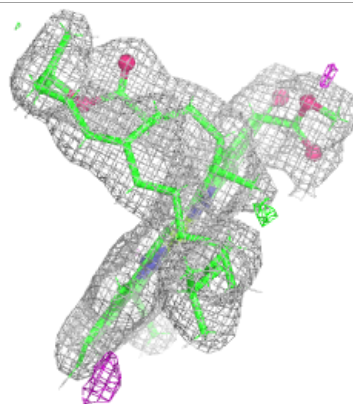
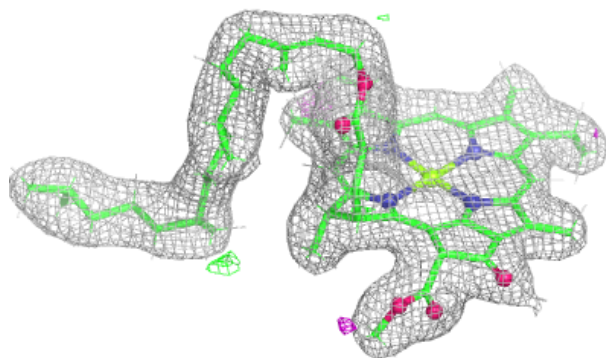
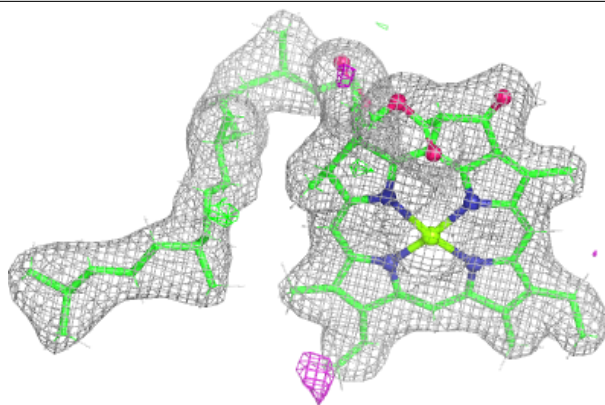
**Electron density around CLA d 403:**

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



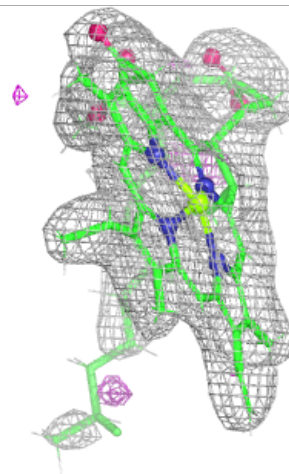
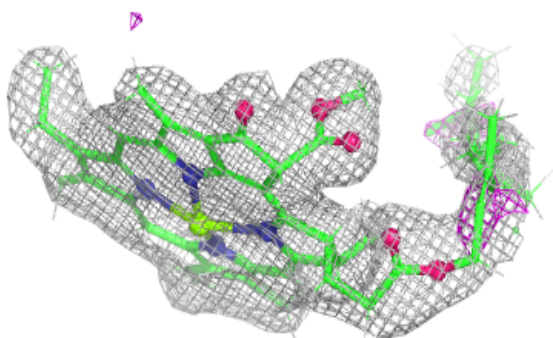
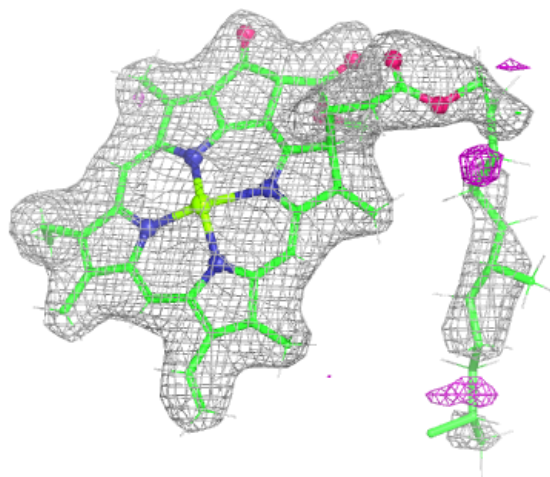
**Electron density around CLA d 404:**

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



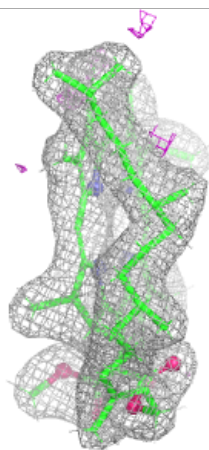
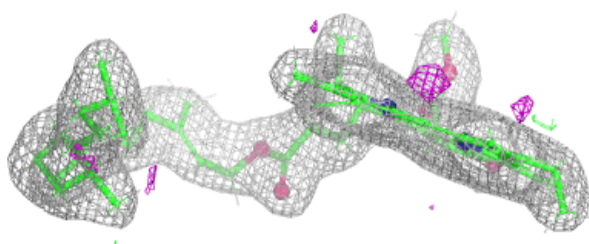
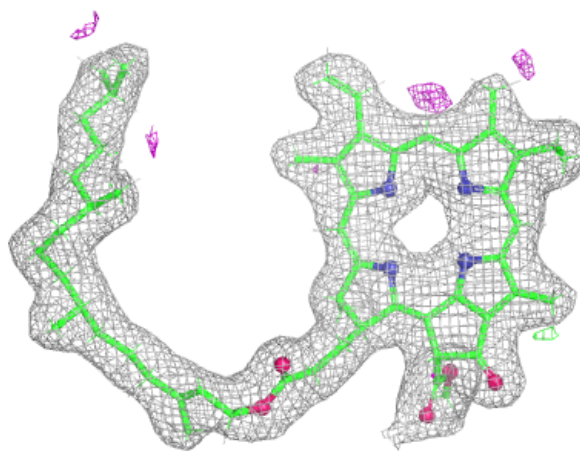
**Electron density around CLA B 616:**

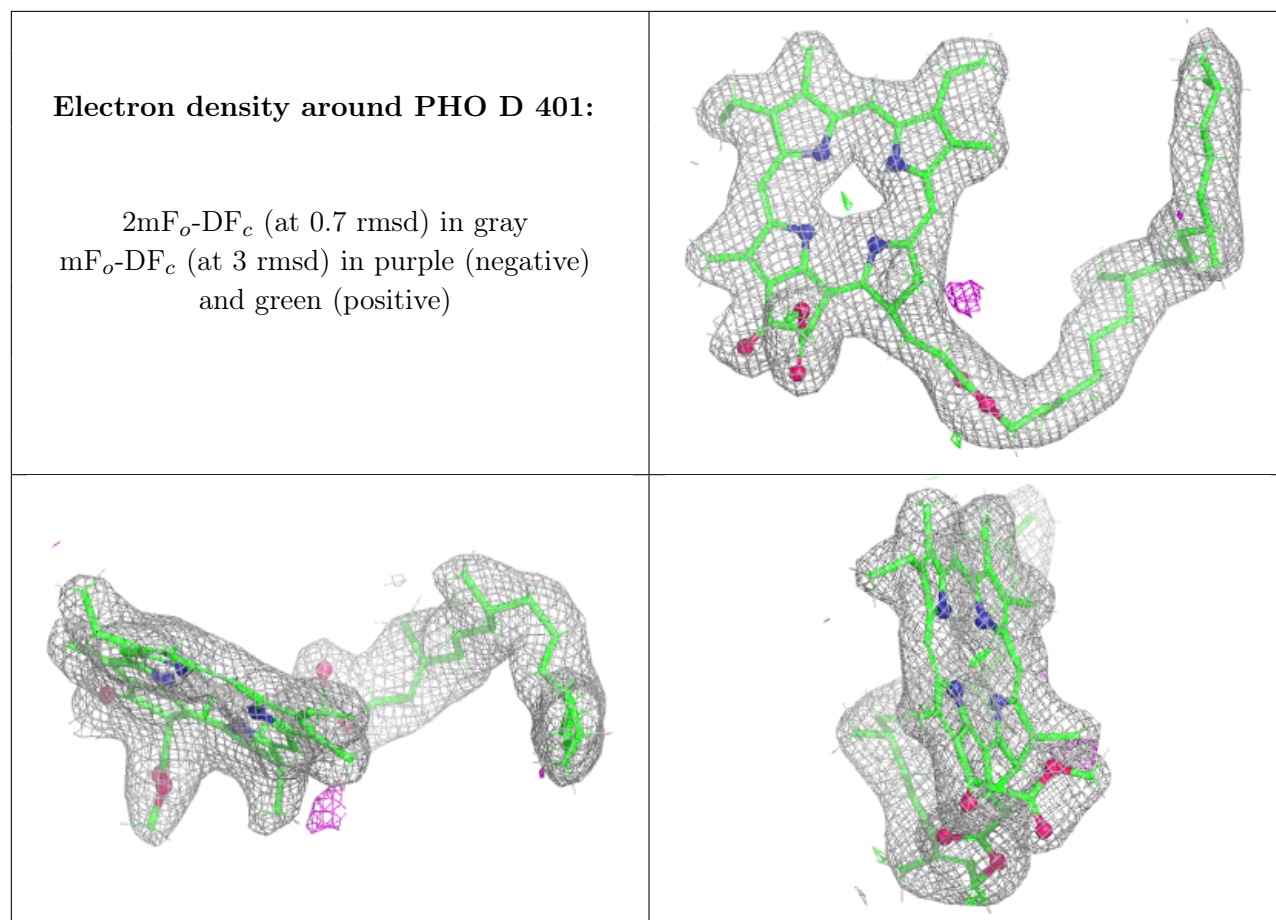
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PHO A 404:**

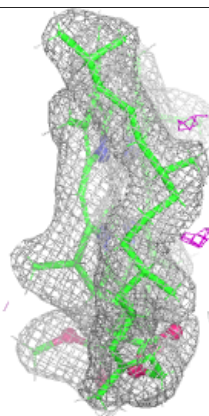
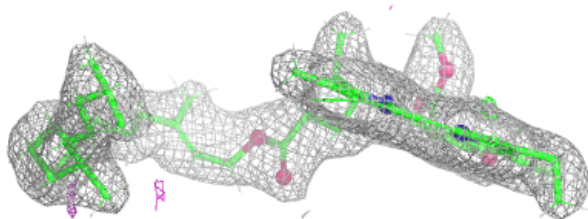
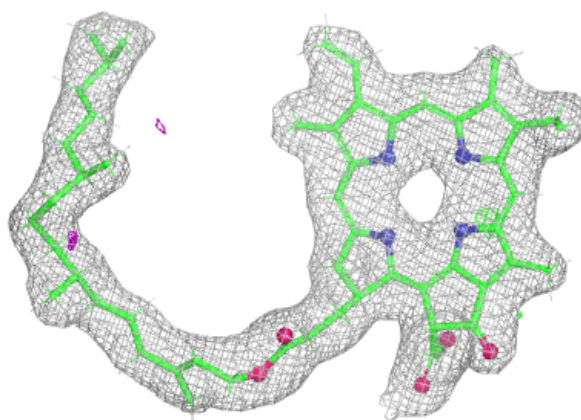
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





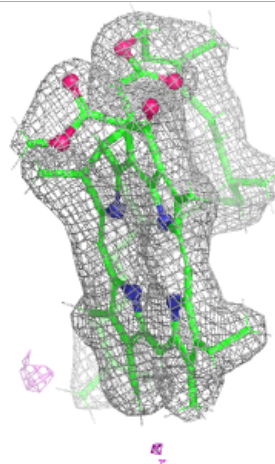
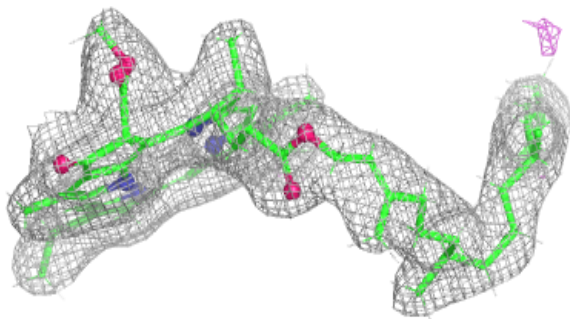
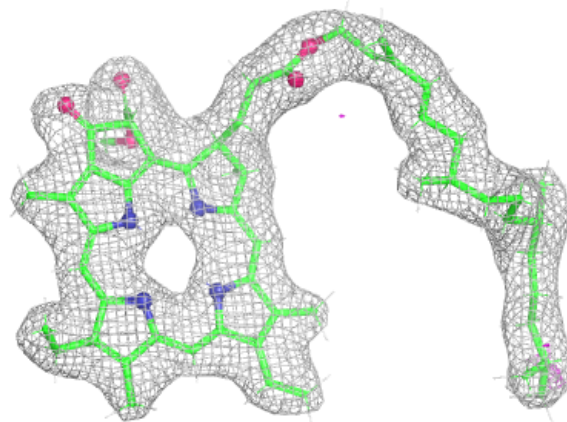
**Electron density around PHO d 401:**

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



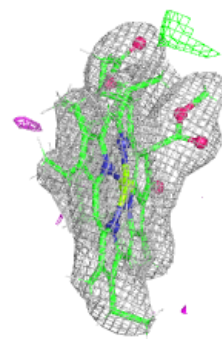
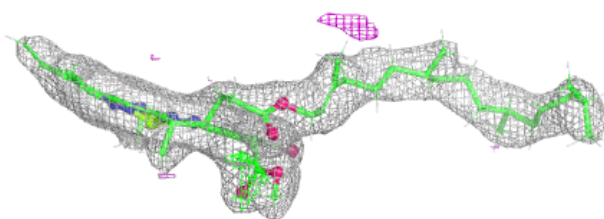
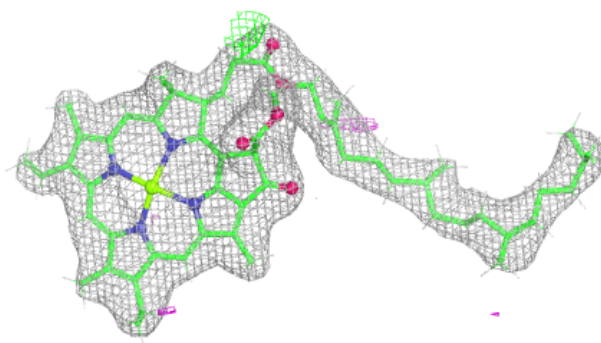
**Electron density around PHO d 402:**

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

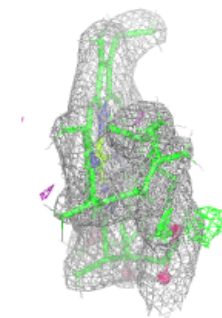
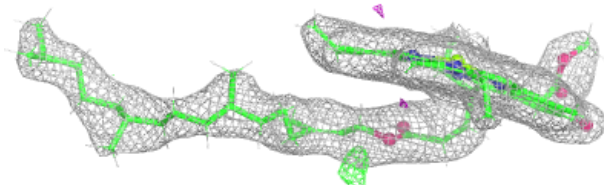
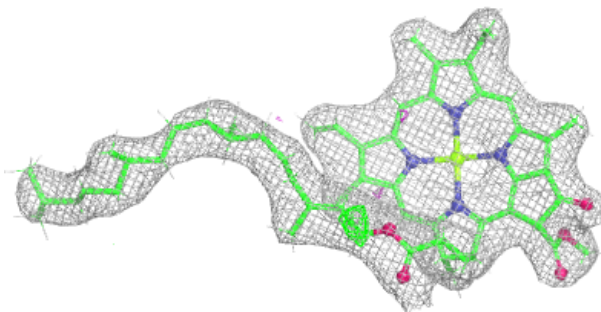


**Electron density around CLA b 602:**

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

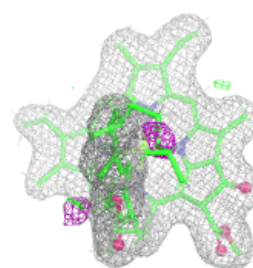
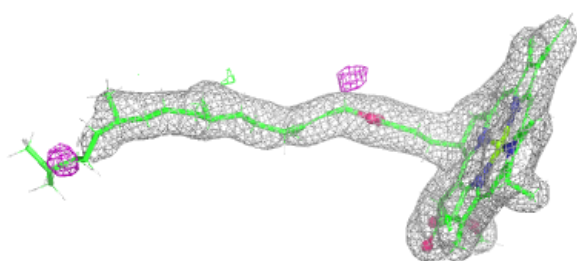
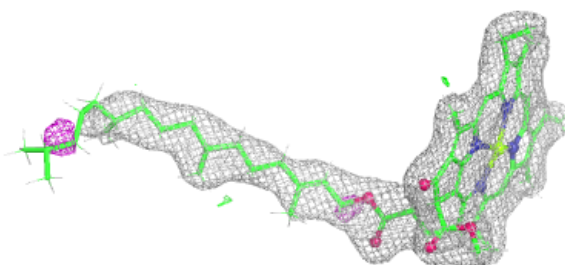
**Electron density around CLA b 603:**

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

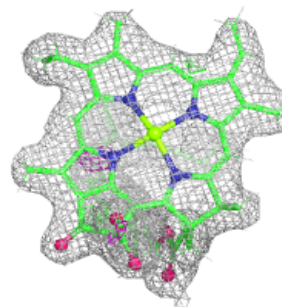
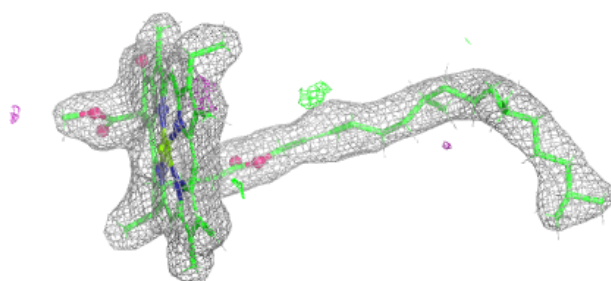
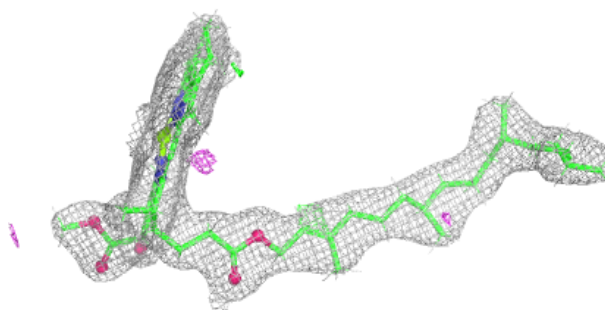


**Electron density around CLA b 604:**

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

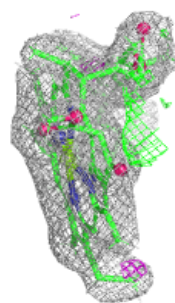
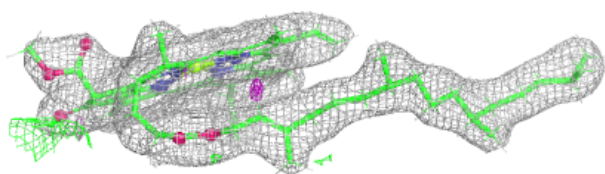
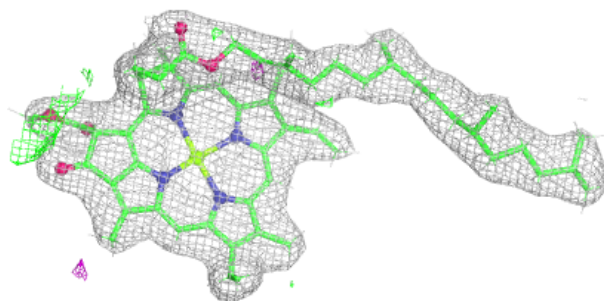
**Electron density around CLA b 605:**

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

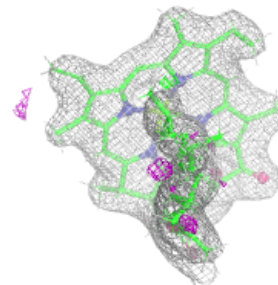
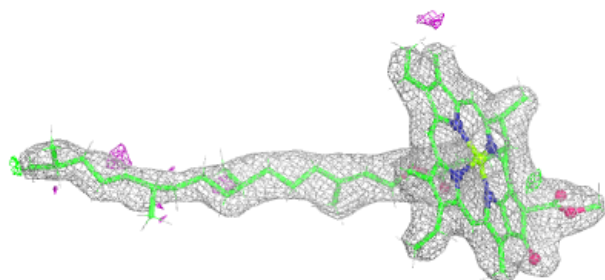
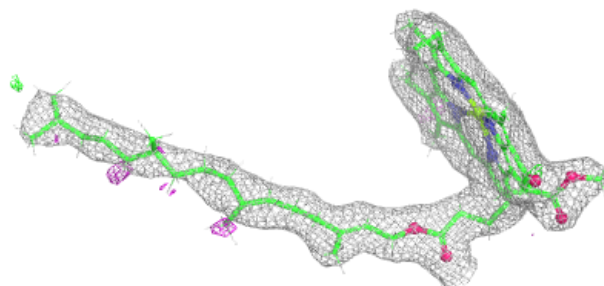


**Electron density around CLA C 501:**

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

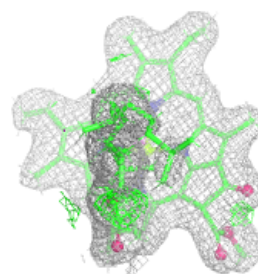
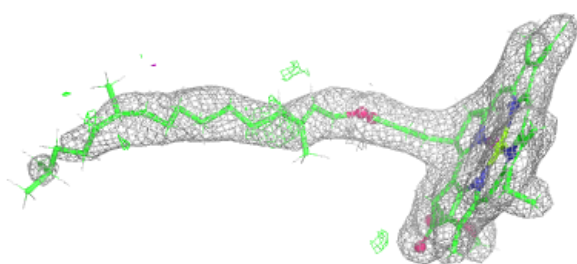
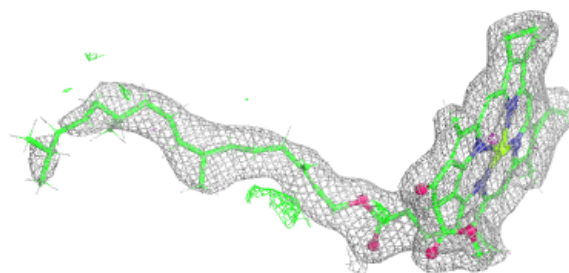
**Electron density around CLA b 607:**

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

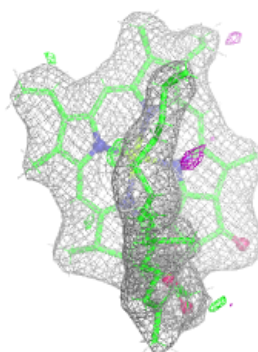
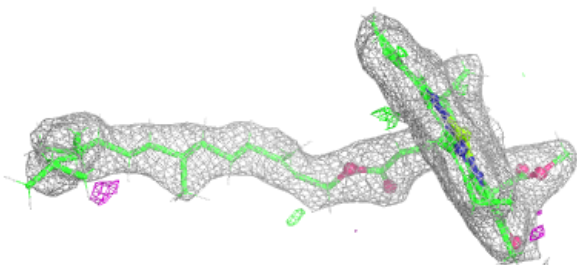
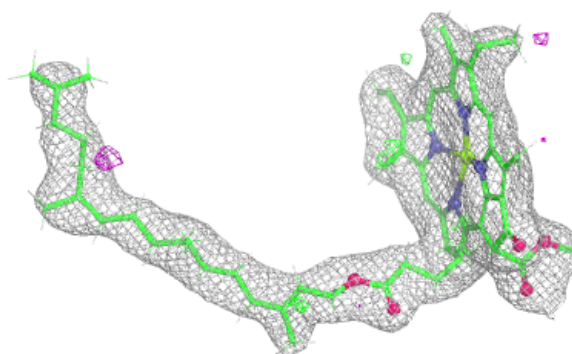


**Electron density around CLA B 604:**

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

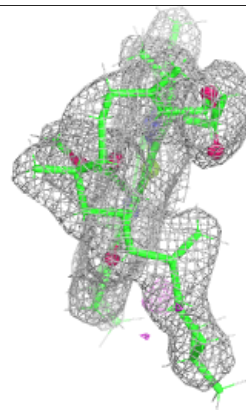
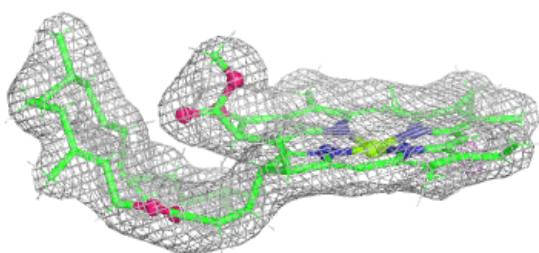
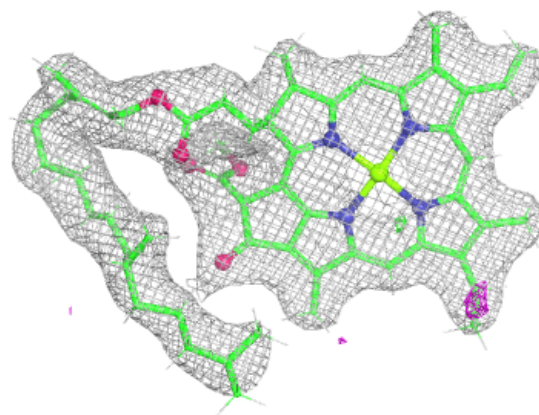
**Electron density around CLA b 609:**

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



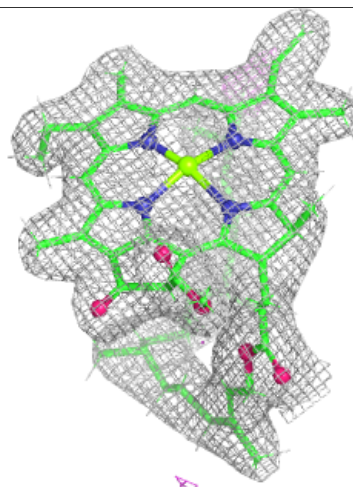
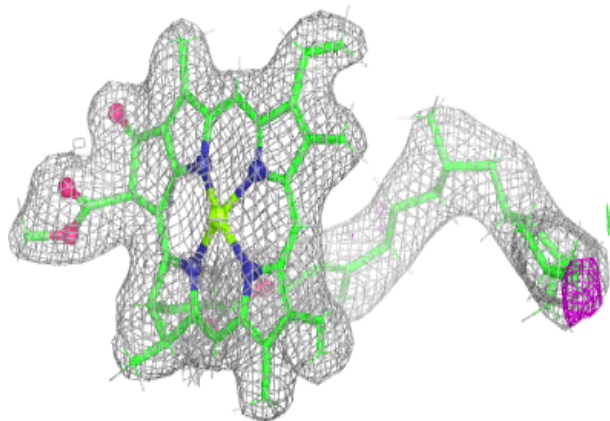
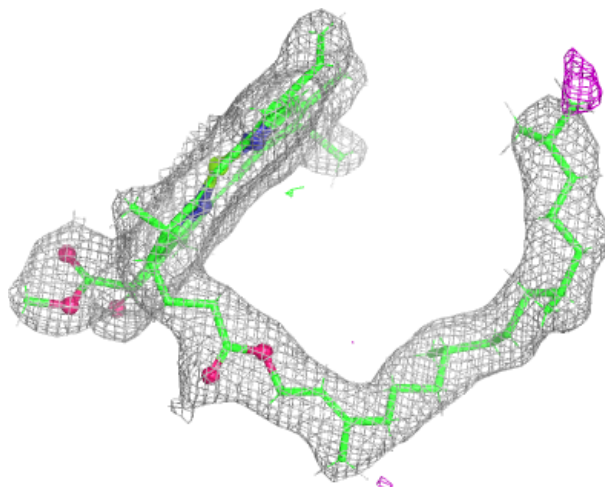
**Electron density around CLA b 610:**

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



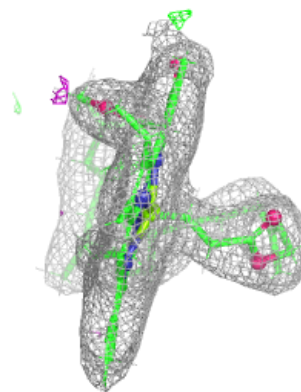
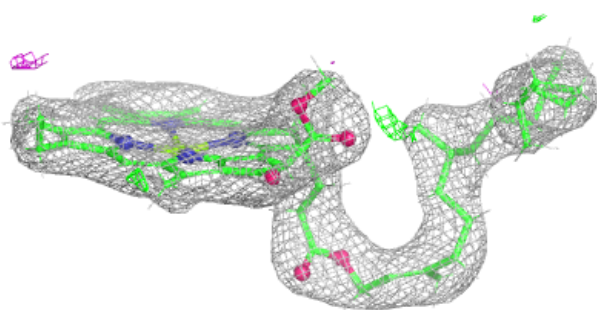
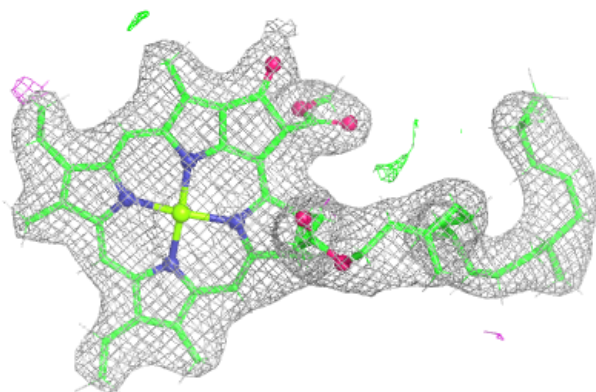
**Electron density around CLA b 611:**

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



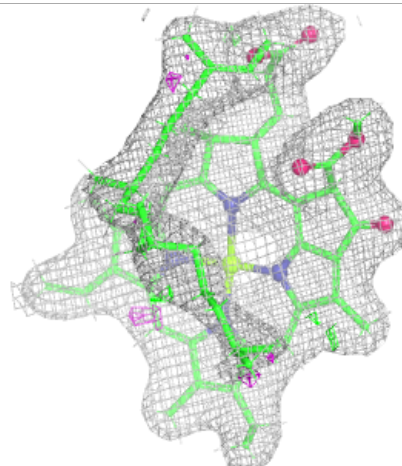
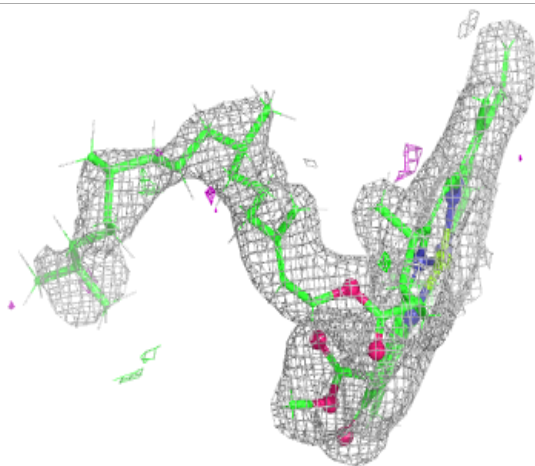
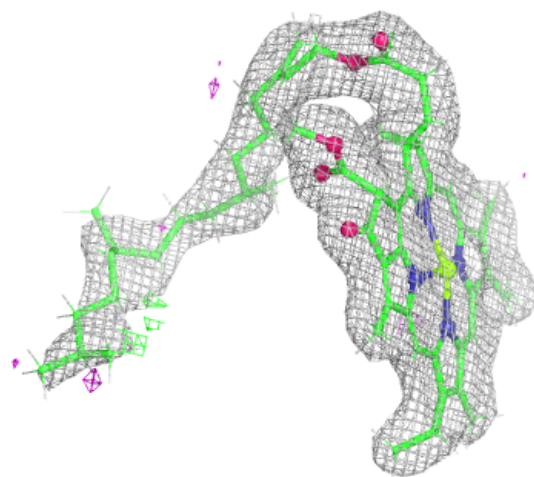
**Electron density around CLA b 612:**

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



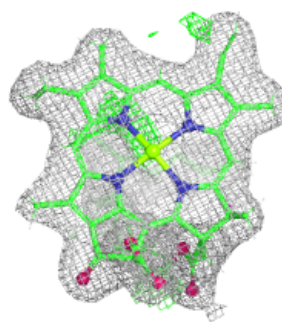
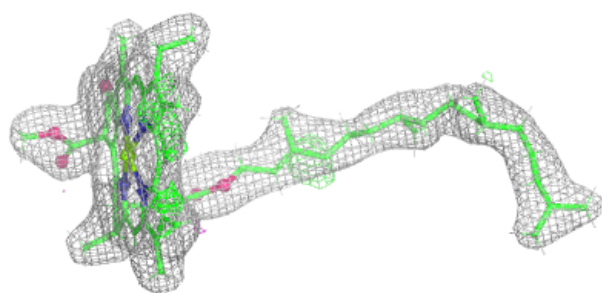
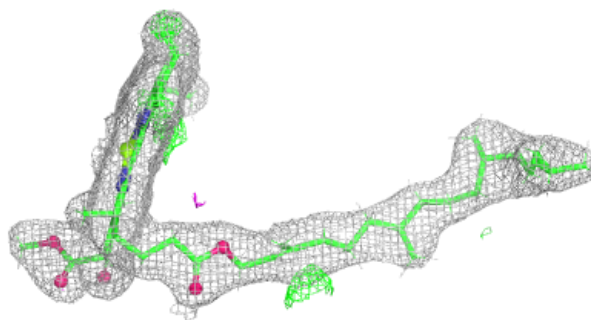
**Electron density around CLA b 613:**

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

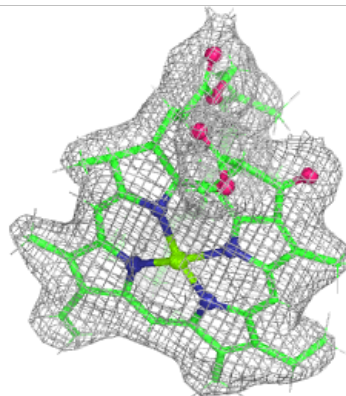
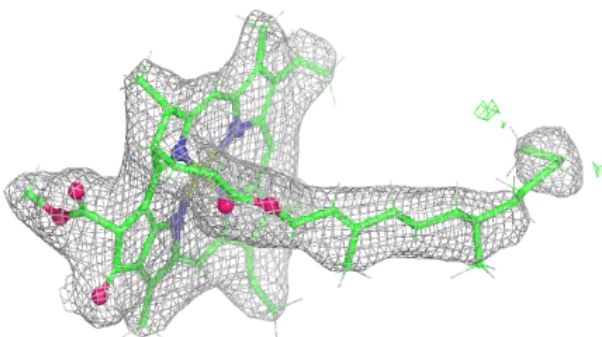
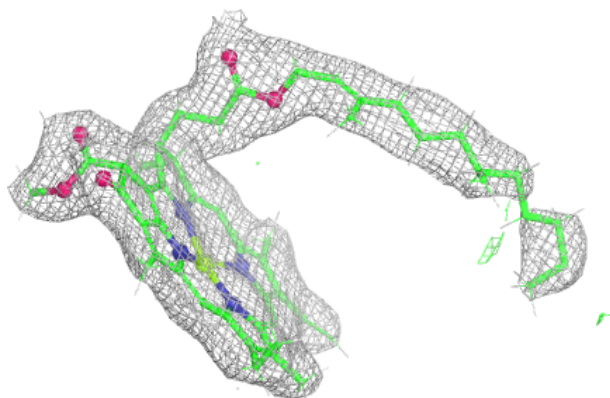


**Electron density around CLA B 605:**

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

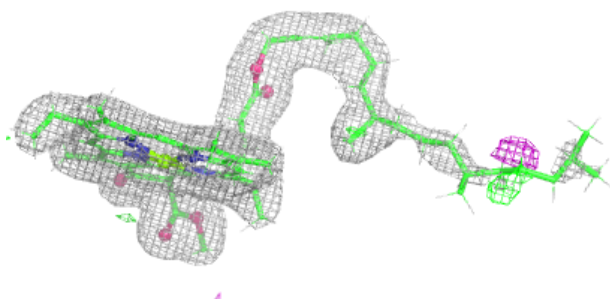
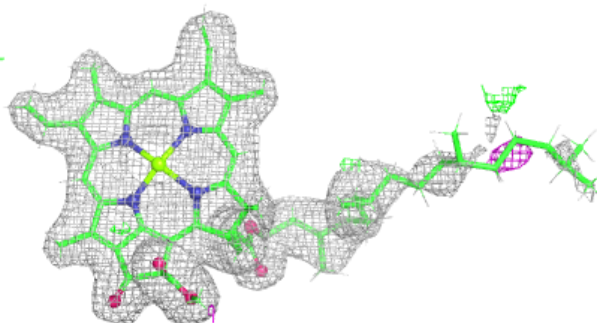
**Electron density around CLA C 504:**

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

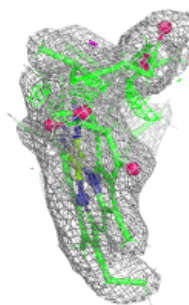
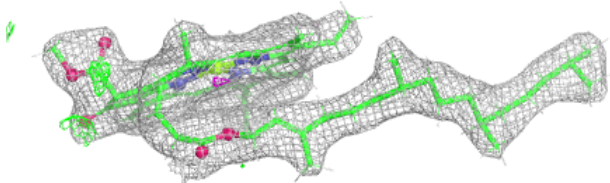
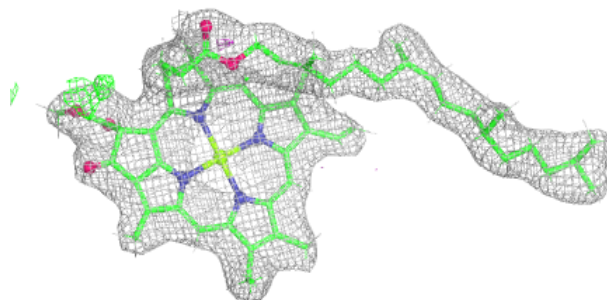


**Electron density around CLA A 403:**

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

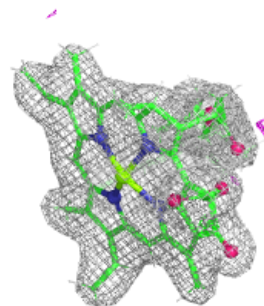
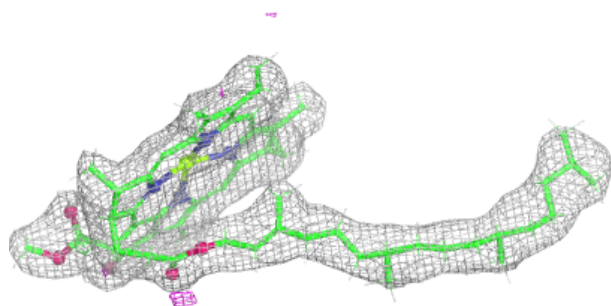
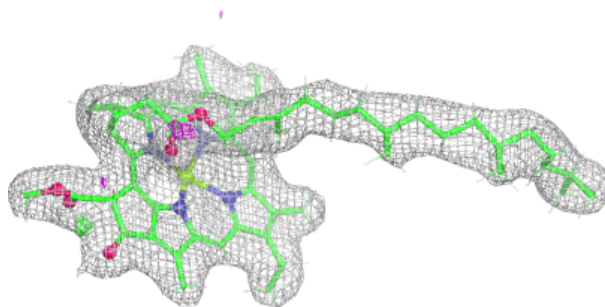
**Electron density around CLA c 501:**

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



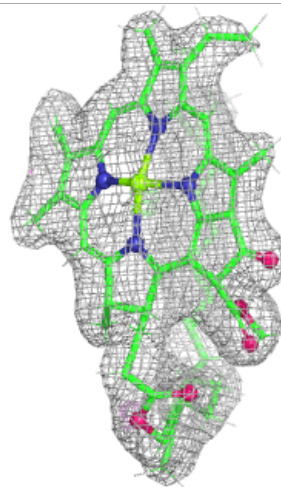
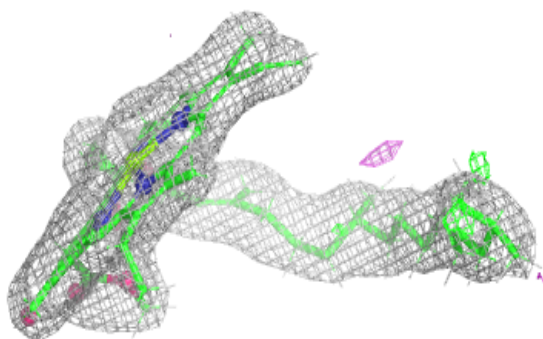
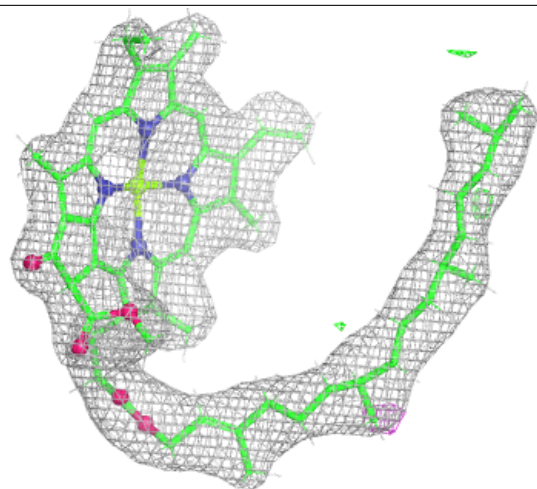
**Electron density around CLA B 608:**

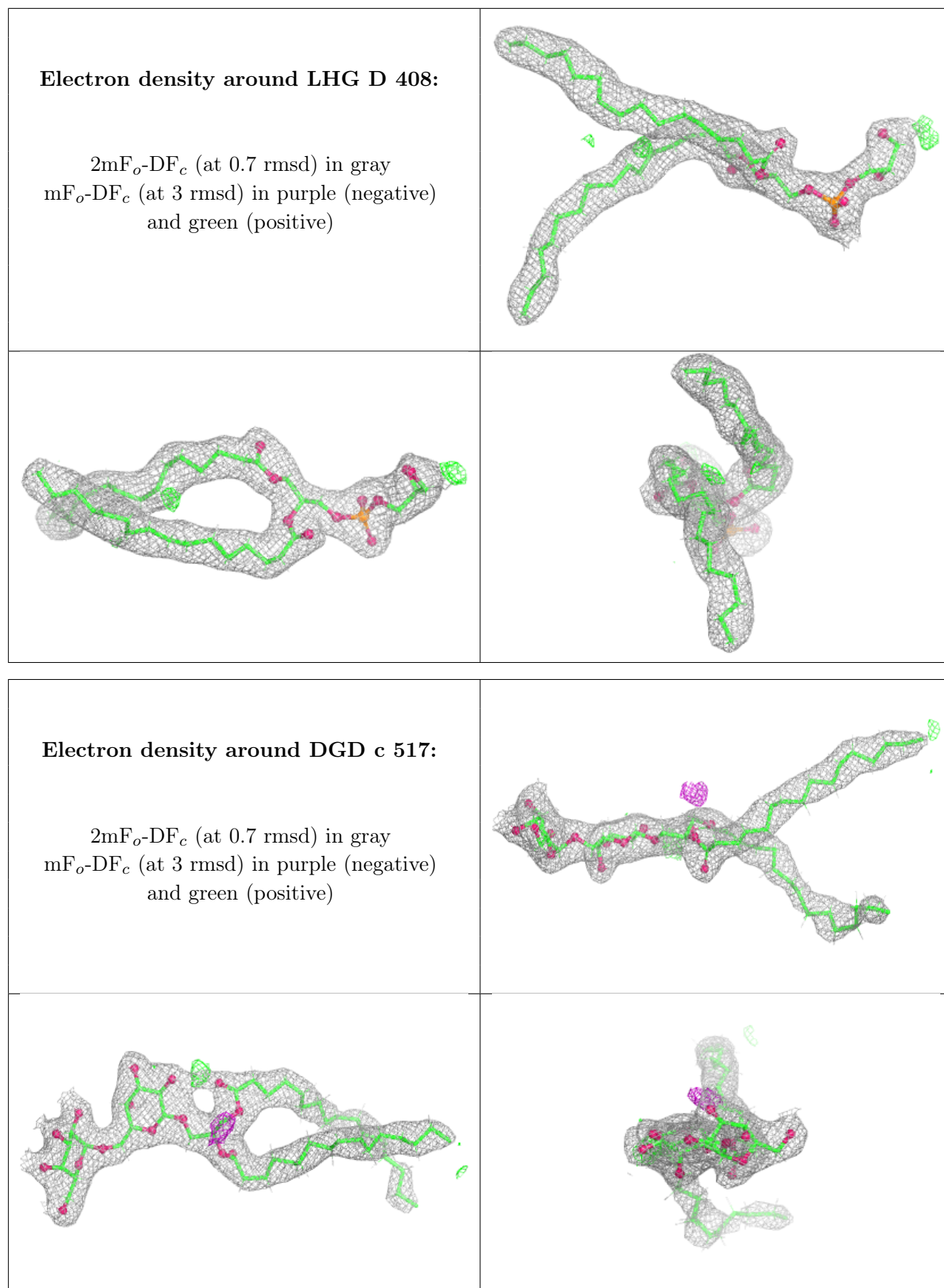
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

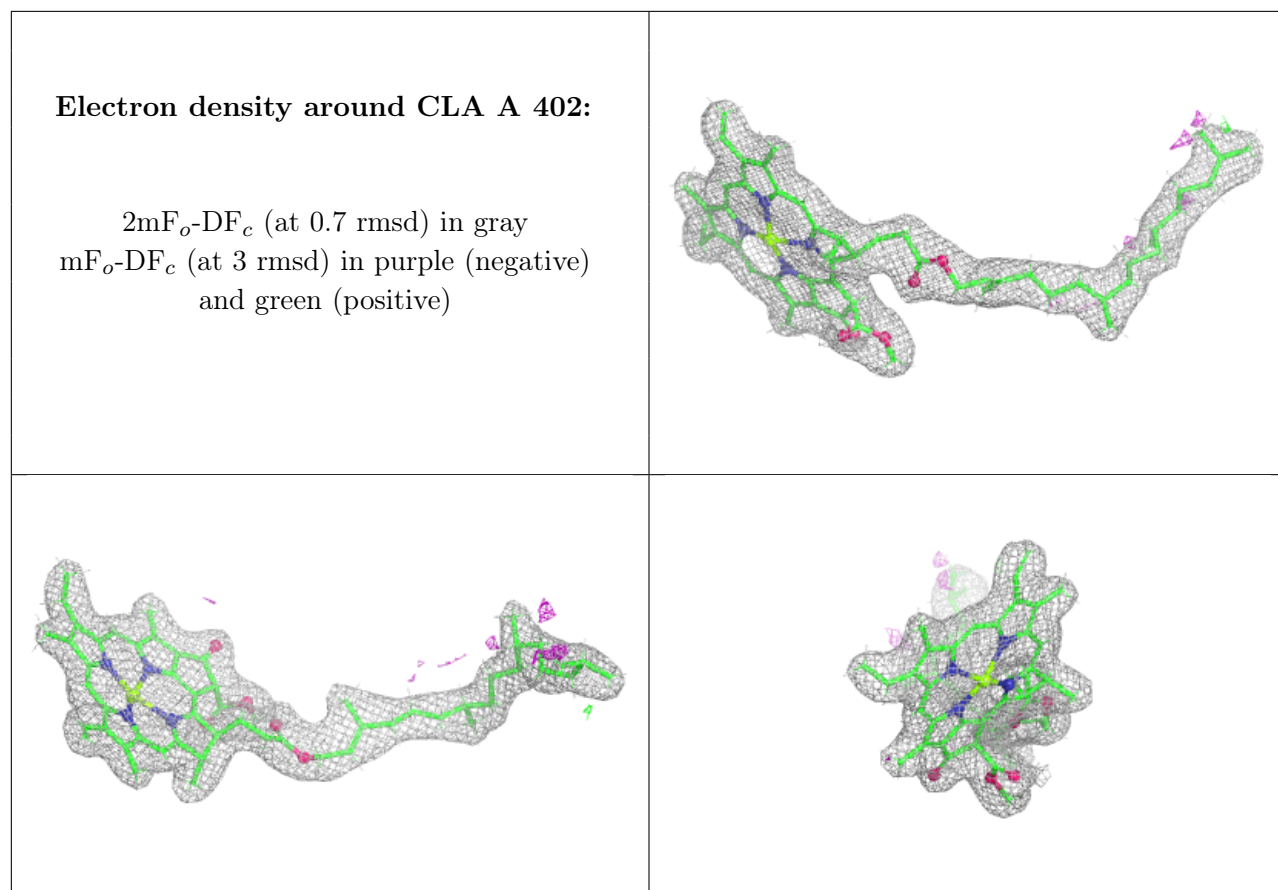


**Electron density around CLA C 507:**

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

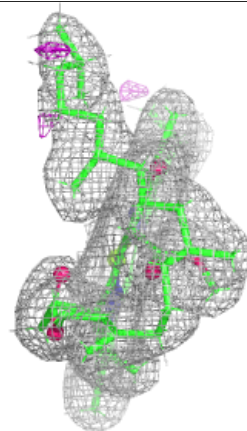
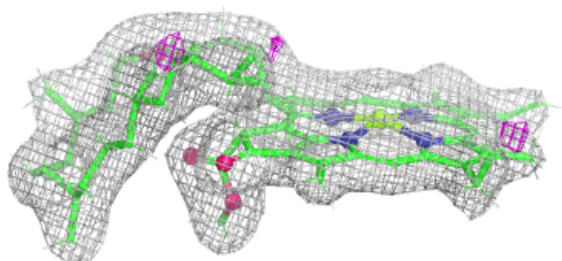
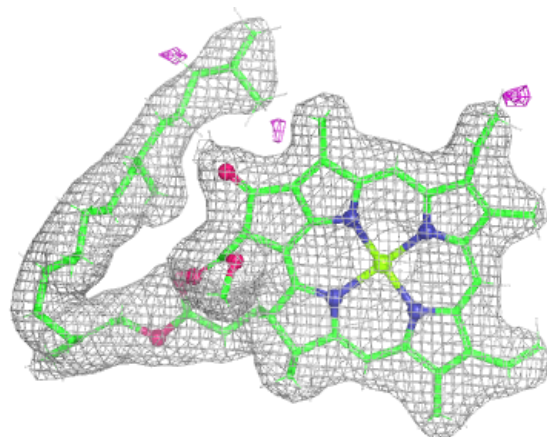






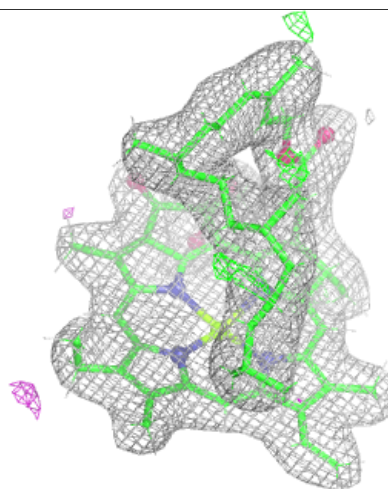
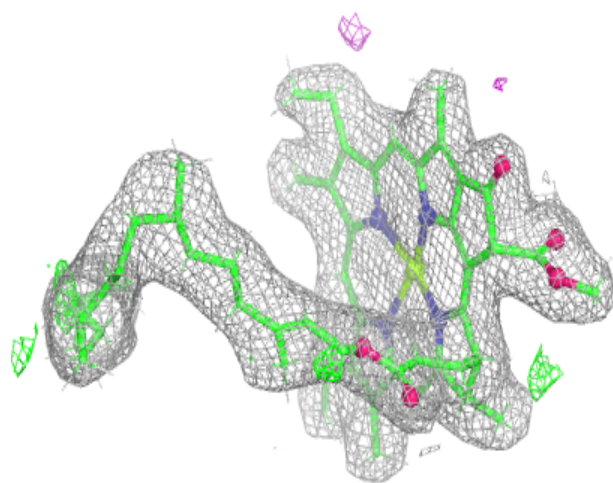
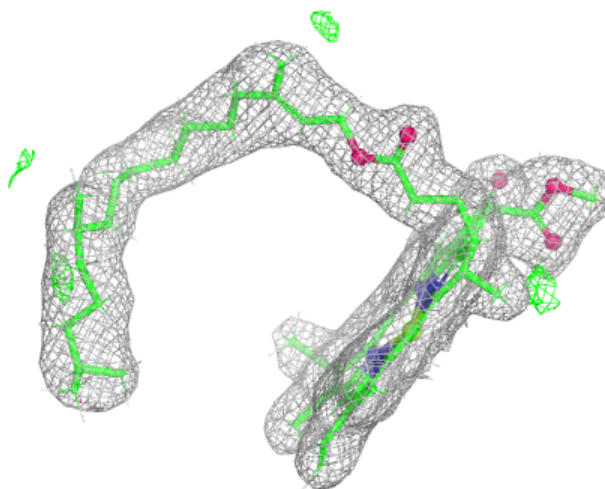
**Electron density around CLA B 610:**

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



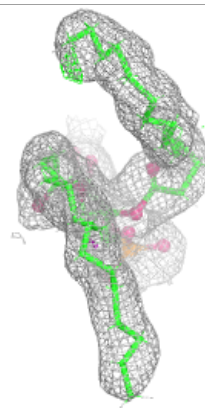
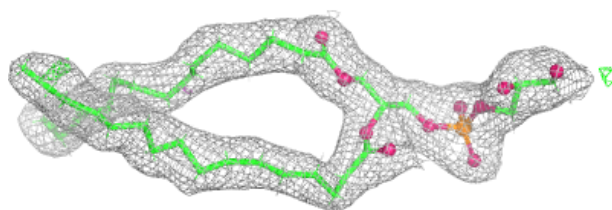
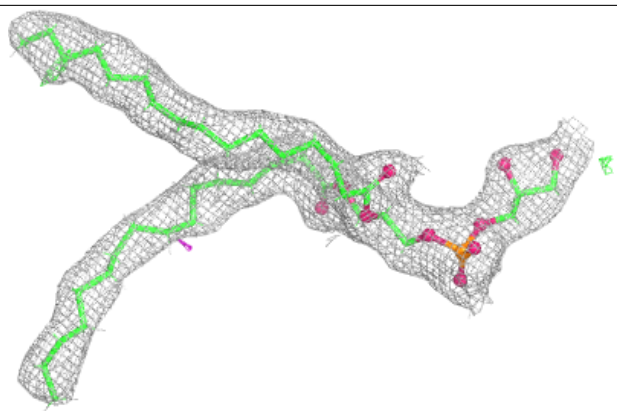
**Electron density around CLA B 611:**

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

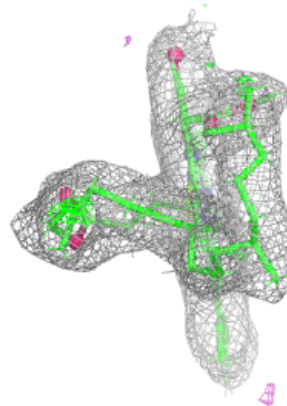
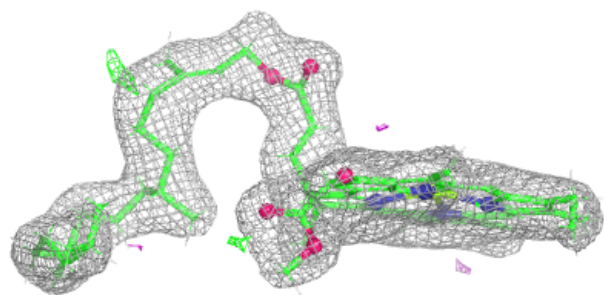
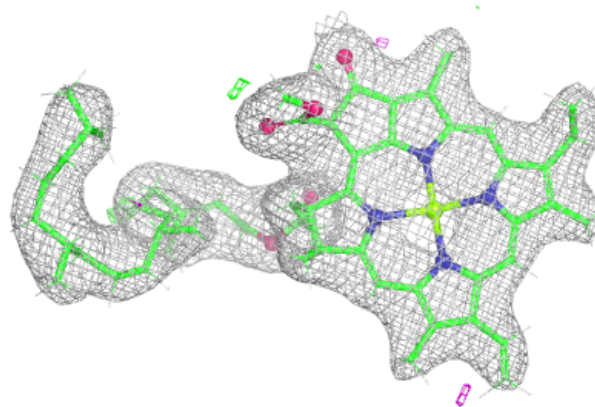


**Electron density around LHG d 409:**

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

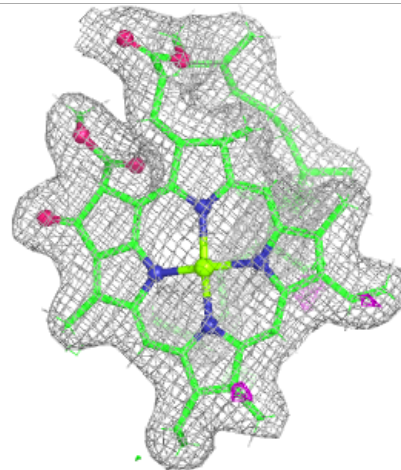
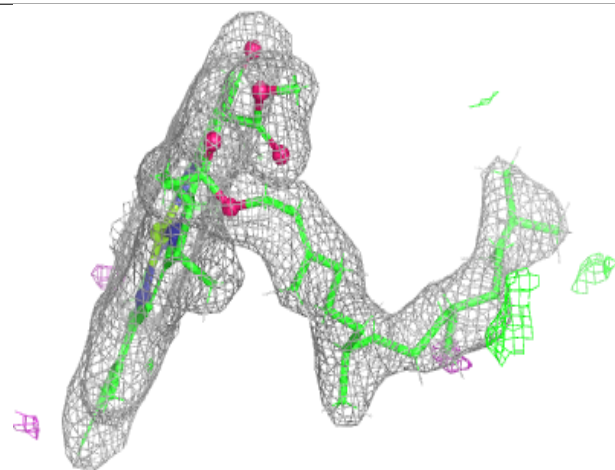
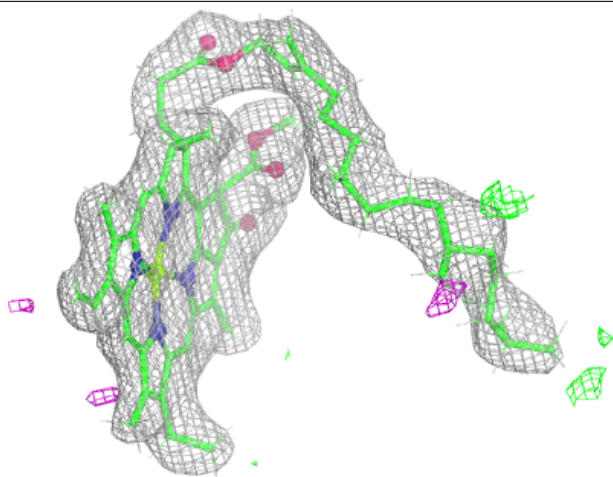
**Electron density around CLA B 612:**

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



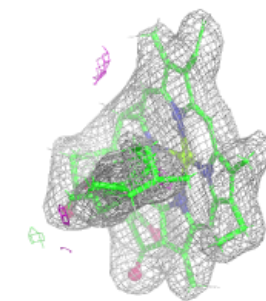
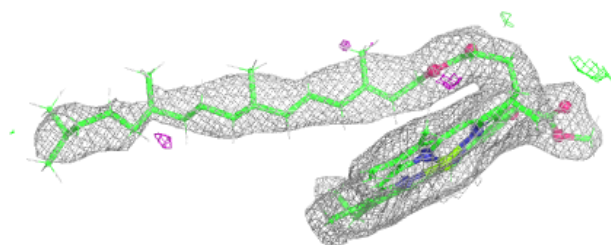
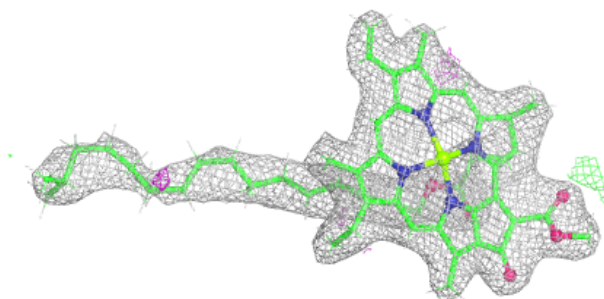
**Electron density around CLA B 613:**

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

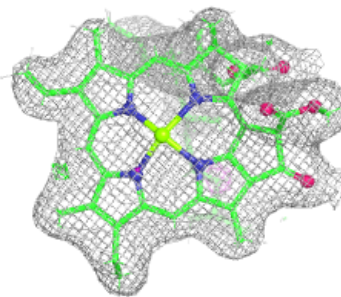
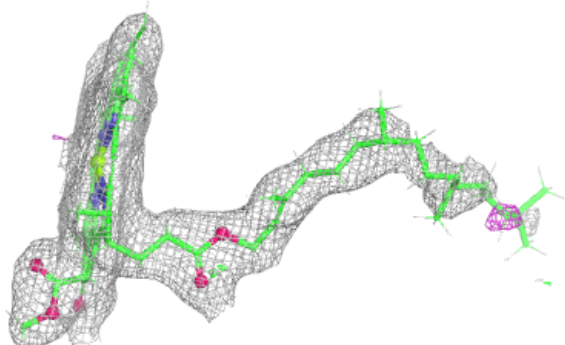
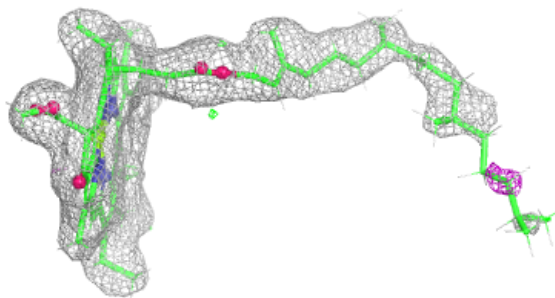


**Electron density around CLA B 614:**

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

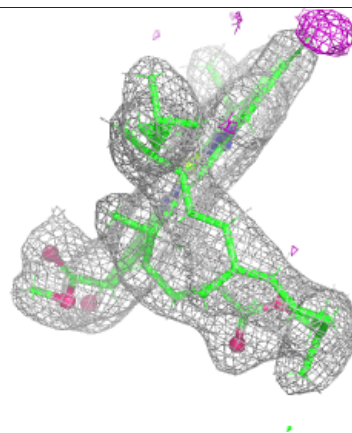
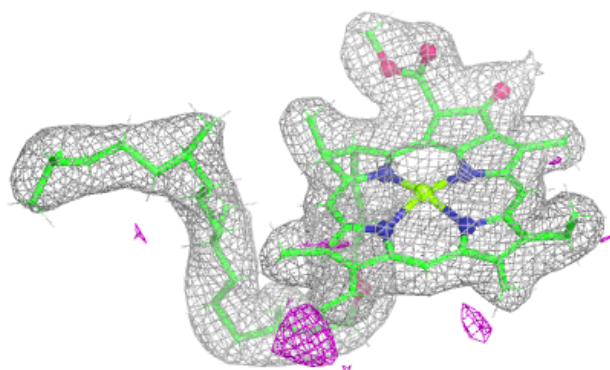
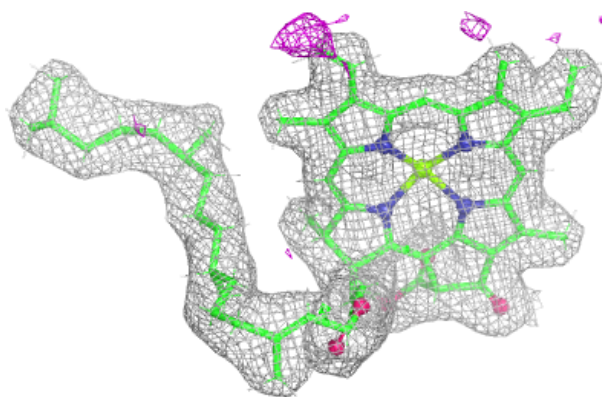
**Electron density around CLA D 404:**

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

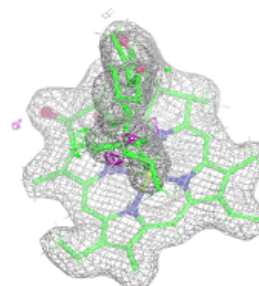
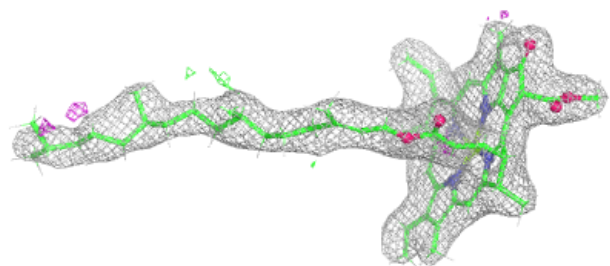
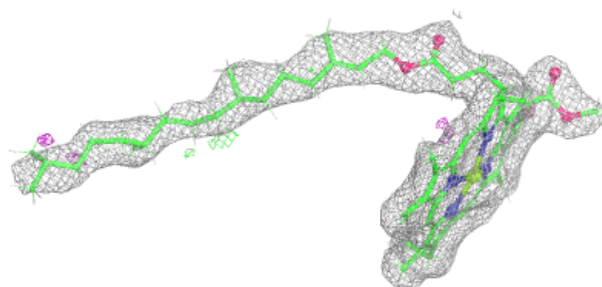


**Electron density around CLA A 410:**

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

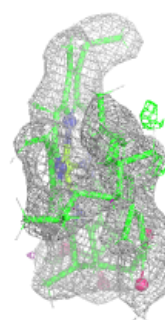
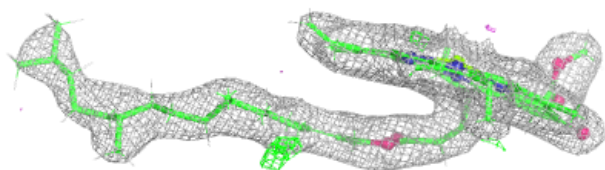
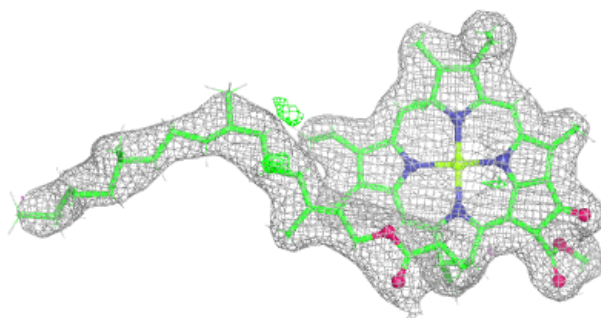
**Electron density around CLA B 607:**

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

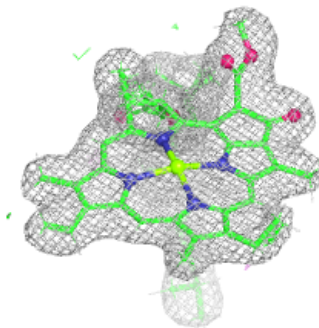
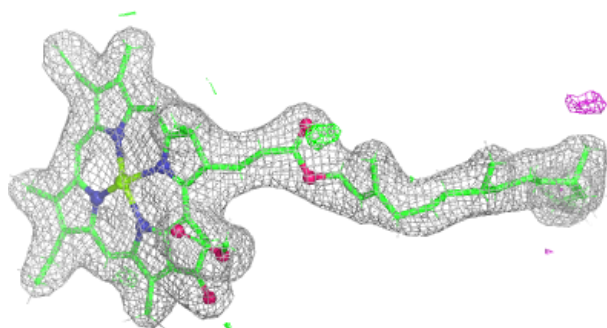
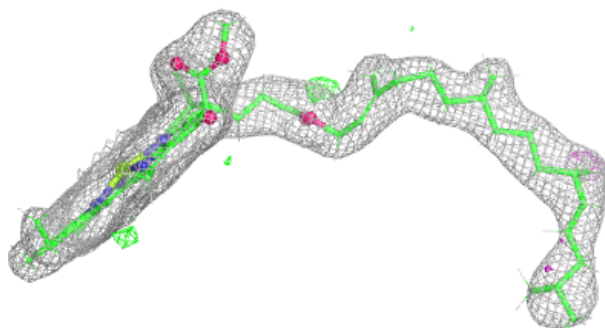


**Electron density around CLA B 603:**

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

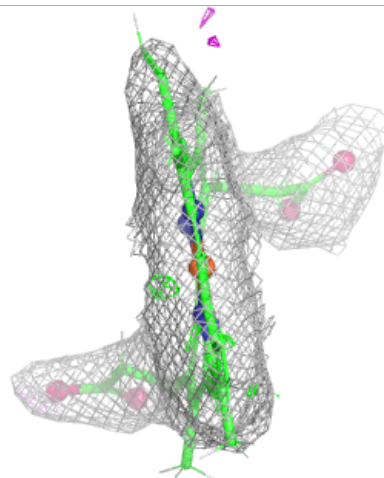
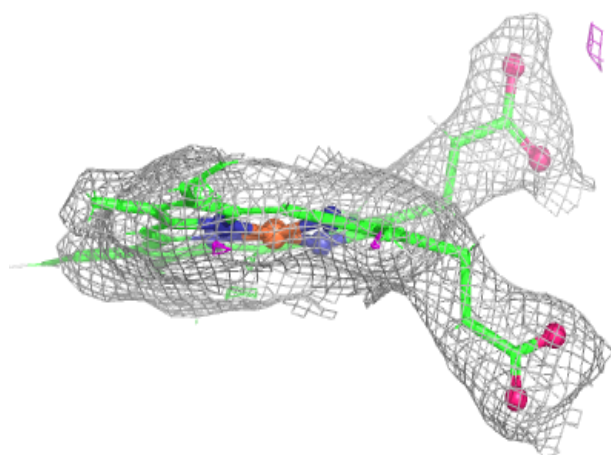
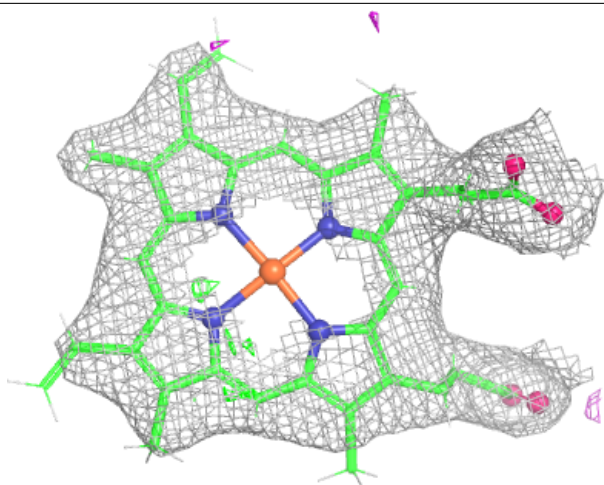
**Electron density around CLA D 403:**

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



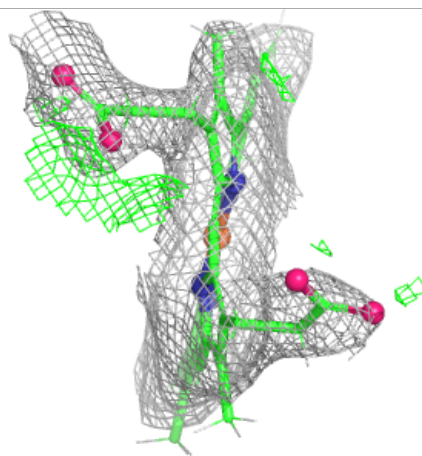
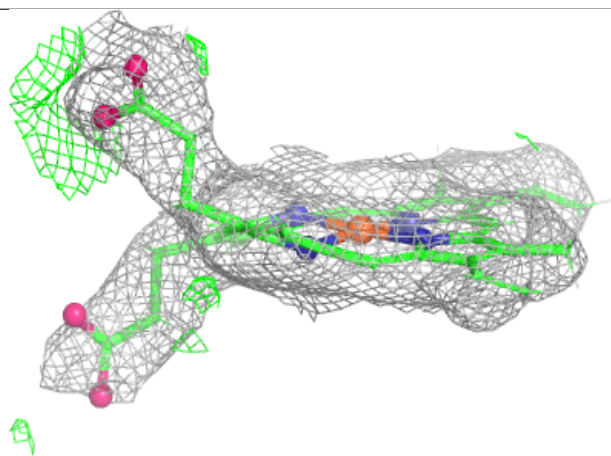
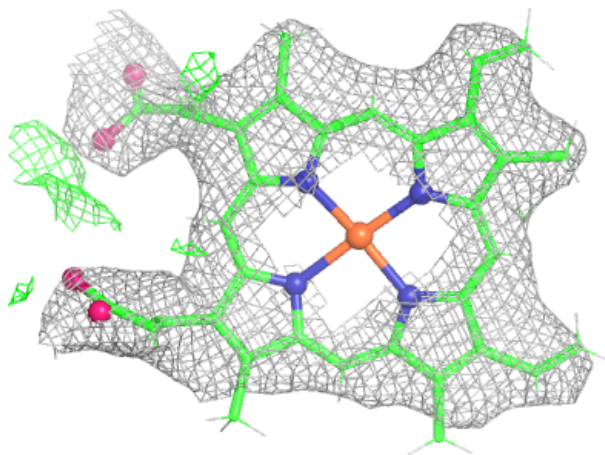
**Electron density around HEM E 101:**

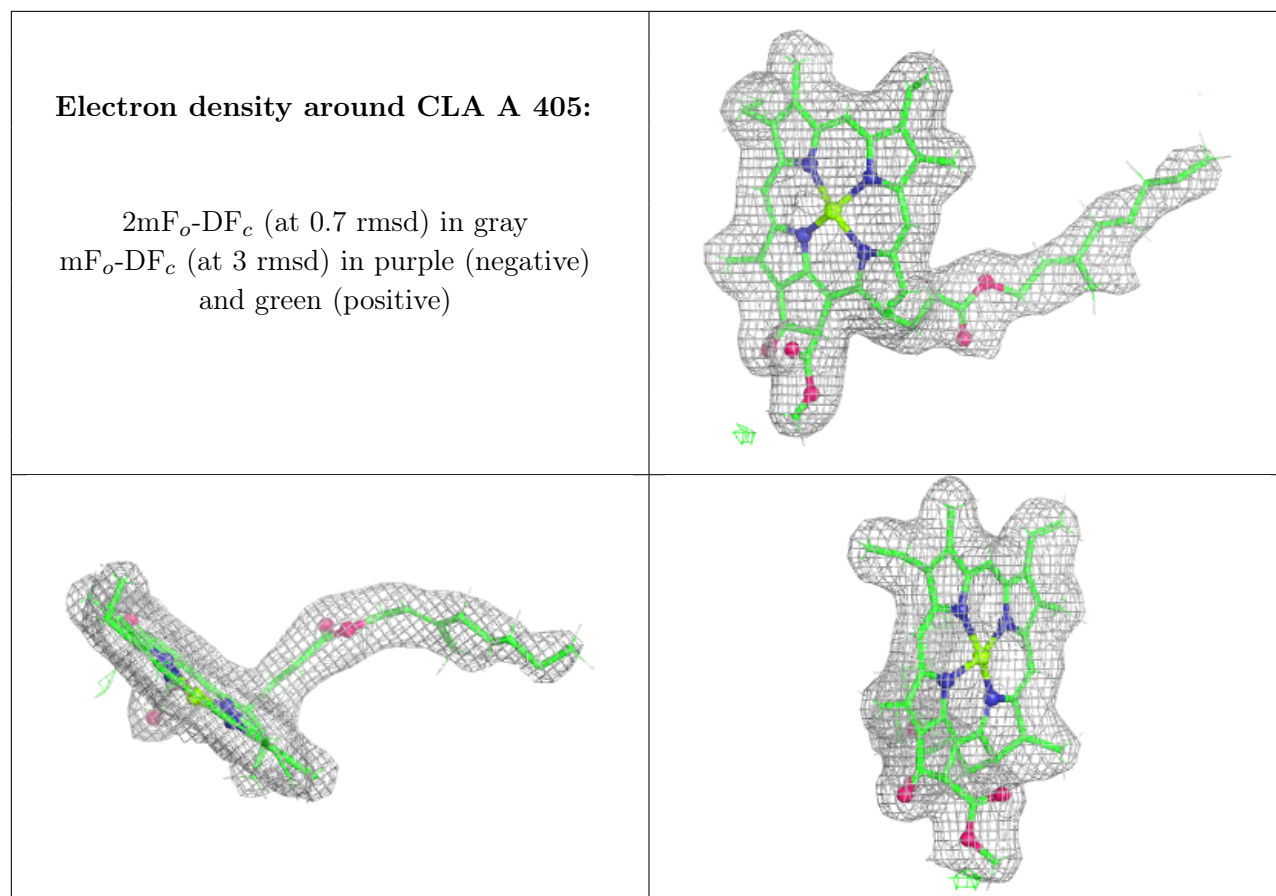
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

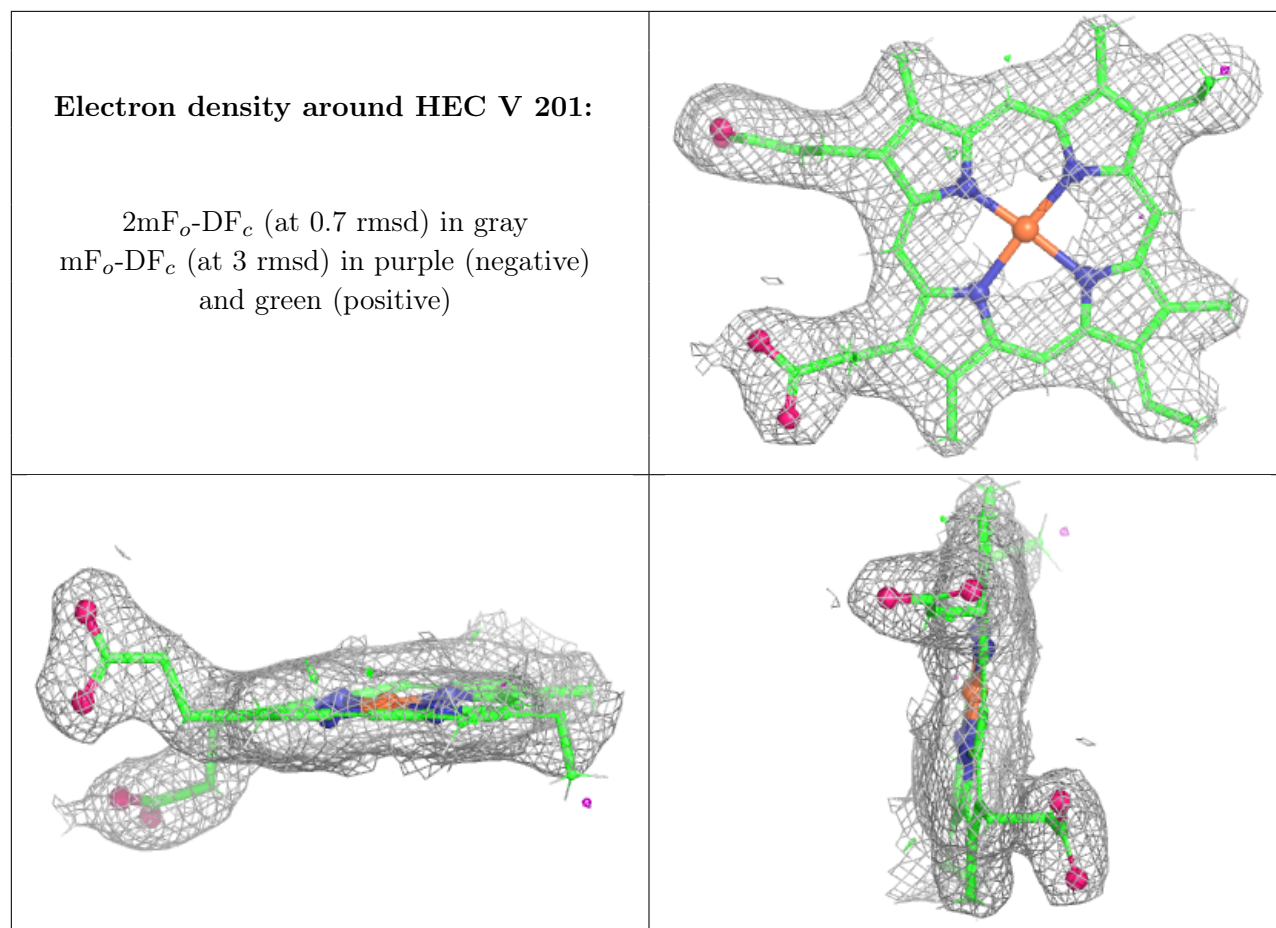


**Electron density around HEM f 101:**

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

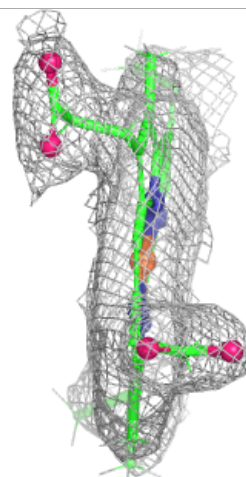
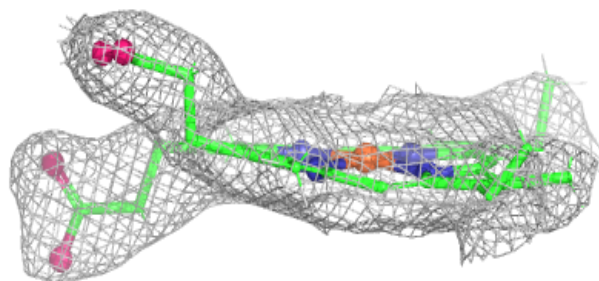
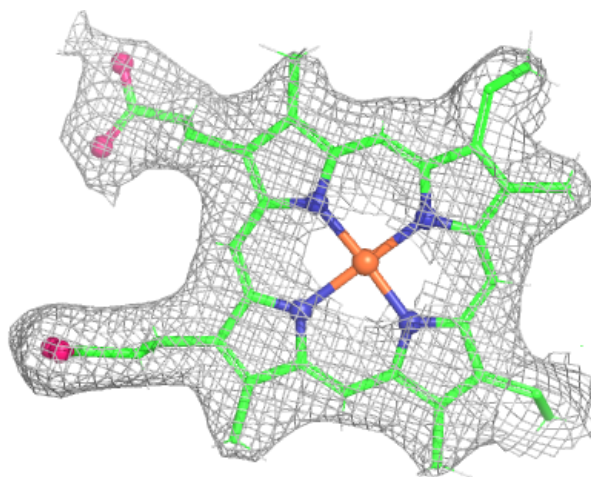






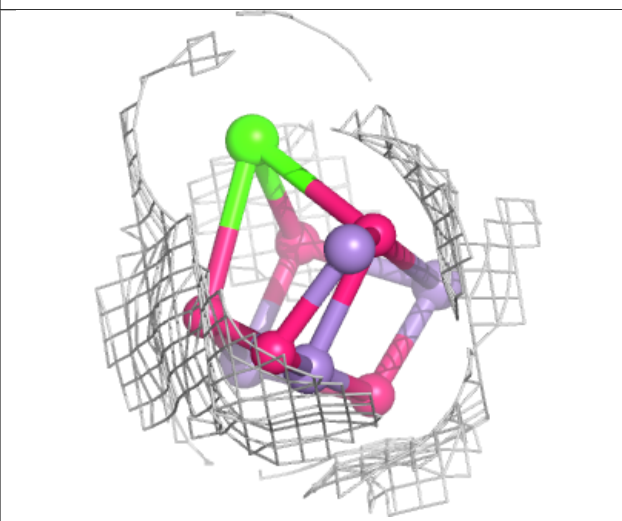
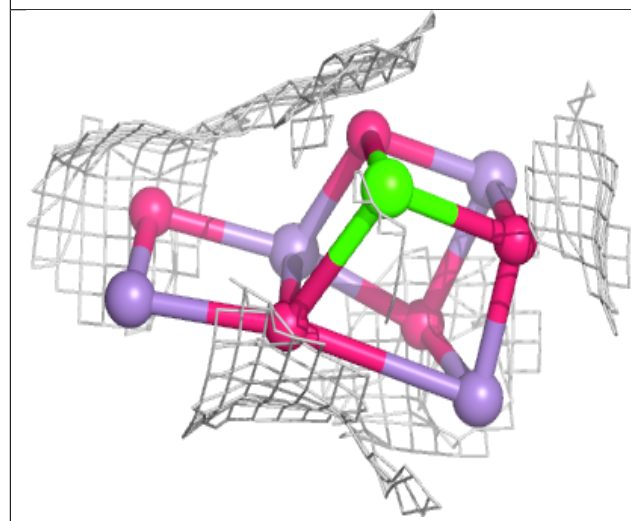
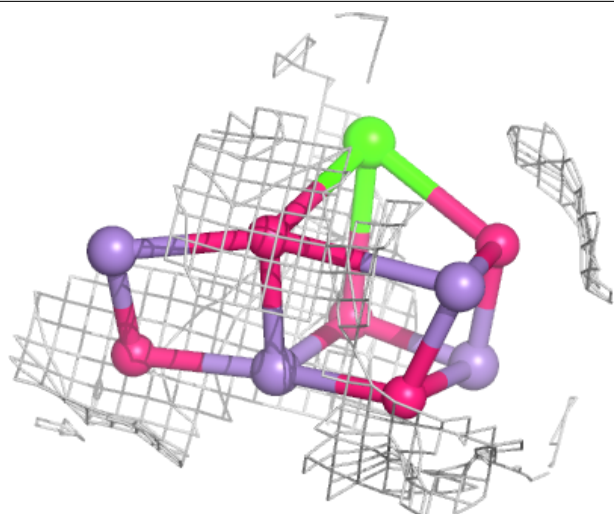
**Electron density around HEC v 201:**

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



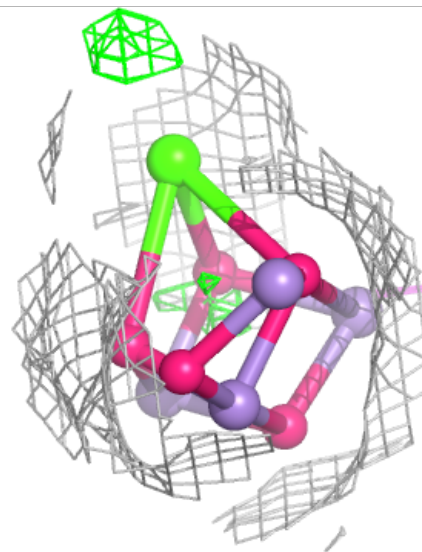
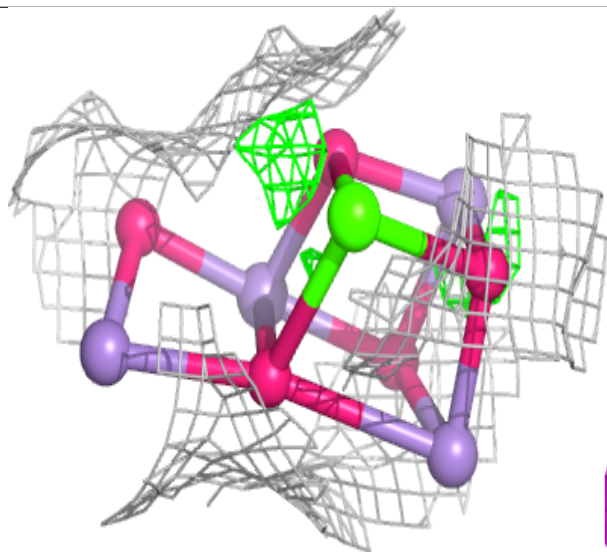
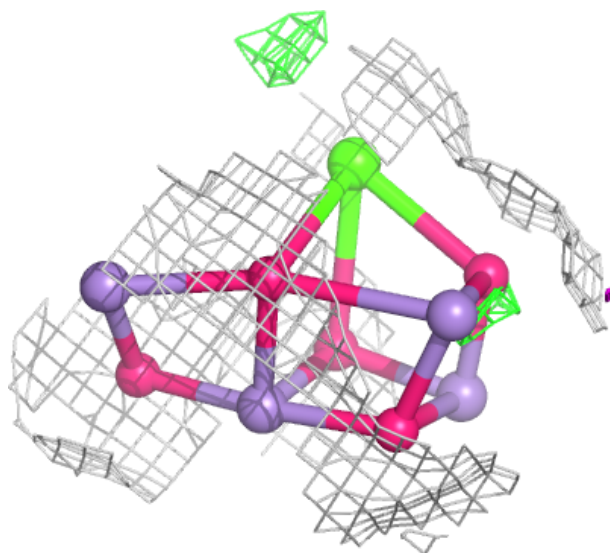
**Electron density around OEX a 416 (A):**

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



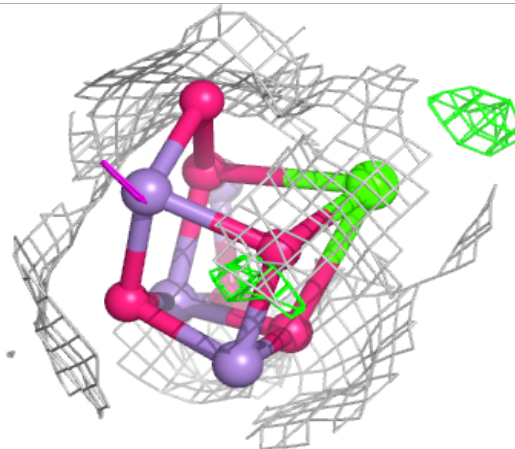
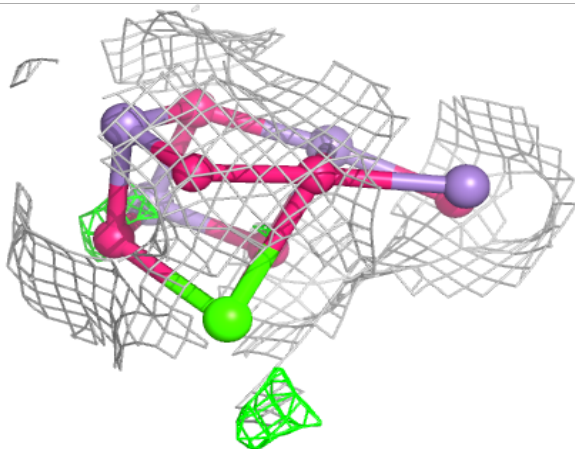
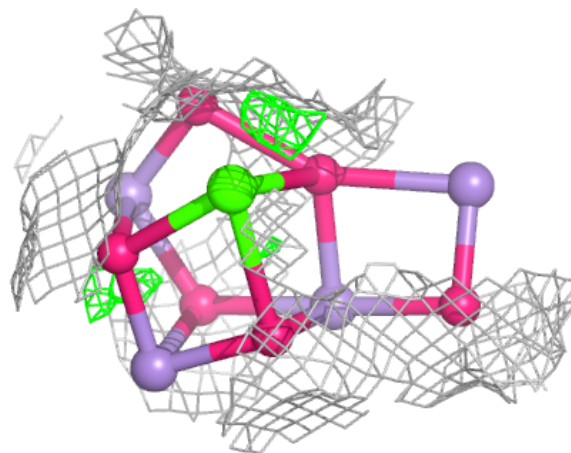
**Electron density around OEX A 416 (A):**

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



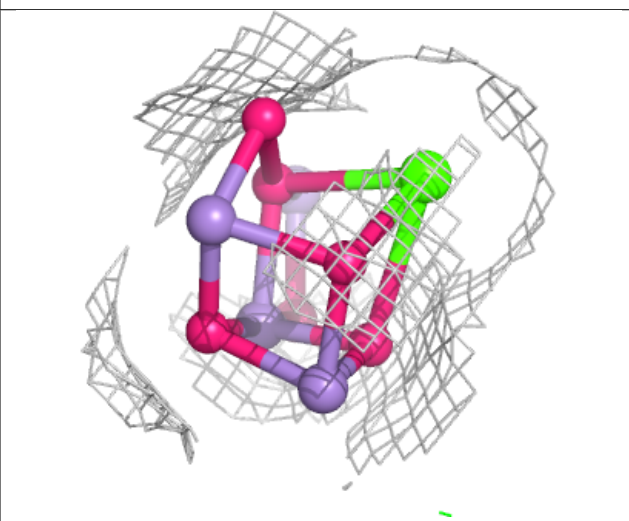
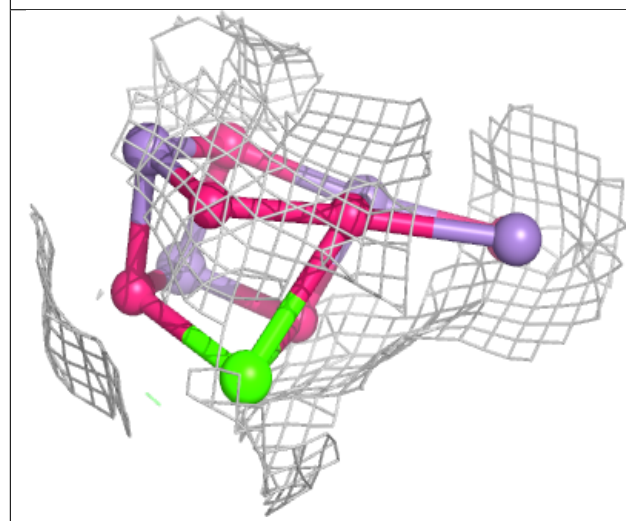
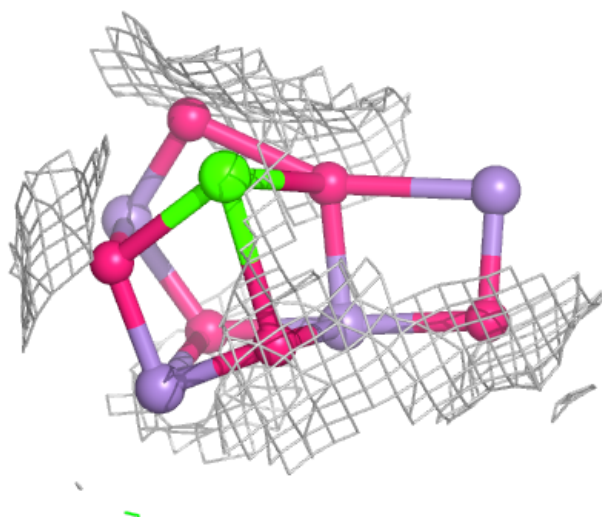
**Electron density around OEY A 415 (B):**

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



**Electron density around OEY a 415 (B):**

$2mF_o-DF_c$  (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.