



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:03 AM UTC

PDB ID : 5B5N / pdb_00005b5n
Title : Crystal structure of the Ba-substituted LH1-RC complex from Tch. tepidum
Authors : Wang-Otomo, Z.-Y.; Yu, L.-J.
Deposited on : 2016-05-12
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

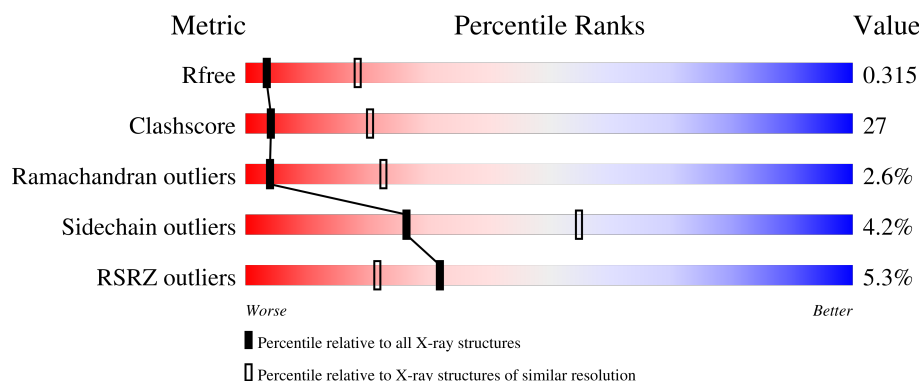
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

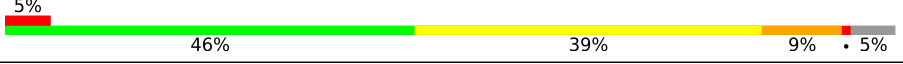
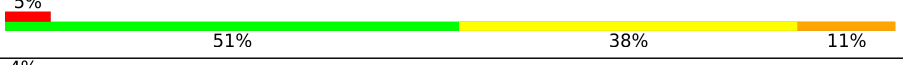
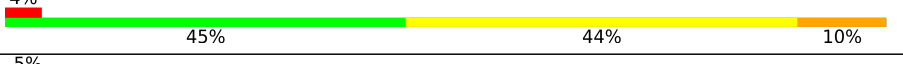
The reported resolution of this entry is 3.30 Å.

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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	C	333	
1	o	333	
2	L	281	
2	x	281	
3	M	319	

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Mol	Chain	Length	Quality of chain
3	y	319	
4	H	259	
4	t	259	
5	1	61	
5	3	61	
5	5	61	
5	7	61	
5	9	61	
5	A	61	
5	AA	61	
5	AC	61	
5	AE	61	
5	AG	61	
5	AI	61	
5	AK	61	
5	D	61	
5	F	61	
5	I	61	
5	K	61	
5	O	61	
5	Q	61	
5	S	61	
5	U	61	
5	W	61	
5	Y	61	

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Mol	Chain	Length	Quality of chain
5	d	61	
5	f	61	
5	h	61	
5	j	61	
5	l	61	
5	m	61	
5	p	61	
5	r	61	
5	u	61	
5	w	61	
6	0	47	
6	2	47	
6	4	47	
6	6	47	
6	8	47	
6	AB	47	
6	AD	47	
6	AF	47	
6	AH	47	
6	AJ	47	
6	AL	47	
6	B	47	
6	E	47	
6	G	47	
6	J	47	

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Mol	Chain	Length	Quality of chain
6	N	47	
6	P	47	
6	R	47	
6	T	47	
6	V	47	
6	X	47	
6	Z	47	
6	c	47	
6	e	47	
6	g	47	
6	i	47	
6	k	47	
6	n	47	
6	q	47	
6	s	47	
6	v	47	
6	z	47	

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
15	CRT	X	101	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 51893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			
1	o	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	280	Total	C	N	O	S	0	0	0
			2231	1501	359	361	10			
2	x	280	Total	C	N	O	S	0	0	0
			2231	1501	359	361	10			

- Molecule 3 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	318	Total	C	N	O	S	0	0	0
			2546	1710	416	409	11			
3	y	318	Total	C	N	O	S	0	0	0
			2546	1710	416	409	11			

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	0	0	0
			1982	1275	339	363	5			
4	t	258	Total	C	N	O	S	0	0	0
			1982	1275	339	363	5			

- Molecule 5 is a protein called LH1 alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	D	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	F	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	I	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	K	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	O	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	Q	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	S	60	Total 481	C 318	N 78	O 83	S 2	0	1	0
5	U	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	W	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	Y	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	1	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	3	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	5	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	7	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	9	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	m	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	p	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	r	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	u	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	w	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	AA	60	Total 475	C 315	N 77	O 81	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AC	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	AE	60	Total	C	N	O	S	0	1	0
			481	318	78	83	2			
5	AG	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	AI	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	AK	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	d	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	f	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	h	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	j	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			
5	l	60	Total	C	N	O	S	0	0	0
			475	315	77	81	2			

- Molecule 6 is a protein called LH1 beta polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	E	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	G	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	J	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	N	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	P	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	R	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	T	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	V	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	X	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	Z	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	2	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	4	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	6	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	8	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	0	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	n	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	q	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	s	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	v	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	z	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	AB	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	AD	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	AF	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	AH	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	AJ	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	AL	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	e	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	g	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	i	40	Total 337	C 228	N 52	O 55	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	k	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	c	40	Total 337	C 228	N 52	O 55	S 2	0	0	0

- # HEM

- Molecule 8 is BARIUM ION (CCD ID: BA) (formula: Ba).

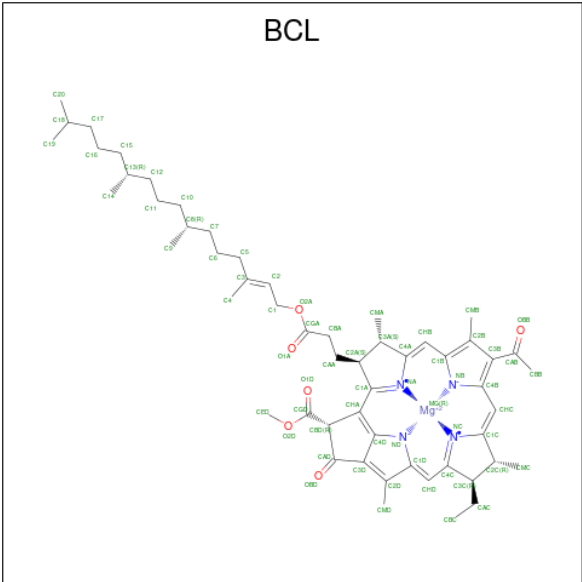
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Ba 1 1	0	0
8	L	2	Total Ba 2 2	0	0
8	A	2	Total Ba 2 2	0	0
8	D	1	Total Ba 1 1	0	0
8	F	1	Total Ba 1 1	0	0
8	I	1	Total Ba 1 1	0	0
8	K	1	Total Ba 1 1	0	0
8	O	1	Total Ba 1 1	0	0
8	Q	1	Total Ba 1 1	0	0
8	S	1	Total Ba 1 1	0	0
8	U	1	Total Ba 1 1	0	0
8	W	1	Total Ba 1 1	0	0
8	Y	1	Total Ba 1 1	0	0
8	1	1	Total Ba 1 1	0	0
8	3	1	Total Ba 1 1	0	0
8	5	1	Total Ba 1 1	0	0
8	7	1	Total Ba 1 1	0	0
8	o	1	Total Ba 1 1	0	0
8	x	2	Total Ba 2 2	0	0
8	m	2	Total Ba 2 2	0	0
8	p	1	Total Ba 1 1	0	0
8	r	1	Total Ba 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	u	1	Total	Ba	0	0
			1	1		
8	w	1	Total	Ba	0	0
			1	1		
8	AA	1	Total	Ba	0	0
			1	1		
8	AC	1	Total	Ba	0	0
			1	1		
8	AE	1	Total	Ba	0	0
			1	1		
8	AG	1	Total	Ba	0	0
			1	1		
8	AI	1	Total	Ba	0	0
			1	1		
8	AK	1	Total	Ba	0	0
			1	1		
8	d	1	Total	Ba	0	0
			1	1		
8	f	1	Total	Ba	0	0
			1	1		
8	h	1	Total	Ba	0	0
			1	1		
8	j	1	Total	Ba	0	0
			1	1		

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	G	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	N	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	P	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	T	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	U	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	V	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	W	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	X	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	2	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	3	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	4	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	5	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	6	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	7	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	8	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	9	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	0	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	x	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	x	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	x	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	y	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	m	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	m	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	p	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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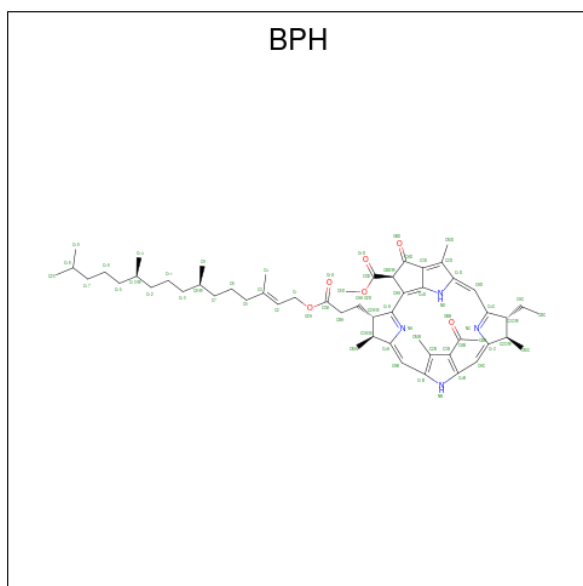
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9	r	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	s	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	u	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	u	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	w	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	z	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AC	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AH	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	d	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	e	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	f	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	g	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	h	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	i	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	j	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	k	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	l	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	c	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



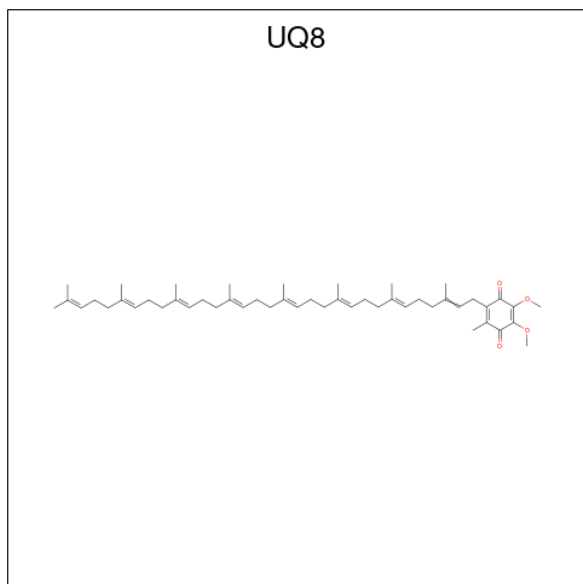
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		
10	x	1	Total	C	N	O	0	0
			65	55	4	6		

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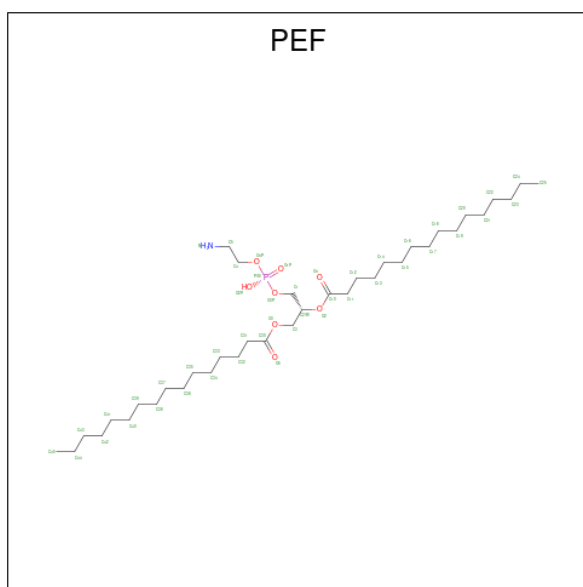
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	y	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			53	49	4		
11	x	1	Total	C	O	0	0
			53	49	4		

- Molecule 12 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	L	1	Total	C	N	O	P	0	0
			12	5	1	5	1		
12	M	1	Total	C	N	O	P	0	0
			16	7	1	7	1		
12	M	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	x	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	y	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	y	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	y	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	t	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	t	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

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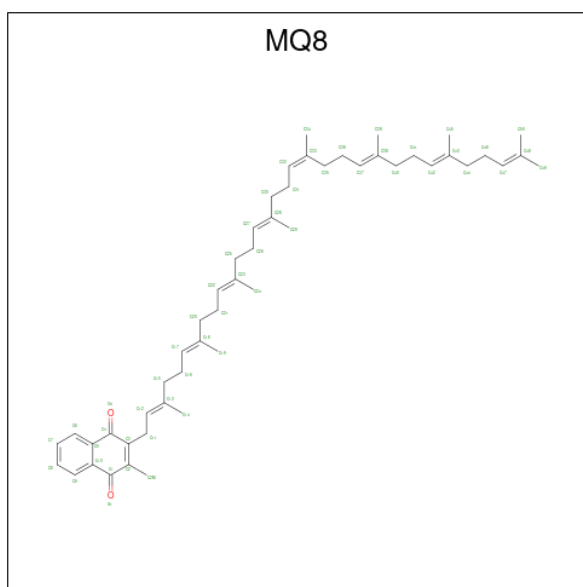
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	m	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	p	1	Total	C	N	O	P	0	0
			16	7	1	7	1		

- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe).

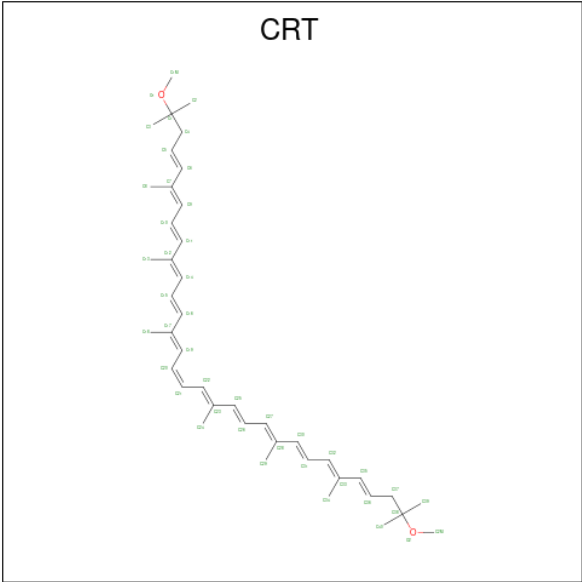
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	1	Total	Fe	0	0
			1	1		
13	x	1	Total	Fe	0	0
			1	1		

- Molecule 14 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			53	51	2		
14	y	1	Total	C	O	0	0
			53	51	2		

- Molecule 15 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



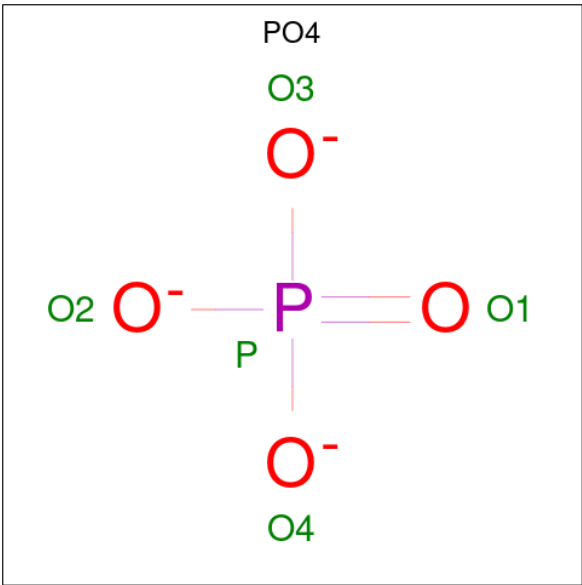
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			44	42	2		
15	E	1	Total	C	O	0	0
			44	42	2		
15	G	1	Total	C	O	0	0
			44	42	2		
15	I	1	Total	C	O	0	0
			44	42	2		
15	O	1	Total	C	O	0	0
			44	42	2		
15	P	1	Total	C	O	0	0
			44	42	2		
15	R	1	Total	C	O	0	0
			44	42	2		
15	T	1	Total	C	O	0	0
			44	42	2		
15	V	1	Total	C	O	0	0
			44	42	2		
15	X	1	Total	C	O	0	0
			44	42	2		
15	Z	1	Total	C	O	0	0
			44	42	2		
15	2	1	Total	C	O	0	0
			44	42	2		
15	4	1	Total	C	O	0	0
			44	42	2		
15	7	1	Total	C	O	0	0
			44	42	2		

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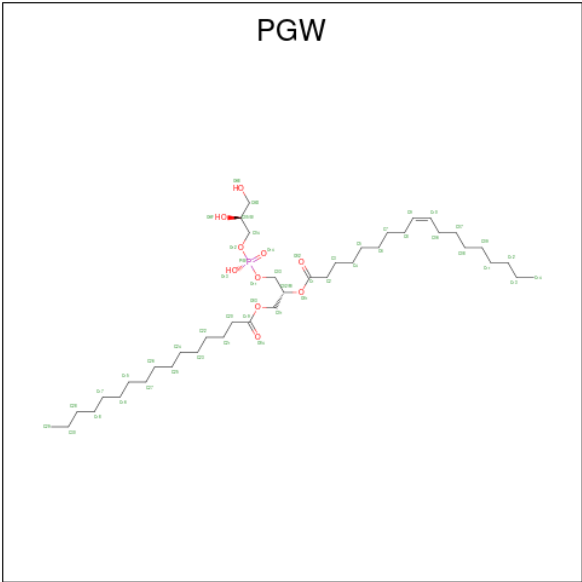
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	7	1	Total	C	O	0	0
			44	42	2		
15	9	1	Total	C	O	0	0
			44	42	2		
15	0	1	Total	C	O	0	0
			44	42	2		
15	y	1	Total	C	O	0	0
			44	42	2		
15	m	1	Total	C	O	0	0
			44	42	2		
15	n	1	Total	C	O	0	0
			44	42	2		
15	q	1	Total	C	O	0	0
			44	42	2		
15	s	1	Total	C	O	0	0
			44	42	2		
15	v	1	Total	C	O	0	0
			44	42	2		
15	z	1	Total	C	O	0	0
			44	42	2		
15	AC	1	Total	C	O	0	0
			44	42	2		
15	AD	1	Total	C	O	0	0
			44	42	2		
15	AF	1	Total	C	O	0	0
			44	42	2		
15	AH	1	Total	C	O	0	0
			44	42	2		
15	AJ	1	Total	C	O	0	0
			44	42	2		
15	AL	1	Total	C	O	0	0
			44	42	2		
15	e	1	Total	C	O	0	0
			44	42	2		
15	g	1	Total	C	O	0	0
			44	42	2		
15	i	1	Total	C	O	0	0
			44	42	2		
15	k	1	Total	C	O	0	0
			44	42	2		

- Molecule 16 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	M	1	Total	O	P	0	0
			5	4	1		
16	H	1	Total	O	P	0	0
			5	4	1		
16	y	1	Total	O	P	0	0
			5	4	1		
16	t	1	Total	O	P	0	0
			5	4	1		

- Molecule 17 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	S	1	Total	C	O	P	0	0
			21	10	10	1		
17	AE	1	Total	C	O	P	0	0
			21	10	10	1		

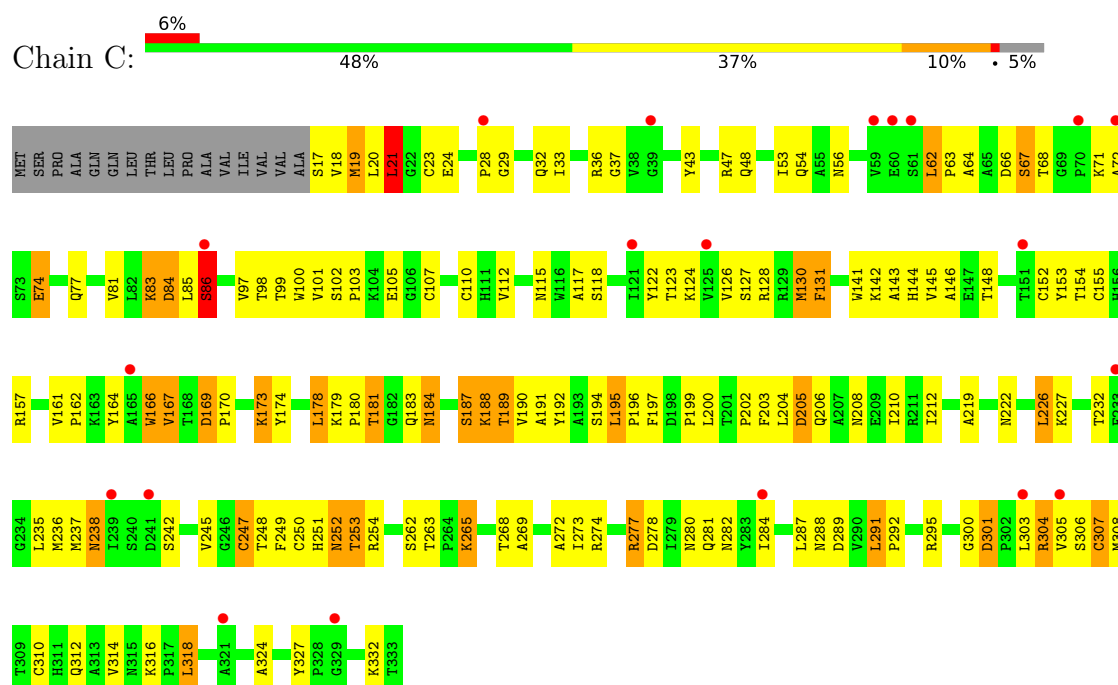
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	2	Total	O	0	0
			2	2		
18	W	1	Total	O	0	0
			1	1		
18	x	2	Total	O	0	0
			2	2		
18	AI	1	Total	O	0	0
			1	1		

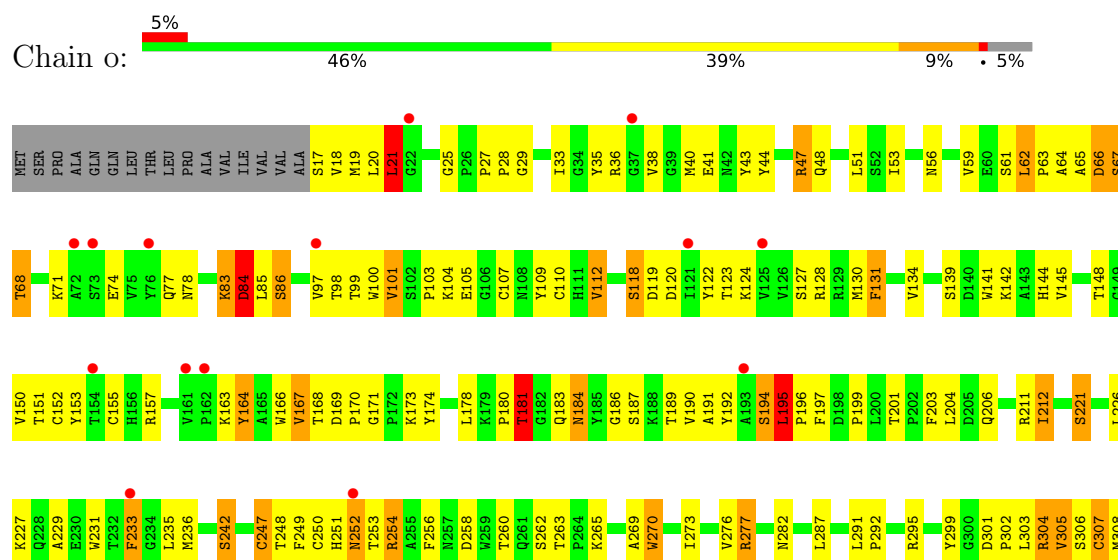
3 Residue-property plots [i](#)

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: Photosynthetic reaction center cytochrome c subunit

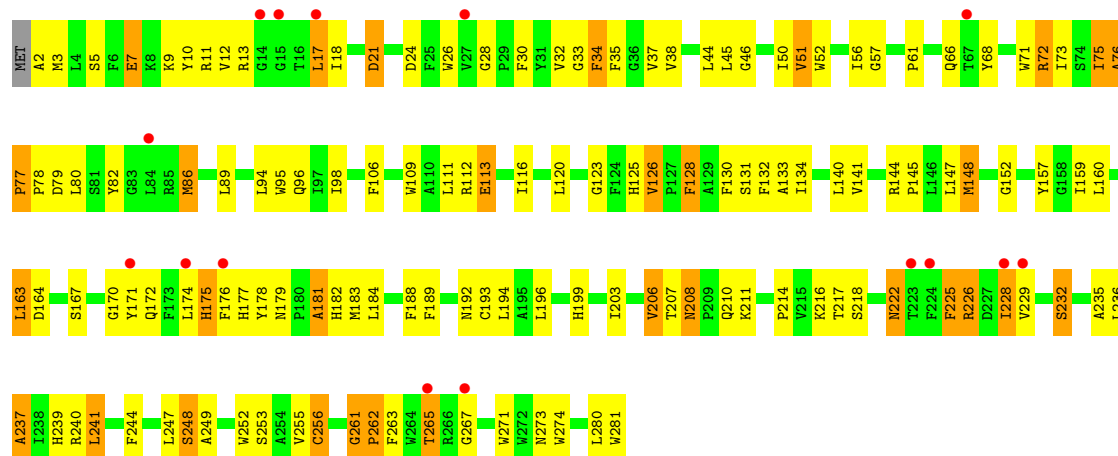


- Molecule 1: Photosynthetic reaction center cytochrome c subunit

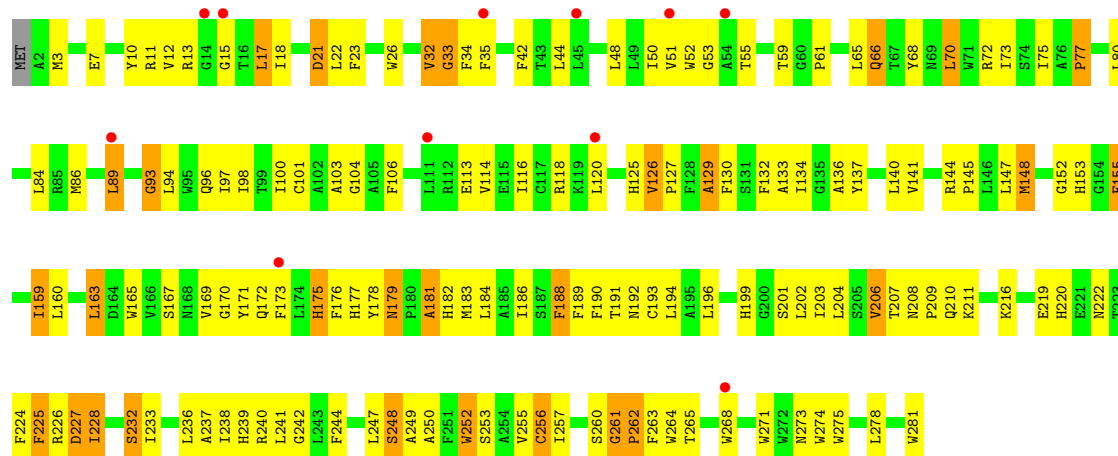




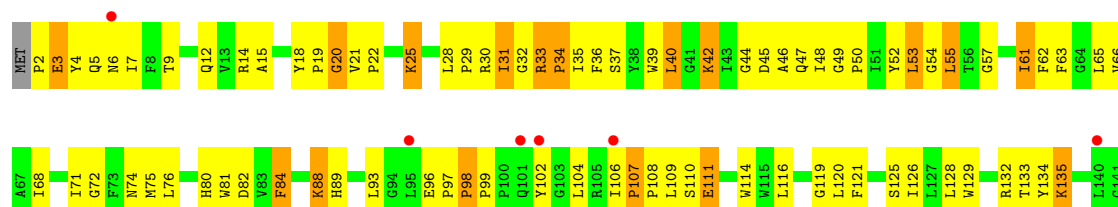
• Molecule 2: Photosynthetic reaction center L subunit

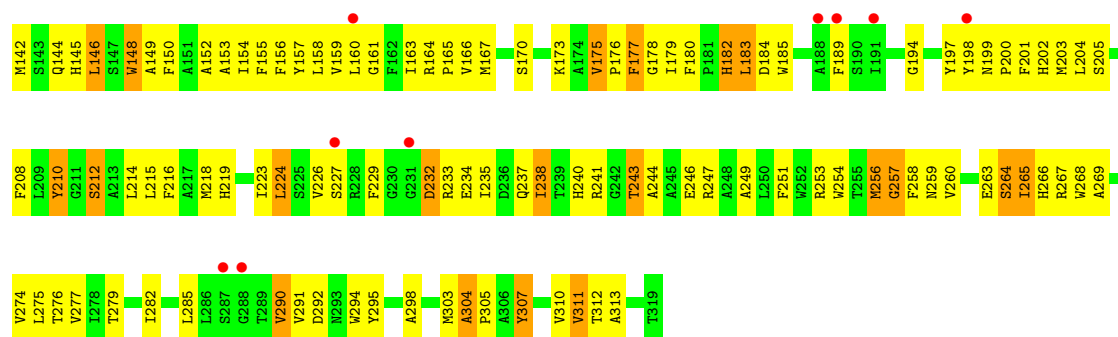


• Molecule 2: Photosynthetic reaction center L subunit

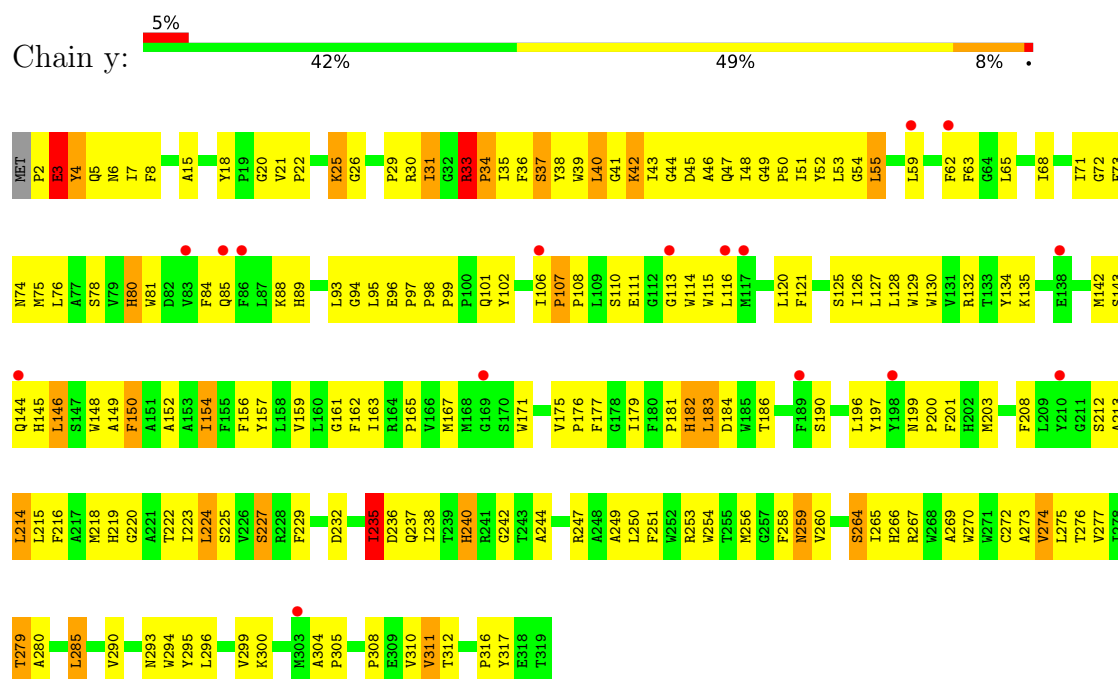


• Molecule 3: Photosynthetic reaction center M subunit

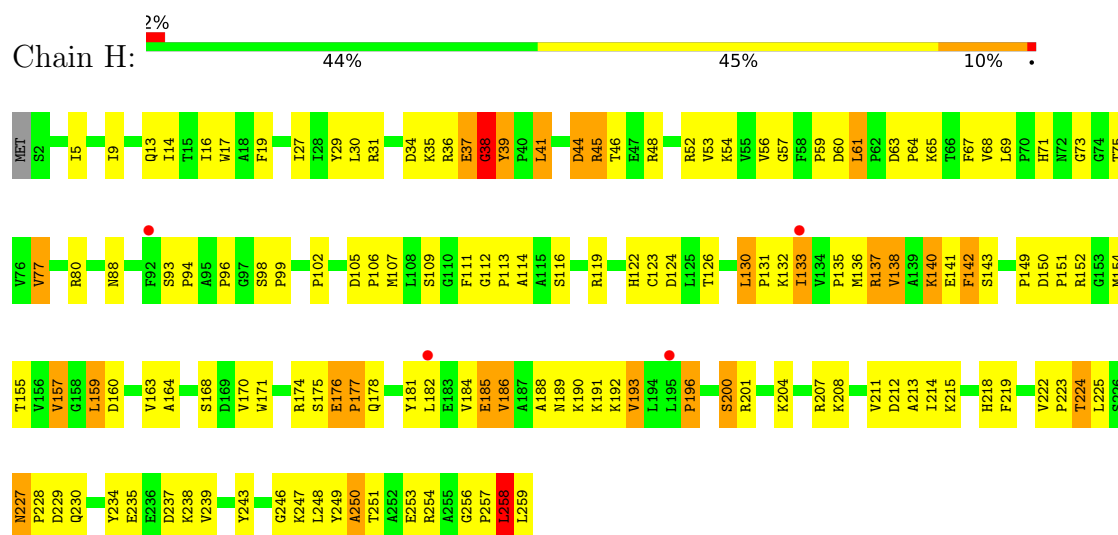




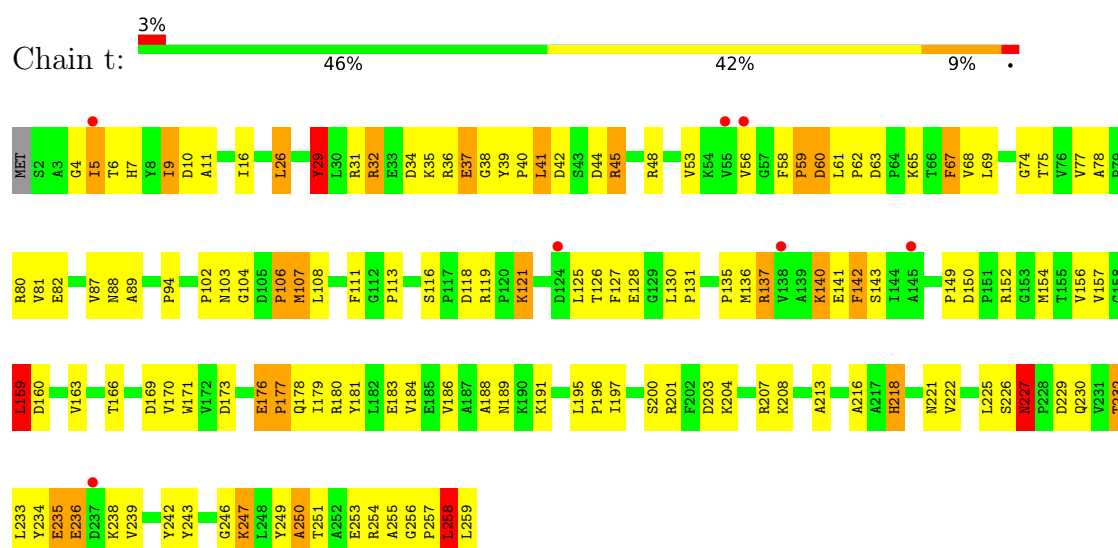
• Molecule 3: Photosynthetic reaction center M subunit



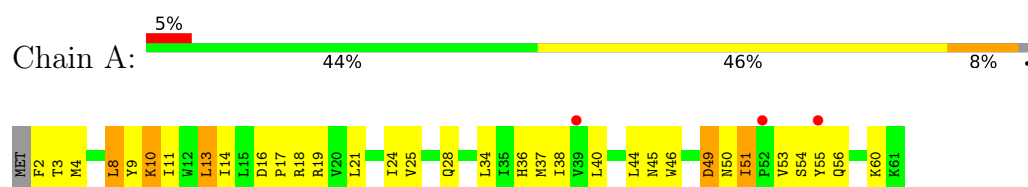
• Molecule 4: Photosynthetic reaction center H subunit



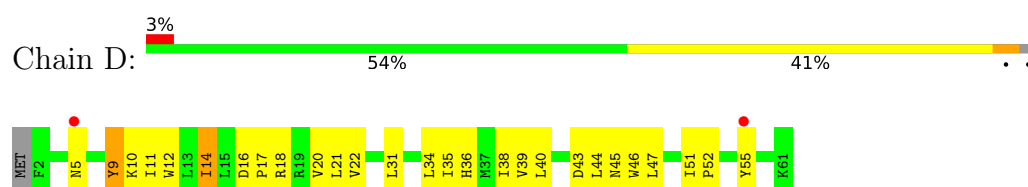
• Molecule 4: Photosynthetic reaction center H subunit



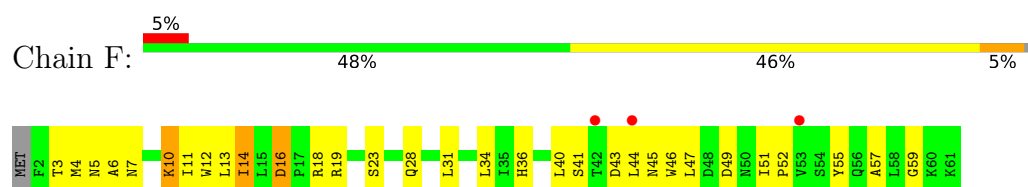
- Molecule 5: LH1 alpha polypeptide



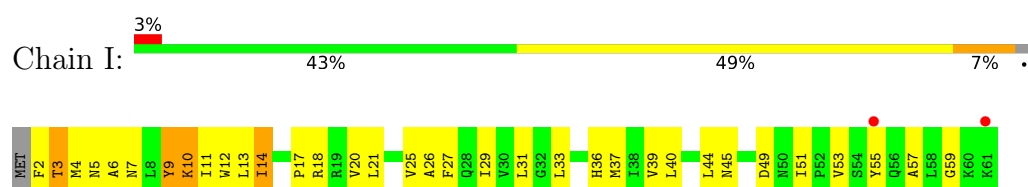
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide





- Molecule 5: LH1 alpha polypeptide



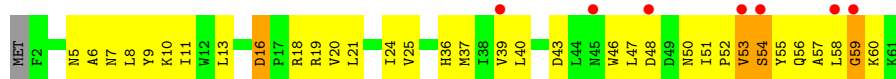
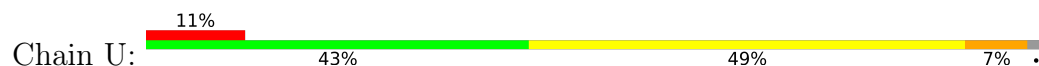
- Molecule 5: LH1 alpha polypeptide



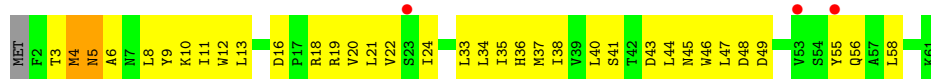
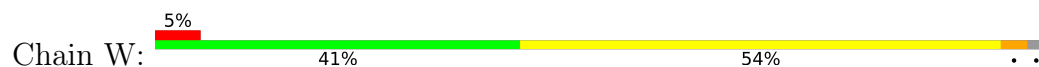
- Molecule 5: LH1 alpha polypeptide



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• Molecule 5: LH1 alpha polypeptide



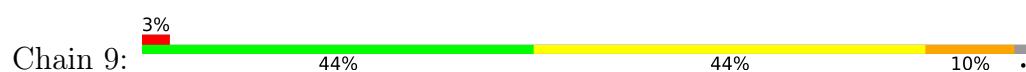
• Molecule 5: LH1 alpha polypeptide



• Molecule 5: LH1 alpha polypeptide



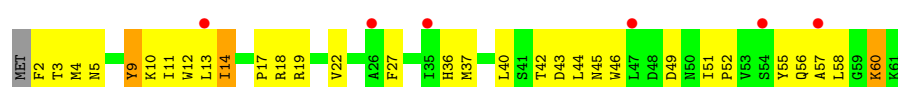
• Molecule 5: LH1 alpha polypeptide



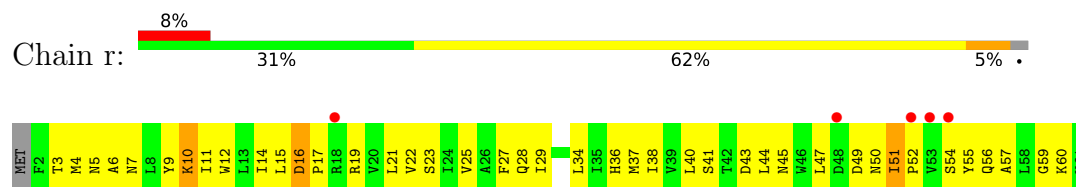
• Molecule 5: LH1 alpha polypeptide



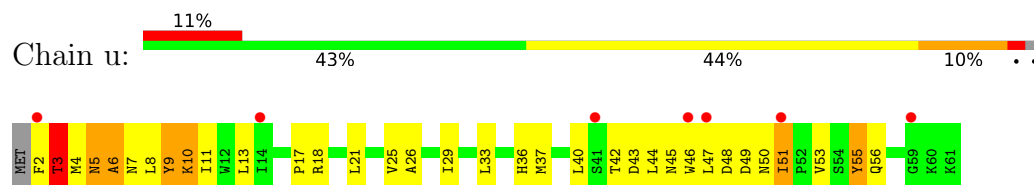
• Molecule 5: LH1 alpha polypeptide



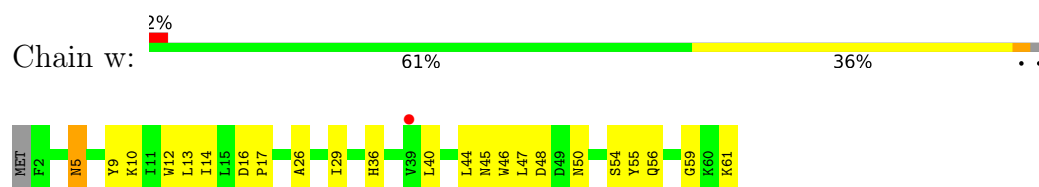
- Molecule 5: LH1 alpha polypeptide



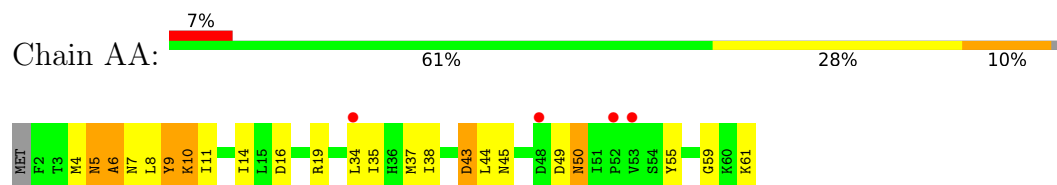
- Molecule 5: LH1 alpha polypeptide



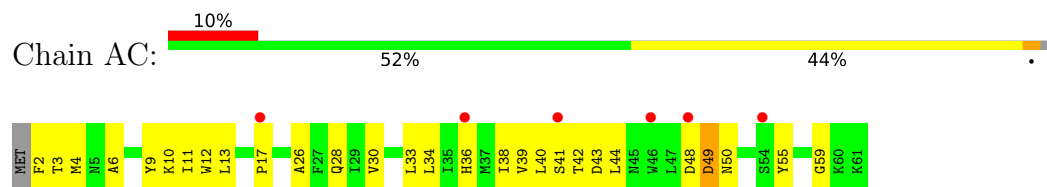
- Molecule 5: LH1 alpha polypeptide



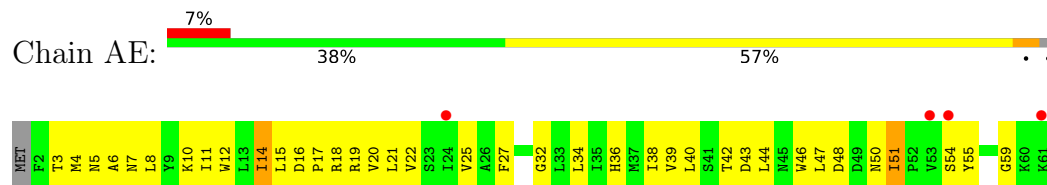
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

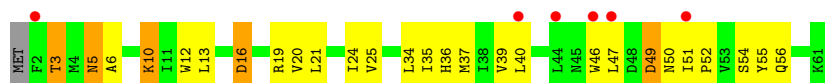


- Molecule 5: LH1 alpha polypeptide

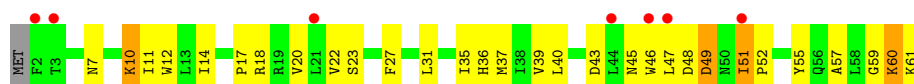




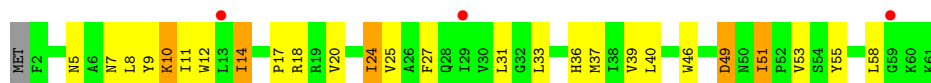
- Molecule 5: LH1 alpha polypeptide



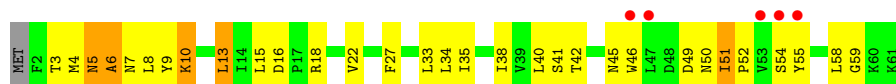
- Molecule 5: LH1 alpha polypeptide



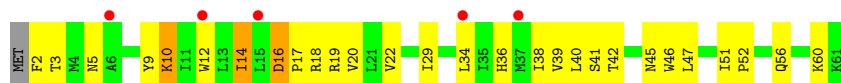
- Molecule 5: LH1 alpha polypeptide



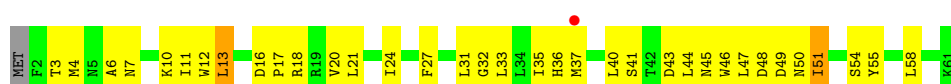
- Molecule 5: LH1 alpha polypeptide



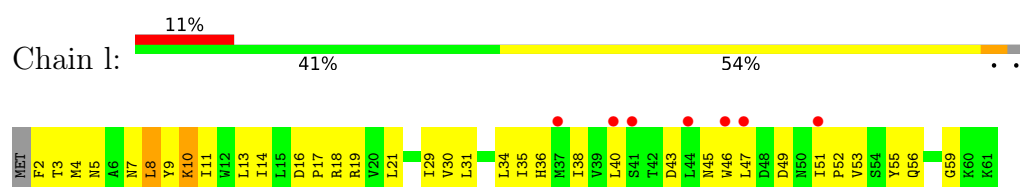
- Molecule 5: LH1 alpha polypeptide



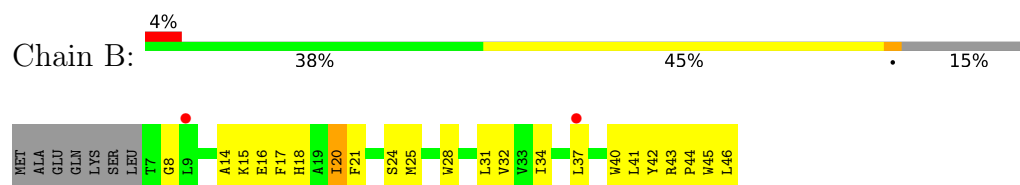
- Molecule 5: LH1 alpha polypeptide



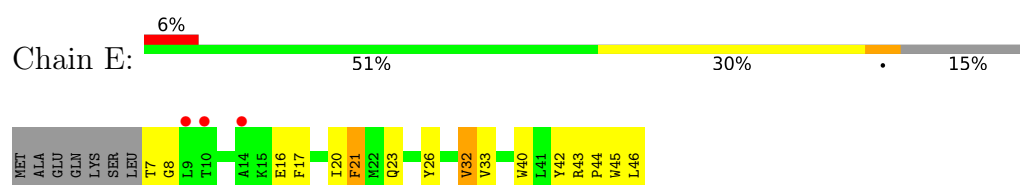
- Molecule 5: LH1 alpha polypeptide



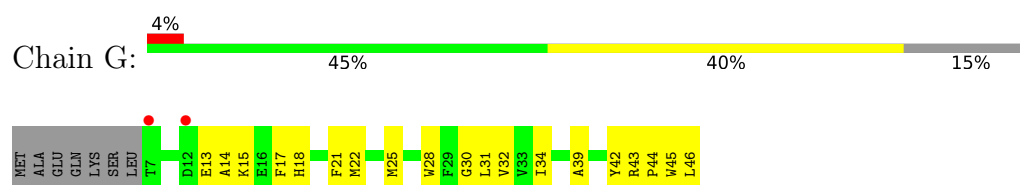
• Molecule 6: LH1 beta polypeptide



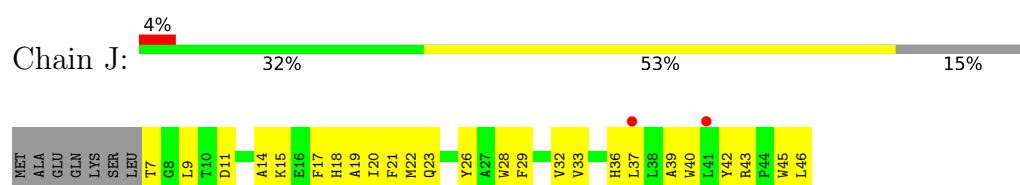
• Molecule 6: LH1 beta polypeptide



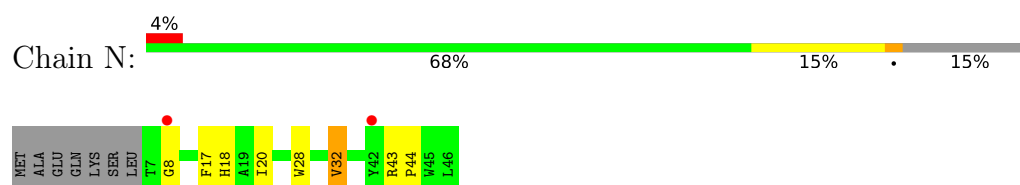
• Molecule 6: LH1 beta polypeptide



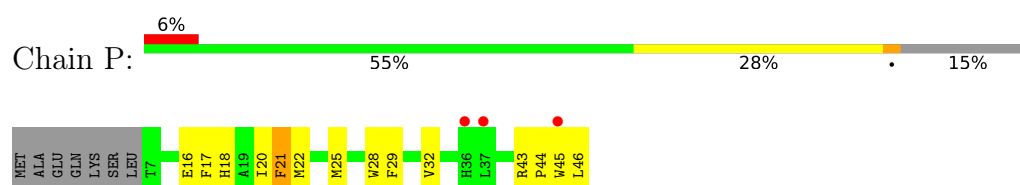
• Molecule 6: LH1 beta polypeptide



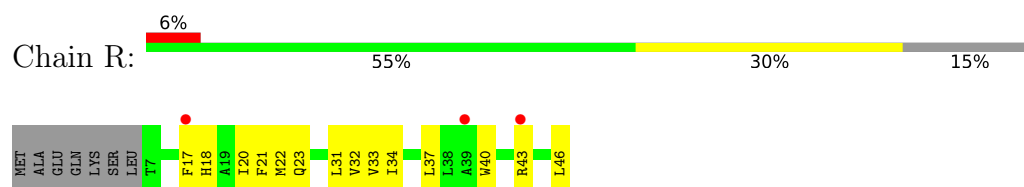
• Molecule 6: LH1 beta polypeptide



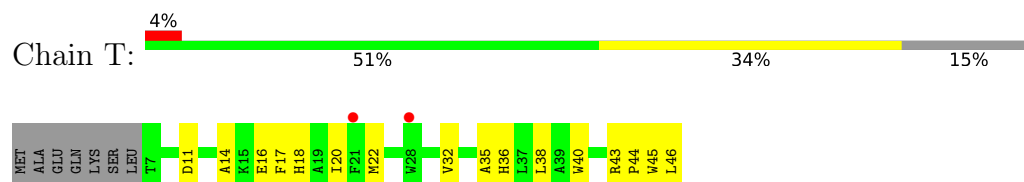
• Molecule 6: LH1 beta polypeptide



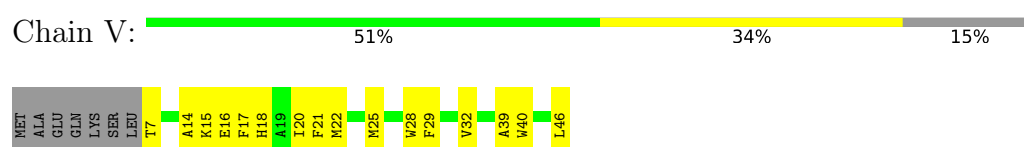
• Molecule 6: LH1 beta polypeptide



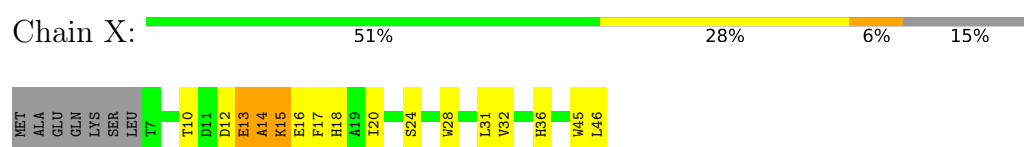
• Molecule 6: LH1 beta polypeptide



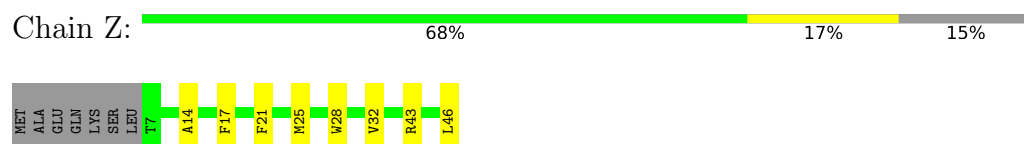
• Molecule 6: LH1 beta polypeptide



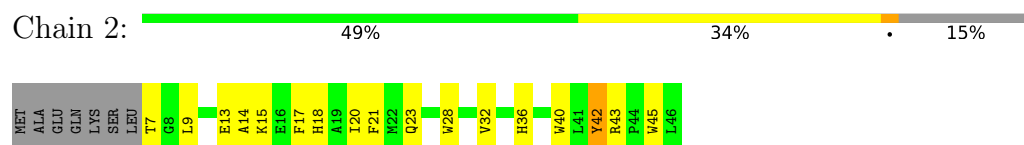
• Molecule 6: LH1 beta polypeptide



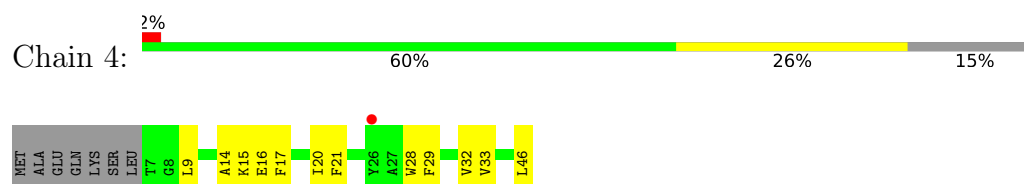
• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide

Chain 6:  57% 26% 15%

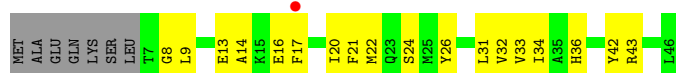
• Molecule 6: LH1 beta polypeptide

Chain 8:  4% 49% 36% 15%

• Molecule 6: LH1 beta polypeptide

Chain 0:  2% 45% 38% 15%

• Molecule 6: LH1 beta polypeptide

Chain n:  2% 47% 38% 15%

• Molecule 6: LH1 beta polypeptide

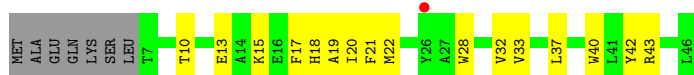
Chain q:  4% 60% 26% 15%

• Molecule 6: LH1 beta polypeptide

Chain s:  2% 51% 34% 15%

• Molecule 6: LH1 beta polypeptide

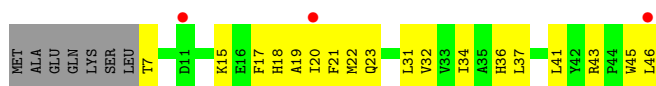
Chain v:  2% 51% 34% 15%



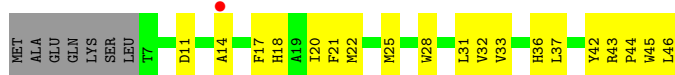
- Molecule 6: LH1 beta polypeptide



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- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



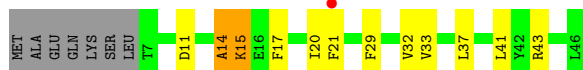
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



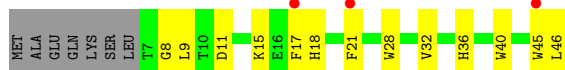
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	163.83Å 148.56Å 210.00Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	49.90 – 3.30 49.90 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (49.90-3.30) 92.5 (49.90-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.279 , 0.313 0.281 , 0.315	Depositor DCC
R_{free} test set	6658 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 96.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	51893	wwPDB-VP
Average B, all atoms (Å ²)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEF, MQ8, HEM, BCL, BA, PGW, PO4, BPH, FE, UQ8, CRT

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	C	0.95	0/2528	1.55	47/3451 (1.4%)
1	o	0.90	0/2528	1.49	40/3451 (1.2%)
2	L	0.98	3/2318 (0.1%)	1.44	37/3167 (1.2%)
2	x	1.02	2/2318 (0.1%)	1.48	35/3167 (1.1%)
3	M	0.93	1/2646 (0.0%)	1.49	53/3621 (1.5%)
3	y	0.92	1/2646 (0.0%)	1.42	28/3621 (0.8%)
4	H	0.95	2/2037 (0.1%)	1.50	29/2776 (1.0%)
4	t	0.99	1/2037 (0.0%)	1.51	29/2776 (1.0%)
5	1	0.72	1/485 (0.2%)	1.34	7/664 (1.1%)
5	3	0.65	0/485	1.19	3/664 (0.5%)
5	5	0.66	0/485	1.12	3/664 (0.5%)
5	7	0.64	0/485	1.23	4/664 (0.6%)
5	9	0.60	0/485	1.09	1/664 (0.2%)
5	A	0.66	0/485	1.22	6/664 (0.9%)
5	AA	0.61	0/485	1.20	4/664 (0.6%)
5	AC	0.63	0/485	1.07	0/664
5	AE	0.58	0/491	1.10	2/672 (0.3%)
5	AG	0.62	0/485	1.14	2/664 (0.3%)
5	AI	0.67	0/485	1.18	5/664 (0.8%)
5	AK	0.72	0/485	1.16	2/664 (0.3%)
5	D	0.60	0/485	1.20	4/664 (0.6%)
5	F	0.59	0/485	1.17	3/664 (0.5%)
5	I	0.64	0/485	1.20	3/664 (0.5%)
5	K	0.61	0/485	1.16	4/664 (0.6%)
5	O	0.62	0/485	1.15	2/664 (0.3%)
5	Q	0.65	0/485	1.27	6/664 (0.9%)
5	S	0.69	0/491	1.03	2/672 (0.3%)
5	U	0.74	0/485	1.17	3/664 (0.5%)
5	W	0.75	0/485	1.20	2/664 (0.3%)
5	Y	0.72	0/485	1.14	2/664 (0.3%)
5	d	0.66	0/485	1.19	3/664 (0.5%)
5	f	0.75	0/485	1.28	7/664 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	h	0.71	0/485	1.21	3/664 (0.5%)
5	j	0.61	0/485	1.19	5/664 (0.8%)
5	l	0.59	0/485	1.11	2/664 (0.3%)
5	m	0.60	0/485	1.15	3/664 (0.5%)
5	p	0.67	0/485	1.20	3/664 (0.5%)
5	r	0.65	0/485	1.16	3/664 (0.5%)
5	u	0.66	0/485	1.13	4/664 (0.6%)
5	w	0.59	0/485	1.18	4/664 (0.6%)
6	0	0.51	0/350	1.07	1/476 (0.2%)
6	2	0.58	0/350	1.10	4/476 (0.8%)
6	4	0.56	0/350	1.01	1/476 (0.2%)
6	6	0.55	0/350	0.97	1/476 (0.2%)
6	8	0.53	0/350	0.92	0/476
6	AB	0.54	0/350	1.04	0/476
6	AD	0.53	0/350	0.95	0/476
6	AF	0.51	0/350	0.92	2/476 (0.4%)
6	AH	0.49	0/350	1.02	2/476 (0.4%)
6	AJ	0.60	0/350	0.94	1/476 (0.2%)
6	AL	0.59	0/350	1.02	1/476 (0.2%)
6	B	0.54	0/350	1.10	3/476 (0.6%)
6	E	0.59	0/350	1.14	1/476 (0.2%)
6	G	0.55	0/350	0.98	1/476 (0.2%)
6	J	0.56	0/350	1.10	1/476 (0.2%)
6	N	0.52	0/350	0.96	1/476 (0.2%)
6	P	0.49	0/350	0.98	0/476
6	R	0.51	0/350	0.97	0/476
6	T	0.56	0/350	1.03	1/476 (0.2%)
6	V	0.55	0/350	0.98	1/476 (0.2%)
6	X	0.58	0/350	1.15	3/476 (0.6%)
6	Z	0.56	0/350	0.89	0/476
6	c	0.54	0/350	0.95	0/476
6	e	0.63	0/350	0.92	2/476 (0.4%)
6	g	0.53	0/350	0.99	2/476 (0.4%)
6	i	0.55	0/350	0.98	2/476 (0.4%)
6	k	0.46	0/350	0.84	0/476
6	n	0.64	0/350	1.04	0/476
6	q	0.59	0/350	1.05	2/476 (0.4%)
6	s	0.59	0/350	0.98	0/476
6	v	0.55	0/350	1.01	1/476 (0.2%)
6	z	0.53	0/350	1.12	1/476 (0.2%)
All	All	0.77	11/45790 (0.0%)	1.28	440/62526 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
3	M	0	1
3	y	0	2
4	t	0	1
6	AJ	0	2
6	X	0	1
All	All	0	8

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	241	LEU	CA-C	-5.75	1.45	1.52
4	H	39	TYR	CA-C	5.74	1.60	1.52
3	y	106	ILE	CA-C	-5.56	1.49	1.53
2	x	252	TRP	C-O	-5.45	1.17	1.24
2	L	237	ALA	C-O	-5.25	1.18	1.24

The worst 5 of 440 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	x	228	ILE	N-CA-C	12.90	122.66	110.53
1	o	195	LEU	CA-C-N	-12.79	105.67	120.13
1	o	195	LEU	C-N-CA	-12.79	105.67	120.13
3	M	33	ARG	CA-C-N	11.09	133.70	119.84
3	M	33	ARG	C-N-CA	11.09	133.70	119.84

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	188	LYS	Mainchain
3	M	265	ILE	Mainchain
6	X	14	ALA	Peptide
3	y	215	LEU	Mainchain
3	y	272	CYS	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2458	0	2385	147	0
1	o	2458	0	2385	152	1
2	L	2231	0	2192	154	0
2	x	2231	0	2192	164	0
3	M	2546	0	2521	197	0
3	y	2546	0	2521	189	0
4	H	1982	0	1981	121	0
4	t	1982	0	1981	113	0
5	1	475	0	486	46	1
5	3	475	0	486	21	0
5	5	475	0	486	26	0
5	7	475	0	486	34	0
5	9	475	0	486	42	0
5	A	475	0	486	38	0
5	AA	475	0	486	21	0
5	AC	475	0	486	36	0
5	AE	481	0	490	35	0
5	AG	475	0	486	30	0
5	AI	475	0	486	28	0
5	AK	475	0	486	30	0
5	D	475	0	486	30	0
5	F	475	0	486	28	0
5	I	475	0	486	52	0
5	K	475	0	486	18	0
5	O	475	0	486	30	0
5	Q	475	0	486	37	0
5	S	481	0	490	39	0
5	U	475	0	486	42	0
5	W	475	0	486	36	0
5	Y	475	0	486	42	0
5	d	475	0	486	32	0
5	f	475	0	486	23	0
5	h	475	0	486	28	0
5	j	475	0	486	37	0
5	l	475	0	486	50	0
5	m	475	0	486	34	0
5	p	475	0	486	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	r	475	0	486	43	0
5	u	475	0	486	48	0
5	w	475	0	486	26	0
6	0	337	0	323	22	0
6	2	337	0	323	17	0
6	4	337	0	323	16	0
6	6	337	0	323	14	0
6	8	337	0	323	17	0
6	AB	337	0	323	18	0
6	AD	337	0	323	23	0
6	AF	337	0	323	20	0
6	AH	337	0	323	17	0
6	AJ	337	0	323	26	0
6	AL	337	0	323	19	0
6	B	337	0	323	37	0
6	E	337	0	323	27	0
6	G	337	0	323	21	0
6	J	337	0	323	31	0
6	N	337	0	323	11	0
6	P	337	0	323	19	0
6	R	337	0	323	19	0
6	T	337	0	323	20	0
6	V	337	0	323	23	0
6	X	337	0	323	23	0
6	Z	337	0	323	13	0
6	c	337	0	323	19	0
6	e	337	0	323	20	0
6	g	337	0	323	15	0
6	i	337	0	323	15	0
6	k	337	0	323	22	0
6	n	337	0	323	31	0
6	q	337	0	323	16	0
6	s	337	0	323	21	0
6	v	337	0	323	20	0
6	z	337	0	323	17	0
7	C	172	0	120	28	0
7	o	172	0	120	30	0
8	1	1	0	0	0	0
8	3	1	0	0	0	0
8	5	1	0	0	0	0
8	7	1	0	0	0	0
8	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AA	1	0	0	0	0
8	AC	1	0	0	0	0
8	AE	1	0	0	0	0
8	AG	1	0	0	0	0
8	AI	1	0	0	0	0
8	AK	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
8	L	2	0	0	0	0
8	O	1	0	0	0	0
8	Q	1	0	0	0	0
8	S	1	0	0	0	0
8	U	1	0	0	0	0
8	W	1	0	0	0	0
8	Y	1	0	0	0	0
8	d	1	0	0	0	0
8	f	1	0	0	0	0
8	h	1	0	0	0	0
8	j	1	0	0	0	0
8	m	2	0	0	0	0
8	o	1	0	0	0	0
8	p	1	0	0	0	0
8	r	1	0	0	0	0
8	u	1	0	0	0	0
8	w	1	0	0	0	0
8	x	2	0	0	0	0
9	0	66	0	74	5	0
9	1	66	0	74	10	0
9	2	66	0	74	9	0
9	3	66	0	74	10	0
9	4	66	0	74	10	0
9	5	66	0	74	12	0
9	6	66	0	74	10	0
9	7	66	0	74	7	0
9	8	66	0	74	12	0
9	9	66	0	74	8	0
9	A	132	0	148	16	0
9	AB	132	0	148	18	0
9	AC	132	0	148	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AE	66	0	74	9	0
9	AF	66	0	74	8	0
9	AG	66	0	74	6	0
9	AH	66	0	74	8	0
9	AI	132	0	148	22	0
9	AK	66	0	74	9	0
9	AL	66	0	74	11	0
9	D	132	0	148	16	0
9	F	66	0	74	4	0
9	G	66	0	74	12	0
9	I	132	0	148	22	0
9	K	66	0	74	6	0
9	L	132	0	148	28	0
9	M	132	0	148	21	0
9	N	66	0	74	4	0
9	O	66	0	74	6	0
9	P	66	0	74	6	0
9	Q	66	0	74	3	0
9	R	66	0	74	5	0
9	S	66	0	74	11	0
9	T	66	0	74	12	0
9	U	66	0	74	9	0
9	V	66	0	74	8	0
9	W	66	0	74	8	0
9	X	66	0	74	8	0
9	Y	66	0	74	9	0
9	Z	66	0	74	16	0
9	c	66	0	74	14	0
9	d	66	0	74	12	0
9	e	66	0	74	12	0
9	f	66	0	74	7	0
9	g	66	0	74	6	0
9	h	66	0	74	8	0
9	i	66	0	74	8	0
9	j	66	0	74	8	0
9	k	66	0	74	12	0
9	l	66	0	74	8	0
9	m	132	0	148	16	0
9	p	66	0	74	12	0
9	q	66	0	74	11	0
9	r	66	0	74	11	0
9	s	66	0	74	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	u	132	0	148	19	0
9	w	66	0	74	8	0
9	x	198	0	222	26	0
9	y	66	0	74	16	0
9	z	66	0	74	6	0
10	L	65	0	76	5	0
10	M	65	0	76	14	0
10	x	65	0	76	4	0
10	y	65	0	76	10	0
11	L	53	0	74	12	0
11	x	53	0	74	18	0
12	A	19	0	11	2	0
12	H	76	0	44	26	0
12	L	12	0	9	0	0
12	M	35	0	22	2	0
12	m	19	0	11	3	0
12	p	16	0	11	7	0
12	t	38	0	22	7	0
12	x	19	0	11	11	0
12	y	57	0	33	8	0
13	L	1	0	0	0	0
13	x	1	0	0	0	0
14	M	53	0	72	4	0
14	y	53	0	72	8	0
15	0	44	0	60	12	0
15	2	44	0	60	7	0
15	4	44	0	60	14	0
15	7	88	0	120	20	0
15	9	44	0	60	16	0
15	AC	44	0	60	11	0
15	AD	44	0	60	8	0
15	AF	44	0	60	14	0
15	AH	44	0	60	9	0
15	AJ	44	0	60	12	0
15	AL	44	0	60	10	0
15	E	44	0	60	14	0
15	G	44	0	60	9	0
15	I	44	0	60	10	0
15	M	44	0	60	13	0
15	O	44	0	60	9	0
15	P	44	0	60	9	0
15	R	44	0	60	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	T	44	0	60	11	0
15	V	44	0	60	10	0
15	X	44	0	60	21	0
15	Z	44	0	60	8	0
15	e	44	0	60	10	0
15	g	44	0	60	12	0
15	i	44	0	60	4	0
15	k	44	0	60	15	0
15	m	44	0	60	8	0
15	n	44	0	60	17	0
15	q	44	0	60	9	0
15	s	44	0	60	10	0
15	v	44	0	60	7	0
15	y	44	0	60	11	0
15	z	44	0	60	6	0
16	H	5	0	0	0	0
16	M	5	0	0	1	0
16	t	5	0	0	0	0
16	y	5	0	0	1	0
17	AE	21	0	12	2	0
17	S	21	0	12	3	0
18	AI	1	0	0	0	0
18	L	2	0	0	0	0
18	W	1	0	0	1	0
18	x	2	0	0	0	0
All	All	51893	0	52456	2857	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 2857 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:AA:45:ASN:O	5:AA:49:ASP:OD2	1.57	1.23
5:7:45:ASN:O	5:7:49:ASP:OD2	1.71	1.06
3:M:277:VAL:HG11	10:M:403:BPH:HAC2	1.42	0.98
3:y:25:LYS:HD3	3:y:26:GLY:H	1.27	0.98
5:p:56:GLN:O	5:p:58:LEU:N	1.98	0.96

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:52:PRO:O	1:o:77:GLN:NE2[1_554]	2.15	0.05

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	C	315/333 (95%)	274 (87%)	33 (10%)	8 (2%)	4	23
1	o	315/333 (95%)	277 (88%)	30 (10%)	8 (2%)	4	23
2	L	278/281 (99%)	248 (89%)	26 (9%)	4 (1%)	9	33
2	x	278/281 (99%)	247 (89%)	28 (10%)	3 (1%)	11	39
3	M	316/319 (99%)	282 (89%)	30 (10%)	4 (1%)	9	35
3	y	316/319 (99%)	286 (90%)	26 (8%)	4 (1%)	9	35
4	H	256/259 (99%)	216 (84%)	31 (12%)	9 (4%)	3	18
4	t	256/259 (99%)	214 (84%)	32 (12%)	10 (4%)	2	16
5	1	58/61 (95%)	44 (76%)	12 (21%)	2 (3%)	3	18
5	3	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	7
5	5	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	18
5	7	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1	11
5	9	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	0	4
5	A	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	18
5	AA	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	1	11
5	AC	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	7
5	AE	59/61 (97%)	49 (83%)	7 (12%)	3 (5%)	1	11
5	AG	58/61 (95%)	53 (91%)	3 (5%)	2 (3%)	3	18
5	AI	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	AK	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	D	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	1	11
5	I	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1	11
5	K	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	30
5	O	58/61 (95%)	46 (79%)	8 (14%)	4 (7%)	1	7
5	Q	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	7
5	S	59/61 (97%)	49 (83%)	8 (14%)	2 (3%)	3	18
5	U	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	1	11
5	W	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	30
5	Y	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	1	11
5	d	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	18
5	f	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	7
5	h	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	18
5	j	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	18
5	l	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	1	11
5	m	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7	30
5	p	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	18
5	r	58/61 (95%)	46 (79%)	7 (12%)	5 (9%)	0	4
5	u	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1	11
5	w	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	30
6	0	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
6	2	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	4	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	6	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	8	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AB	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AD	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AF	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AH	38/47 (81%)	37 (97%)	0	1 (3%)	4	23
6	AJ	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AL	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	B	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	38/47 (81%)	38 (100%)	0	0	100	100
6	G	38/47 (81%)	38 (100%)	0	0	100	100
6	J	38/47 (81%)	38 (100%)	0	0	100	100
6	N	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
6	P	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	R	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	T	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	V	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	X	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	Z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	c	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	e	38/47 (81%)	38 (100%)	0	0	100	100
6	g	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	i	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	k	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	n	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	q	38/47 (81%)	38 (100%)	0	0	100	100
6	s	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	v	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
All	All	5404/5840 (92%)	4783 (88%)	483 (9%)	138 (3%)	4	23

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	ASP
1	C	195	LEU
2	L	262	PRO
4	H	142	PHE
4	H	250	ALA

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	265/278 (95%)	243 (92%)	22 (8%)	10	34
1	o	265/278 (95%)	246 (93%)	19 (7%)	13	40
2	L	228/229 (100%)	214 (94%)	14 (6%)	17	45
2	x	228/229 (100%)	214 (94%)	14 (6%)	17	45
3	M	256/257 (100%)	239 (93%)	17 (7%)	15	43
3	y	256/257 (100%)	238 (93%)	18 (7%)	14	41
4	H	210/211 (100%)	192 (91%)	18 (9%)	10	33
4	t	210/211 (100%)	188 (90%)	22 (10%)	6	25
5	1	52/56 (93%)	49 (94%)	3 (6%)	18	47
5	3	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	5	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	7	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	9	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	A	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	AA	52/56 (93%)	49 (94%)	3 (6%)	18	47
5	AC	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	AE	53/56 (95%)	52 (98%)	1 (2%)	50	68
5	AG	52/56 (93%)	49 (94%)	3 (6%)	18	47
5	AI	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	AK	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	D	52/56 (93%)	52 (100%)	0	100	100
5	F	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	I	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	K	52/56 (93%)	52 (100%)	0	100	100
5	O	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	Q	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	S	53/56 (95%)	52 (98%)	1 (2%)	50	68
5	U	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	W	52/56 (93%)	50 (96%)	2 (4%)	29	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Y	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	d	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	f	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	h	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	j	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	l	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	m	52/56 (93%)	52 (100%)	0	100	100
5	p	52/56 (93%)	52 (100%)	0	100	100
5	r	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	u	52/56 (93%)	49 (94%)	3 (6%)	18	47
5	w	52/56 (93%)	51 (98%)	1 (2%)	50	68
6	0	33/39 (85%)	33 (100%)	0	100	100
6	2	33/39 (85%)	33 (100%)	0	100	100
6	4	33/39 (85%)	33 (100%)	0	100	100
6	6	33/39 (85%)	33 (100%)	0	100	100
6	8	33/39 (85%)	33 (100%)	0	100	100
6	AB	33/39 (85%)	33 (100%)	0	100	100
6	AD	33/39 (85%)	33 (100%)	0	100	100
6	AF	33/39 (85%)	33 (100%)	0	100	100
6	AH	33/39 (85%)	33 (100%)	0	100	100
6	AJ	33/39 (85%)	32 (97%)	1 (3%)	36	61
6	AL	33/39 (85%)	33 (100%)	0	100	100
6	B	33/39 (85%)	32 (97%)	1 (3%)	36	61
6	E	33/39 (85%)	32 (97%)	1 (3%)	36	61
6	G	33/39 (85%)	33 (100%)	0	100	100
6	J	33/39 (85%)	33 (100%)	0	100	100
6	N	33/39 (85%)	33 (100%)	0	100	100
6	P	33/39 (85%)	32 (97%)	1 (3%)	36	61
6	R	33/39 (85%)	33 (100%)	0	100	100
6	T	33/39 (85%)	33 (100%)	0	100	100
6	V	33/39 (85%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	X	33/39 (85%)	32 (97%)	1 (3%)	36	61
6	Z	33/39 (85%)	33 (100%)	0	100	100
6	c	33/39 (85%)	33 (100%)	0	100	100
6	e	33/39 (85%)	33 (100%)	0	100	100
6	g	33/39 (85%)	33 (100%)	0	100	100
6	i	33/39 (85%)	33 (100%)	0	100	100
6	k	33/39 (85%)	33 (100%)	0	100	100
6	n	33/39 (85%)	33 (100%)	0	100	100
6	q	33/39 (85%)	33 (100%)	0	100	100
6	s	33/39 (85%)	33 (100%)	0	100	100
6	v	33/39 (85%)	33 (100%)	0	100	100
6	z	33/39 (85%)	33 (100%)	0	100	100
All	All	4640/4990 (93%)	4444 (96%)	196 (4%)	26	55

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	o	307	CYS
3	y	274	VAL
2	x	94	LEU
2	x	256	CYS
4	t	60	ASP

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

Mol	Chain	Res	Type
2	x	182	HIS
5	r	56	GLN
3	y	74	ASN
5	m	7	ASN
5	w	50	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 40 are monoatomic - leaving 144 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
15	CRT	AC	101	-	43,43,43	0.70	0	48,54,54	2.35	18 (37%)
7	HEM	o	502	1	50,50,50	2.48	9 (18%)	67,82,82	2.17	24 (35%)
9	BCL	m	102	-	69,74,74	1.78	15 (21%)	79,115,115	2.08	25 (31%)
9	BCL	j	101	-	69,74,74	1.71	13 (18%)	79,115,115	2.12	26 (32%)
9	BCL	AG	101	-	69,74,74	1.71	12 (17%)	79,115,115	2.20	30 (37%)
9	BCL	y	401	-	69,74,74	1.80	14 (20%)	79,115,115	2.09	29 (36%)
12	PEF	p	101	-	15,15,46	0.95	1 (6%)	17,19,51	0.98	1 (5%)
15	CRT	4	101	-	43,43,43	0.83	0	48,54,54	2.41	24 (50%)
12	PEF	M	408	-	18,18,46	1.79	2 (11%)	21,23,51	1.63	2 (9%)
9	BCL	AK	101	-	69,74,74	1.72	13 (18%)	79,115,115	2.11	29 (36%)
12	PEF	x	306	-	18,18,46	1.75	2 (11%)	21,23,51	1.34	3 (14%)
10	BPH	L	302	-	59,70,70	0.55	1 (1%)	59,101,101	1.97	13 (22%)
15	CRT	7	103	-	43,43,43	0.99	2 (4%)	48,54,54	1.87	10 (20%)
9	BCL	W	101	-	69,74,74	1.74	14 (20%)	79,115,115	1.98	25 (31%)
9	BCL	u	101	-	69,74,74	1.74	15 (21%)	79,115,115	2.09	27 (34%)
9	BCL	A	103	-	69,74,74	1.78	16 (23%)	79,115,115	2.11	28 (35%)
9	BCL	P	101	-	69,74,74	1.74	15 (21%)	79,115,115	2.07	27 (34%)
9	BCL	AB	102	-	69,74,74	1.69	15 (21%)	79,115,115	2.07	31 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	p	102	-	69,74,74	1.72	14 (20%)	79,115,115	2.11	26 (32%)
9	BCL	z	102	-	69,74,74	1.69	12 (17%)	79,115,115	2.03	28 (35%)
9	BCL	0	102	-	69,74,74	1.78	14 (20%)	79,115,115	2.06	26 (32%)
9	BCL	x	301	-	69,74,74	1.78	14 (20%)	79,115,115	2.27	25 (31%)
12	PEF	H	305	-	18,18,46	1.47	2 (11%)	21,23,51	1.55	3 (14%)
7	HEM	C	502	1	50,50,50	2.49	10 (20%)	67,82,82	2.07	20 (29%)
9	BCL	U	101	-	69,74,74	1.77	14 (20%)	79,115,115	2.04	28 (35%)
9	BCL	r	101	-	69,74,74	1.78	15 (21%)	79,115,115	1.98	27 (34%)
9	BCL	w	101	-	69,74,74	1.76	13 (18%)	79,115,115	2.10	29 (36%)
9	BCL	AL	102	-	69,74,74	1.78	15 (21%)	79,115,115	2.04	28 (35%)
9	BCL	9	102	-	69,74,74	1.70	13 (18%)	79,115,115	2.00	22 (27%)
9	BCL	I	103	-	69,74,74	1.74	14 (20%)	79,115,115	2.08	26 (32%)
11	UQ8	x	304	-	53,53,53	1.57	4 (7%)	66,67,67	1.94	19 (28%)
12	PEF	t	301	-	18,18,46	1.60	2 (11%)	21,23,51	1.30	3 (14%)
10	BPH	M	403	-	59,70,70	0.74	1 (1%)	59,101,101	1.79	7 (11%)
9	BCL	AC	103	-	69,74,74	1.65	13 (18%)	79,115,115	2.11	26 (32%)
9	BCL	O	102	-	69,74,74	1.72	12 (17%)	79,115,115	2.18	33 (41%)
15	CRT	M	405	-	43,43,43	0.78	0	48,54,54	2.17	13 (27%)
15	CRT	O	101	-	43,43,43	0.65	0	48,54,54	2.48	18 (37%)
12	PEF	m	101	-	18,18,46	1.55	2 (11%)	21,23,51	1.64	3 (14%)
15	CRT	Z	101	-	43,43,43	0.79	0	48,54,54	2.18	18 (37%)
7	HEM	o	503	1	50,50,50	2.55	10 (20%)	67,82,82	2.00	19 (28%)
9	BCL	m	103	-	69,74,74	1.73	15 (21%)	79,115,115	2.03	28 (35%)
15	CRT	AD	101	-	43,43,43	0.85	0	48,54,54	2.35	17 (35%)
9	BCL	2	102	-	69,74,74	1.78	14 (20%)	79,115,115	2.13	27 (34%)
17	PGW	S	101	-	20,20,50	1.04	1 (5%)	23,26,56	1.32	1 (4%)
15	CRT	T	101	-	43,43,43	0.71	0	48,54,54	2.27	14 (29%)
9	BCL	7	102	-	69,74,74	1.66	12 (17%)	79,115,115	2.07	27 (34%)
12	PEF	y	407	-	18,18,46	1.68	2 (11%)	21,23,51	1.27	3 (14%)
15	CRT	V	101	-	43,43,43	0.71	0	48,54,54	2.44	16 (33%)
12	PEF	A	101	-	18,18,46	1.46	2 (11%)	21,23,51	1.97	4 (19%)
9	BCL	q	102	-	69,74,74	1.78	16 (23%)	79,115,115	2.07	26 (32%)
12	PEF	H	302	-	18,18,46	1.57	2 (11%)	21,23,51	1.82	2 (9%)
12	PEF	H	304	-	18,18,46	1.65	2 (11%)	21,23,51	1.61	2 (9%)
9	BCL	6	101	-	69,74,74	1.78	14 (20%)	79,115,115	2.10	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	h	101	-	69,74,74	1.71	13 (18%)	79,115,115	2.06	27 (34%)
9	BCL	G	102	-	69,74,74	1.73	13 (18%)	79,115,115	2.00	25 (31%)
15	CRT	AL	101	-	43,43,43	0.79	0	48,54,54	2.04	15 (31%)
17	PGW	AE	101	-	20,20,50	1.00	1 (5%)	23,26,56	1.38	3 (13%)
15	CRT	AH	102	-	43,43,43	0.74	0	48,54,54	2.11	13 (27%)
9	BCL	R	102	-	69,74,74	1.71	15 (21%)	79,115,115	2.22	30 (37%)
15	CRT	g	101	-	43,43,43	0.83	0	48,54,54	2.33	14 (29%)
9	BCL	d	101	-	69,74,74	1.81	15 (21%)	79,115,115	2.06	28 (35%)
12	PEF	L	305	-	11,11,46	0.79	0	13,14,51	1.15	1 (7%)
15	CRT	n	101	-	43,43,43	0.77	0	48,54,54	2.42	21 (43%)
15	CRT	R	101	-	43,43,43	0.85	0	48,54,54	2.17	14 (29%)
9	BCL	L	303	-	69,74,74	1.80	15 (21%)	79,115,115	2.15	26 (32%)
9	BCL	s	102	-	69,74,74	1.80	14 (20%)	79,115,115	2.18	27 (34%)
15	CRT	I	102	-	43,43,43	0.76	0	48,54,54	2.38	14 (29%)
15	CRT	v	101	-	43,43,43	0.70	0	48,54,54	2.55	18 (37%)
9	BCL	e	102	-	69,74,74	1.76	13 (18%)	79,115,115	2.08	28 (35%)
9	BCL	f	101	-	69,74,74	1.83	16 (23%)	79,115,115	2.08	26 (32%)
15	CRT	0	101	-	43,43,43	0.76	0	48,54,54	2.34	20 (41%)
9	BCL	g	102	-	69,74,74	1.73	15 (21%)	79,115,115	2.15	31 (39%)
12	PEF	t	303	-	18,18,46	1.46	2 (11%)	21,23,51	2.28	8 (38%)
7	HEM	C	501	1	50,50,50	2.57	8 (16%)	67,82,82	2.18	22 (32%)
9	BCL	l	101	-	69,74,74	1.74	14 (20%)	79,115,115	2.05	24 (30%)
15	CRT	AJ	101	-	43,43,43	0.79	0	48,54,54	2.38	14 (29%)
9	BCL	AI	101	-	69,74,74	1.75	14 (20%)	79,115,115	2.12	30 (37%)
9	BCL	Q	101	-	69,74,74	1.75	13 (18%)	79,115,115	2.12	28 (35%)
9	BCL	M	401	-	69,74,74	1.72	14 (20%)	79,115,115	2.20	25 (31%)
9	BCL	AB	101	-	69,74,74	1.72	12 (17%)	79,115,115	2.05	26 (32%)
9	BCL	x	305	-	69,74,74	1.81	13 (18%)	79,115,115	2.26	28 (35%)
9	BCL	k	102	-	69,74,74	1.75	14 (20%)	79,115,115	2.16	30 (37%)
9	BCL	u	102	-	69,74,74	1.77	14 (20%)	79,115,115	2.20	25 (31%)
9	BCL	AI	102	-	69,74,74	1.73	13 (18%)	79,115,115	2.08	23 (29%)
9	BCL	A	102	-	69,74,74	1.74	11 (15%)	79,115,115	2.03	26 (32%)
9	BCL	l	101	-	69,74,74	1.69	13 (18%)	79,115,115	2.18	30 (37%)
12	PEF	y	408	-	18,18,46	1.73	2 (11%)	21,23,51	2.44	6 (28%)
16	PO4	M	406	-	4,4,4	0.53	0	6,6,6	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BPH	y	402	-	59,70,70	0.88	3 (5%)	59,101,101	1.59	9 (15%)
15	CRT	i	101	-	43,43,43	0.75	0	48,54,54	2.19	15 (31%)
9	BCL	AE	102	-	69,74,74	1.69	12 (17%)	79,115,115	2.14	29 (36%)
7	HEM	o	504	1	50,50,50	2.55	11 (22%)	67,82,82	1.81	16 (23%)
9	BCL	I	101	-	69,74,74	1.76	14 (20%)	79,115,115	2.08	28 (35%)
9	BCL	Y	101	-	69,74,74	1.76	11 (15%)	79,115,115	2.03	25 (31%)
9	BCL	T	102	-	69,74,74	1.72	14 (20%)	79,115,115	2.23	31 (39%)
9	BCL	AF	101	-	69,74,74	1.75	13 (18%)	79,115,115	2.04	28 (35%)
7	HEM	C	504	1	50,50,50	2.54	10 (20%)	67,82,82	1.93	16 (23%)
15	CRT	AF	102	-	43,43,43	0.70	0	48,54,54	2.33	14 (29%)
14	MQ8	M	404	-	54,54,54	1.03	6 (11%)	67,69,69	1.46	11 (16%)
15	CRT	X	101	-	43,43,43	0.90	0	48,54,54	1.94	10 (20%)
15	CRT	q	101	-	43,43,43	0.73	0	48,54,54	2.13	14 (29%)
12	PEF	M	407	-	15,15,46	1.10	1 (6%)	17,19,51	1.15	1 (5%)
15	CRT	P	102	-	43,43,43	0.66	0	48,54,54	2.15	15 (31%)
15	CRT	9	101	-	43,43,43	0.72	0	48,54,54	2.43	19 (39%)
9	BCL	3	101	-	69,74,74	1.71	14 (20%)	79,115,115	2.06	26 (32%)
15	CRT	m	104	-	43,43,43	0.67	0	48,54,54	2.34	20 (41%)
9	BCL	i	102	-	69,74,74	1.73	13 (18%)	79,115,115	2.15	34 (43%)
15	CRT	k	101	-	43,43,43	0.76	0	48,54,54	2.15	14 (29%)
9	BCL	L	301	-	69,74,74	1.79	15 (21%)	79,115,115	2.19	32 (40%)
14	MQ8	y	403	-	54,54,54	1.10	5 (9%)	67,69,69	1.59	17 (25%)
9	BCL	X	102	-	69,74,74	1.76	12 (17%)	79,115,115	2.21	29 (36%)
12	PEF	H	301	-	18,18,46	1.46	2 (11%)	21,23,51	1.67	3 (14%)
15	CRT	s	101	-	43,43,43	0.77	1 (2%)	48,54,54	2.22	15 (31%)
15	CRT	7	101	-	43,43,43	0.79	0	48,54,54	2.50	17 (35%)
9	BCL	4	102	-	69,74,74	1.76	15 (21%)	79,115,115	2.21	28 (35%)
9	BCL	AH	101	-	69,74,74	1.74	15 (21%)	79,115,115	2.10	27 (34%)
11	UQ8	L	304	-	53,53,53	1.53	4 (7%)	66,67,67	1.71	17 (25%)
16	PO4	H	303	-	4,4,4	0.67	0	6,6,6	0.76	0
16	PO4	y	405	-	4,4,4	0.79	0	6,6,6	1.15	0
15	CRT	G	101	-	43,43,43	0.68	0	48,54,54	2.16	15 (31%)
9	BCL	K	101	-	69,74,74	1.71	12 (17%)	79,115,115	2.09	28 (35%)
9	BCL	x	303	-	69,74,74	1.89	15 (21%)	79,115,115	2.14	28 (35%)
16	PO4	t	302	-	4,4,4	0.92	0	6,6,6	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	Z	102	-	69,74,74	1.73	12 (17%)	79,115,115	2.28	29 (36%)
9	BCL	AC	102	-	69,74,74	1.76	13 (18%)	79,115,115	2.11	28 (35%)
9	BCL	S	102	-	69,74,74	1.74	13 (18%)	79,115,115	2.05	24 (30%)
9	BCL	M	402	-	69,74,74	1.75	13 (18%)	79,115,115	2.33	30 (37%)
15	CRT	E	101	-	43,43,43	0.81	0	48,54,54	2.00	14 (29%)
9	BCL	F	101	-	69,74,74	1.72	14 (20%)	79,115,115	2.12	29 (36%)
9	BCL	D	101	-	69,74,74	1.70	12 (17%)	79,115,115	2.13	24 (30%)
9	BCL	D	102	-	69,74,74	1.73	13 (18%)	79,115,115	2.16	33 (41%)
9	BCL	c	101	-	69,74,74	1.70	13 (18%)	79,115,115	2.06	27 (34%)
9	BCL	5	101	-	69,74,74	1.77	14 (20%)	79,115,115	2.08	25 (31%)
9	BCL	V	102	-	69,74,74	1.73	14 (20%)	79,115,115	2.11	31 (39%)
15	CRT	y	404	-	43,43,43	0.83	0	48,54,54	2.06	12 (25%)
15	CRT	e	101	-	43,43,43	0.68	0	48,54,54	2.15	16 (33%)
10	BPH	x	302	-	59,70,70	0.71	1 (1%)	59,101,101	1.80	13 (22%)
7	HEM	o	501	1	50,50,50	2.58	9 (18%)	67,82,82	1.93	16 (23%)
12	PEF	y	406	-	18,18,46	1.55	2 (11%)	21,23,51	2.10	4 (19%)
9	BCL	N	101	-	69,74,74	1.69	13 (18%)	79,115,115	2.11	27 (34%)
7	HEM	C	503	1	50,50,50	2.55	10 (20%)	67,82,82	2.29	23 (34%)
9	BCL	8	101	-	69,74,74	1.74	14 (20%)	79,115,115	2.12	24 (30%)
15	CRT	2	101	-	43,43,43	0.79	0	48,54,54	1.87	15 (31%)
15	CRT	z	101	-	43,43,43	0.73	0	48,54,54	2.31	19 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	AC	101	-	-	10/51/51/51	-
7	HEM	o	502	1	-	3/14/54/54	-
9	BCL	m	102	-	-	13/41/137/137	-
9	BCL	j	101	-	-	17/41/137/137	-
9	BCL	AG	101	-	-	17/41/137/137	-
9	BCL	y	401	-	-	12/41/137/137	-
12	PEF	p	101	-	-	3/16/16/50	-
15	CRT	4	101	-	-	17/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEF	M	408	-	-	11/20/20/50	-
9	BCL	AK	101	-	-	14/41/137/137	-
12	PEF	x	306	-	-	10/20/20/50	-
10	BPH	L	302	-	-	16/37/105/105	0/5/6/6
15	CRT	7	103	-	-	7/51/51/51	-
9	BCL	W	101	-	-	18/41/137/137	-
9	BCL	u	101	-	-	20/41/137/137	-
9	BCL	A	103	-	-	10/41/137/137	-
9	BCL	P	101	-	-	12/41/137/137	-
9	BCL	AB	102	-	-	16/41/137/137	-
9	BCL	p	102	-	-	12/41/137/137	-
9	BCL	z	102	-	-	17/41/137/137	-
9	BCL	0	102	-	-	16/41/137/137	-
9	BCL	x	301	-	-	12/41/137/137	-
12	PEF	H	305	-	-	10/20/20/50	-
7	HEM	C	502	1	-	5/14/54/54	-
9	BCL	U	101	-	-	16/41/137/137	-
9	BCL	r	101	-	-	17/41/137/137	-
9	BCL	w	101	-	-	15/41/137/137	-
9	BCL	AL	102	-	-	16/41/137/137	-
9	BCL	9	102	-	-	10/41/137/137	-
9	BCL	I	103	-	-	13/41/137/137	-
11	UQ8	x	304	-	-	16/51/75/75	0/1/1/1
12	PEF	t	301	-	-	6/20/20/50	-
10	BPH	M	403	-	-	15/37/105/105	0/5/6/6
9	BCL	AC	103	-	-	16/41/137/137	-
9	BCL	O	102	-	-	14/41/137/137	-
15	CRT	M	405	-	-	13/51/51/51	-
15	CRT	O	101	-	-	7/51/51/51	-
12	PEF	m	101	-	-	8/20/20/50	-
15	CRT	Z	101	-	-	10/51/51/51	-
7	HEM	o	503	1	-	5/14/54/54	-
9	BCL	m	103	-	-	16/41/137/137	-
15	CRT	AD	101	-	-	9/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	2	102	-	-	12/41/137/137	-
17	PGW	S	101	-	-	11/23/23/55	-
15	CRT	T	101	-	-	6/51/51/51	-
9	BCL	7	102	-	-	18/41/137/137	-
12	PEF	y	407	-	-	5/20/20/50	-
15	CRT	V	101	-	-	16/51/51/51	-
12	PEF	A	101	-	-	8/20/20/50	-
9	BCL	q	102	-	-	17/41/137/137	-
12	PEF	H	302	-	-	6/20/20/50	-
12	PEF	H	304	-	-	11/20/20/50	-
9	BCL	6	101	-	-	13/41/137/137	-
9	BCL	h	101	-	-	9/41/137/137	-
9	BCL	G	102	-	-	16/41/137/137	-
15	CRT	AL	101	-	-	8/51/51/51	-
17	PGW	AE	101	-	-	10/23/23/55	-
15	CRT	AH	102	-	-	12/51/51/51	-
9	BCL	R	102	-	-	15/41/137/137	-
15	CRT	g	101	-	-	5/51/51/51	-
9	BCL	d	101	-	-	11/41/137/137	-
12	PEF	L	305	-	-	4/11/11/50	-
15	CRT	n	101	-	-	14/51/51/51	-
15	CRT	R	101	-	-	14/51/51/51	-
9	BCL	L	303	-	-	18/41/137/137	-
9	BCL	s	102	-	-	15/41/137/137	-
15	CRT	I	102	-	-	7/51/51/51	-
15	CRT	v	101	-	-	8/51/51/51	-
9	BCL	e	102	-	-	14/41/137/137	-
9	BCL	f	101	-	-	17/41/137/137	-
15	CRT	0	101	-	-	10/51/51/51	-
9	BCL	g	102	-	-	17/41/137/137	-
12	PEF	t	303	-	-	8/20/20/50	-
7	HEM	C	501	1	-	7/14/54/54	-
9	BCL	1	101	-	-	16/41/137/137	-
15	CRT	AJ	101	-	-	13/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	AI	101	-	-	14/41/137/137	-
9	BCL	Q	101	-	-	14/41/137/137	-
9	BCL	M	401	-	-	16/41/137/137	-
9	BCL	AB	101	-	-	13/41/137/137	-
9	BCL	x	305	-	-	16/41/137/137	-
9	BCL	k	102	-	-	22/41/137/137	-
9	BCL	u	102	-	-	10/41/137/137	-
9	BCL	AI	102	-	-	17/41/137/137	-
9	BCL	A	102	-	-	13/41/137/137	-
9	BCL	l	101	-	-	16/41/137/137	-
12	PEF	y	408	-	-	8/20/20/50	-
10	BPH	y	402	-	-	13/37/105/105	0/5/6/6
15	CRT	i	101	-	-	8/51/51/51	-
9	BCL	AE	102	-	-	13/41/137/137	-
7	HEM	o	504	1	-	3/14/54/54	-
9	BCL	I	101	-	-	9/41/137/137	-
9	BCL	Y	101	-	-	12/41/137/137	-
9	BCL	T	102	-	-	13/41/137/137	-
9	BCL	AF	101	-	-	13/41/137/137	-
7	HEM	C	504	1	-	5/14/54/54	-
15	CRT	AF	102	-	-	5/51/51/51	-
14	MQ8	M	404	-	-	20/47/67/67	0/2/2/2
15	CRT	X	101	-	-	15/51/51/51	-
15	CRT	q	101	-	-	7/51/51/51	-
12	PEF	M	407	-	-	3/16/16/50	-
15	CRT	P	102	-	-	7/51/51/51	-
15	CRT	9	101	-	-	12/51/51/51	-
9	BCL	3	101	-	-	12/41/137/137	-
15	CRT	m	104	-	-	3/51/51/51	-
9	BCL	i	102	-	-	17/41/137/137	-
15	CRT	k	101	-	-	9/51/51/51	-
9	BCL	L	301	-	-	9/41/137/137	-
14	MQ8	y	403	-	-	24/47/67/67	0/2/2/2
9	BCL	X	102	-	-	18/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEF	H	301	-	-	8/20/20/50	-
15	CRT	s	101	-	-	10/51/51/51	-
15	CRT	7	101	-	-	8/51/51/51	-
9	BCL	4	102	-	-	14/41/137/137	-
9	BCL	AH	101	-	-	20/41/137/137	-
11	UQ8	L	304	-	-	10/51/75/75	0/1/1/1
15	CRT	G	101	-	-	12/51/51/51	-
9	BCL	K	101	-	-	11/41/137/137	-
9	BCL	x	303	-	-	16/41/137/137	-
9	BCL	Z	102	-	-	14/41/137/137	-
9	BCL	AC	102	-	-	23/41/137/137	-
9	BCL	S	102	-	-	16/41/137/137	-
9	BCL	M	402	-	-	14/41/137/137	-
15	CRT	E	101	-	-	8/51/51/51	-
9	BCL	F	101	-	-	18/41/137/137	-
9	BCL	D	101	-	-	8/41/137/137	-
9	BCL	D	102	-	-	13/41/137/137	-
9	BCL	c	101	-	-	19/41/137/137	-
9	BCL	5	101	-	-	8/41/137/137	-
9	BCL	V	102	-	-	11/41/137/137	-
15	CRT	y	404	-	-	14/51/51/51	-
15	CRT	e	101	-	-	13/51/51/51	-
10	BPH	x	302	-	-	11/37/105/105	0/5/6/6
7	HEM	o	501	1	-	7/14/54/54	-
12	PEF	y	406	-	-	6/20/20/50	-
9	BCL	N	101	-	-	15/41/137/137	-
7	HEM	C	503	1	-	3/14/54/54	-
9	BCL	8	101	-	-	23/41/137/137	-
15	CRT	2	101	-	-	6/51/51/51	-
15	CRT	z	101	-	-	2/51/51/51	-

The worst 5 of 1118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	504	HEM	FE-NB	14.40	2.39	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	501	HEM	FE-NB	14.11	2.38	1.94
7	C	503	HEM	FE-NB	14.05	2.38	1.94
7	o	503	HEM	FE-NB	13.96	2.37	1.94
7	C	501	HEM	FE-NB	13.85	2.37	1.94

The worst 5 of 2834 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	302	BPH	O2D-CGD-CBD	10.00	121.93	110.95
10	M	403	BPH	O2D-CGD-CBD	9.51	121.39	110.95
15	g	101	CRT	C31-C32-C33	-9.13	114.47	127.28
15	AJ	101	CRT	C37-C36-C35	-8.66	112.75	124.91
15	s	101	CRT	C37-C36-C35	-8.23	113.36	124.91

There are no chirality outliers.

5 of 1681 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	502	HEM	C2B-C3B-CAB-CBB
7	C	502	HEM	C3D-CAD-CBD-CGD
7	C	503	HEM	C2B-C3B-CAB-CBB
7	C	503	HEM	C4B-C3B-CAB-CBB
7	o	502	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

141 monomers are involved in 1144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	AC	101	CRT	11	0
7	o	502	HEM	6	0
9	m	102	BCL	5	0
9	j	101	BCL	8	0
9	AG	101	BCL	6	0
9	y	401	BCL	16	0
12	p	101	PEF	7	0
15	4	101	CRT	14	0
12	M	408	PEF	2	0
9	AK	101	BCL	9	0
12	x	306	PEF	11	0
10	L	302	BPH	5	0
15	7	103	CRT	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	101	BCL	8	0
9	u	101	BCL	10	0
9	A	103	BCL	7	0
9	P	101	BCL	6	0
9	AB	102	BCL	9	0
9	p	102	BCL	12	0
9	z	102	BCL	6	0
9	0	102	BCL	5	0
9	x	301	BCL	14	0
12	H	305	PEF	7	0
7	C	502	HEM	4	0
9	U	101	BCL	9	0
9	r	101	BCL	11	0
9	w	101	BCL	8	0
9	AL	102	BCL	11	0
9	9	102	BCL	8	0
9	I	103	BCL	15	0
11	x	304	UQ8	18	0
12	t	301	PEF	3	0
10	M	403	BPH	14	0
9	AC	103	BCL	6	0
9	O	102	BCL	6	0
15	M	405	CRT	13	0
15	O	101	CRT	9	0
12	m	101	PEF	3	0
15	Z	101	CRT	8	0
7	o	503	HEM	5	0
9	m	103	BCL	12	0
15	AD	101	CRT	8	0
9	2	102	BCL	9	0
17	S	101	PGW	3	0
15	T	101	CRT	11	0
9	7	102	BCL	7	0
12	y	407	PEF	3	0
15	V	101	CRT	10	0
12	A	101	PEF	2	0
9	q	102	BCL	11	0
12	H	302	PEF	11	0
12	H	304	PEF	2	0
9	6	101	BCL	10	0
9	h	101	BCL	8	0
9	G	102	BCL	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	AL	101	CRT	10	0
17	AE	101	PGW	2	0
15	AH	102	CRT	9	0
9	R	102	BCL	5	0
15	g	101	CRT	12	0
9	d	101	BCL	12	0
15	n	101	CRT	17	0
15	R	101	CRT	11	0
9	L	303	BCL	10	0
9	s	102	BCL	11	0
15	I	102	CRT	10	0
15	v	101	CRT	7	0
9	e	102	BCL	12	0
9	f	101	BCL	7	0
15	0	101	CRT	12	0
9	g	102	BCL	6	0
12	t	303	PEF	4	0
7	C	501	HEM	11	0
9	1	101	BCL	10	0
15	AJ	101	CRT	12	0
9	AI	101	BCL	15	0
9	Q	101	BCL	3	0
9	M	401	BCL	7	0
9	AB	101	BCL	10	0
9	x	305	BCL	6	0
9	k	102	BCL	12	0
9	u	102	BCL	11	0
9	AI	102	BCL	8	0
9	A	102	BCL	9	0
9	l	101	BCL	8	0
12	y	408	PEF	2	0
16	M	406	PO4	1	0
10	y	402	BPH	10	0
15	i	101	CRT	4	0
9	AE	102	BCL	9	0
7	o	504	HEM	12	0
9	I	101	BCL	8	0
9	Y	101	BCL	9	0
9	T	102	BCL	12	0
9	AF	101	BCL	8	0
7	C	504	HEM	8	0
15	AF	102	CRT	14	0

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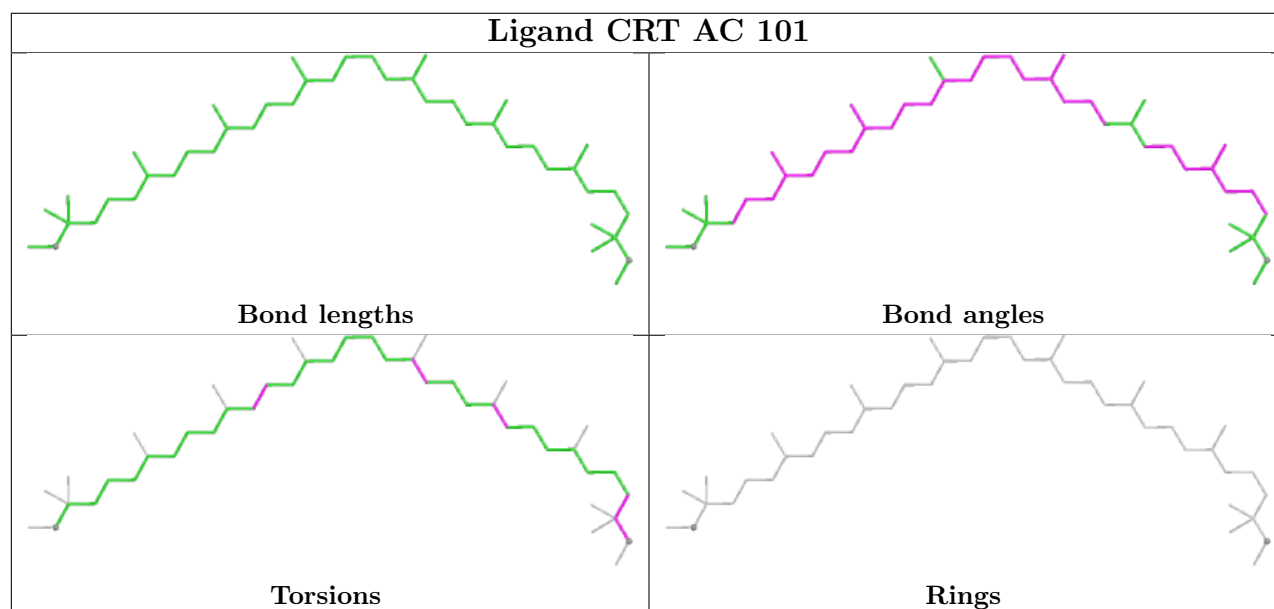
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	M	404	MQ8	4	0
15	X	101	CRT	21	0
15	q	101	CRT	9	0
12	M	407	PEF	1	0
15	P	102	CRT	9	0
15	9	101	CRT	16	0
9	3	101	BCL	10	0
15	m	104	CRT	8	0
9	i	102	BCL	8	0
15	k	101	CRT	15	0
9	L	301	BCL	18	0
14	y	403	MQ8	8	0
9	X	102	BCL	8	0
12	H	301	PEF	6	0
15	s	101	CRT	10	0
15	7	101	CRT	9	0
9	4	102	BCL	10	0
9	AH	101	BCL	8	0
11	L	304	UQ8	12	0
16	y	405	PO4	1	0
15	G	101	CRT	9	0
9	K	101	BCL	6	0
9	x	303	BCL	8	0
9	Z	102	BCL	16	0
9	AC	102	BCL	10	0
9	S	102	BCL	11	0
9	M	402	BCL	14	0
15	E	101	CRT	14	0
9	F	101	BCL	4	0
9	D	101	BCL	10	0
9	D	102	BCL	7	0
9	c	101	BCL	14	0
9	5	101	BCL	12	0
9	V	102	BCL	8	0
15	y	404	CRT	11	0
15	e	101	CRT	10	0
10	x	302	BPH	4	0
7	o	501	HEM	7	0
12	y	406	PEF	4	0
9	N	101	BCL	4	0
7	C	503	HEM	5	0
9	8	101	BCL	12	0

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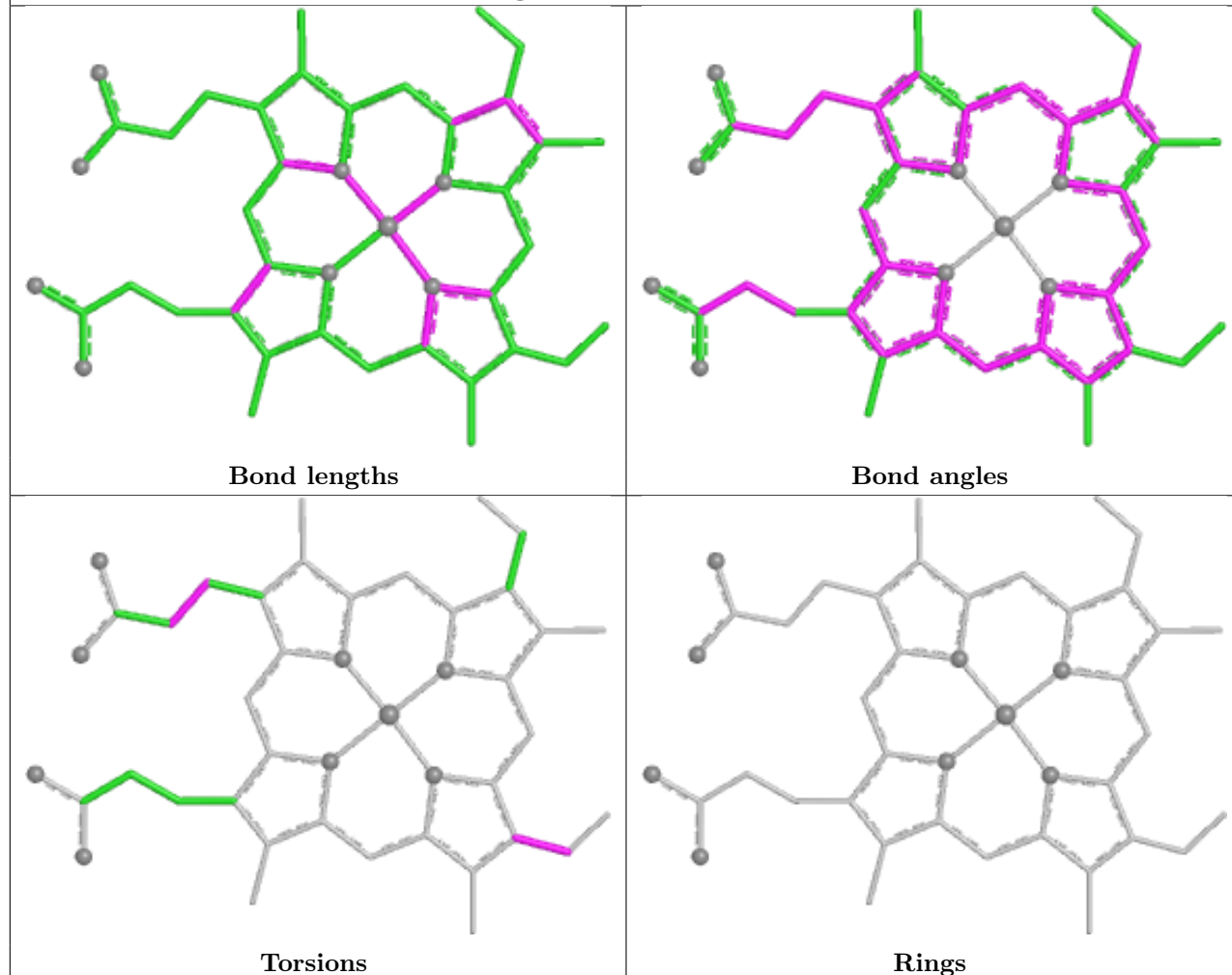
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	2	101	CRT	7	0
15	z	101	CRT	6	0

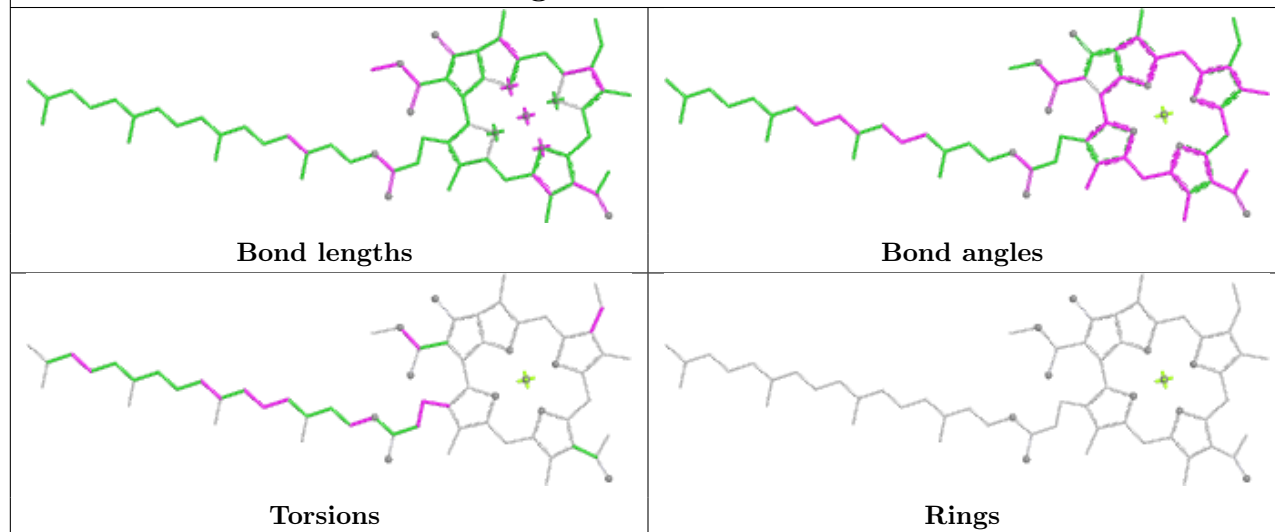
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

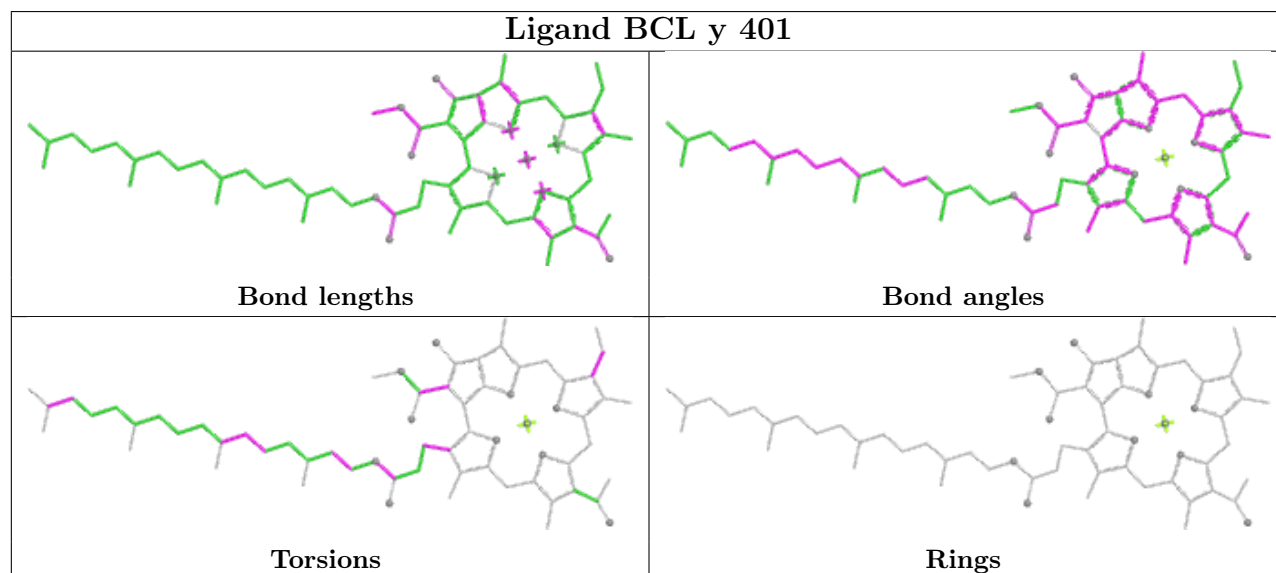
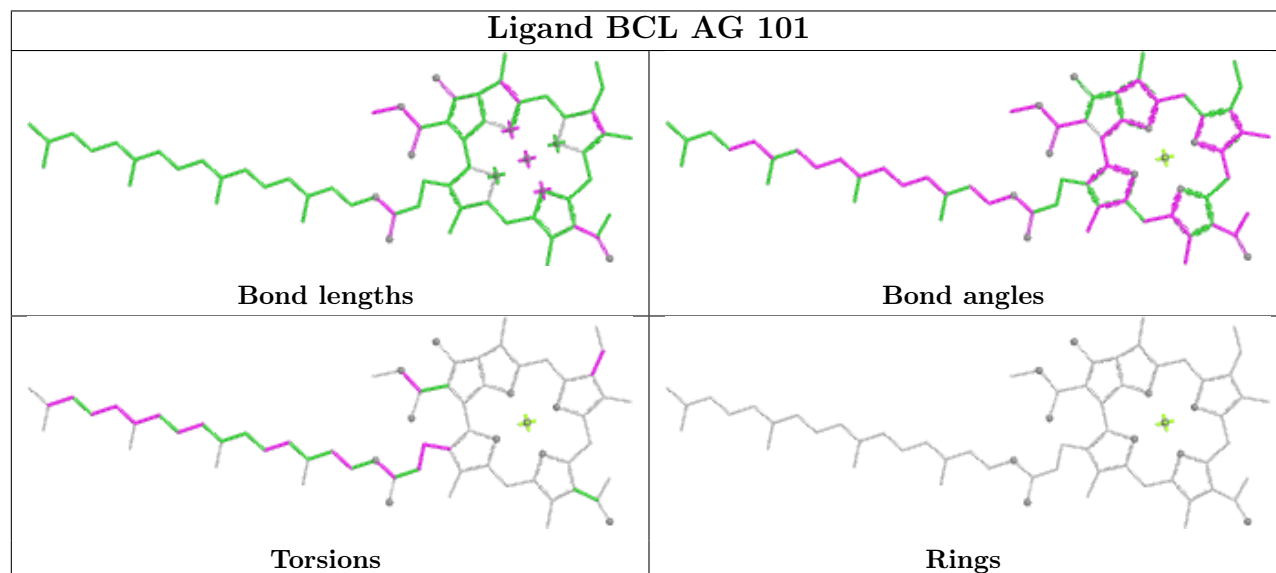
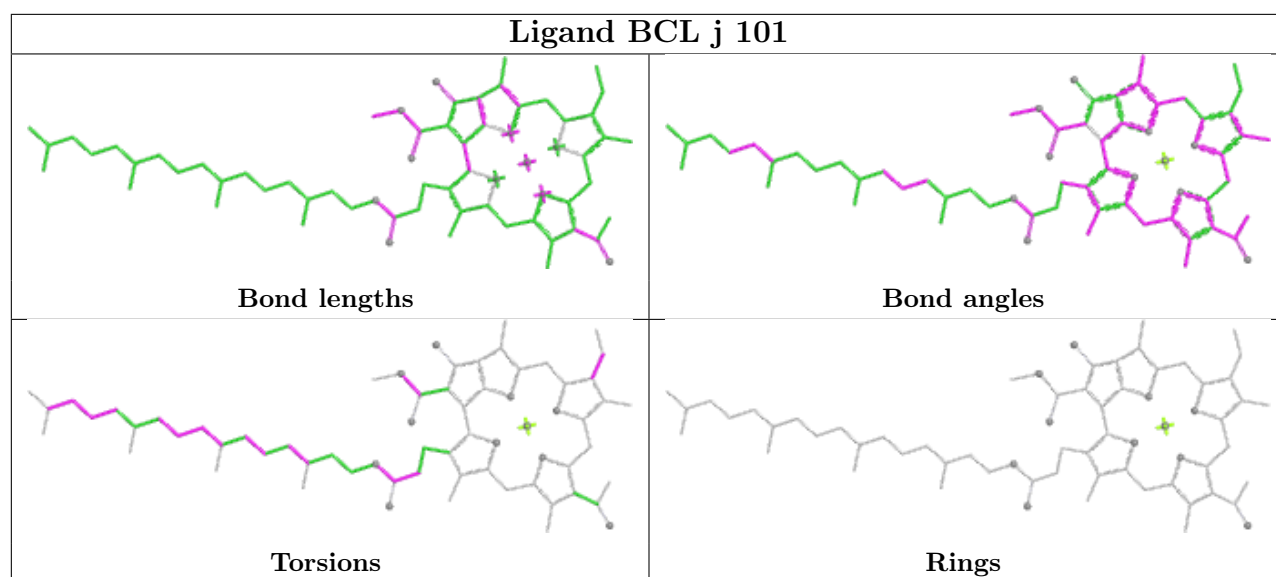


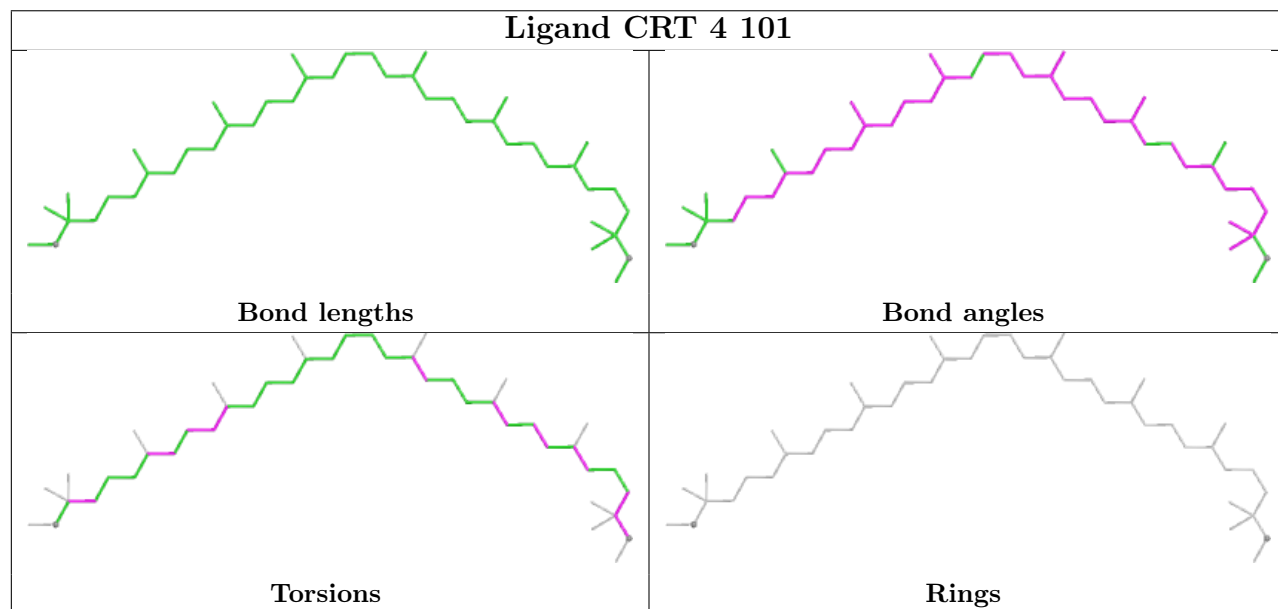
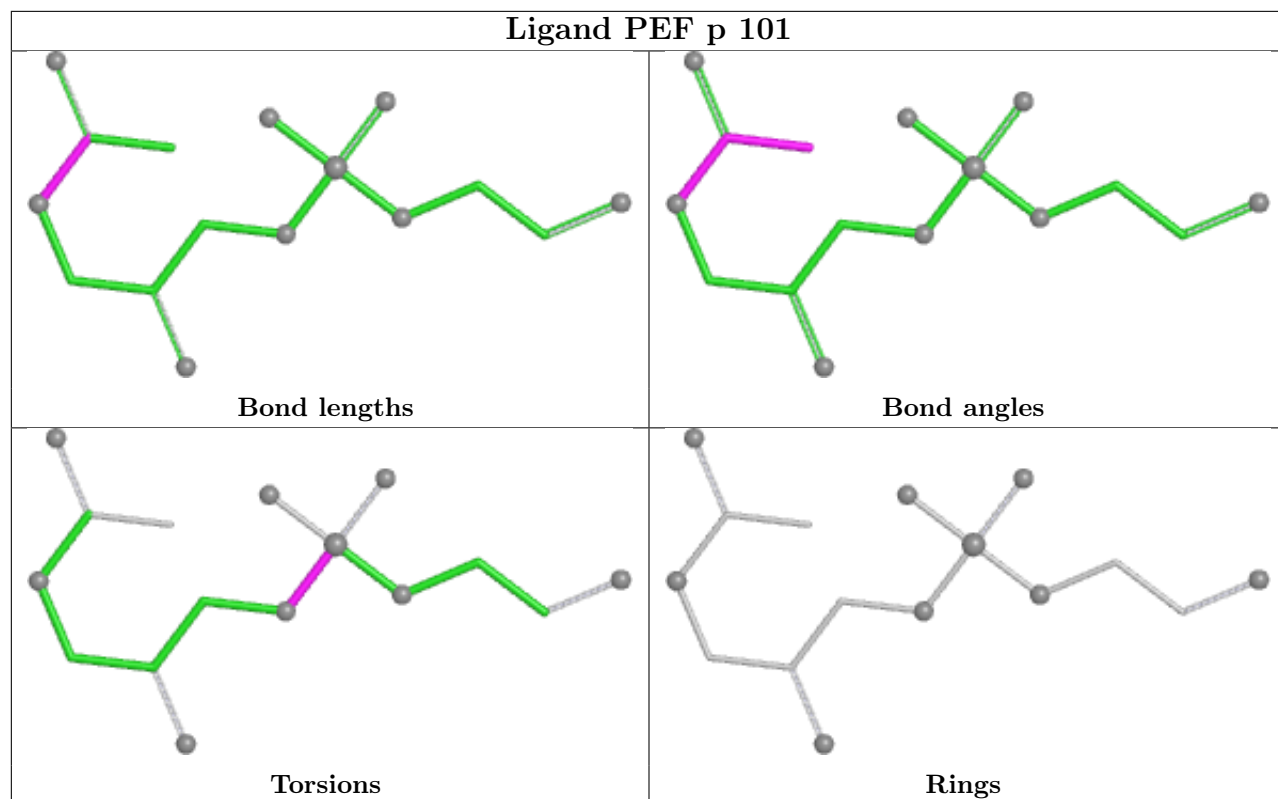
Ligand HEM o 502

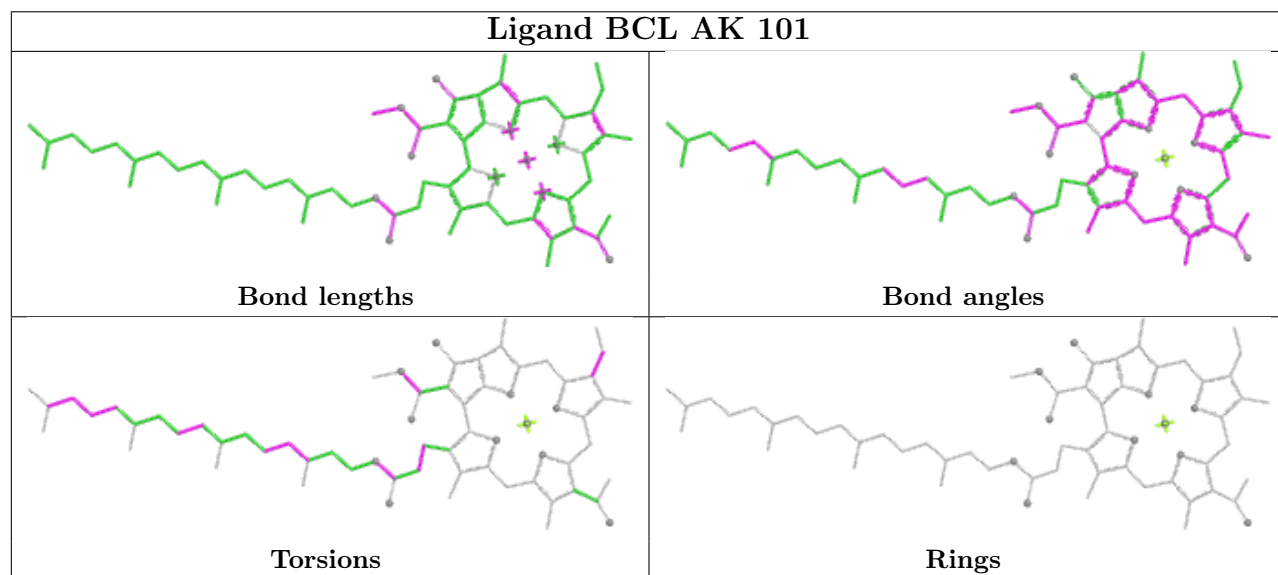
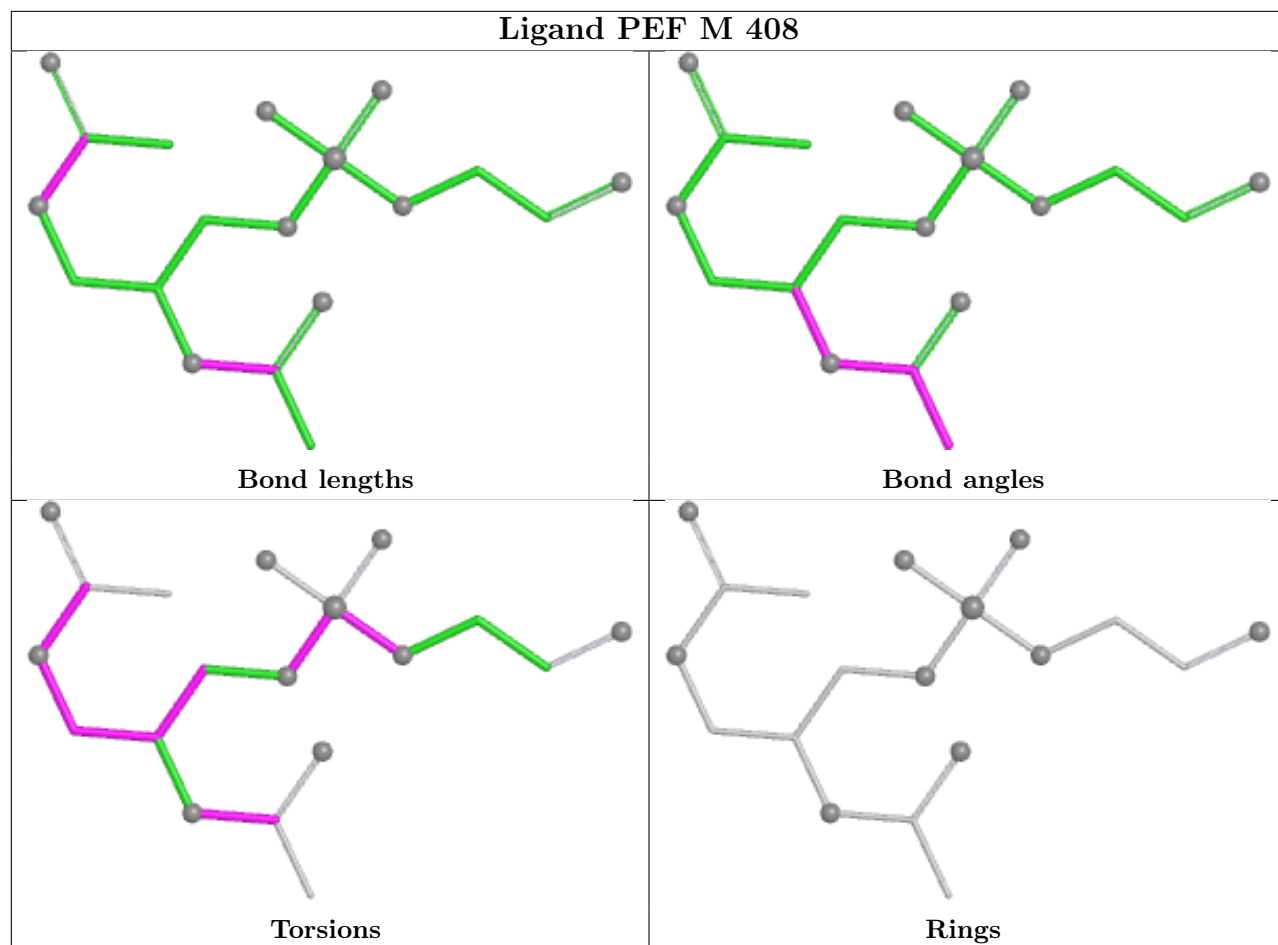


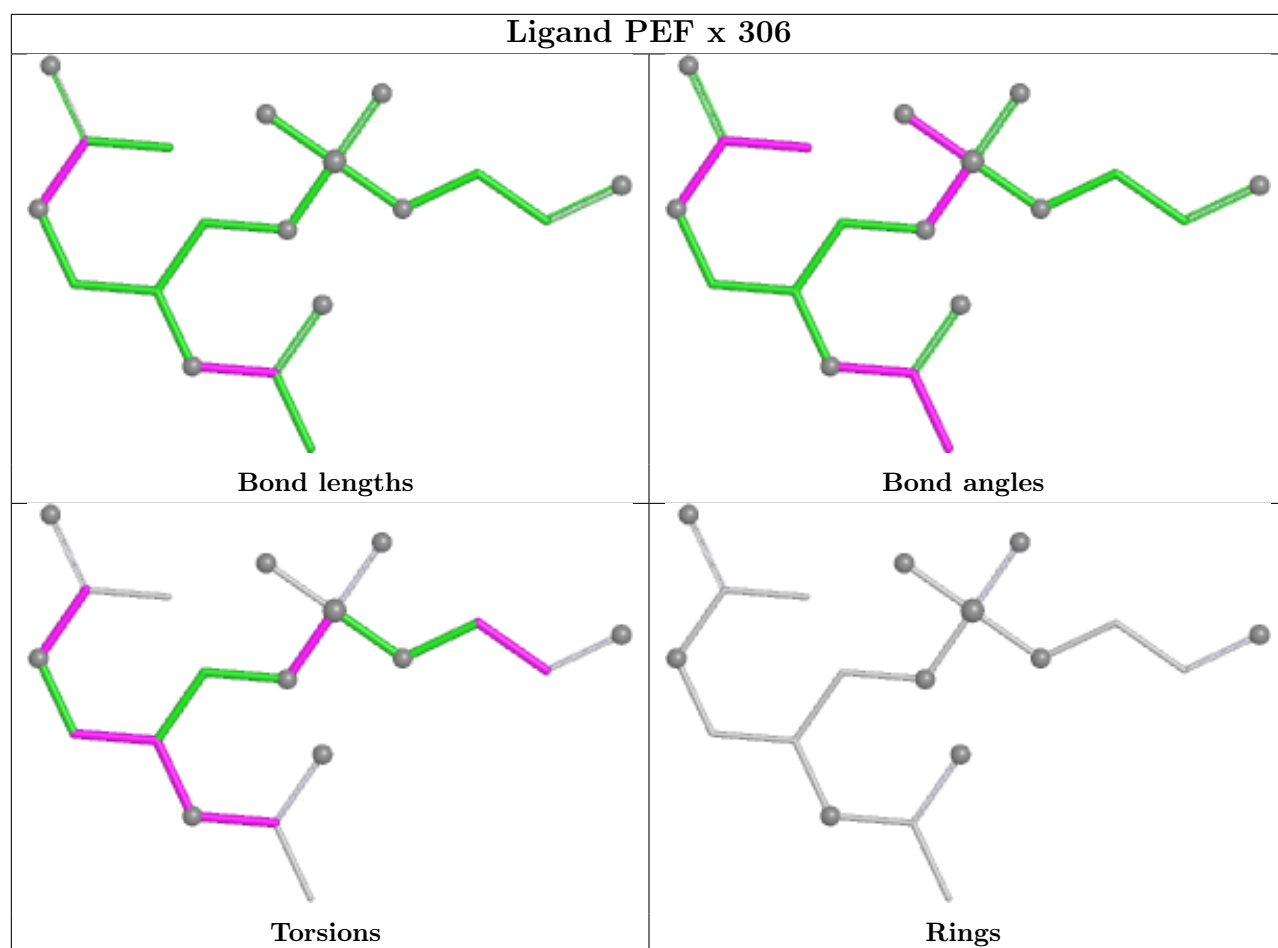
Ligand BCL m 102



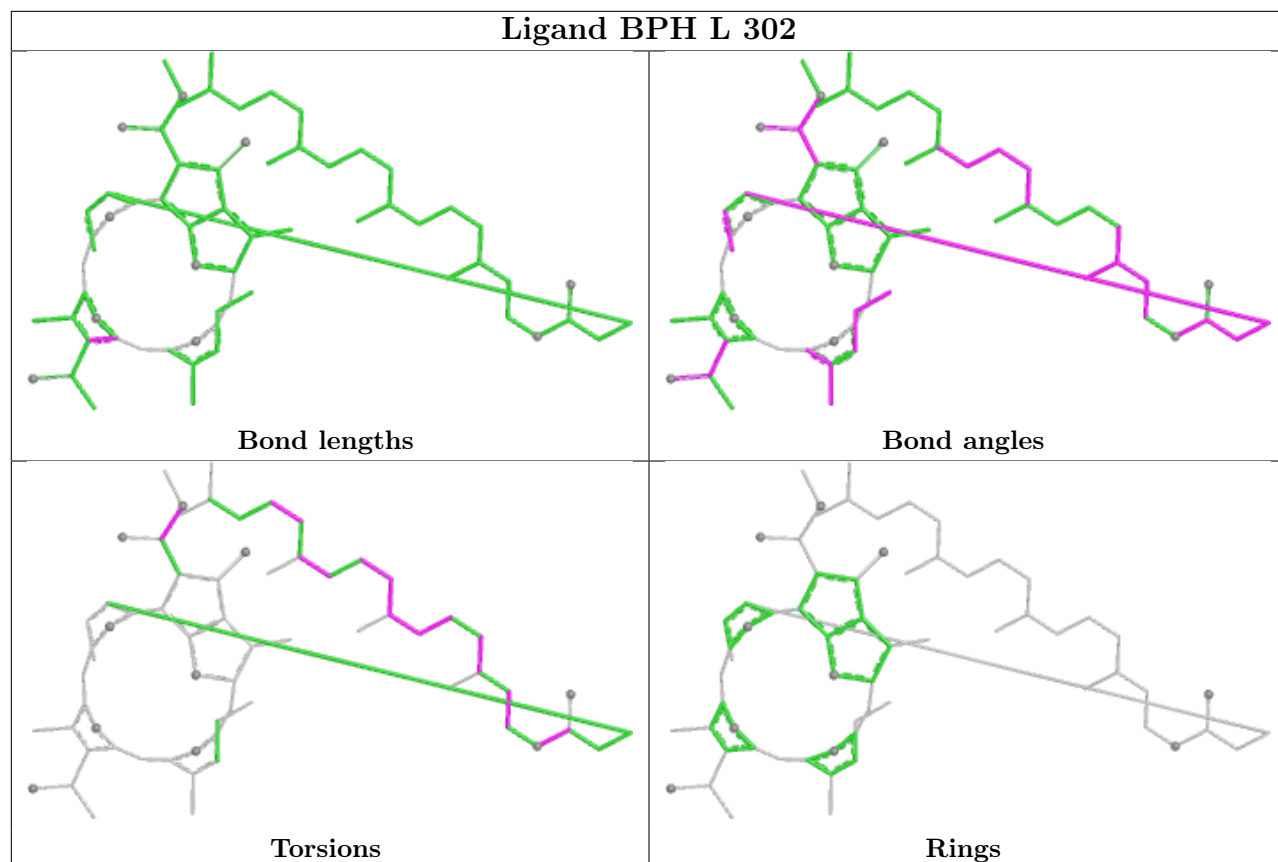




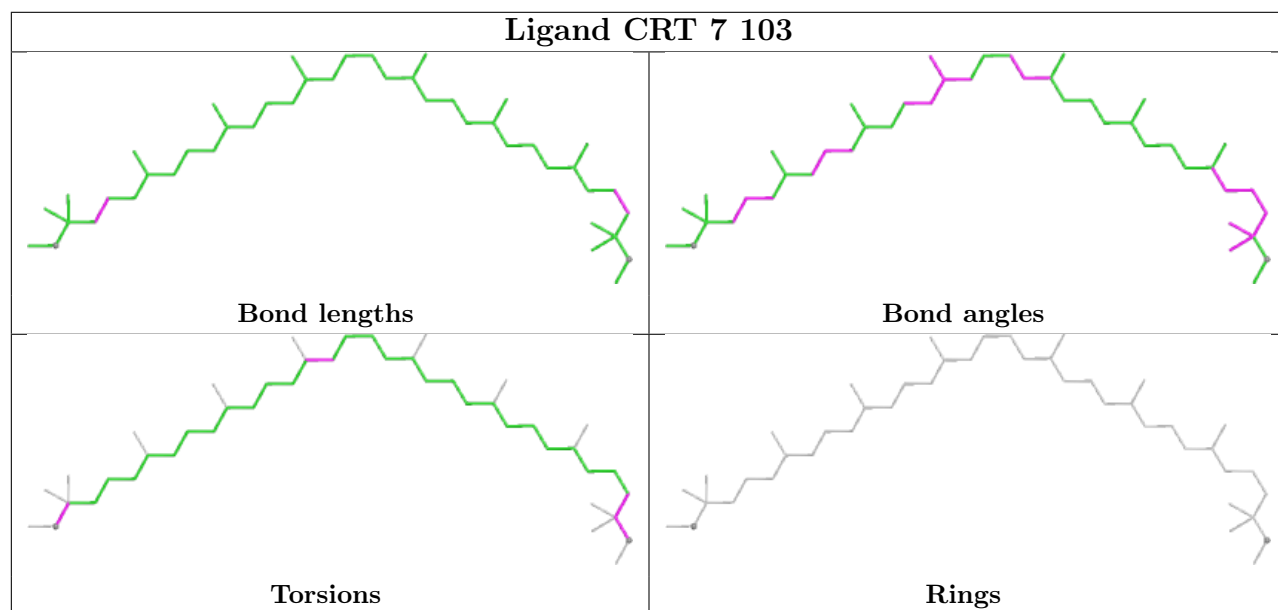


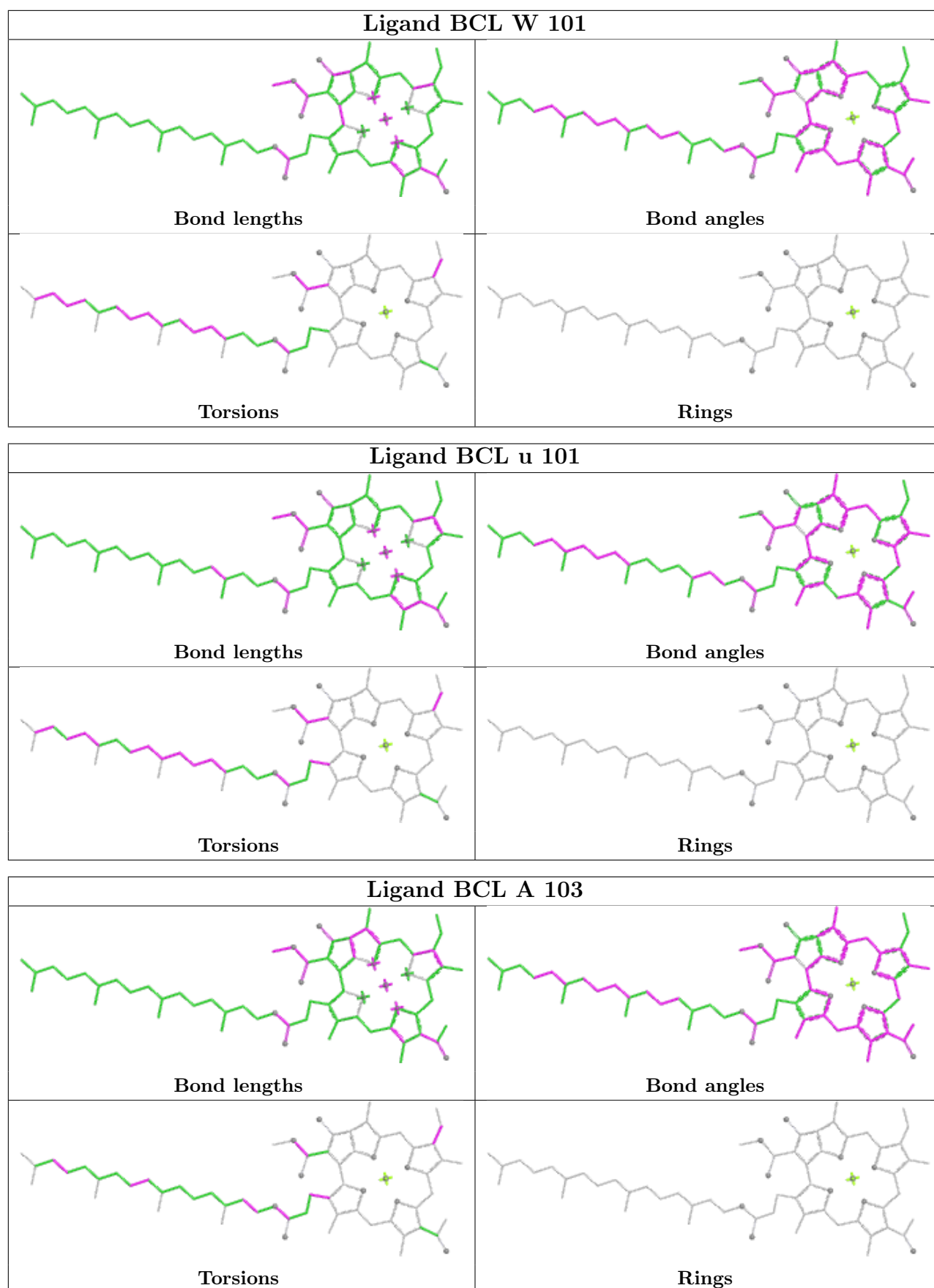


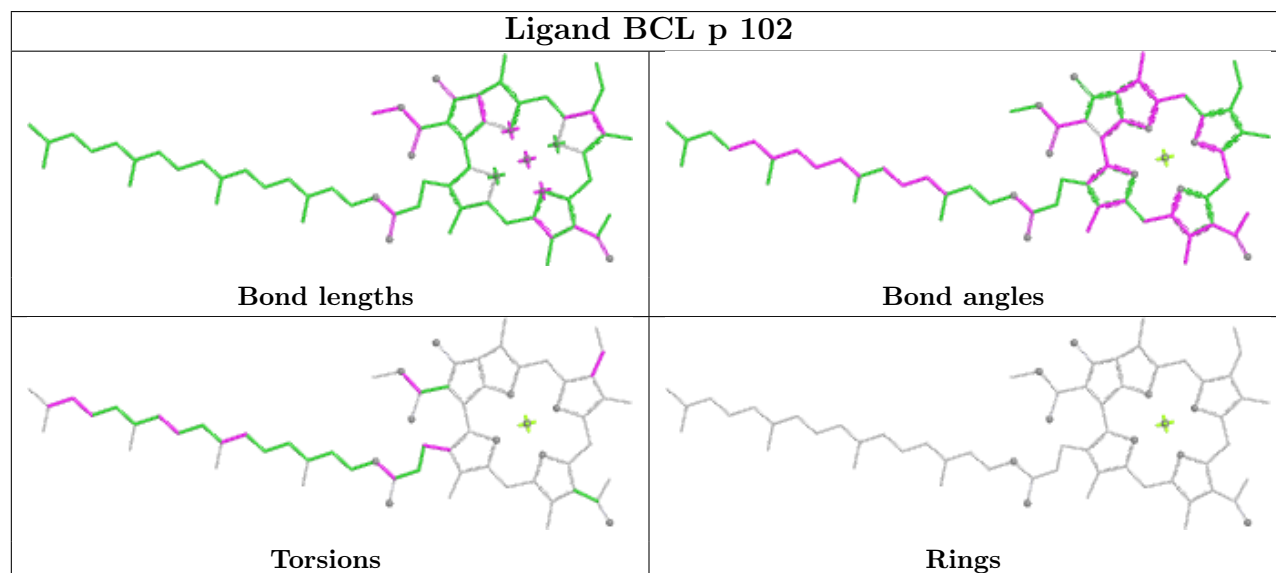
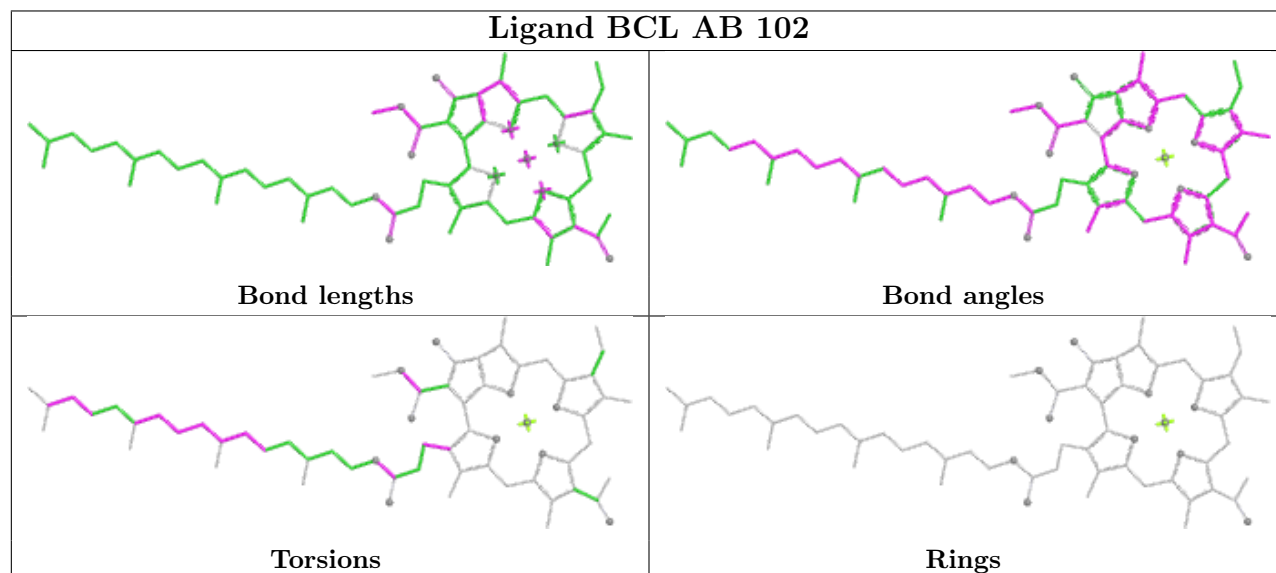
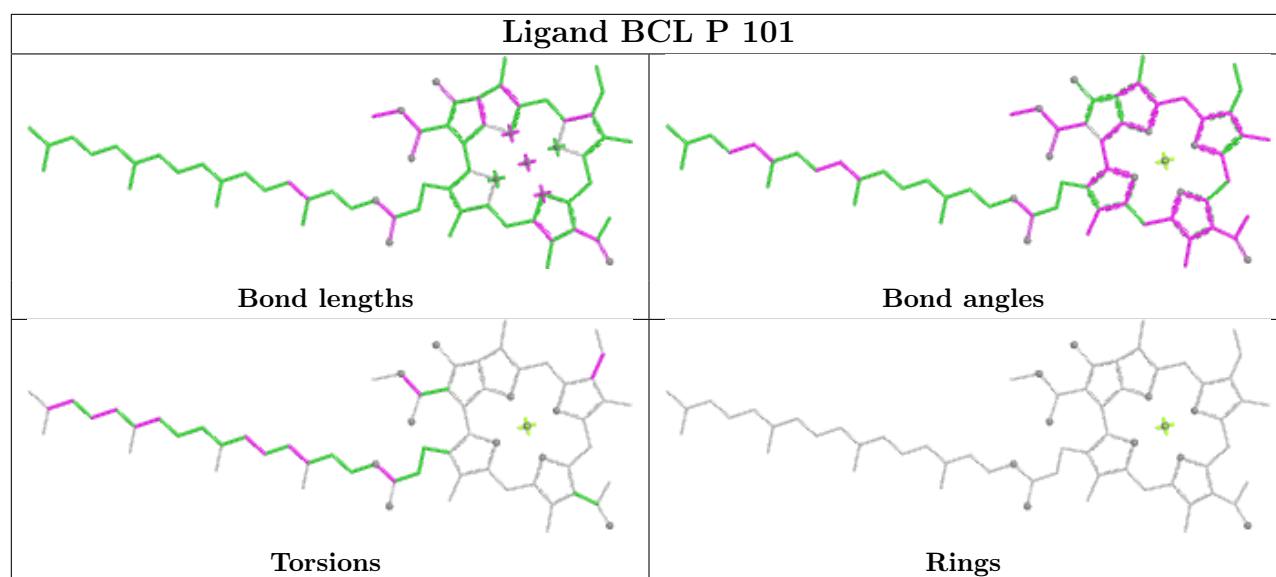
Ligand BPH L 302

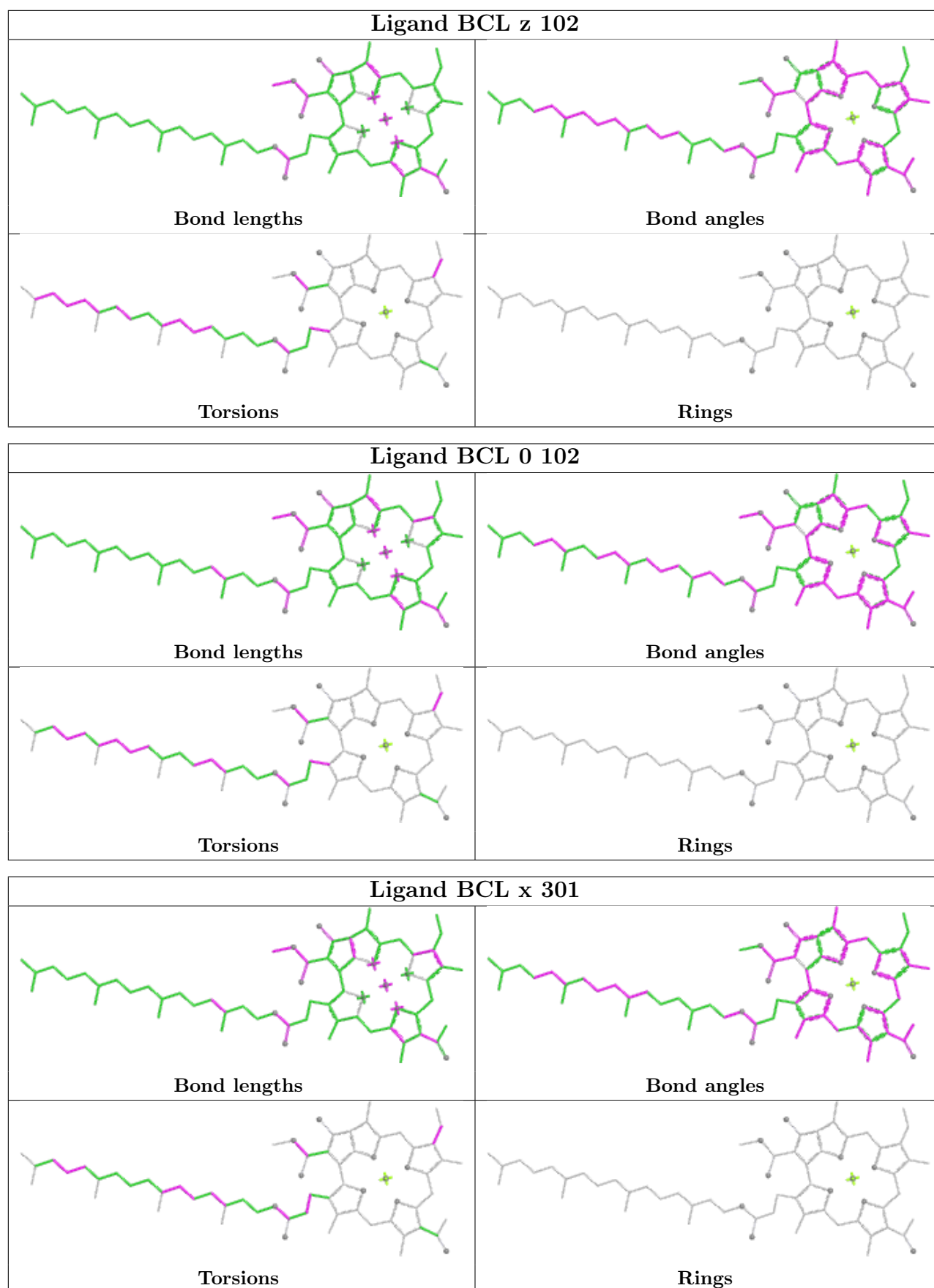


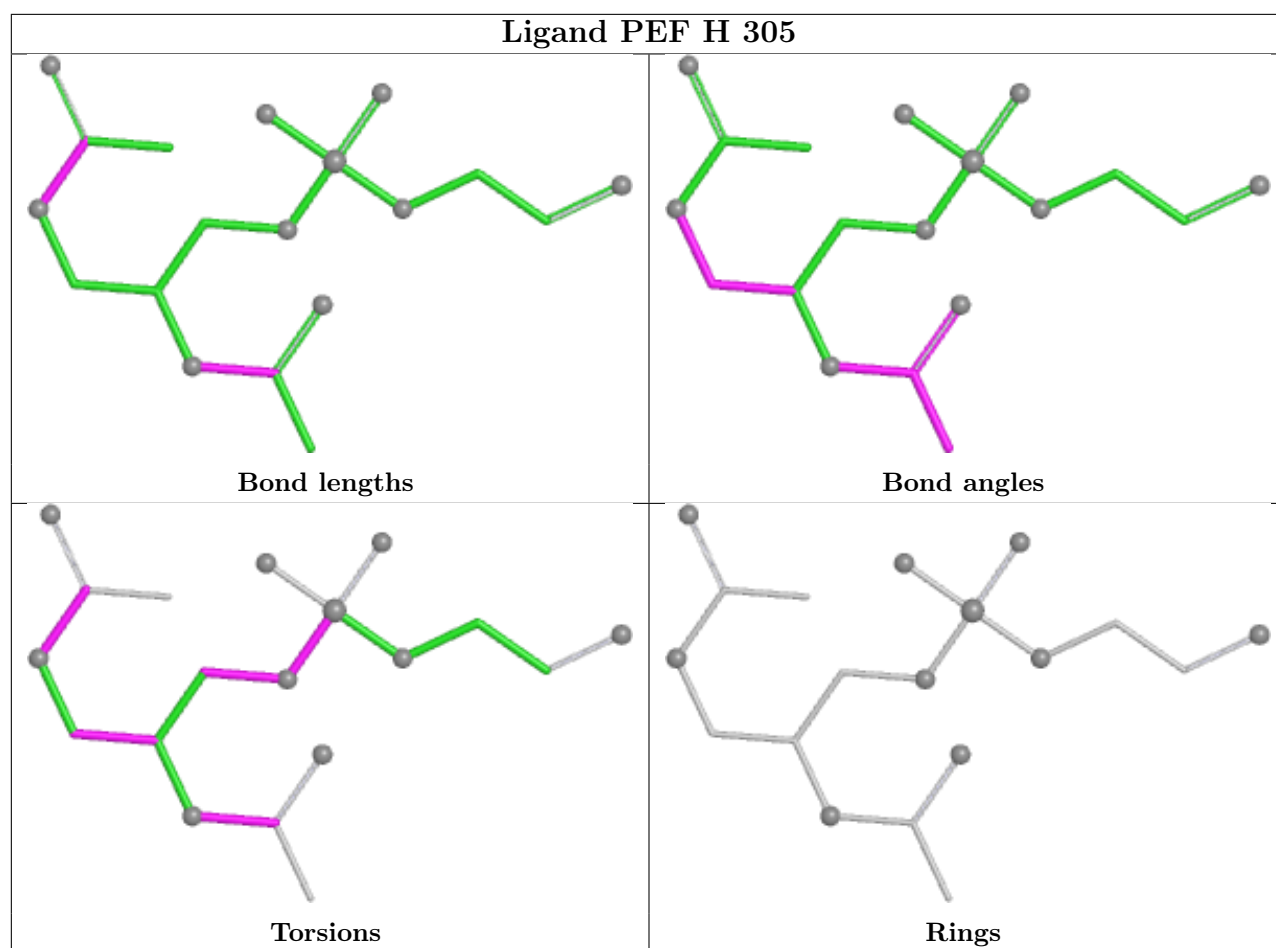
Ligand CRT 7 103

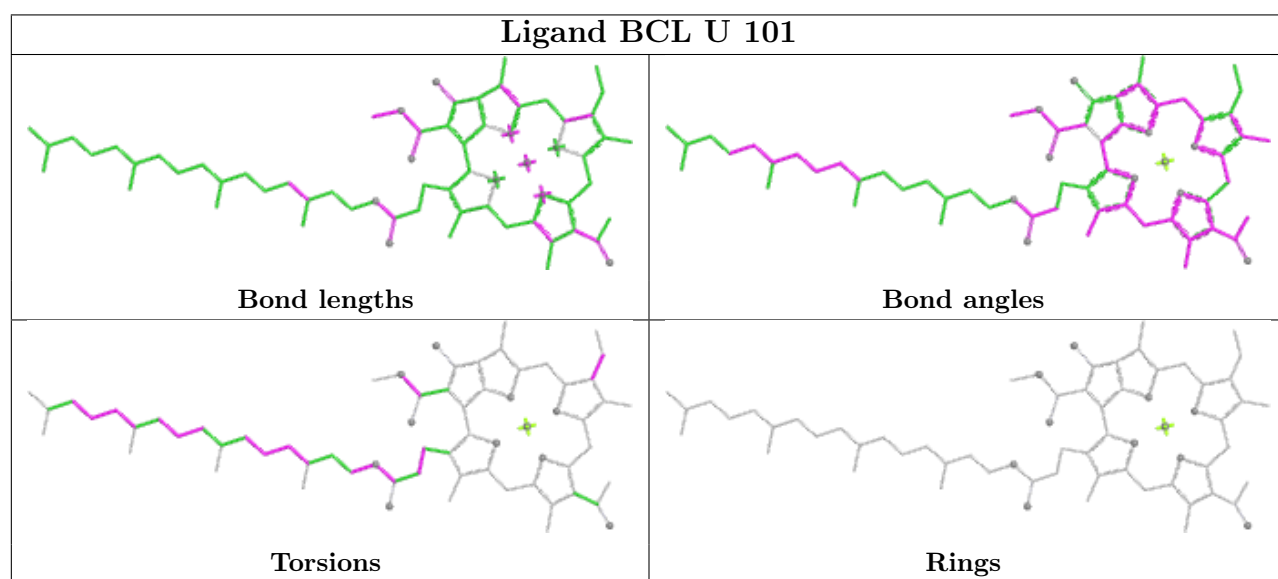
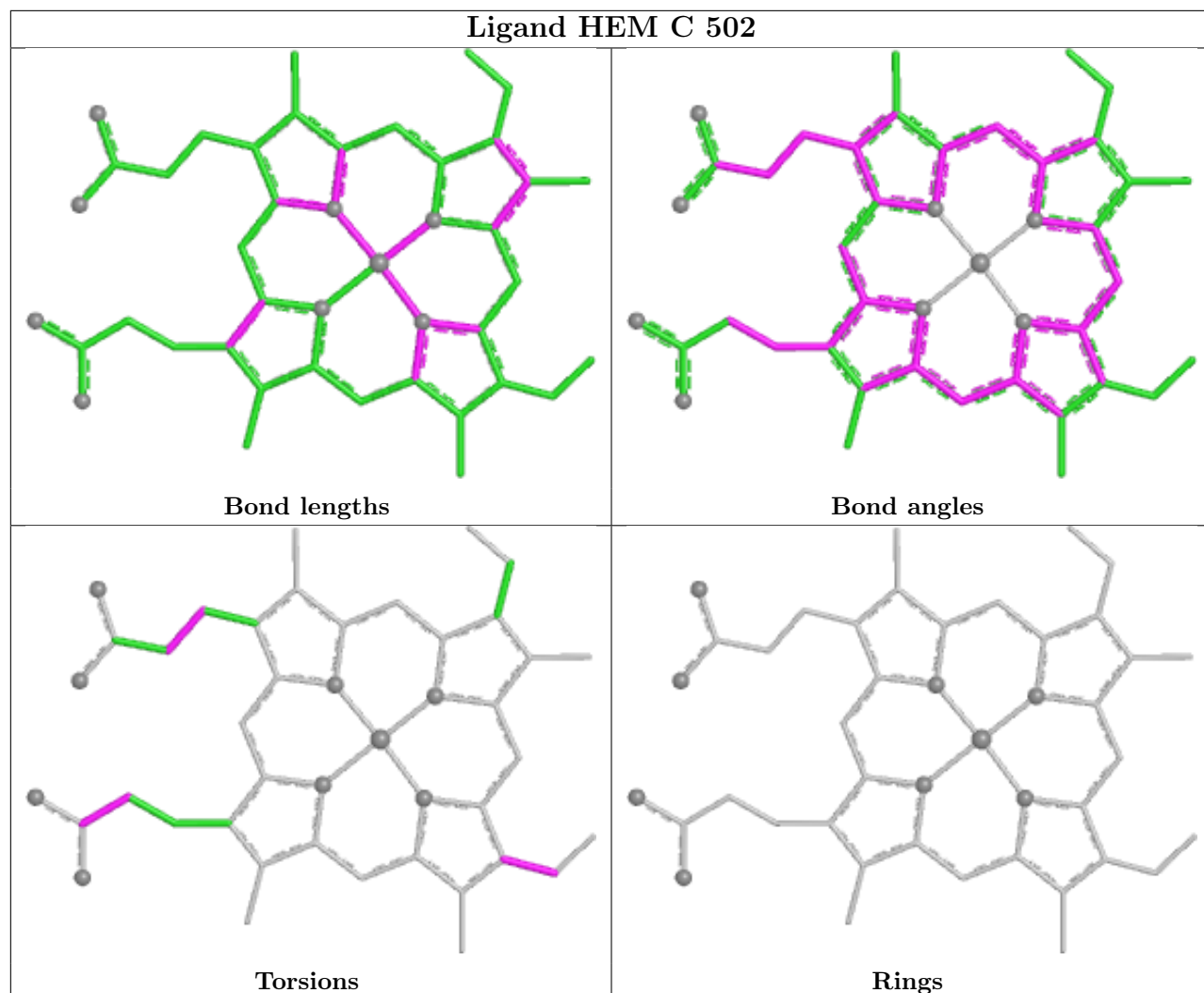


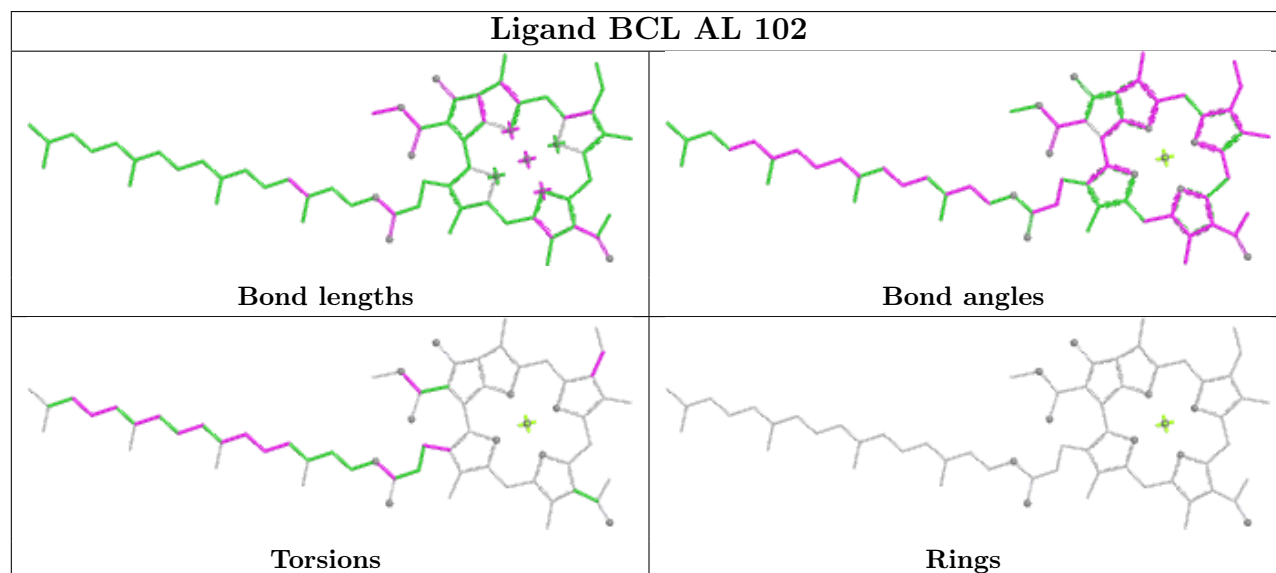
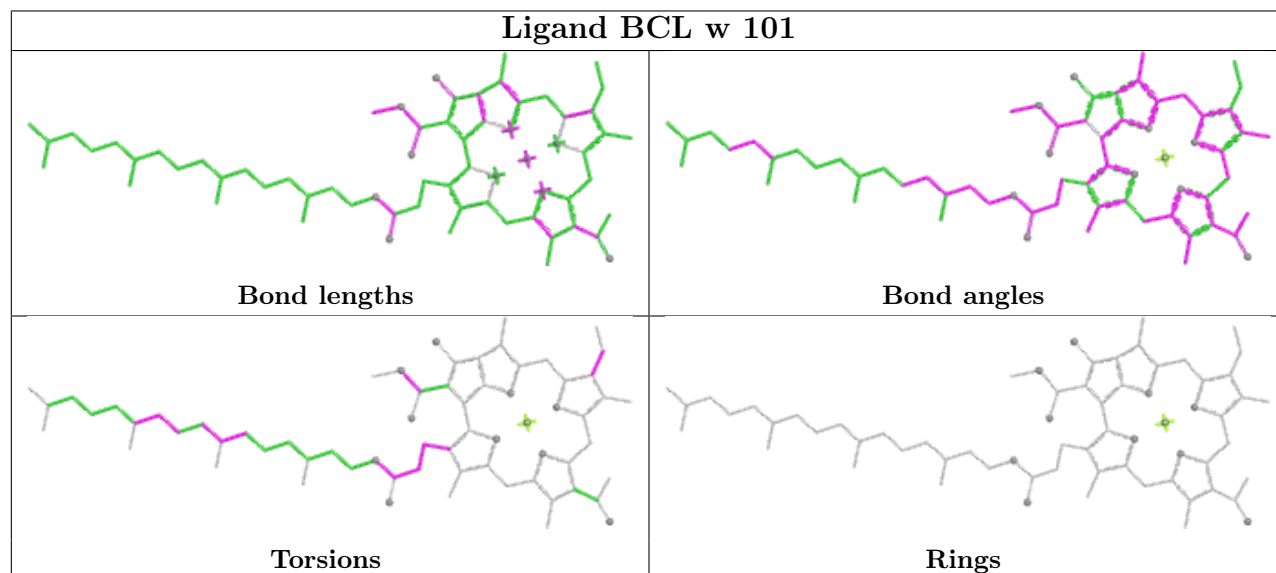
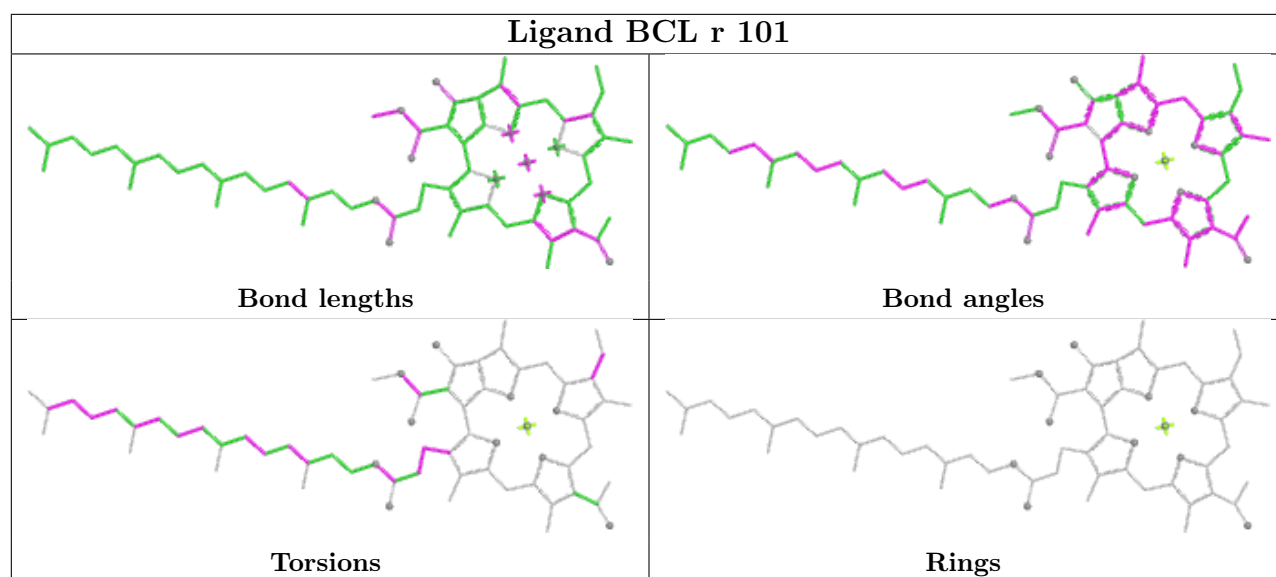


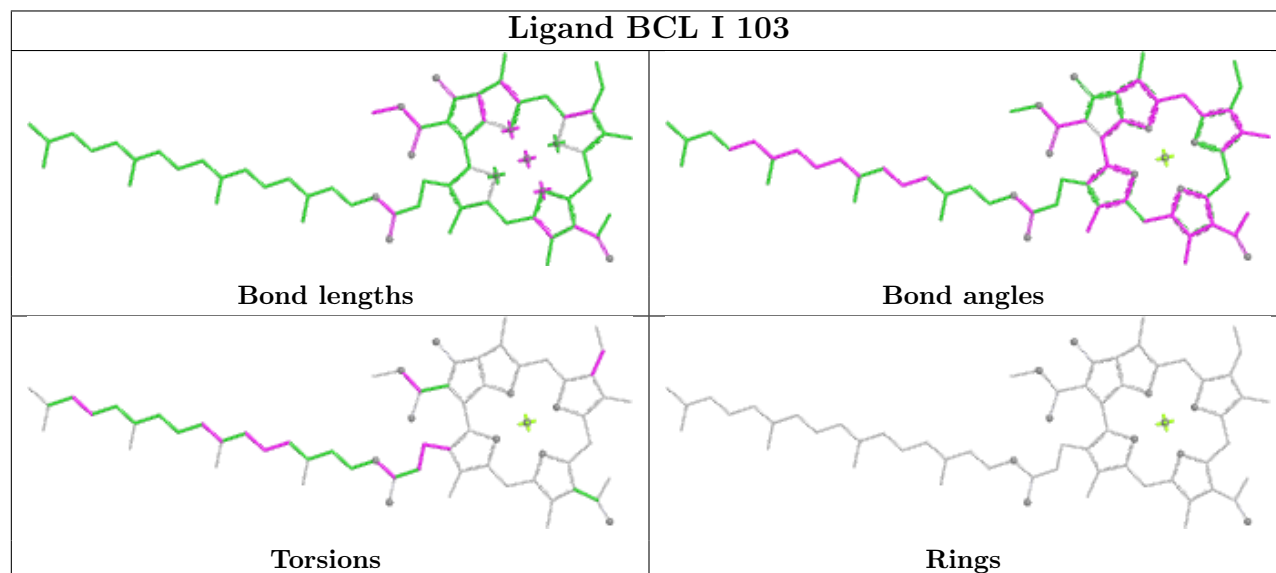
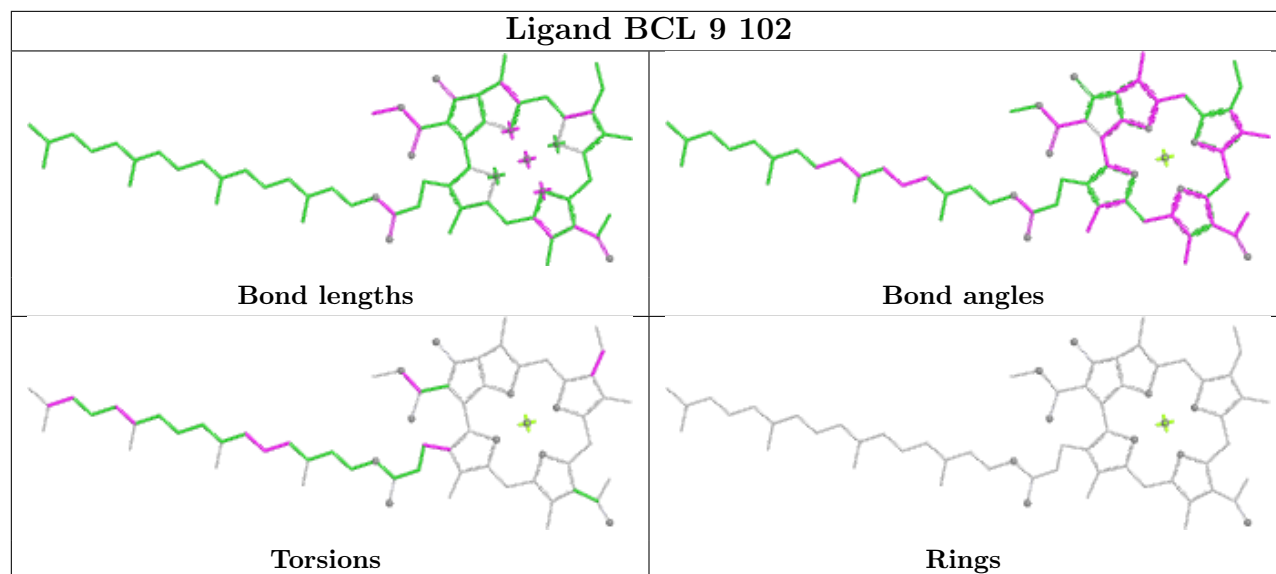




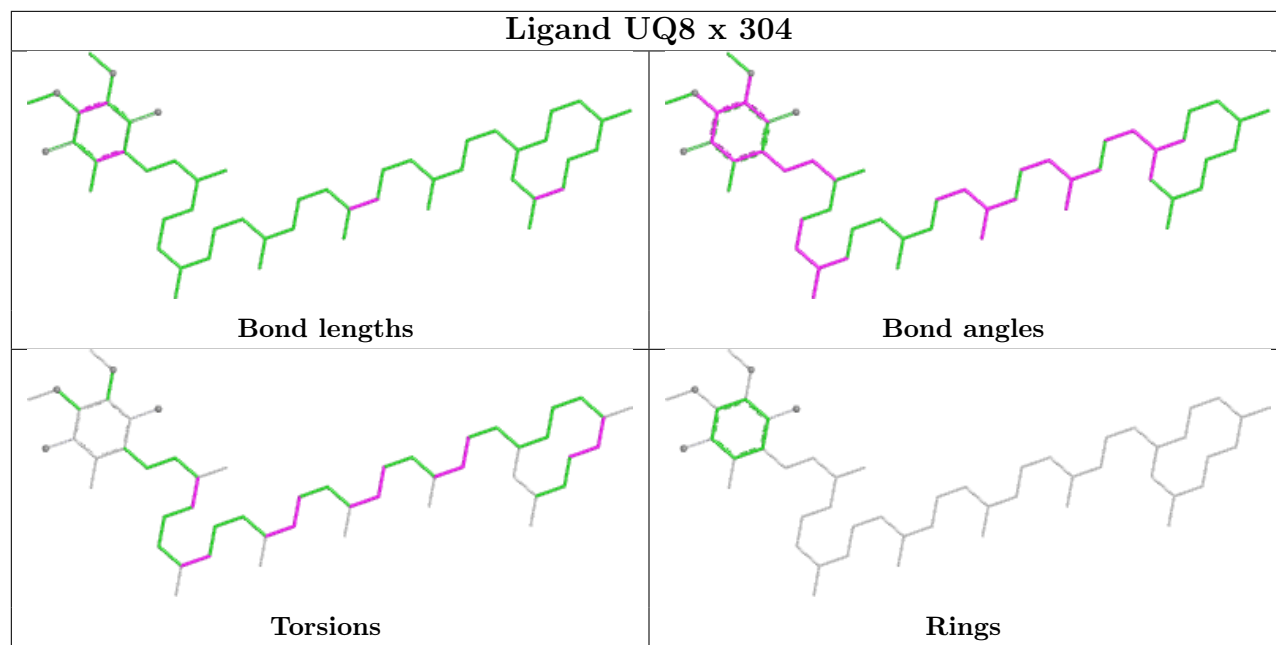




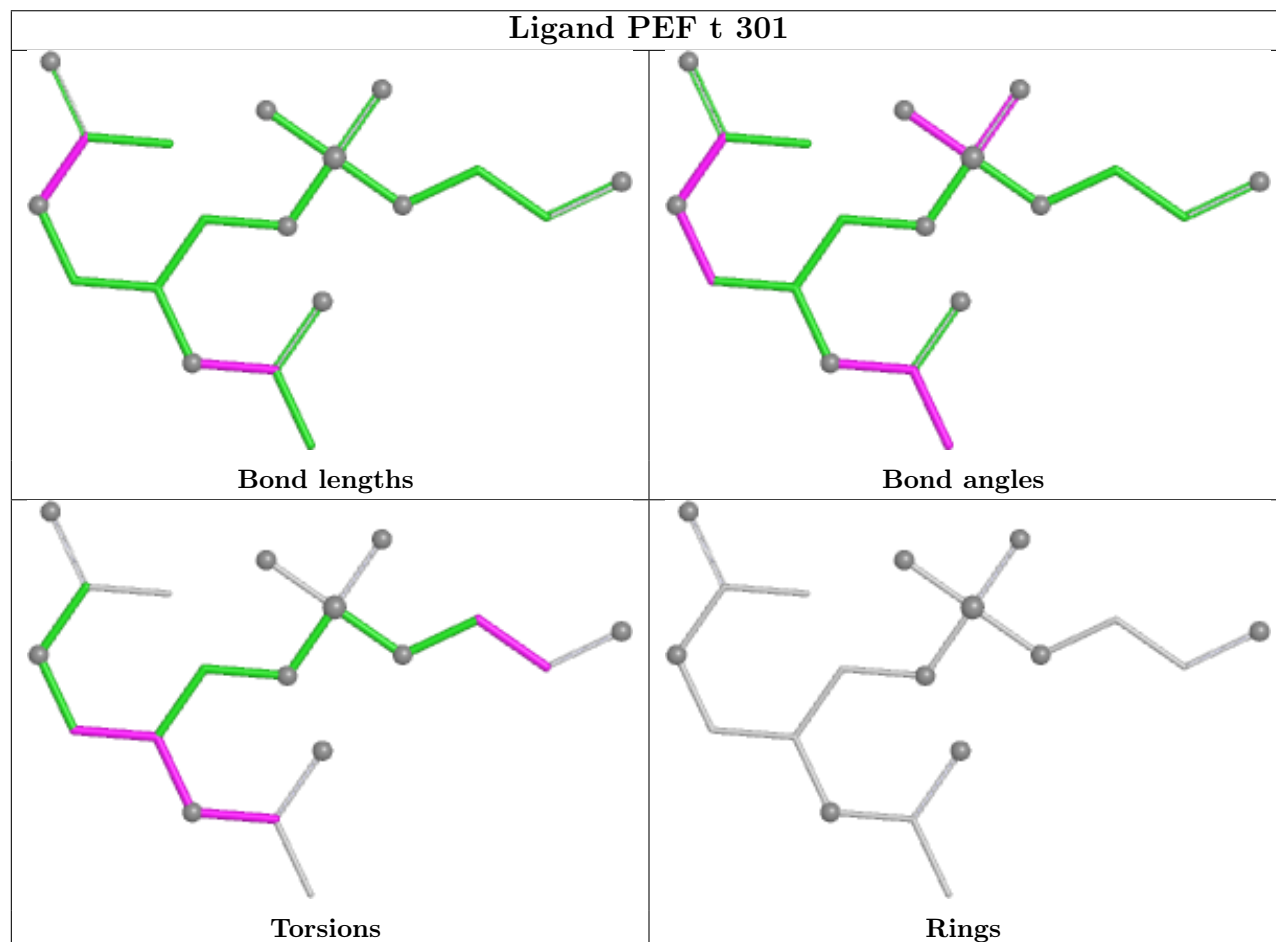


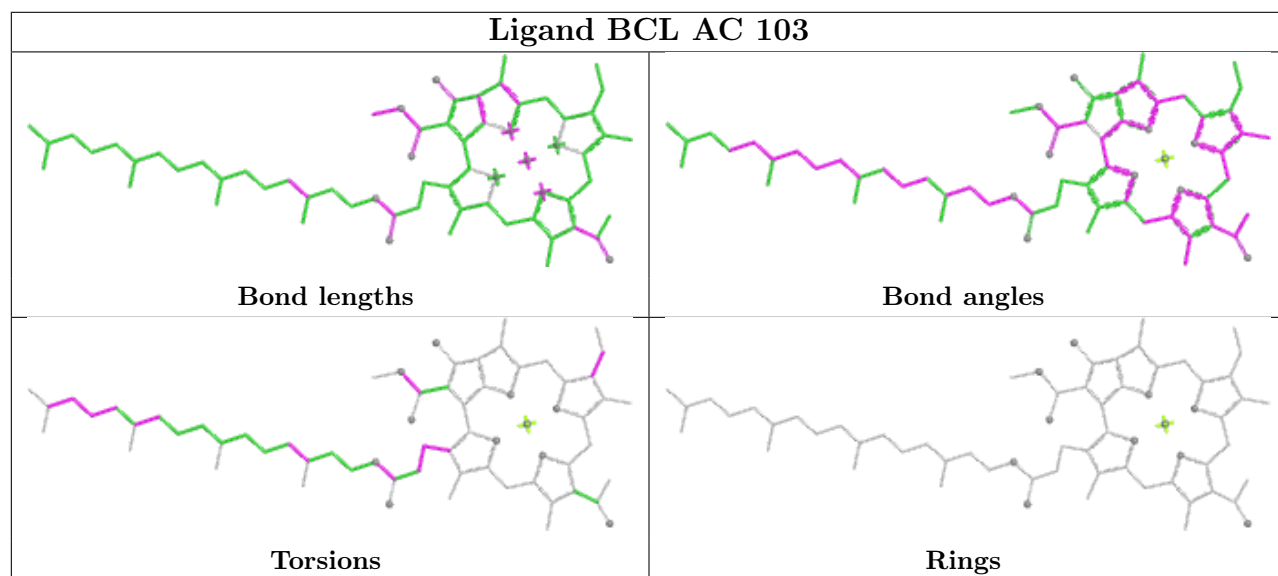
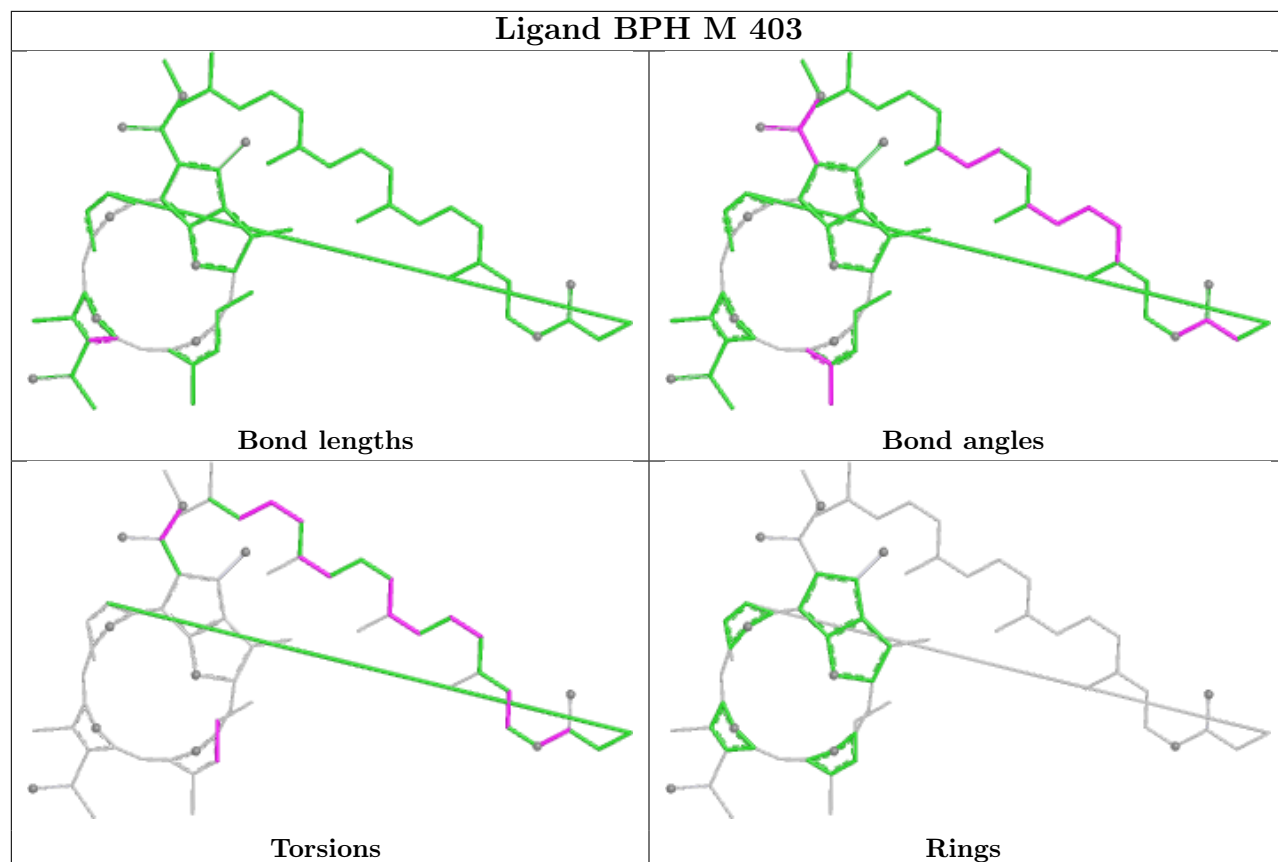


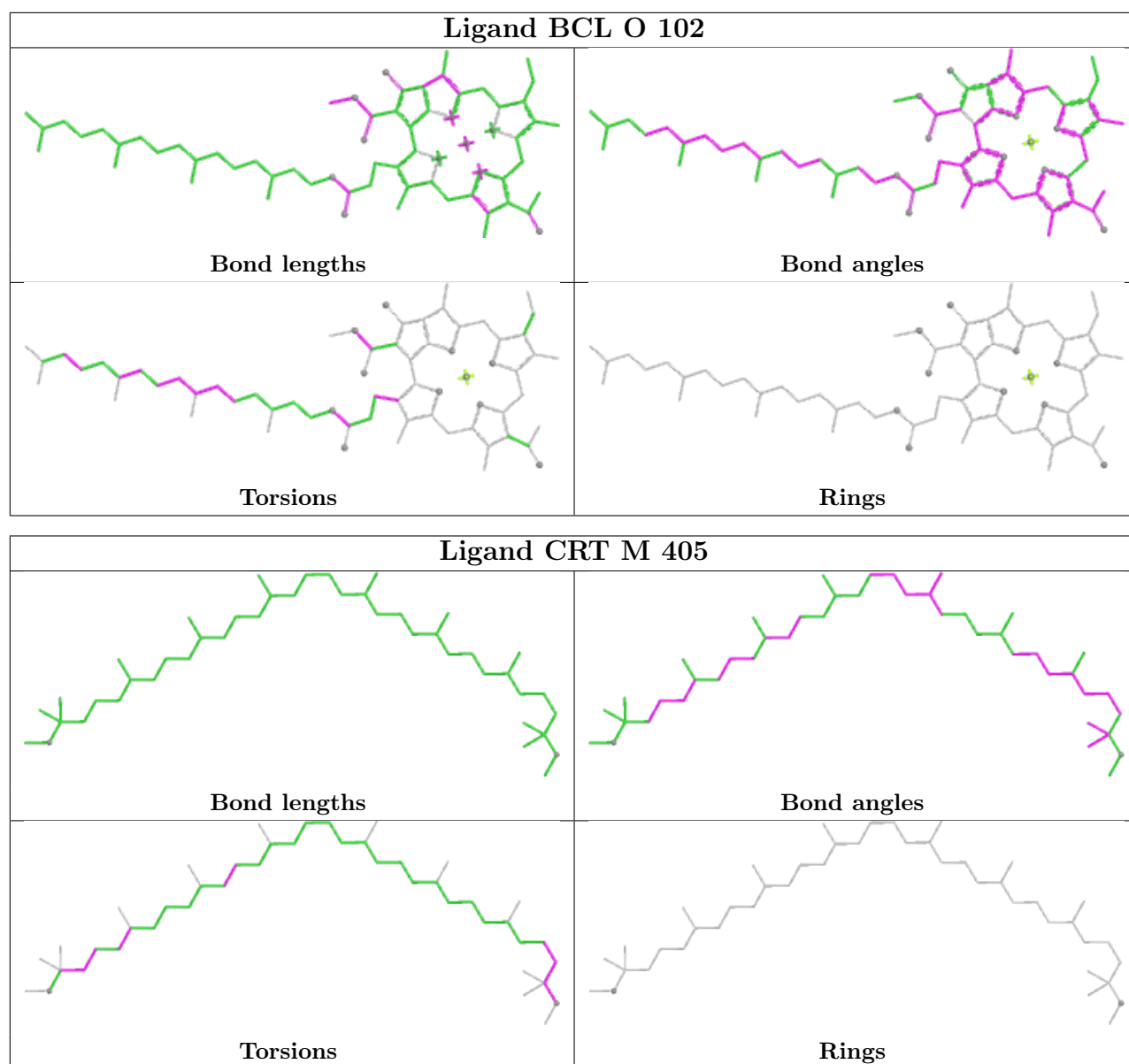
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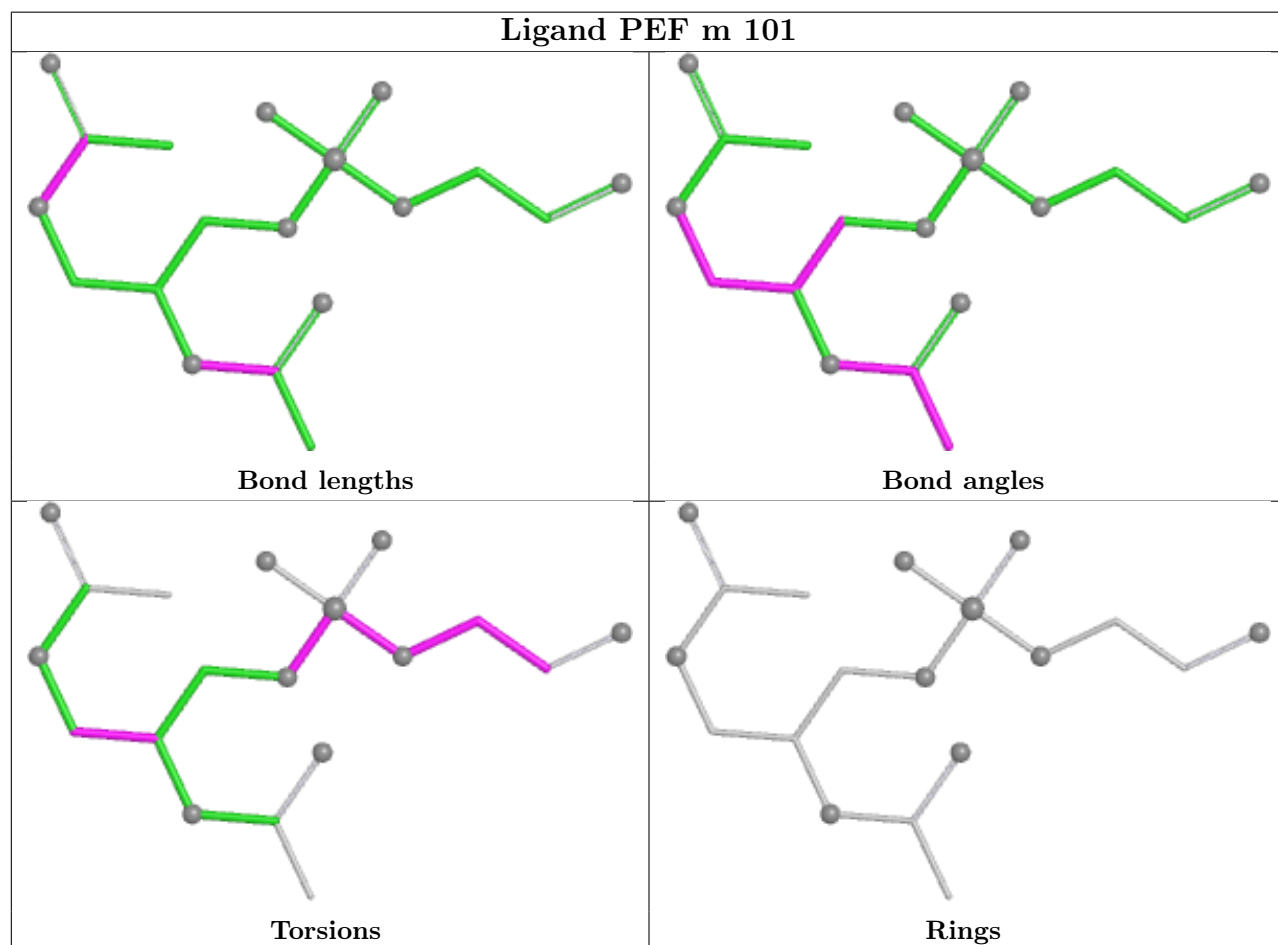
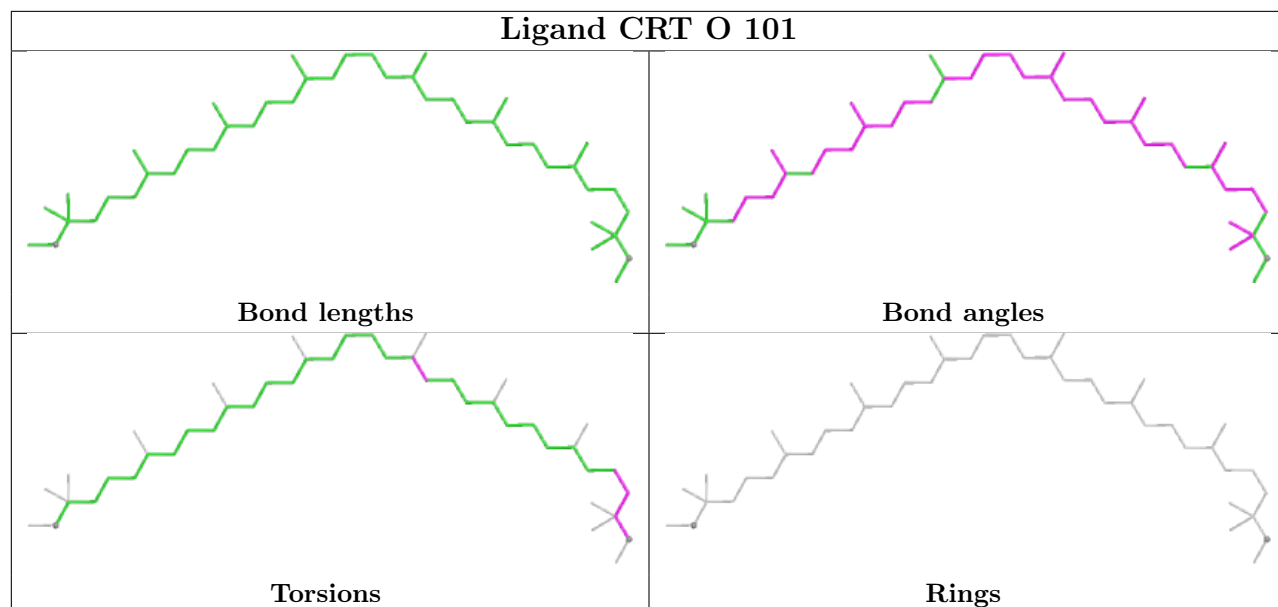


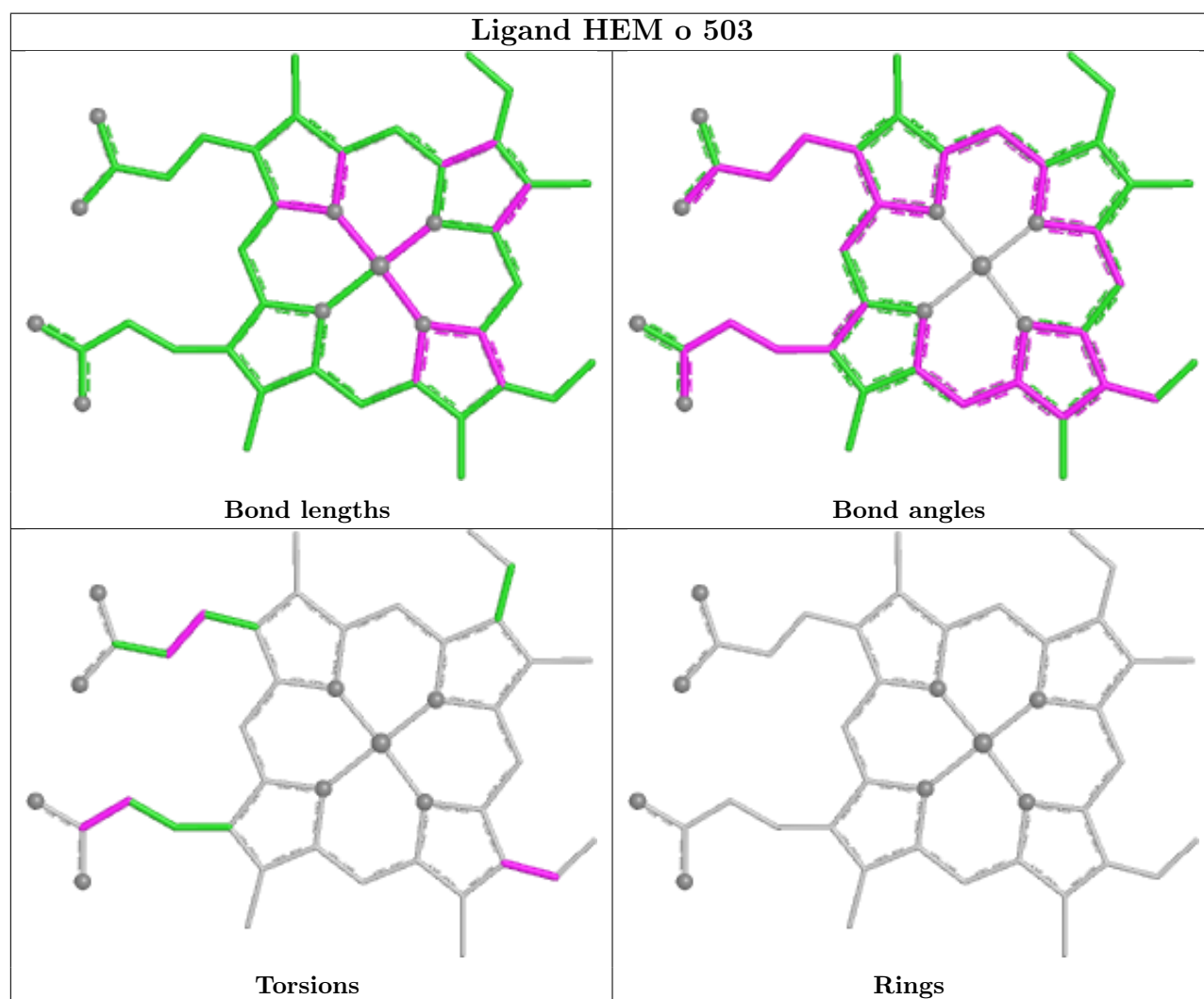
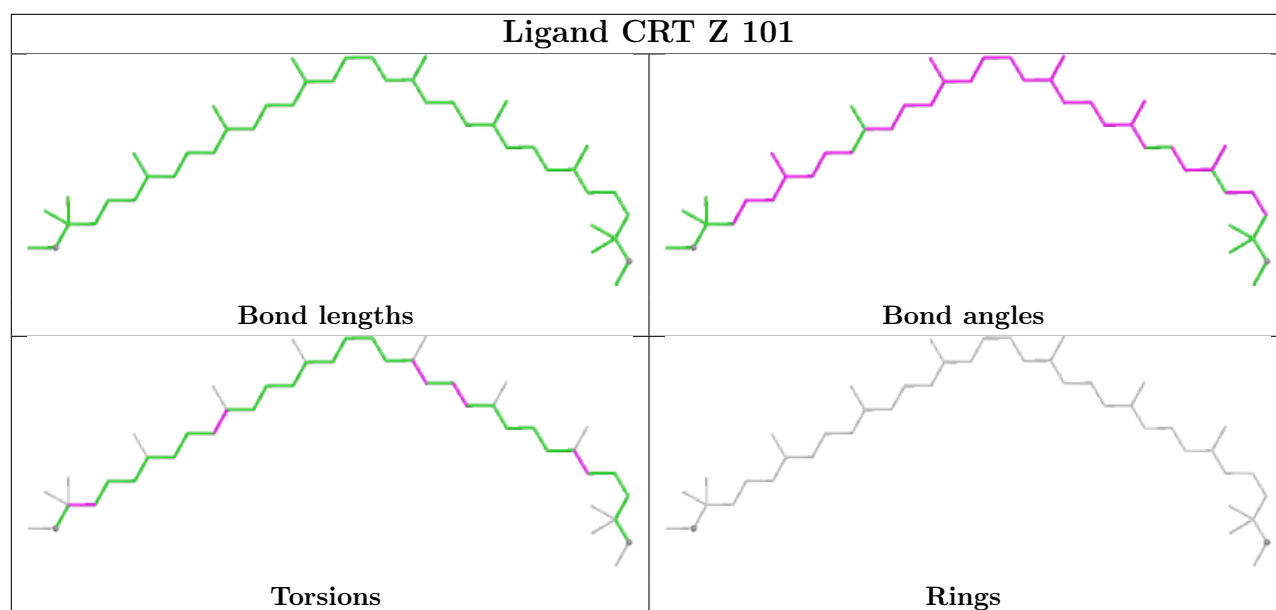
Ligand PEF t 301

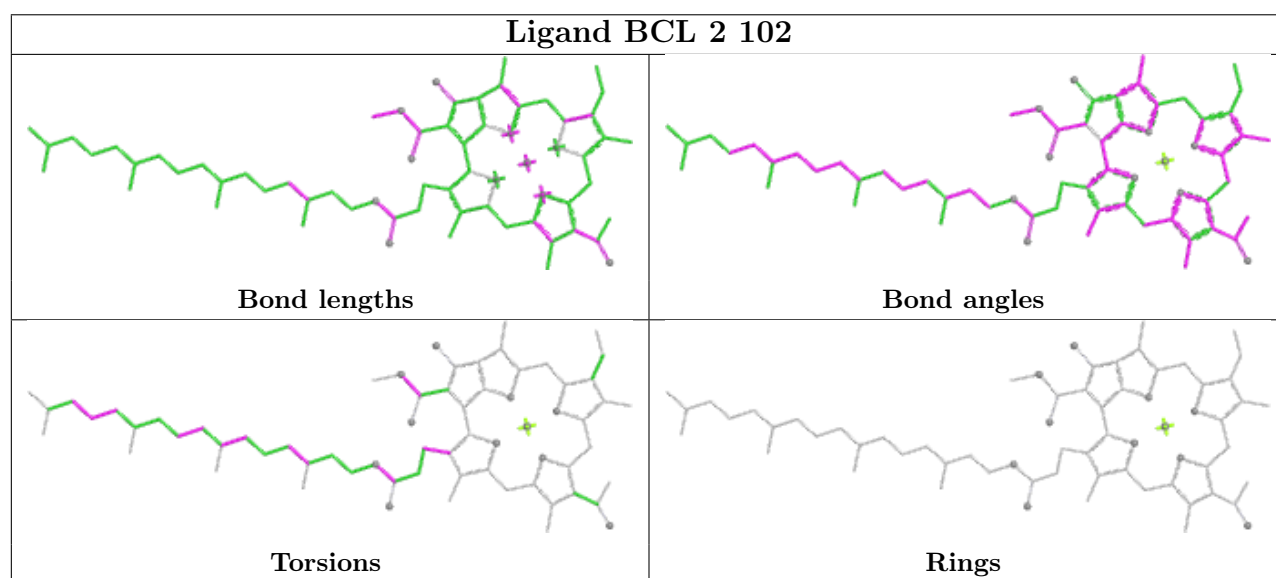
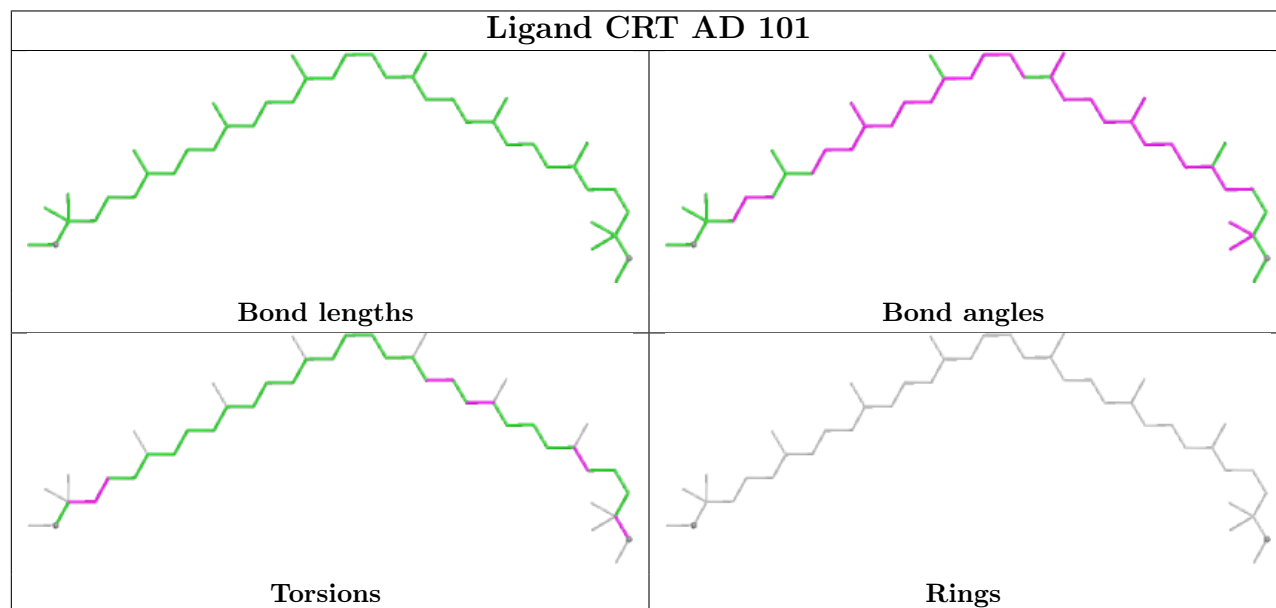
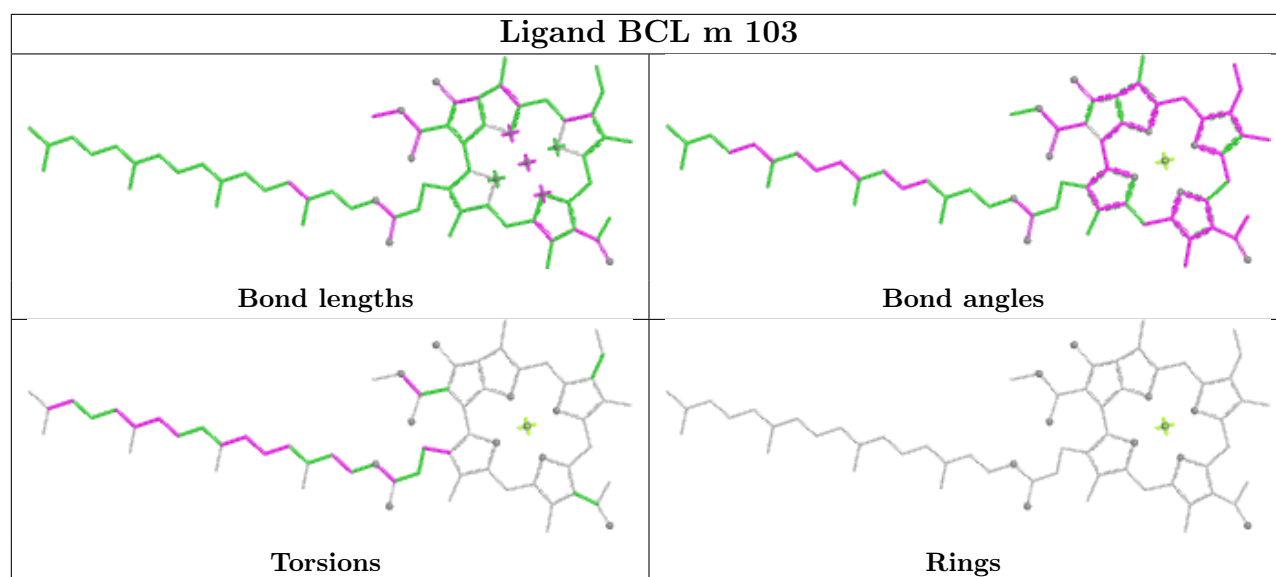


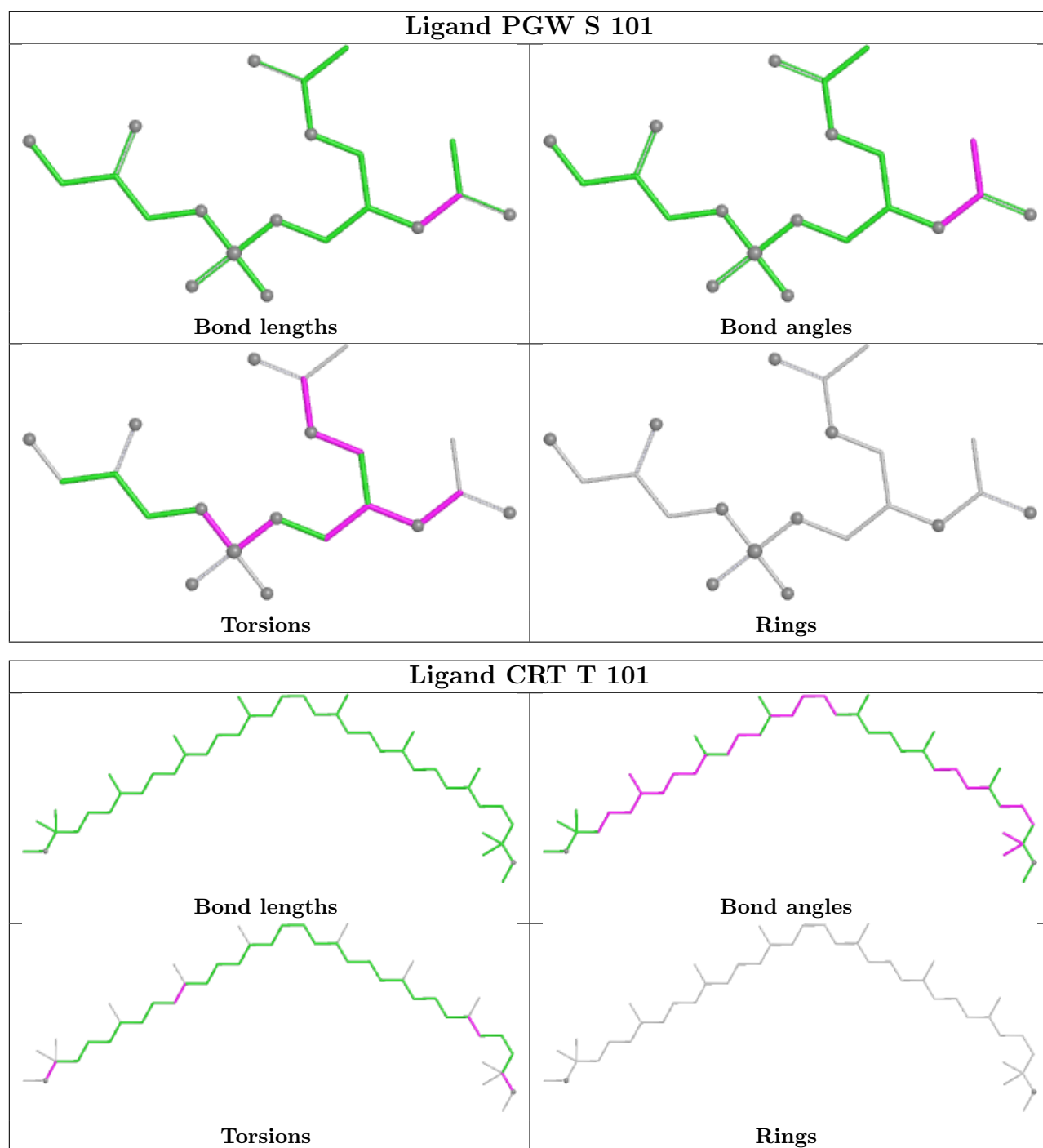




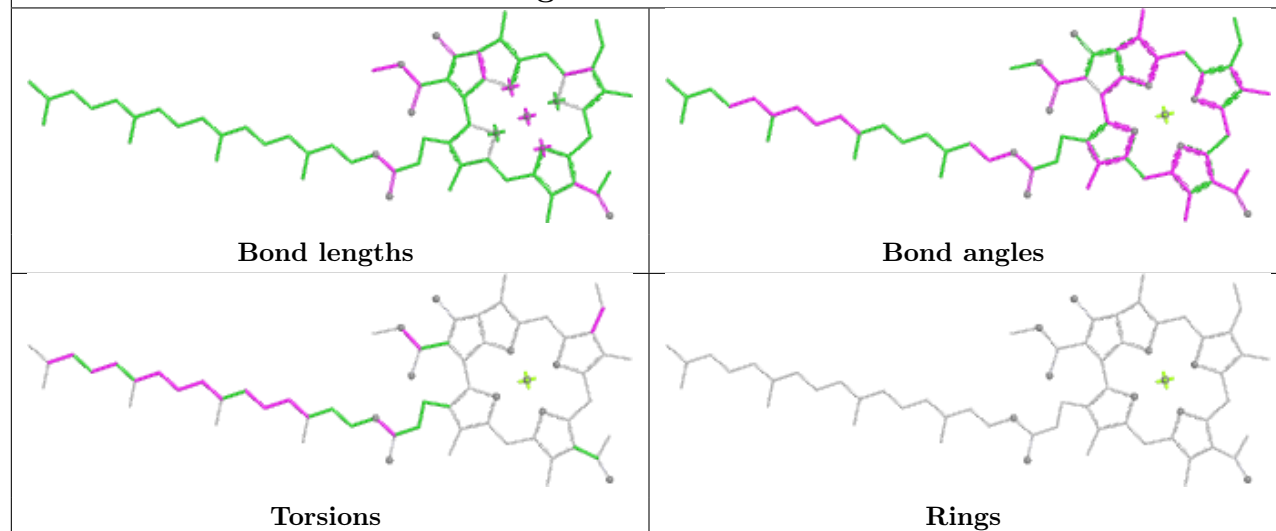




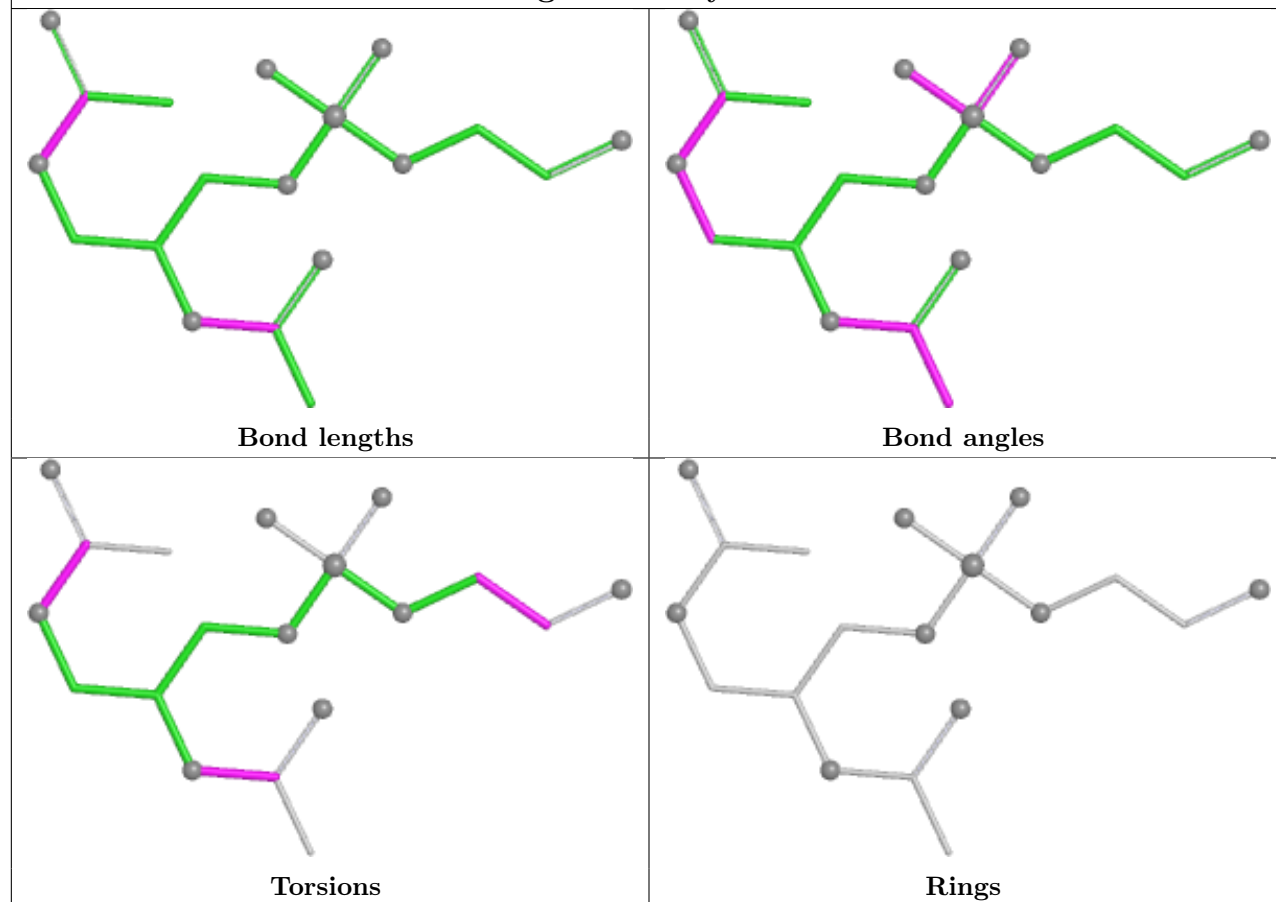


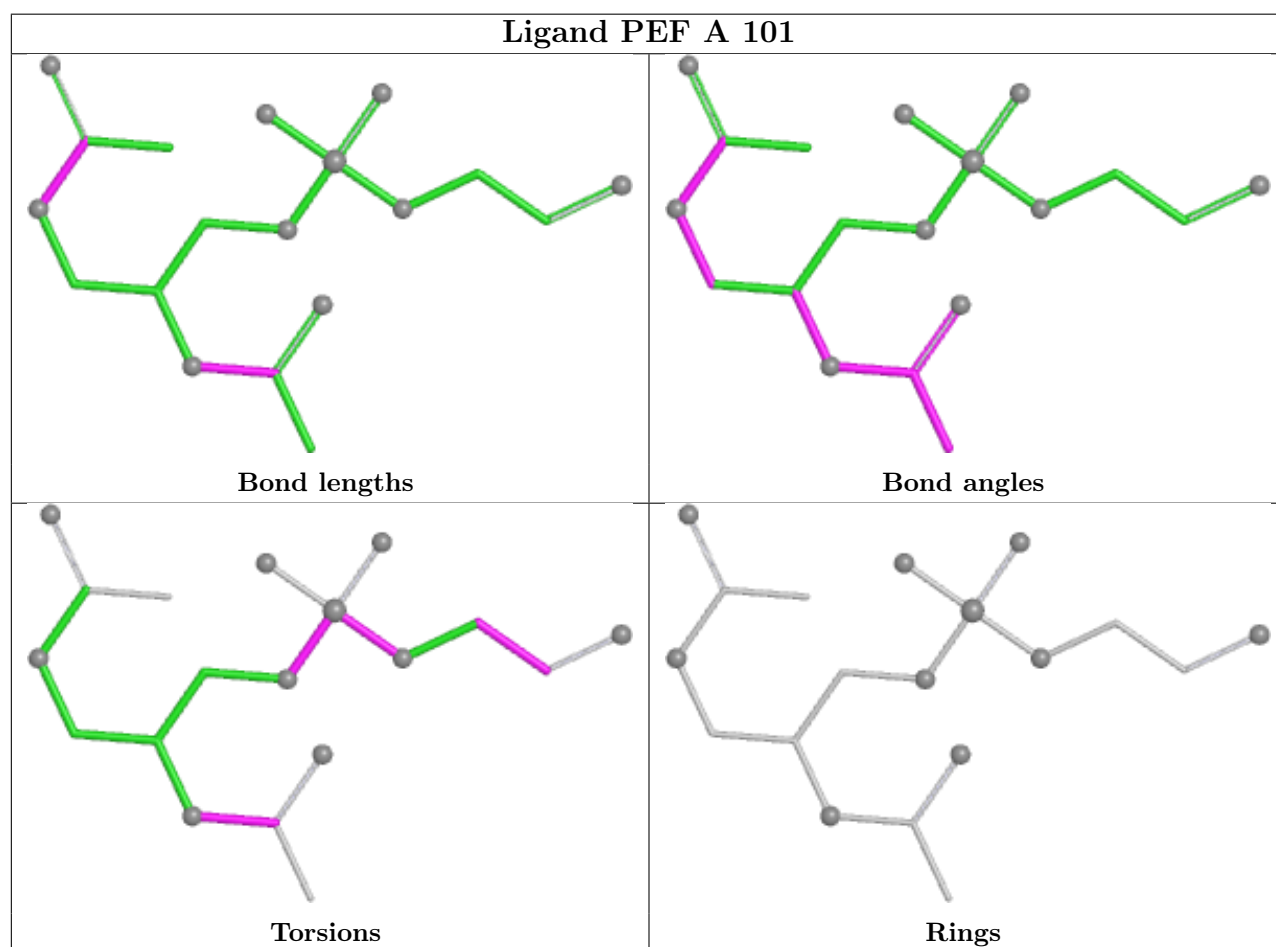
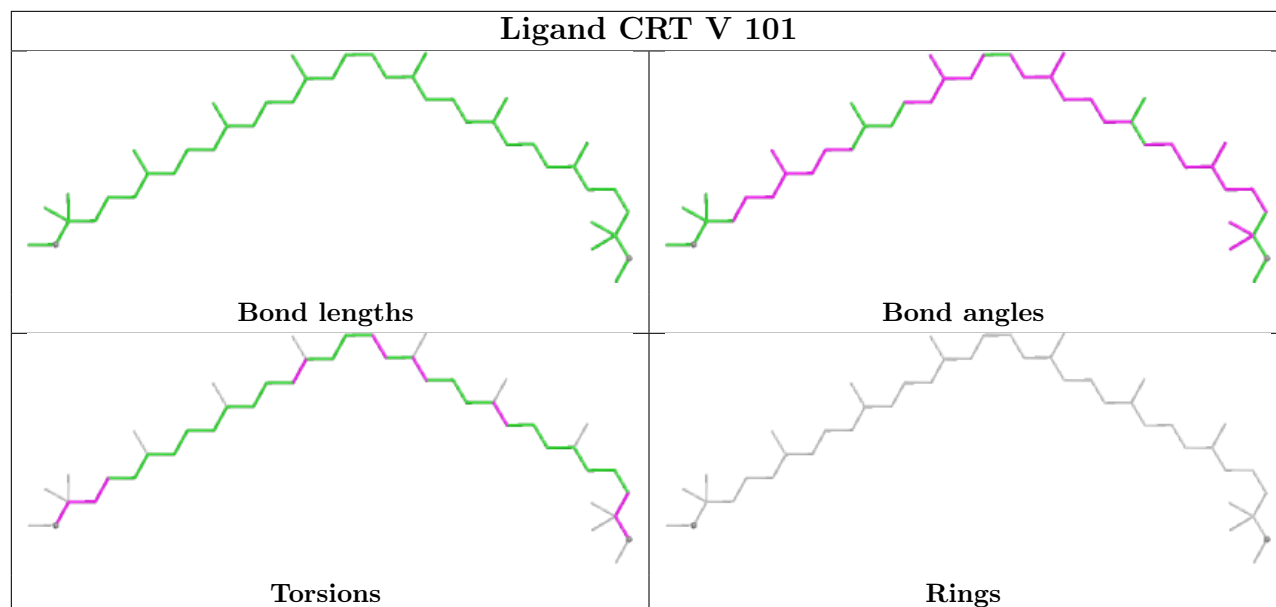


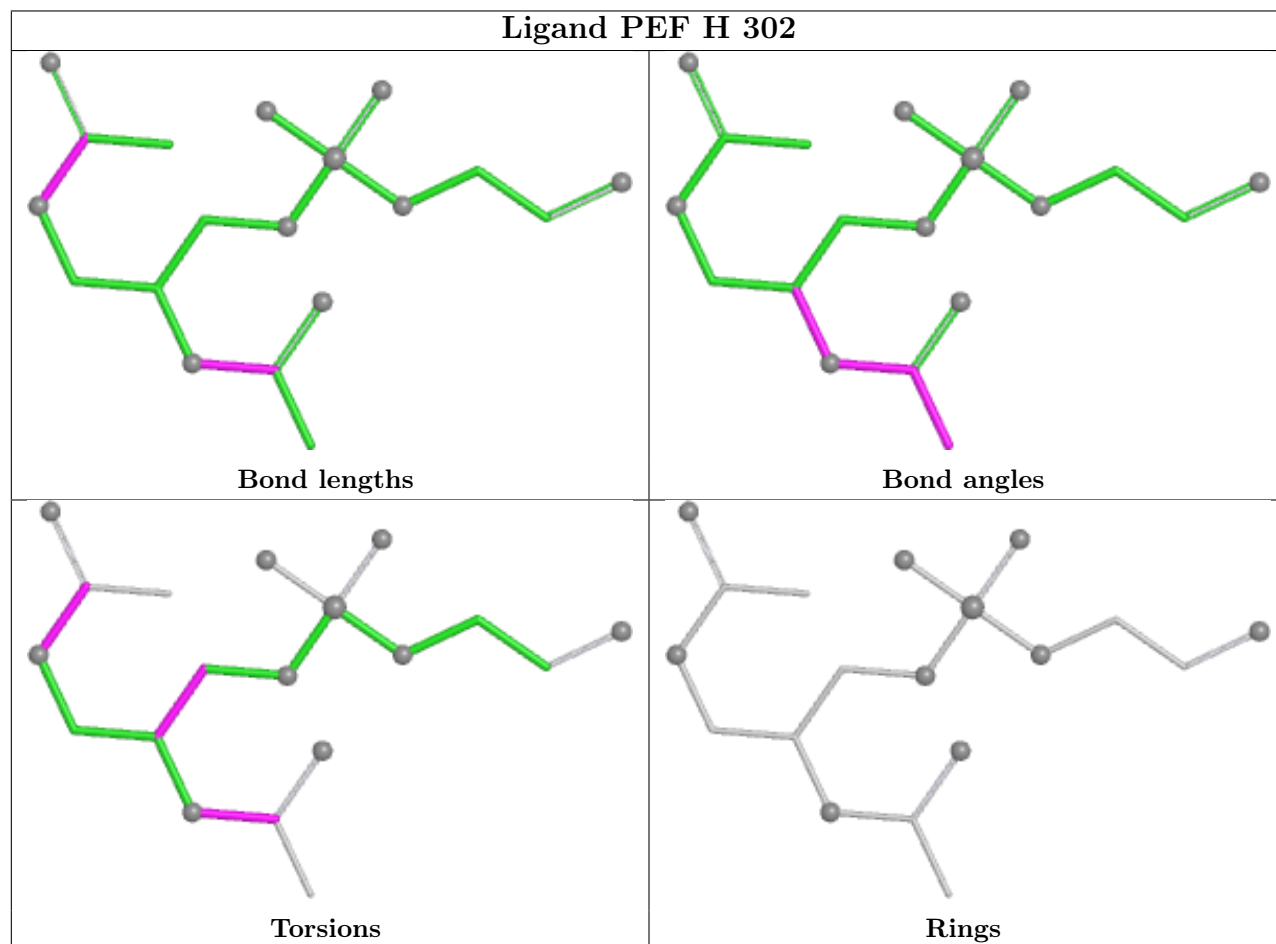
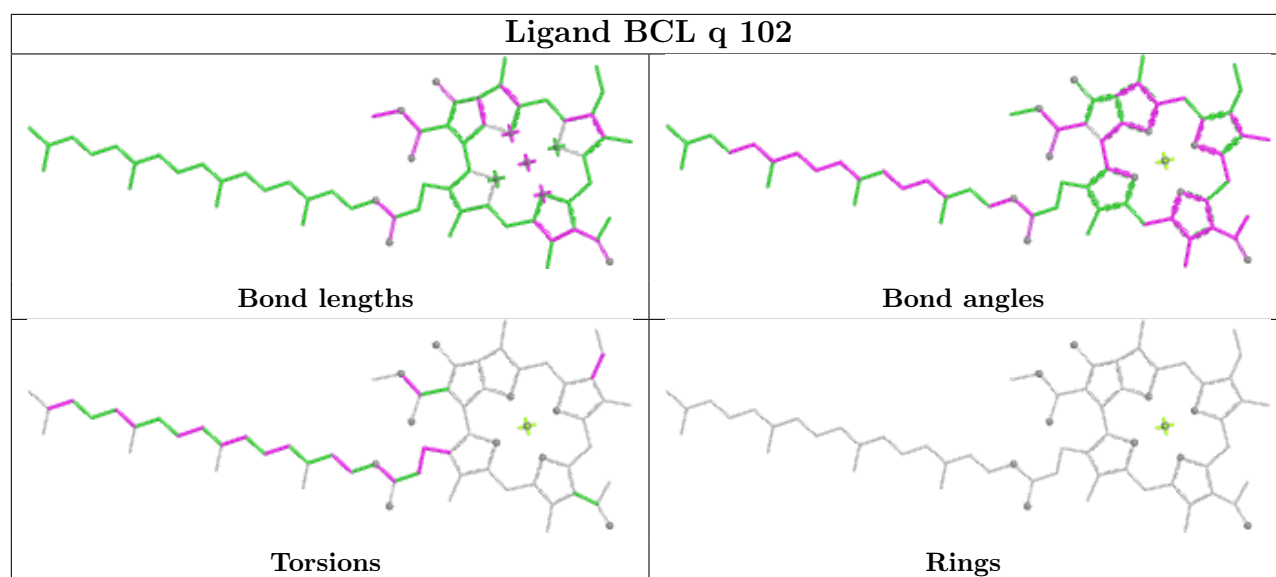
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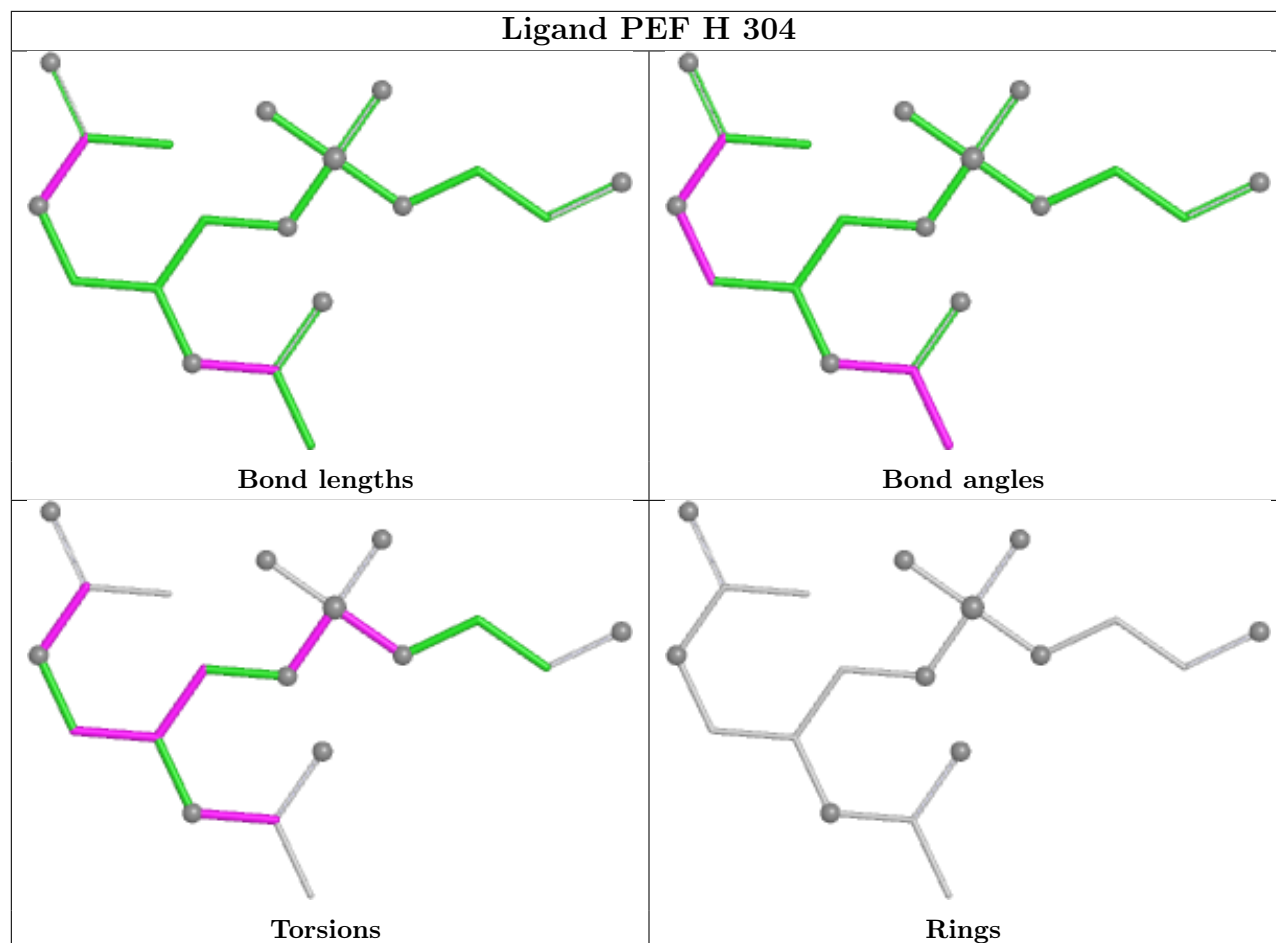
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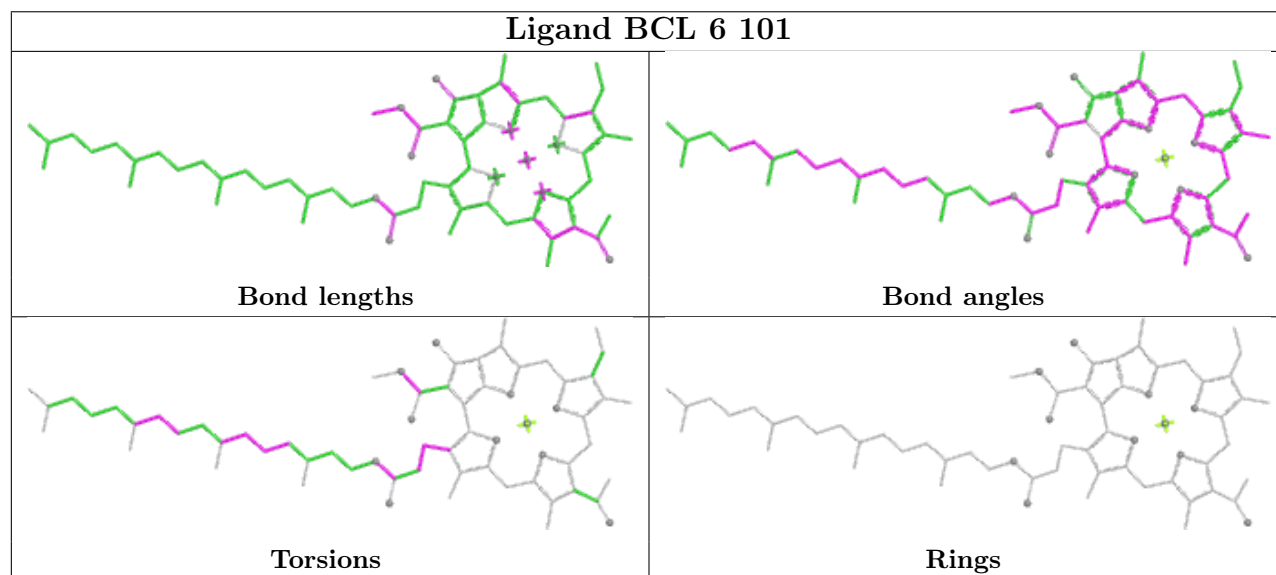


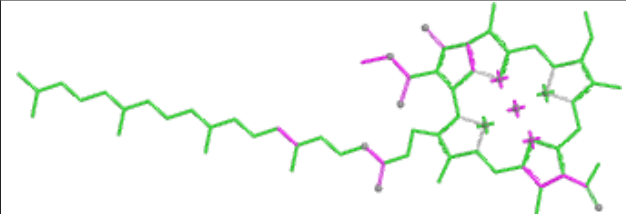
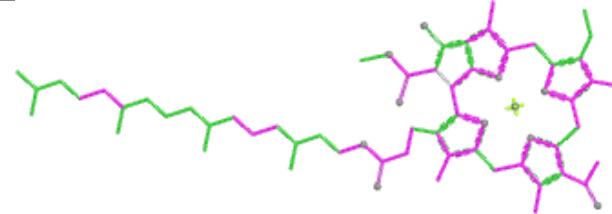
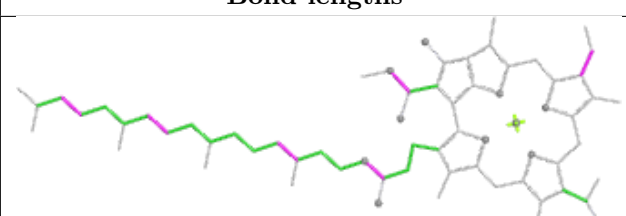
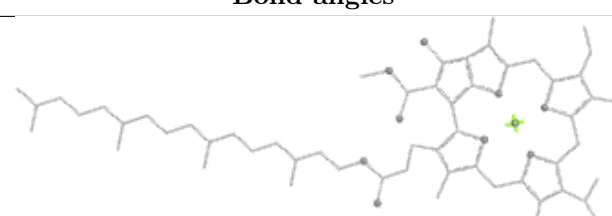


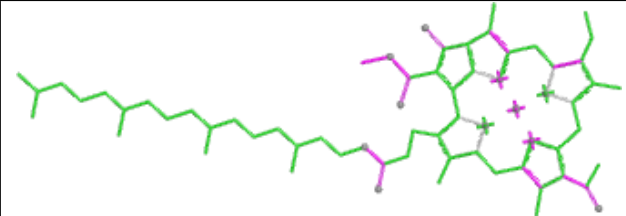
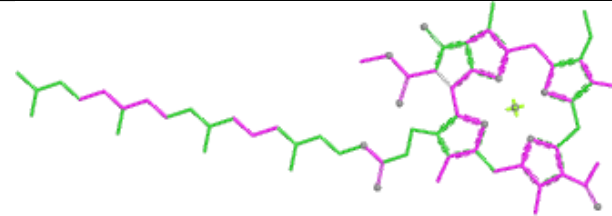
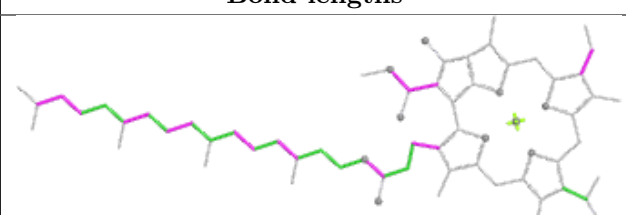
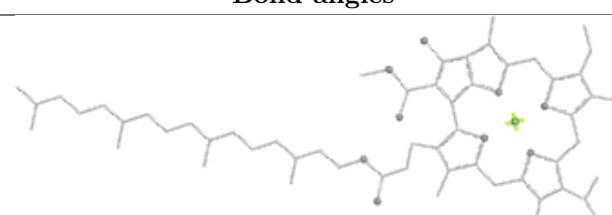
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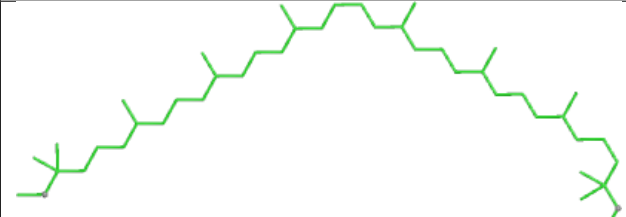
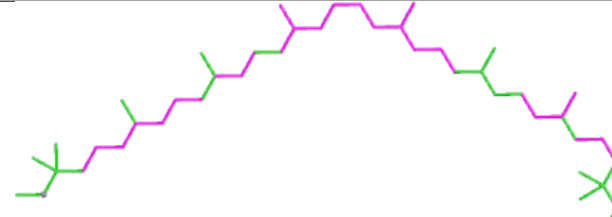
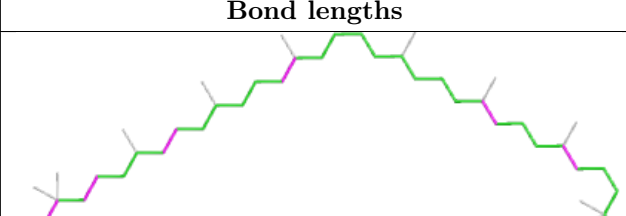
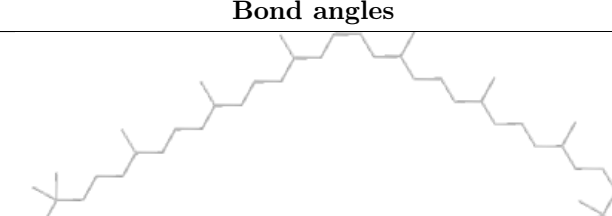


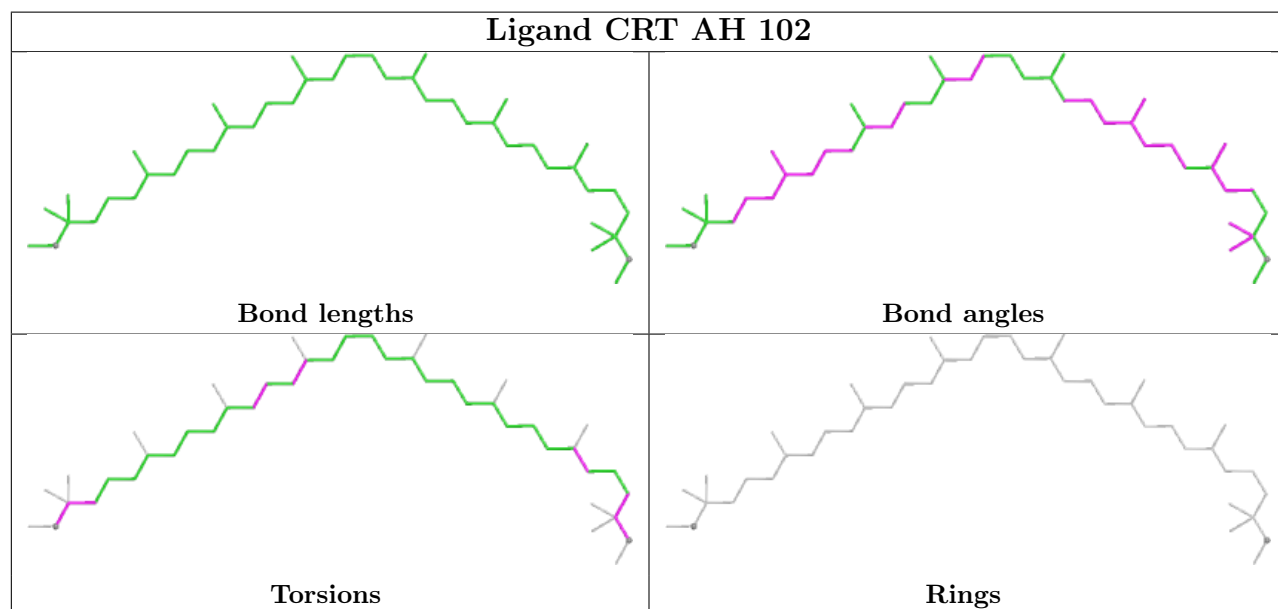
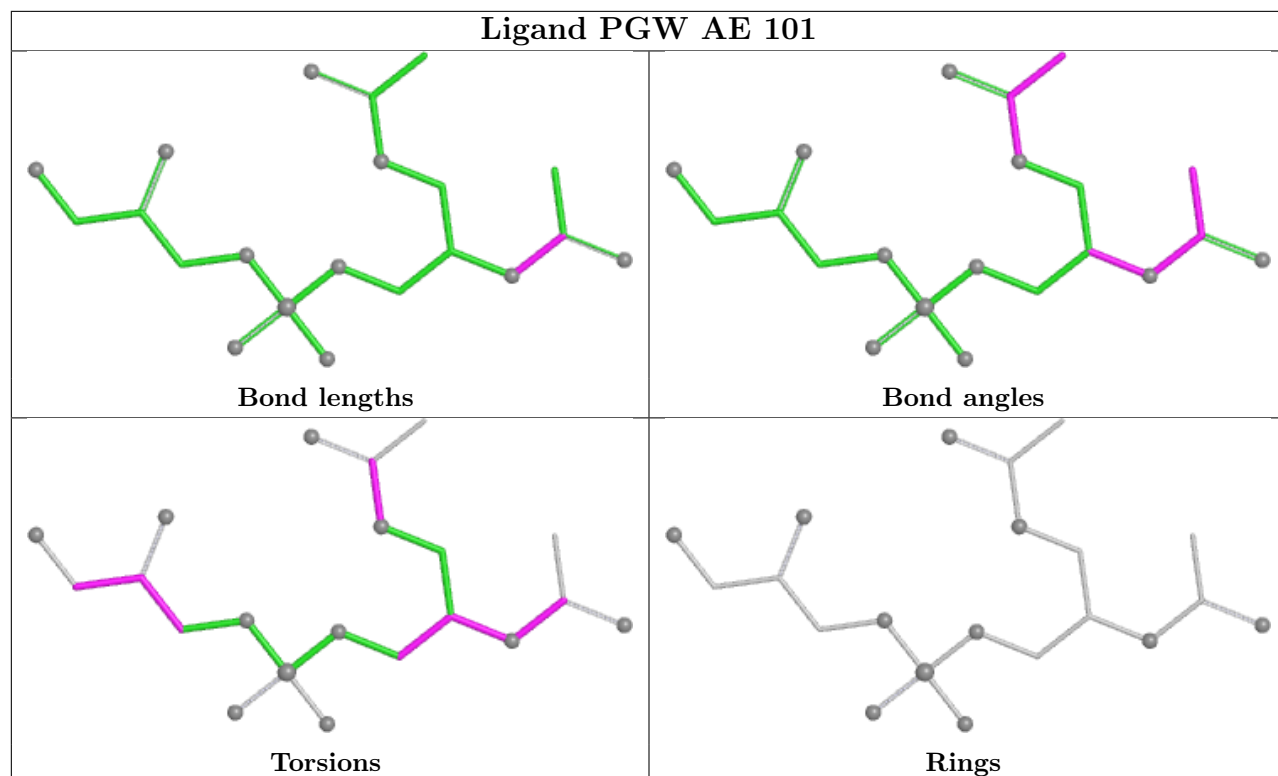
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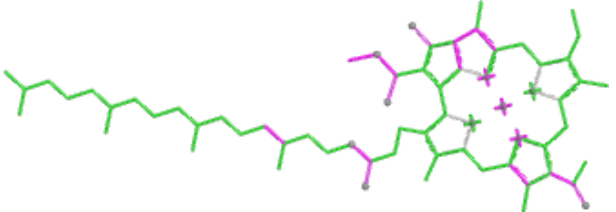
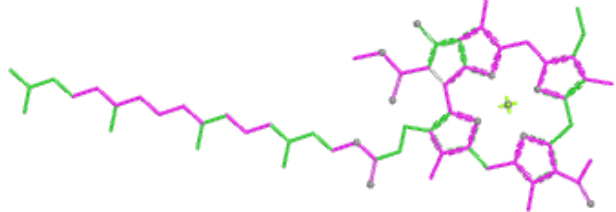
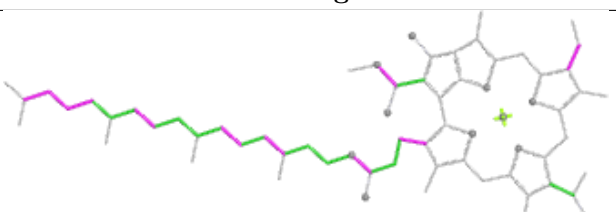
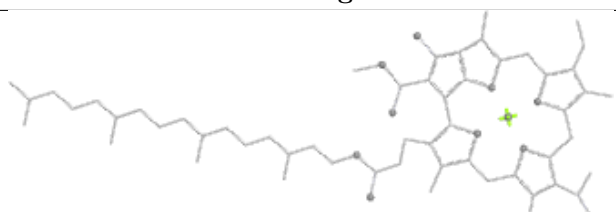
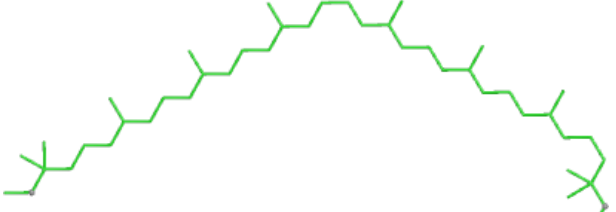
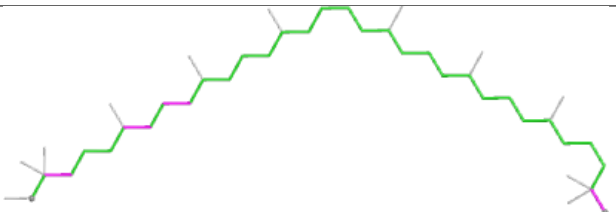
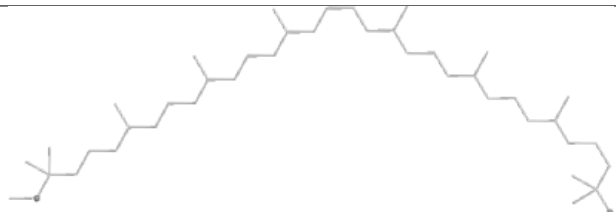
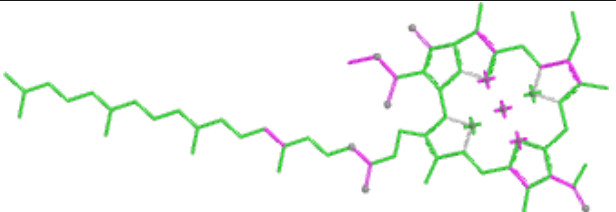
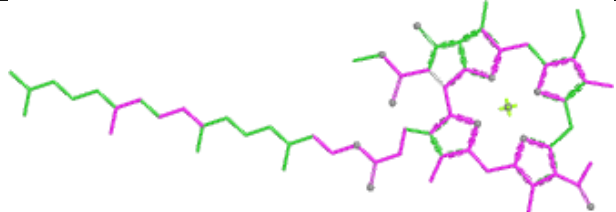
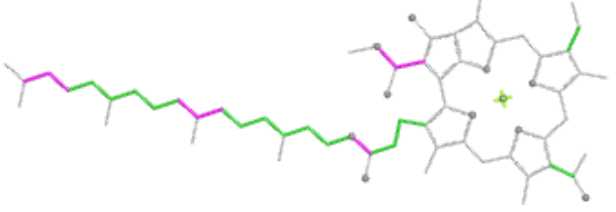
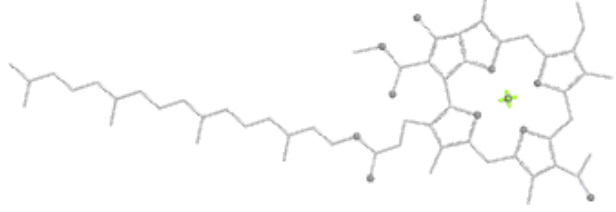


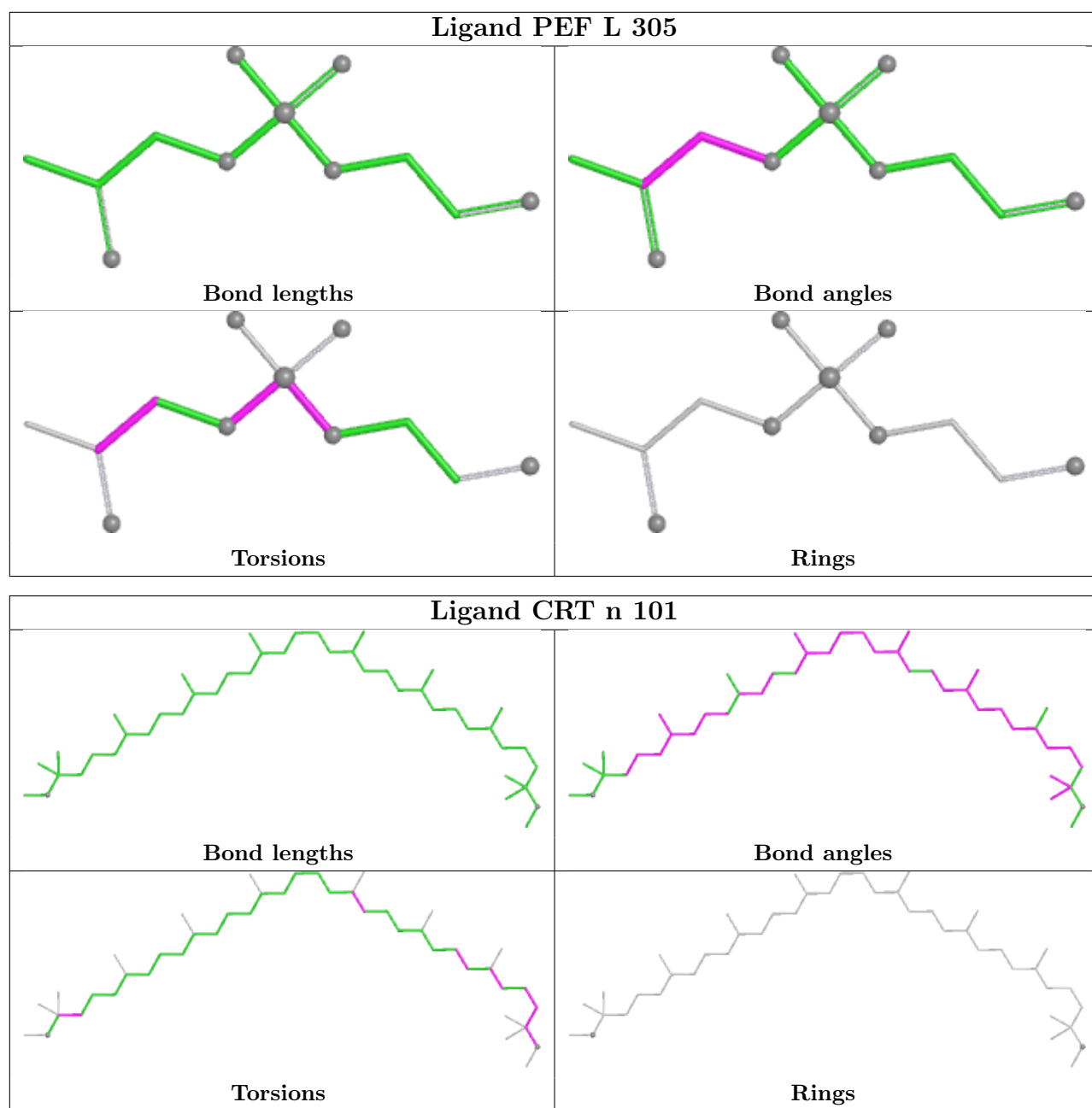
Ligand BCL h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

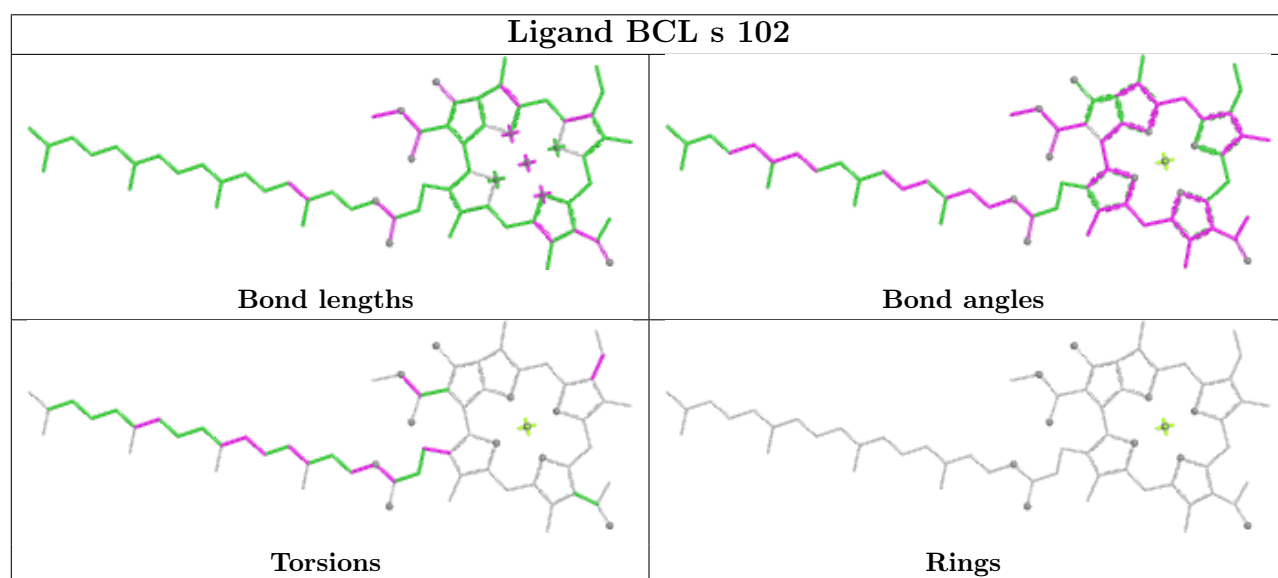
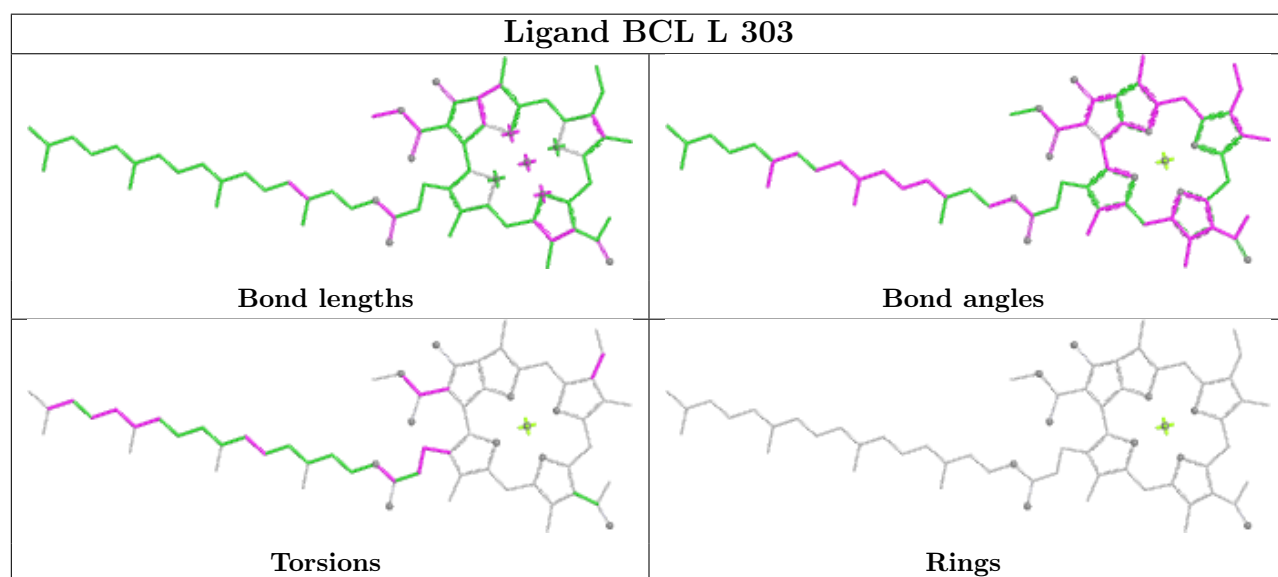
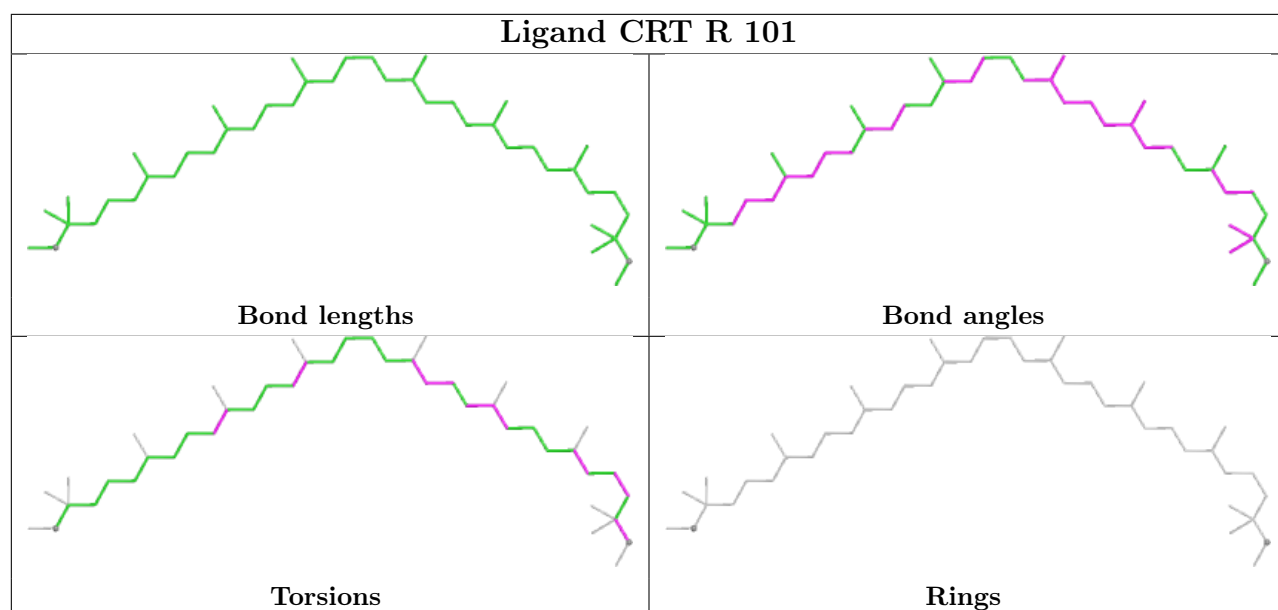
Ligand BCL G 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

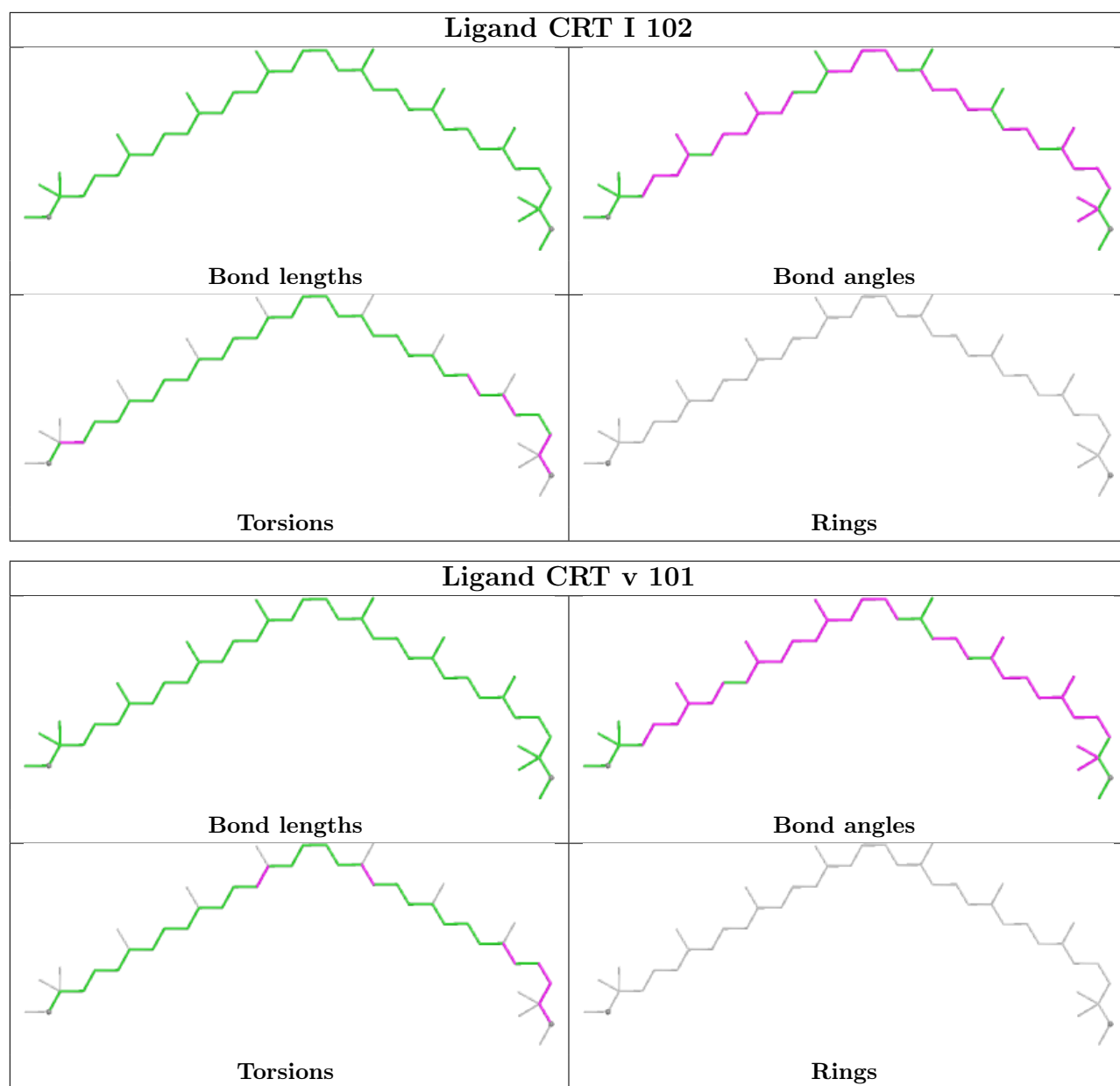
Ligand CRT AL 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

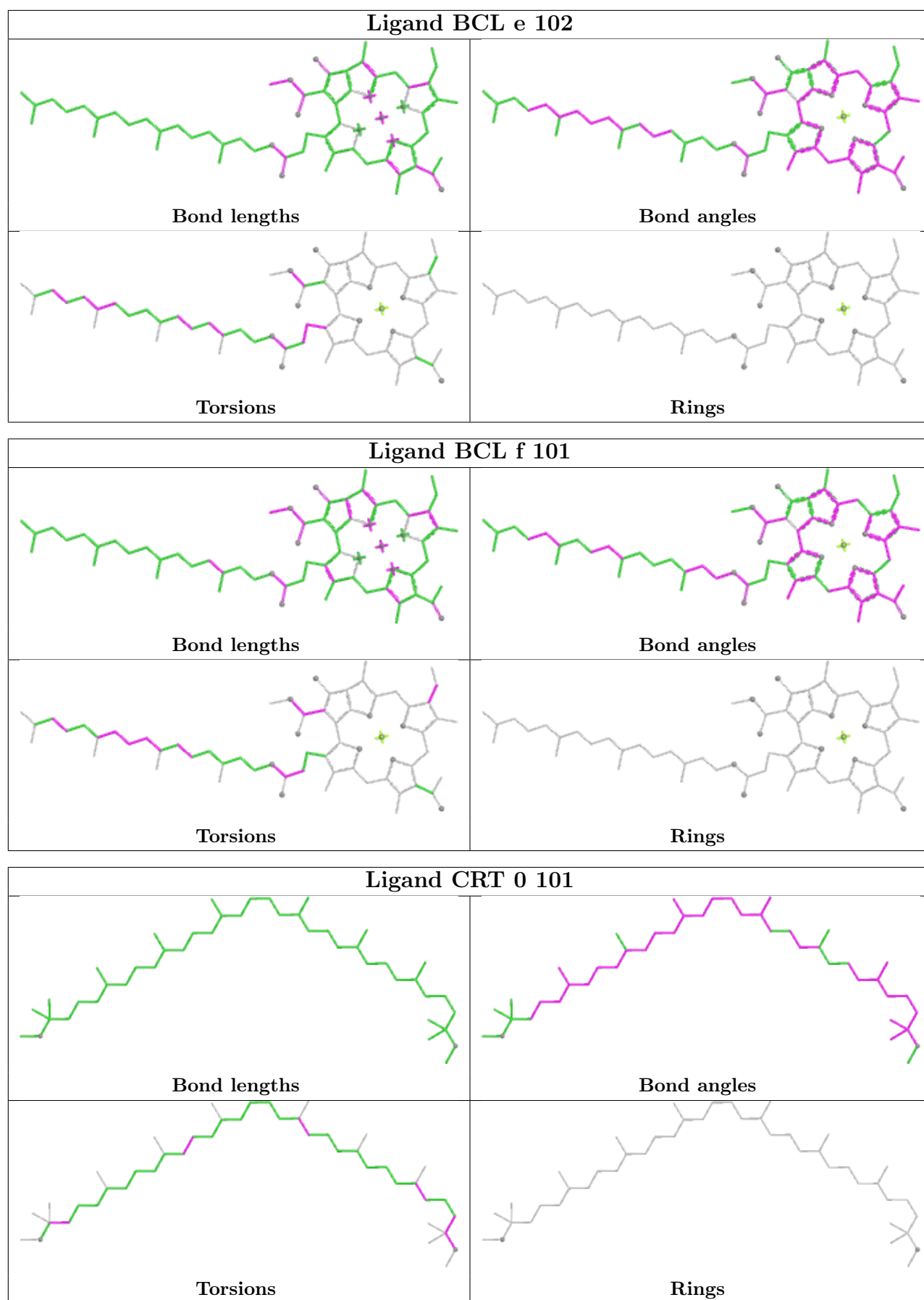


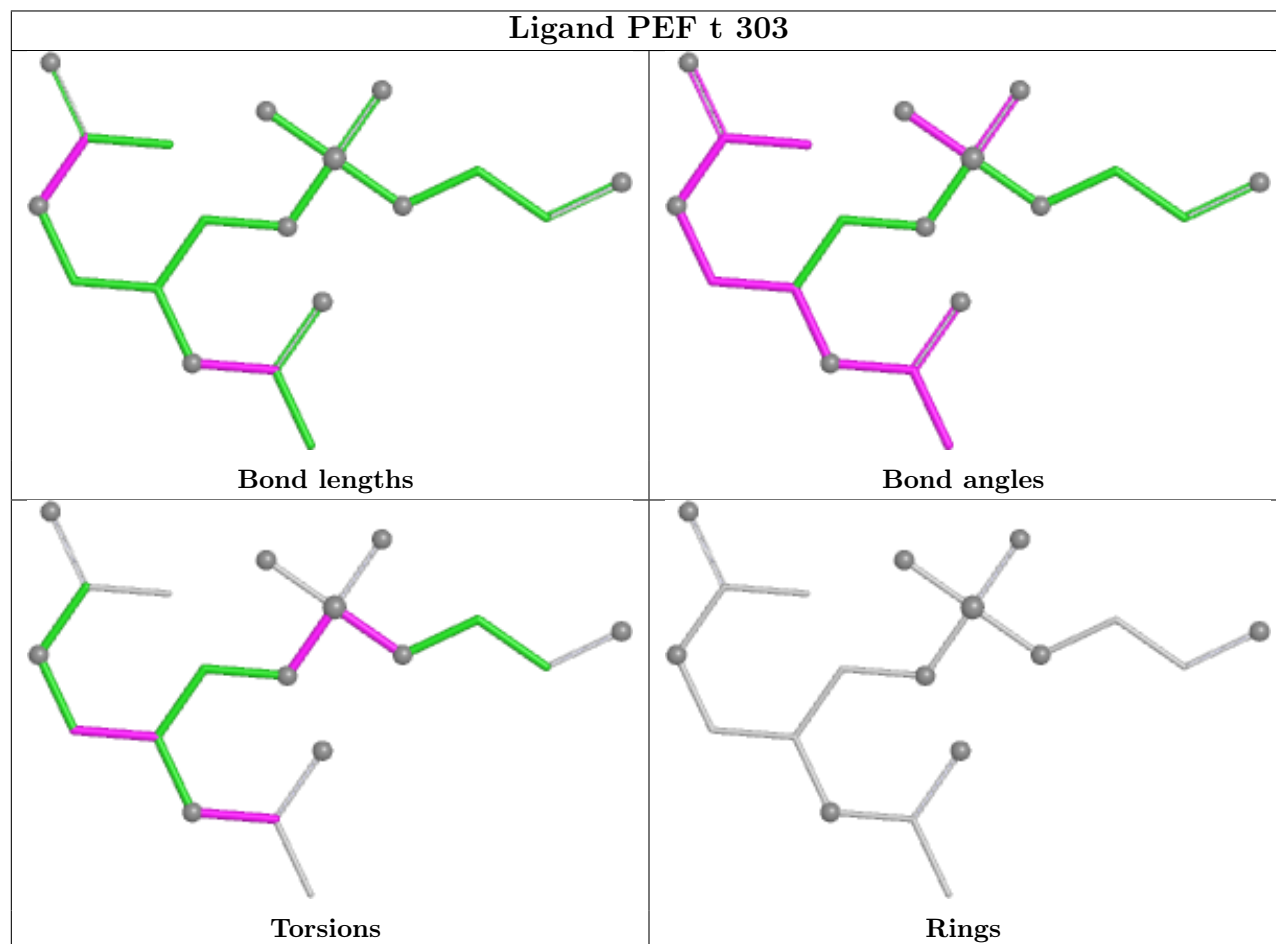
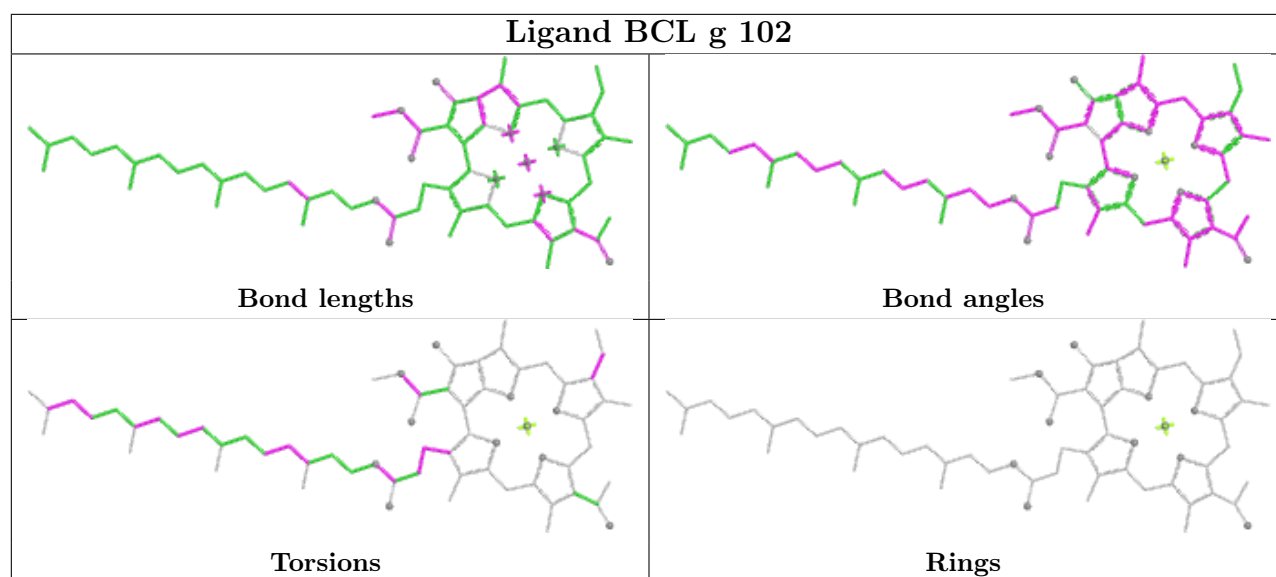
Ligand BCL R 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CRT g 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL d 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

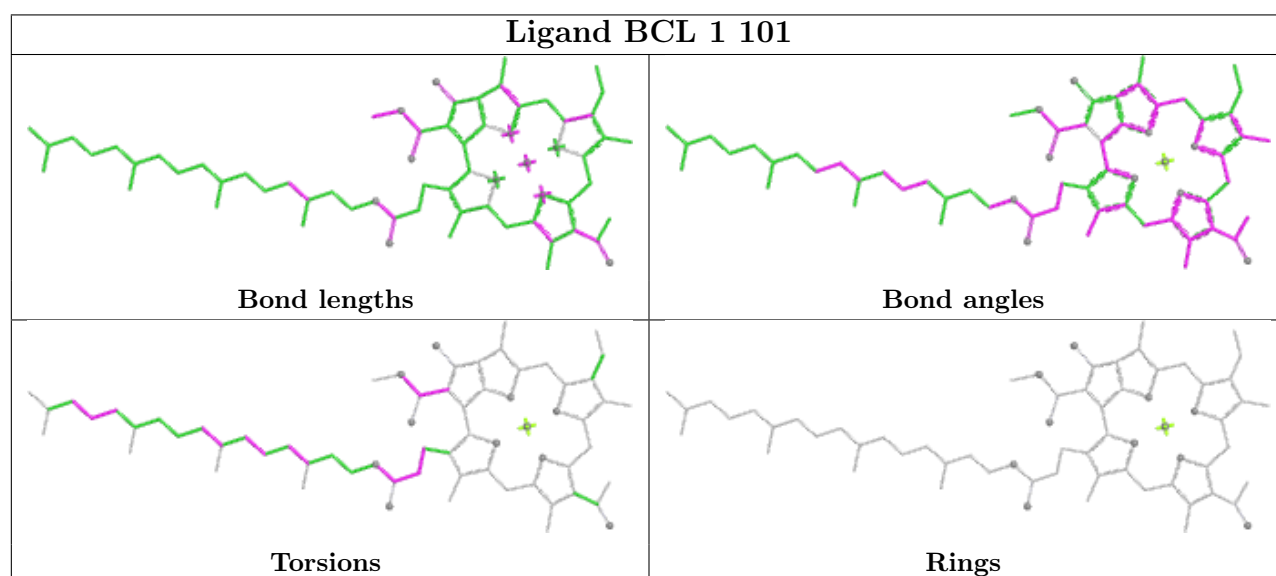
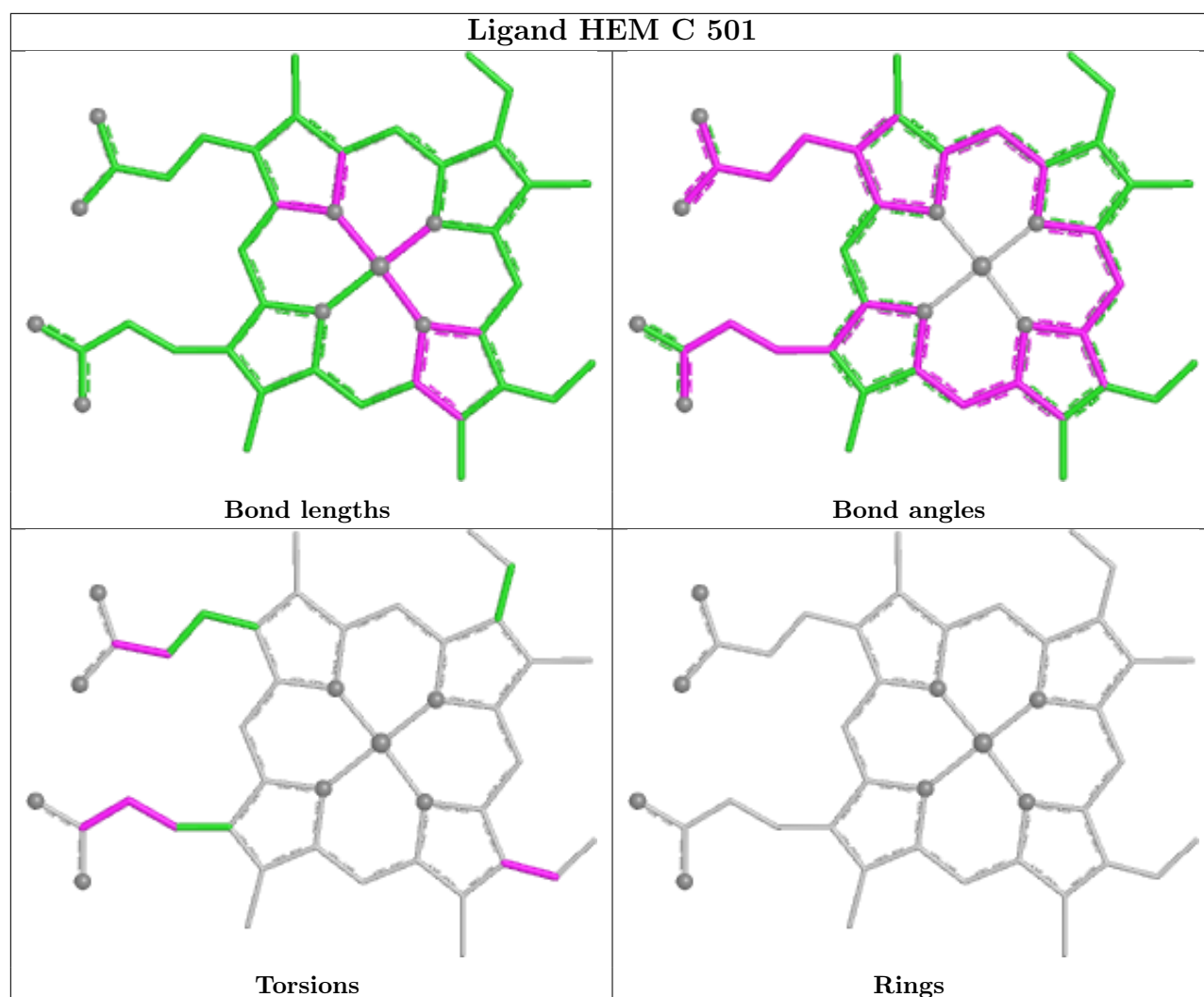


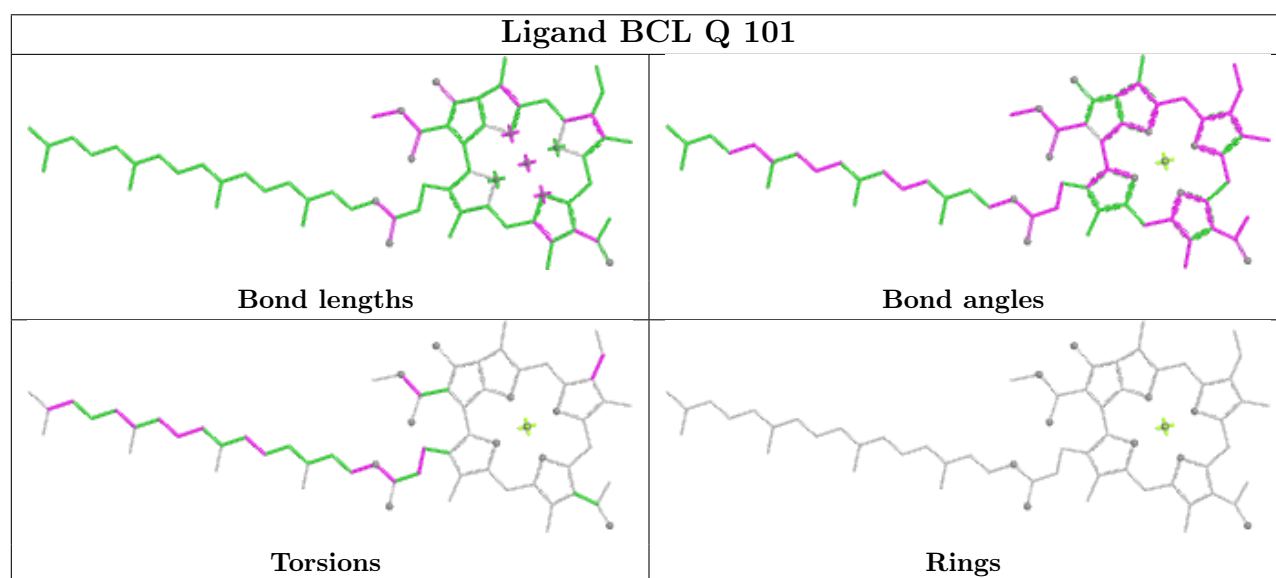
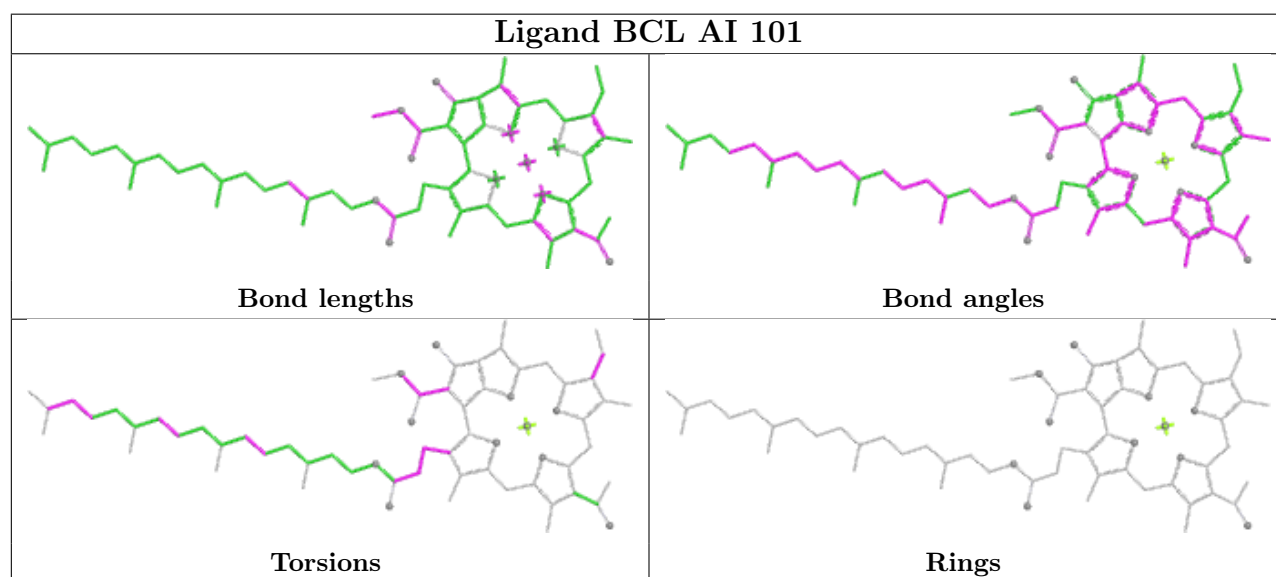
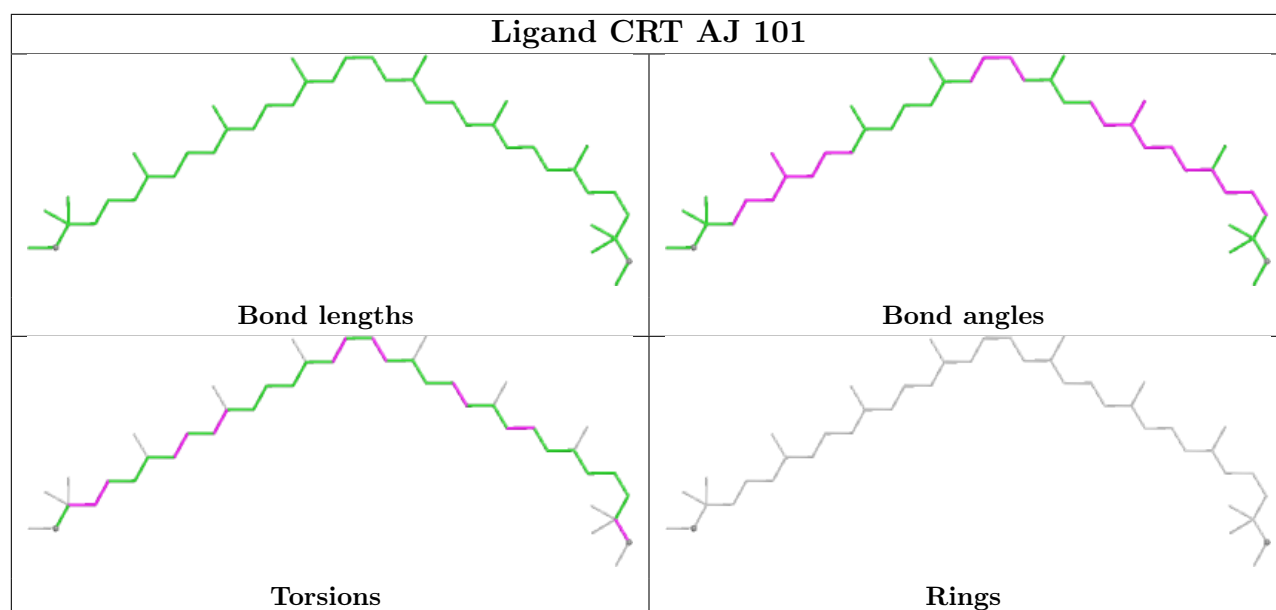


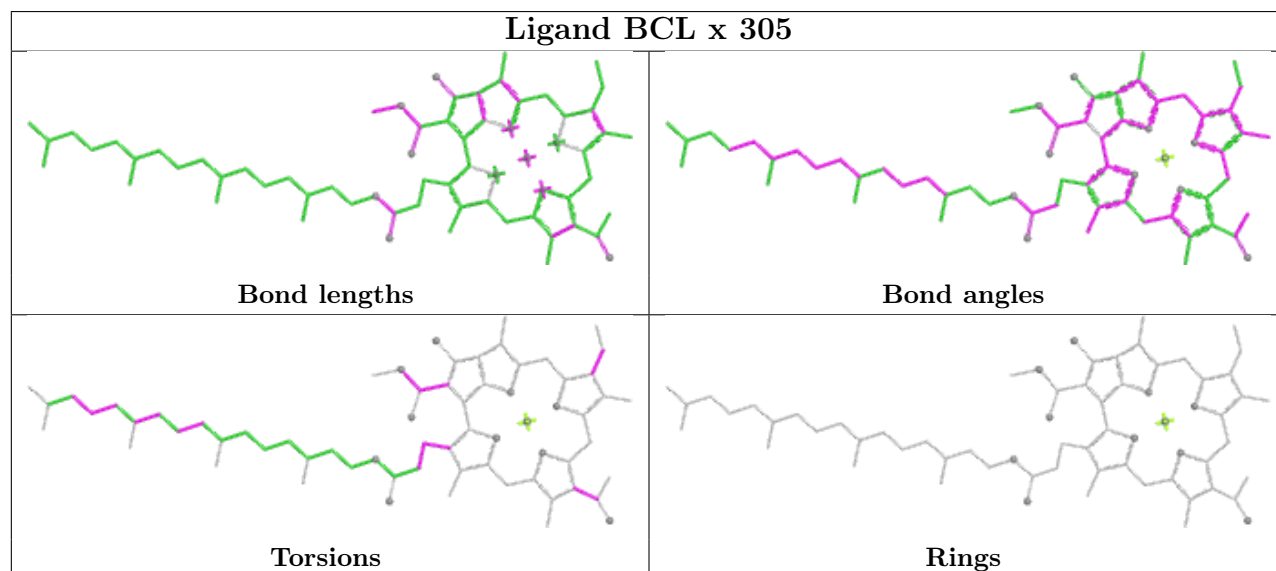
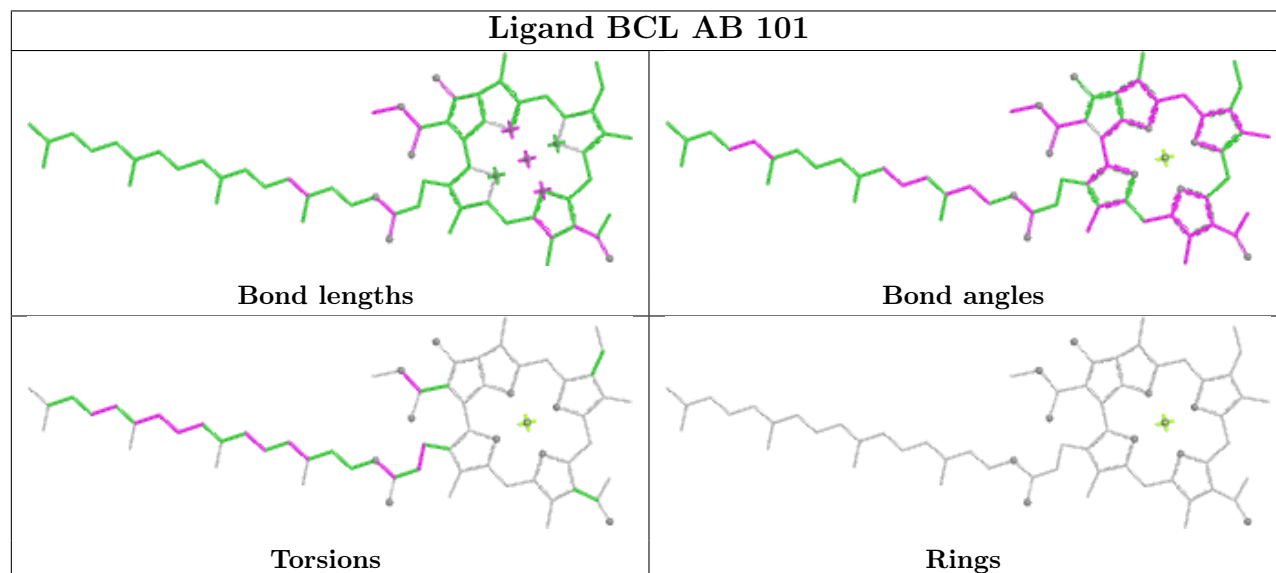
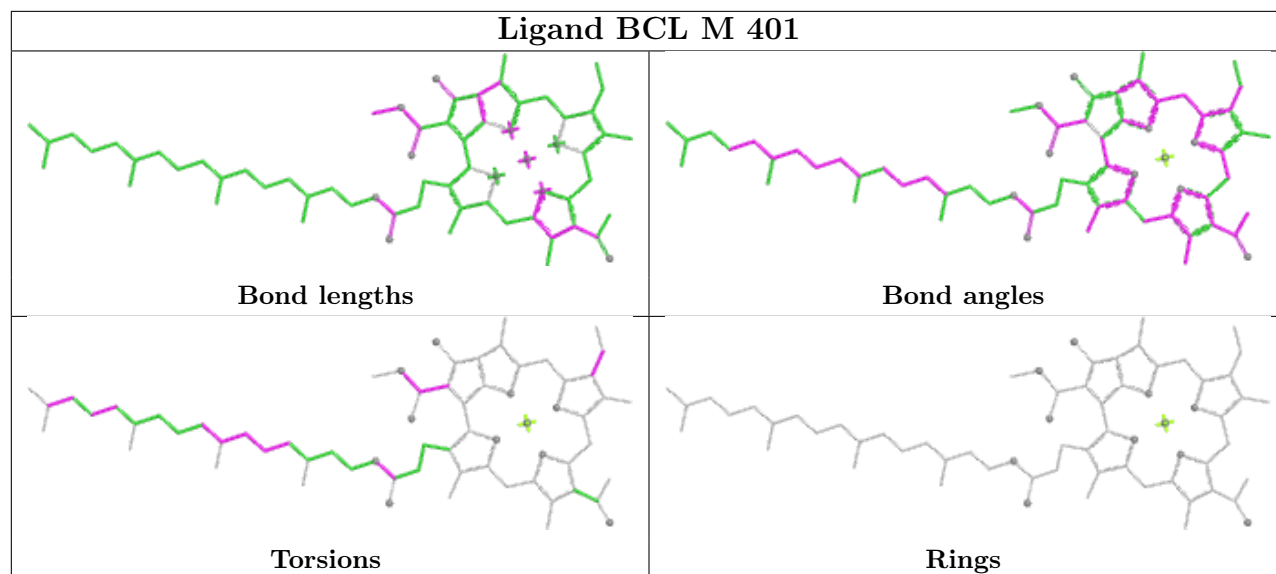


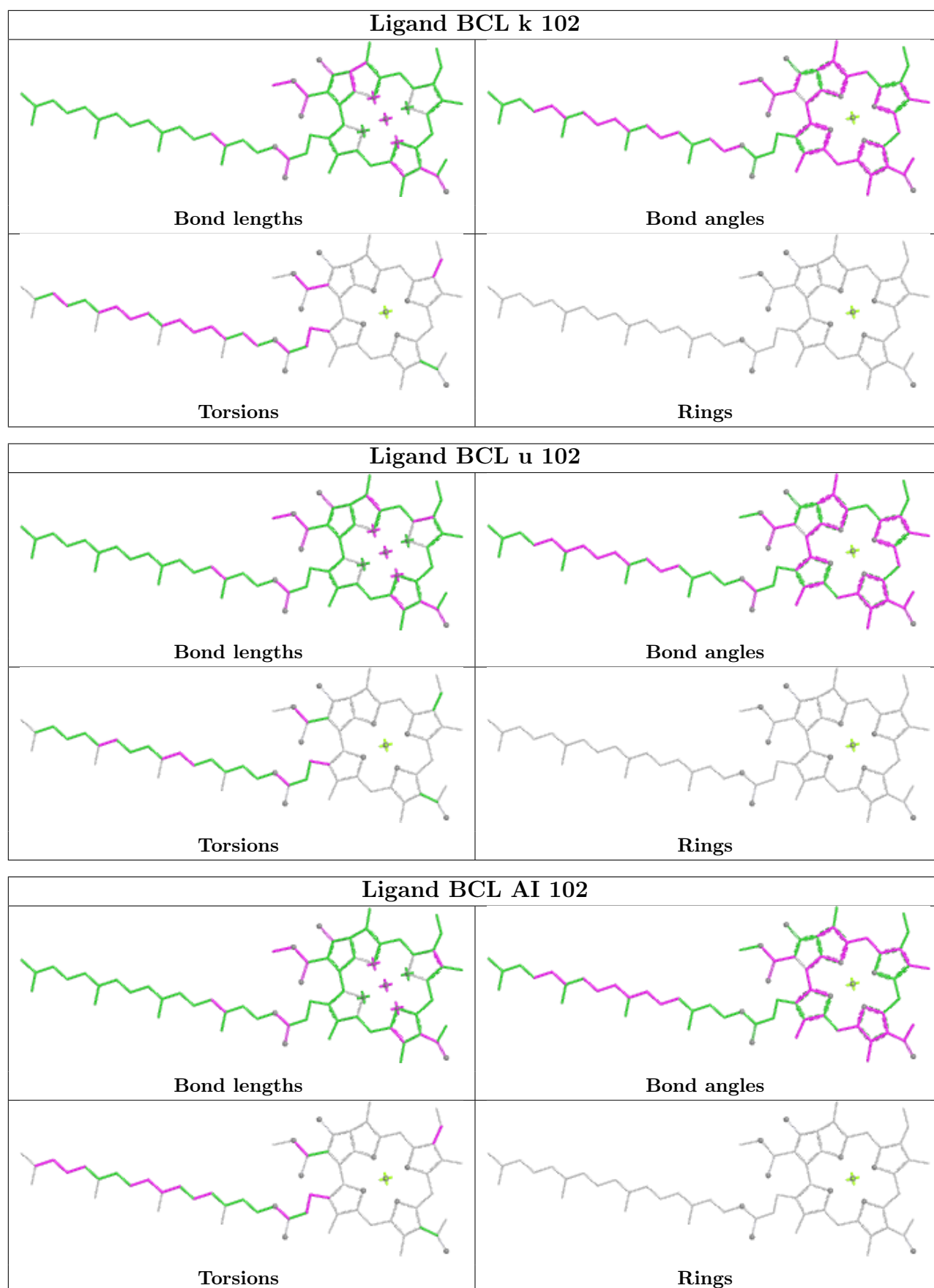


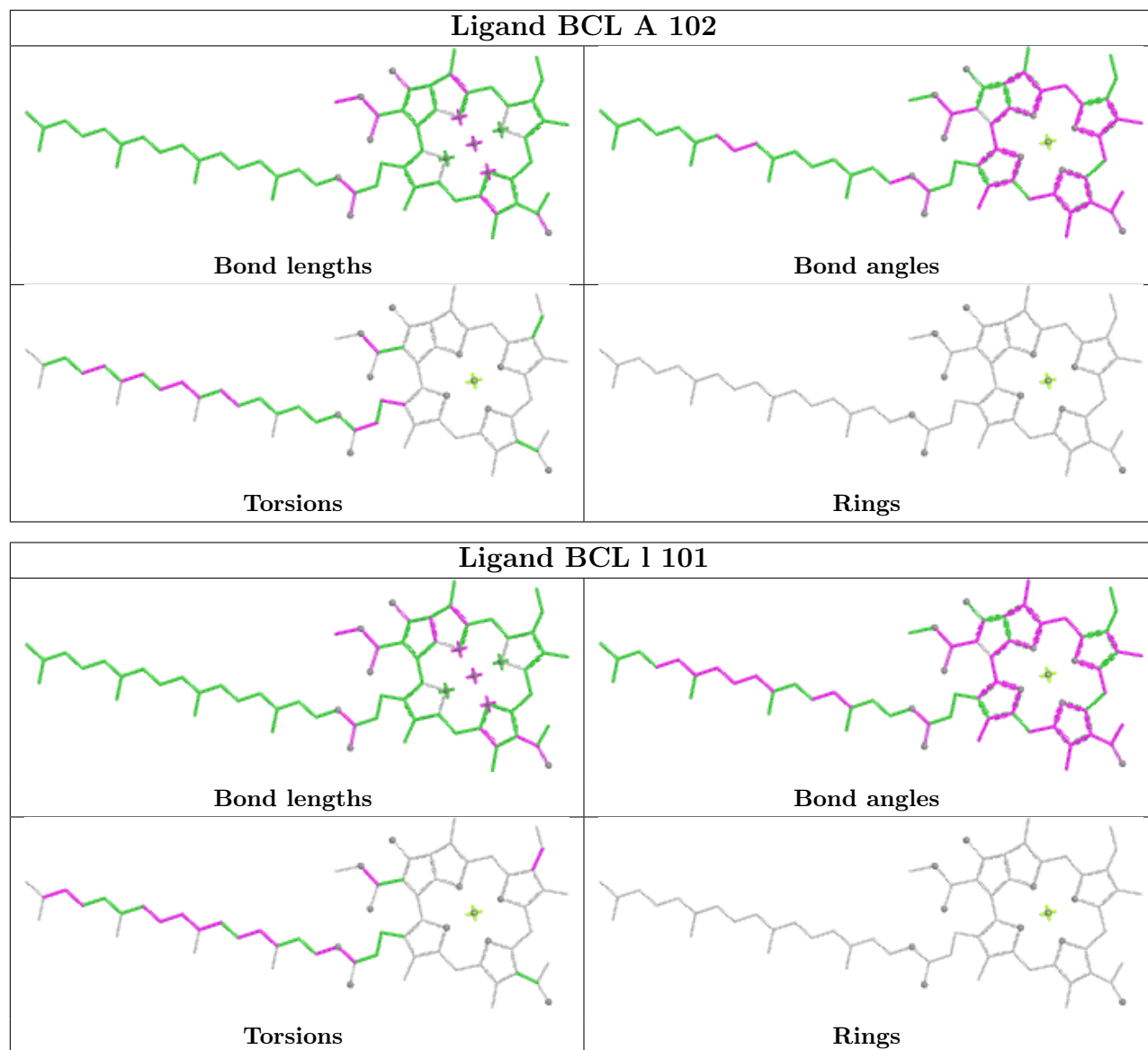


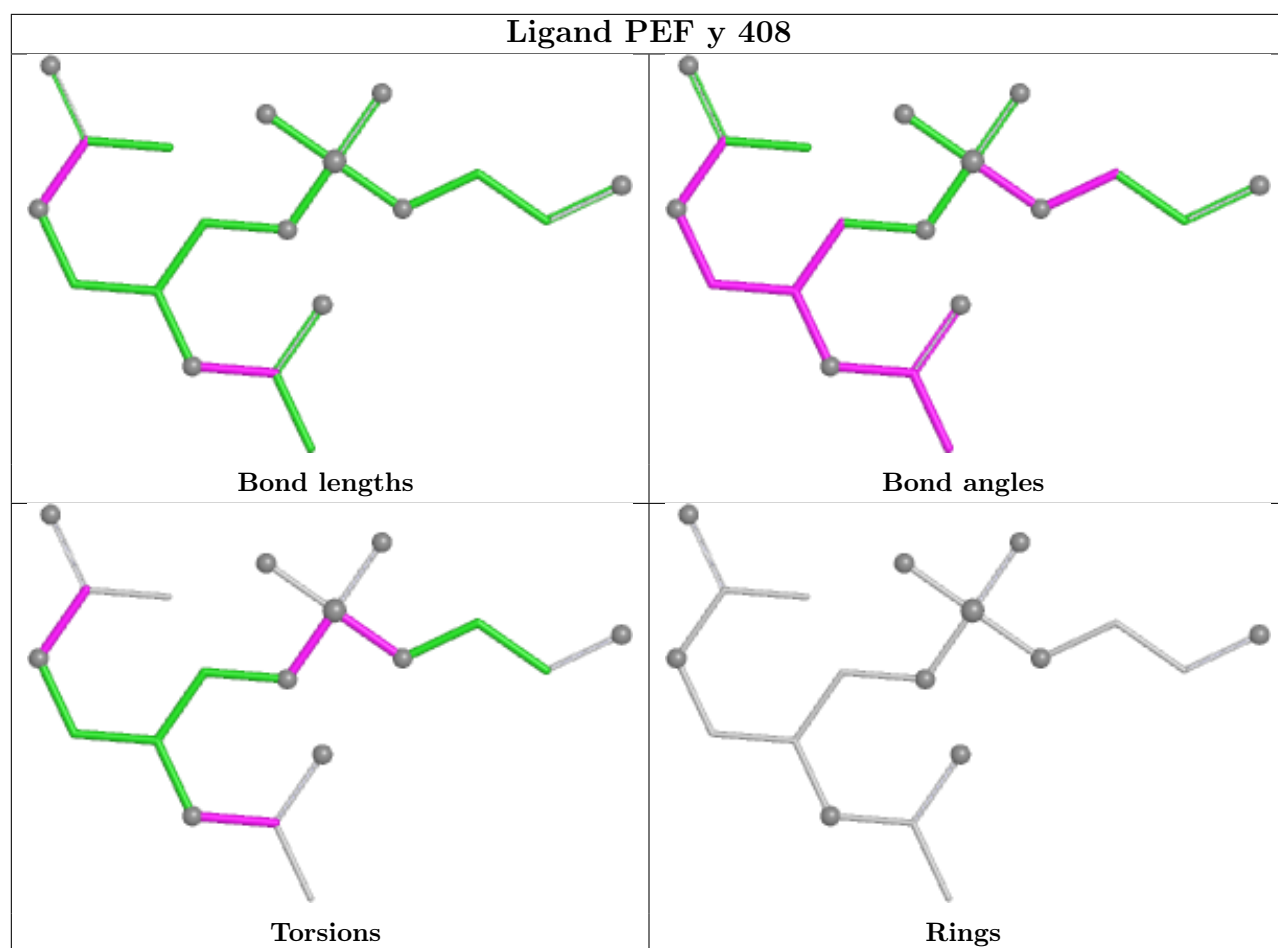




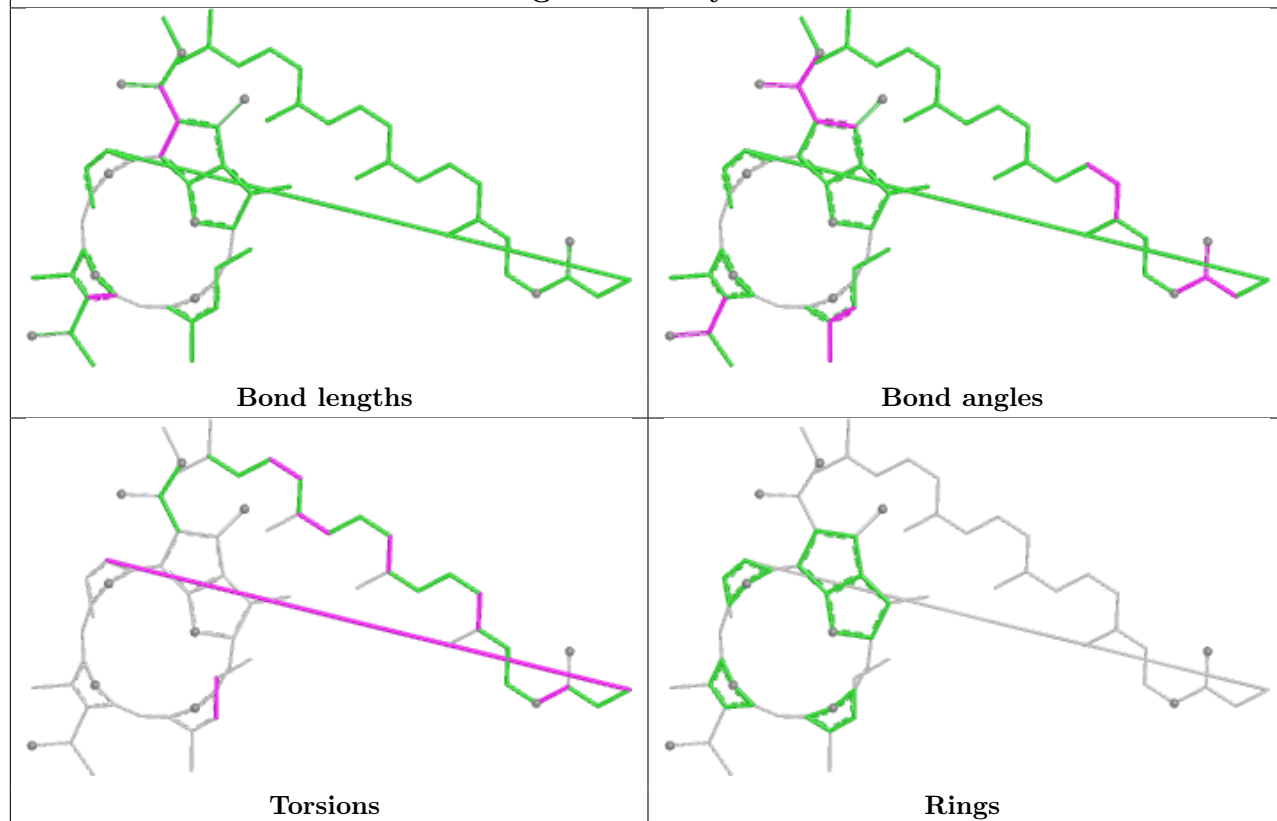




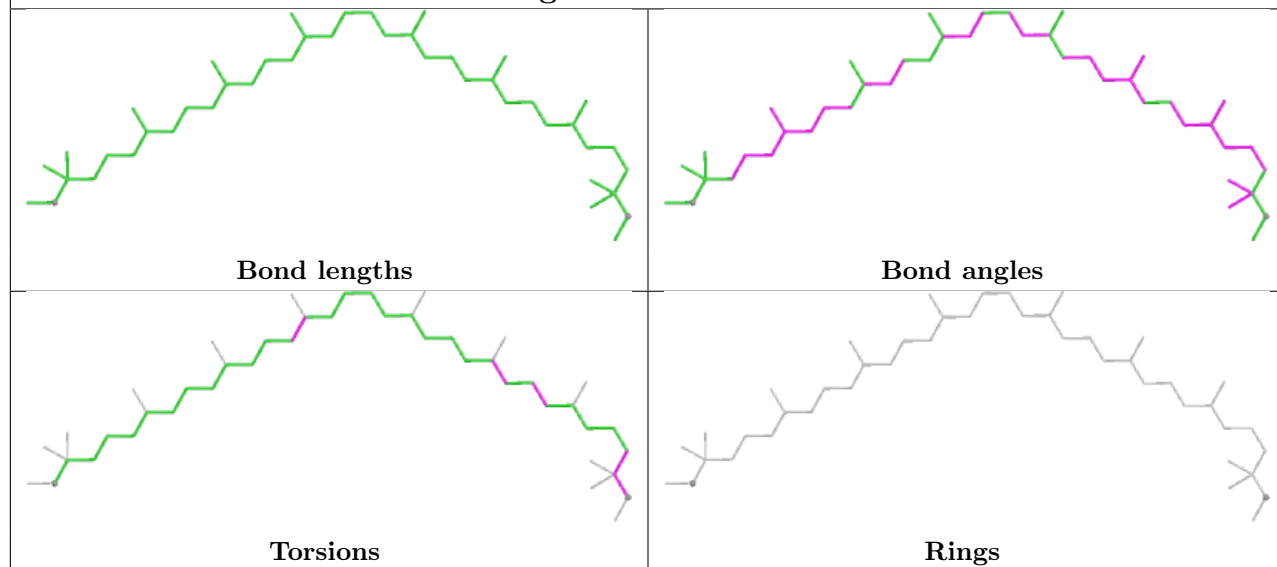




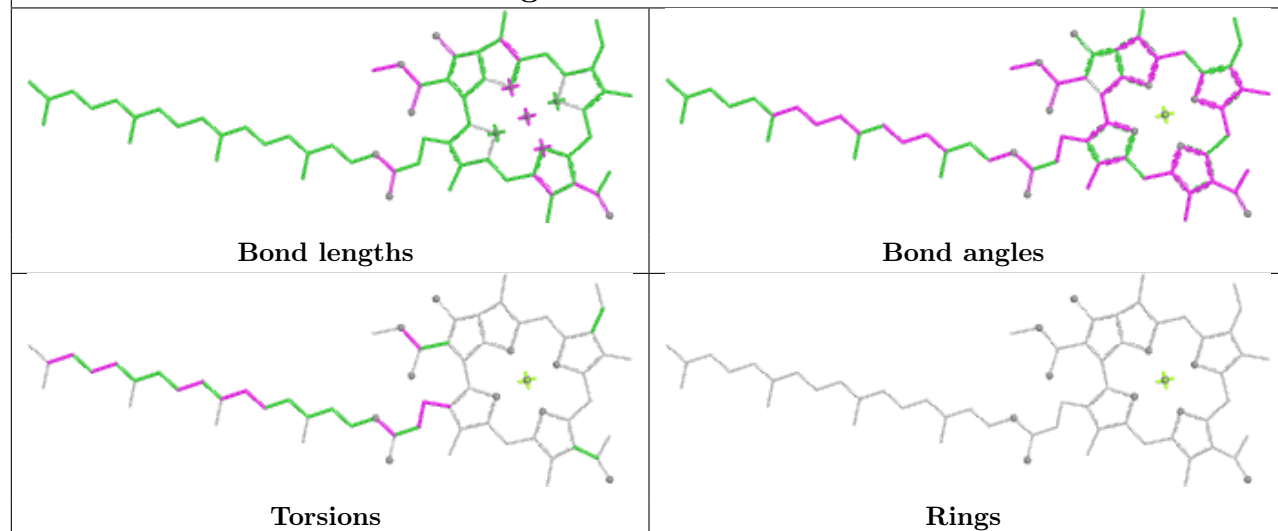
Ligand BPH y 402



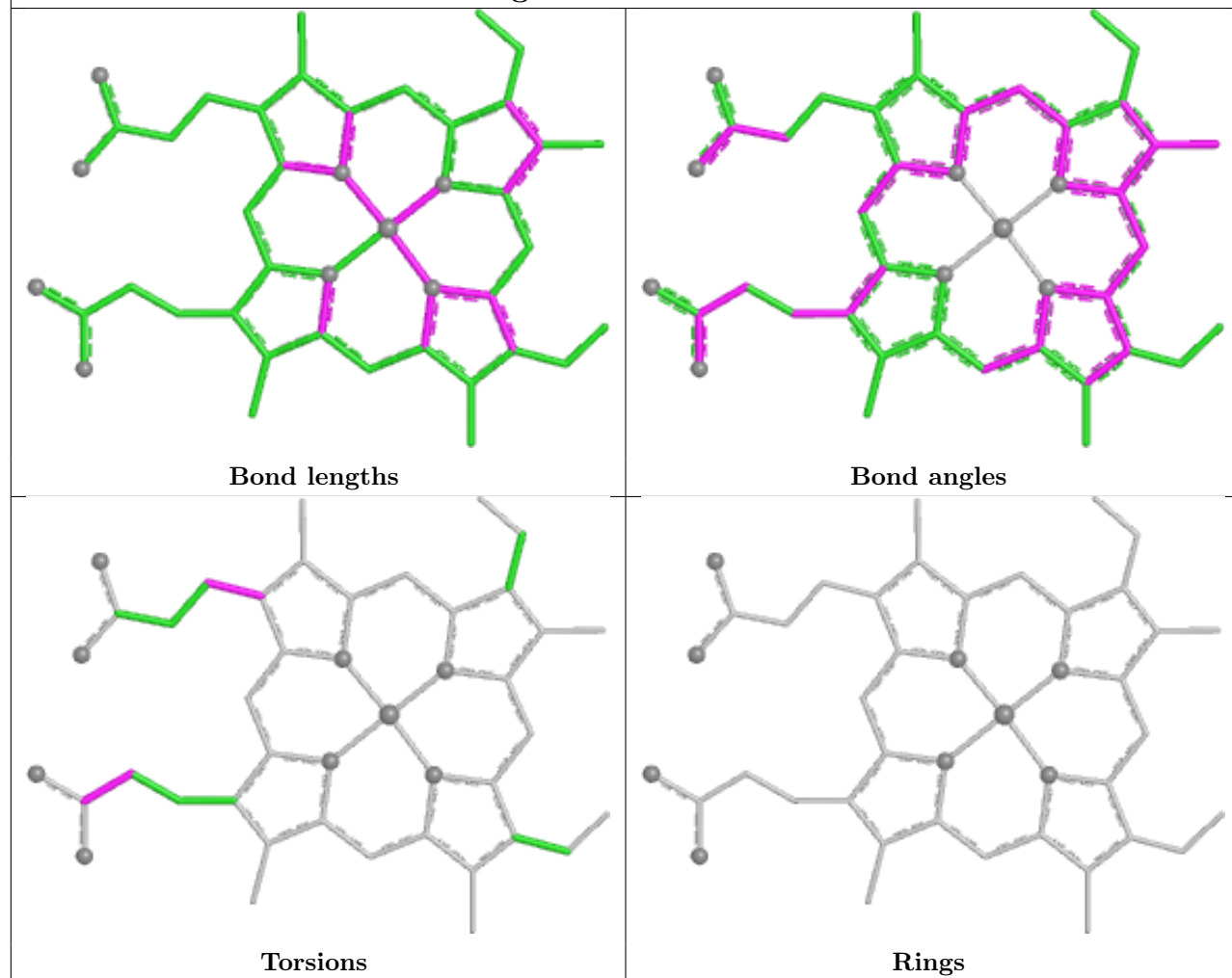
Ligand CRT i 101

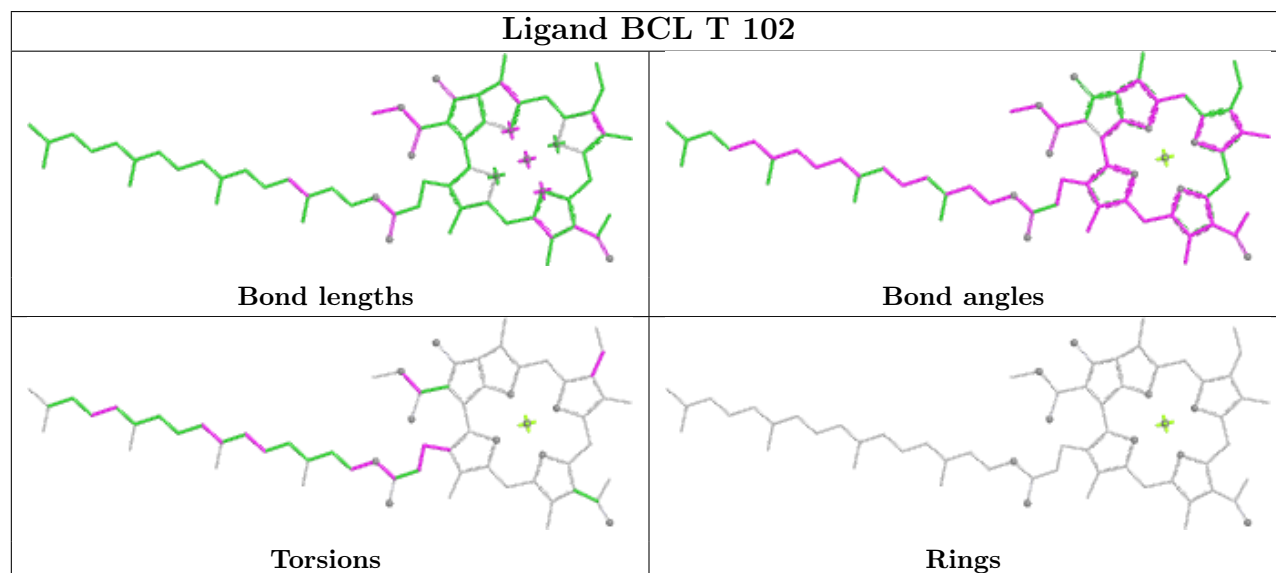
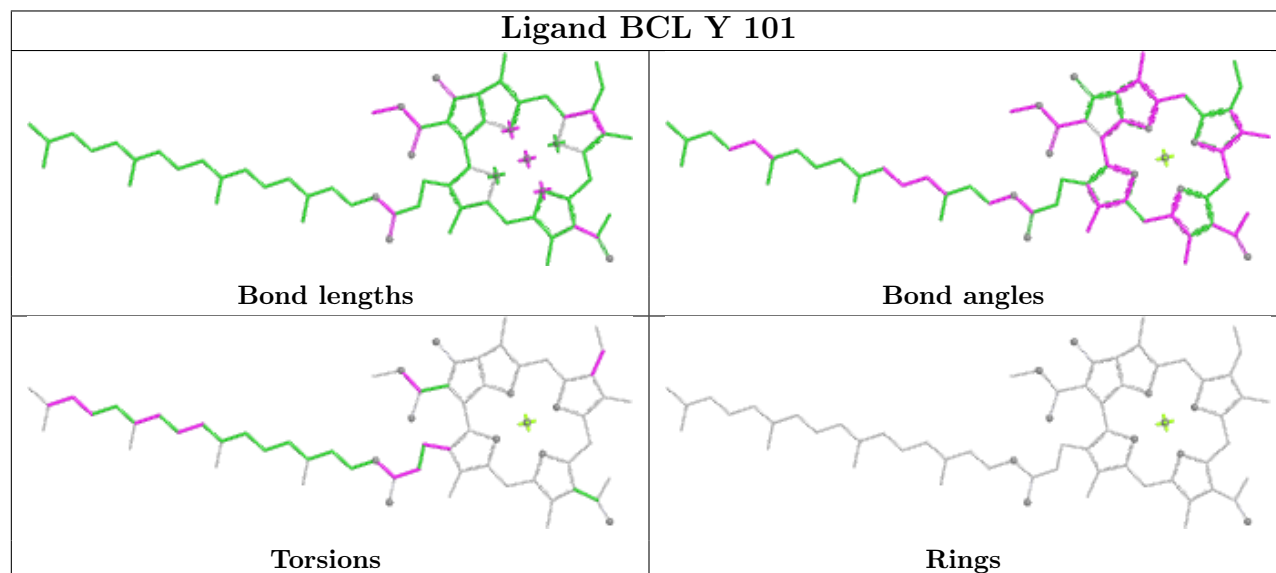
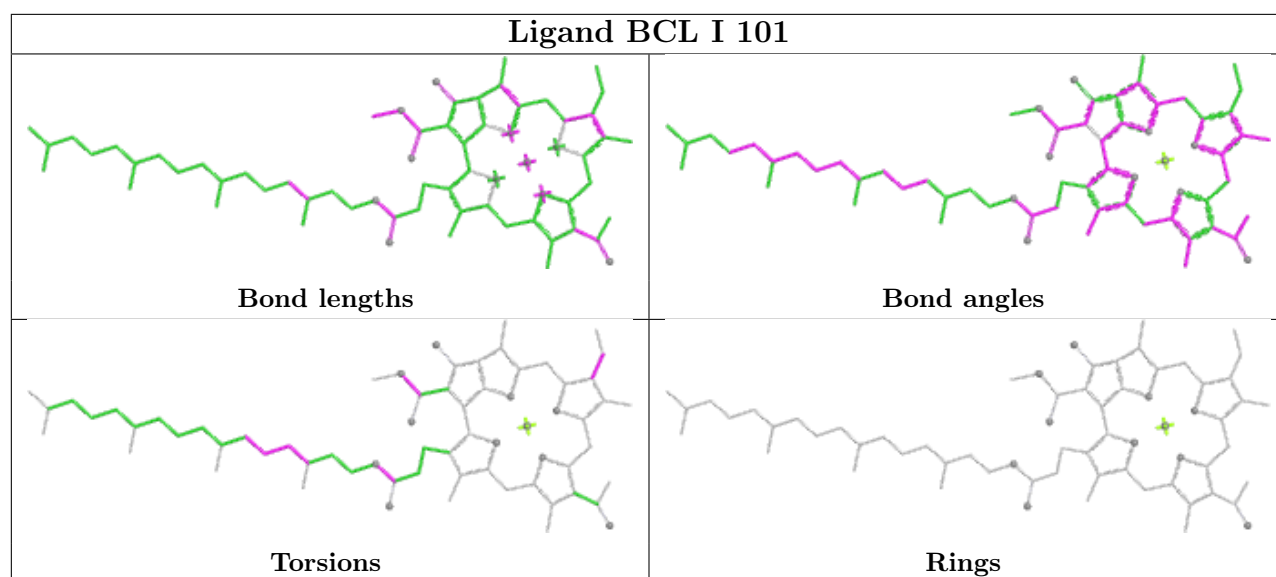


Ligand BCL AE 102

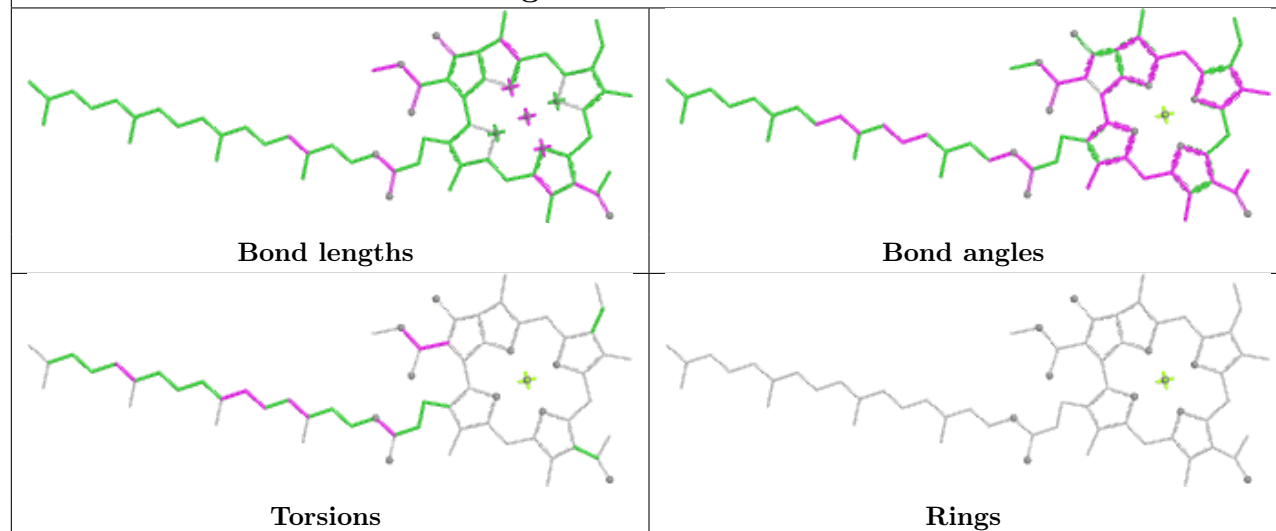


Ligand HEM o 504

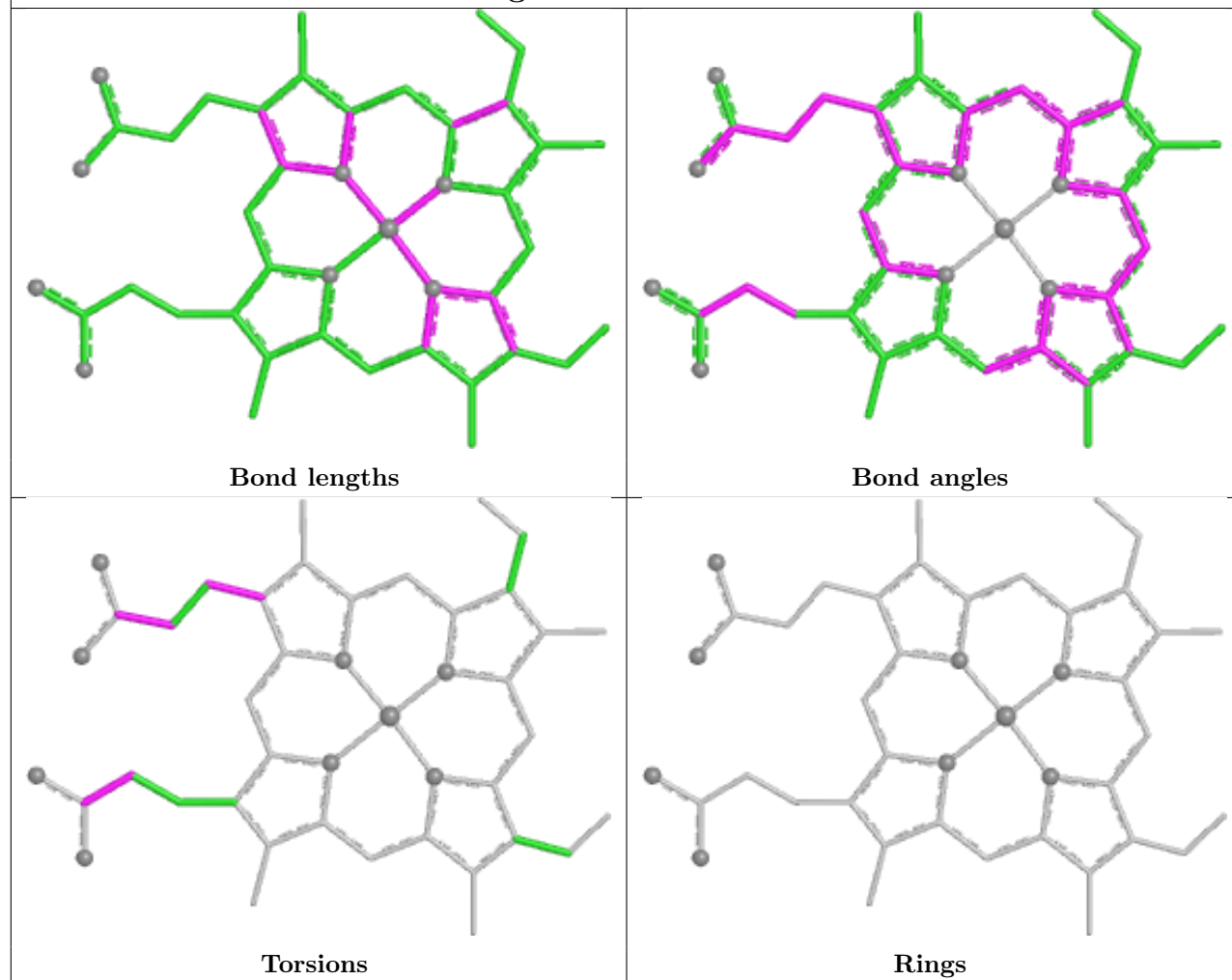


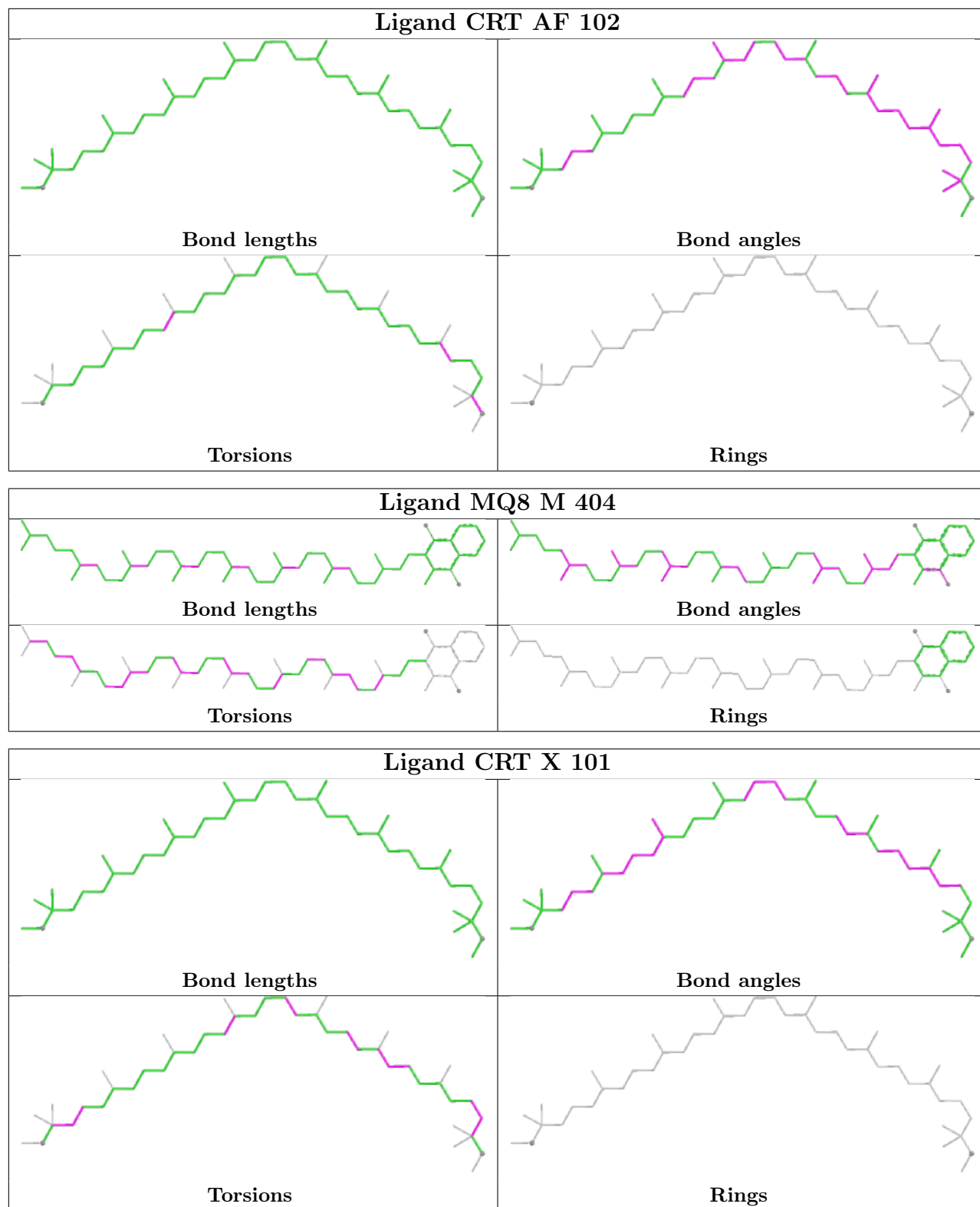


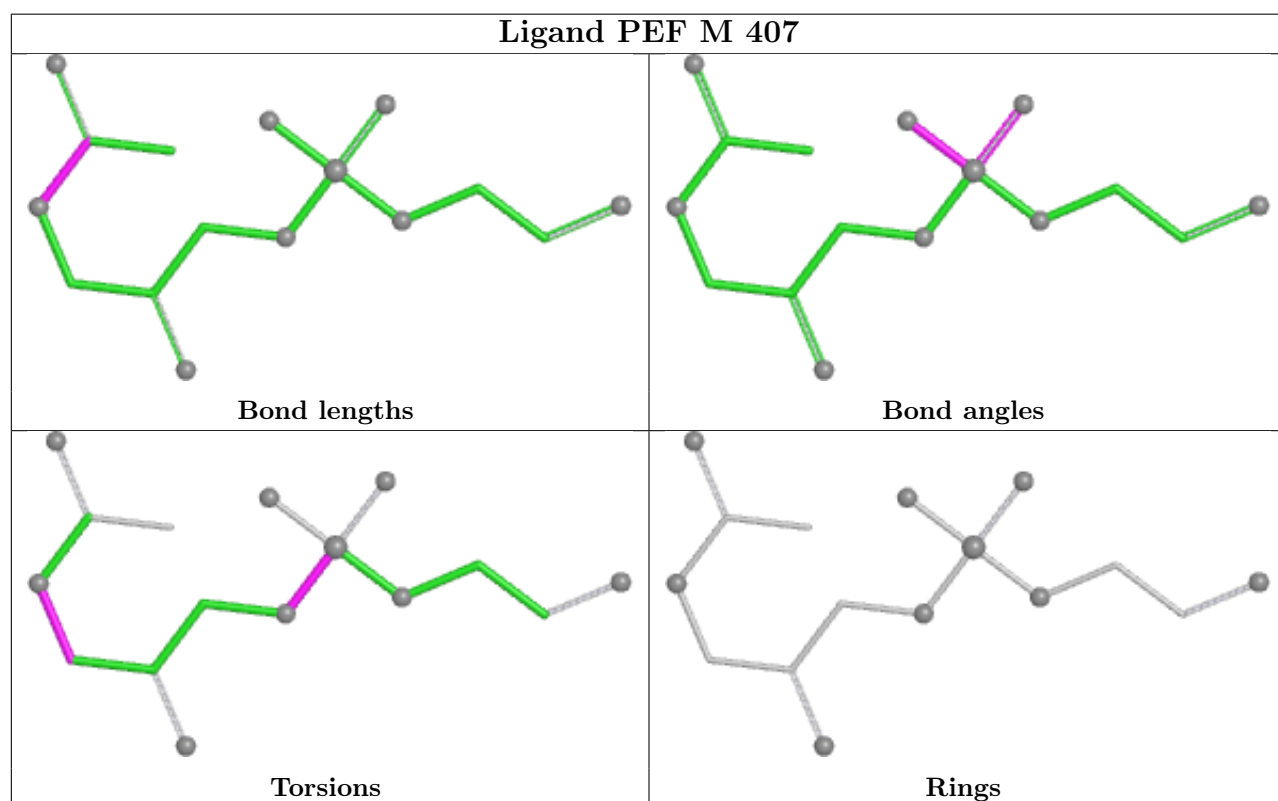
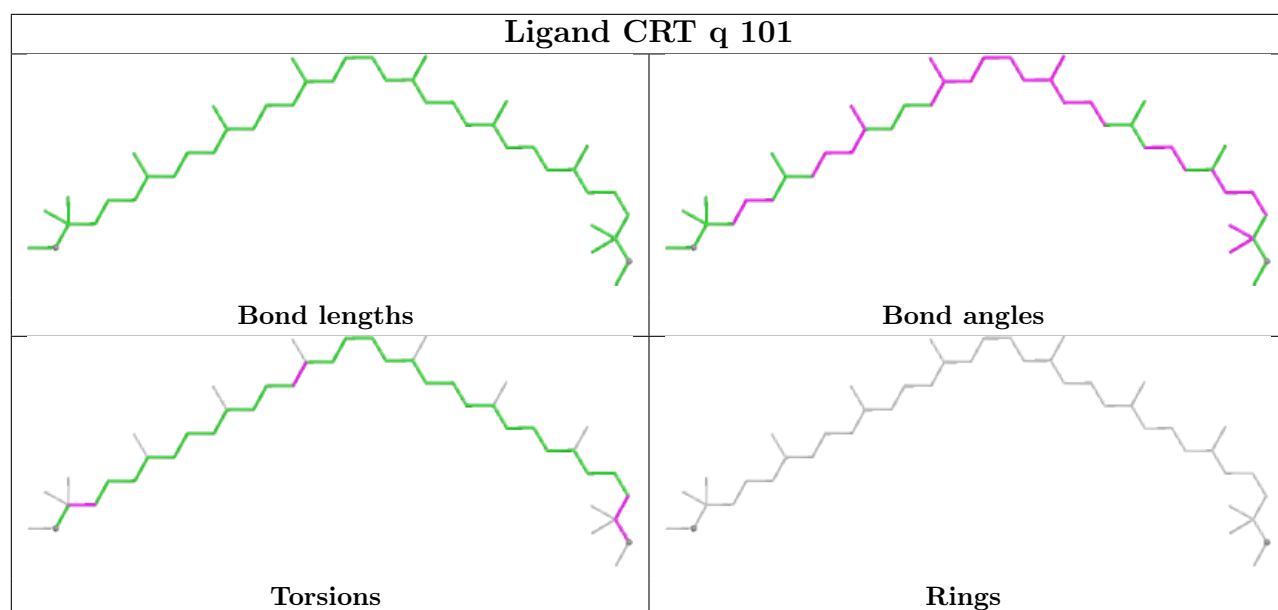
Ligand BCL AF 101

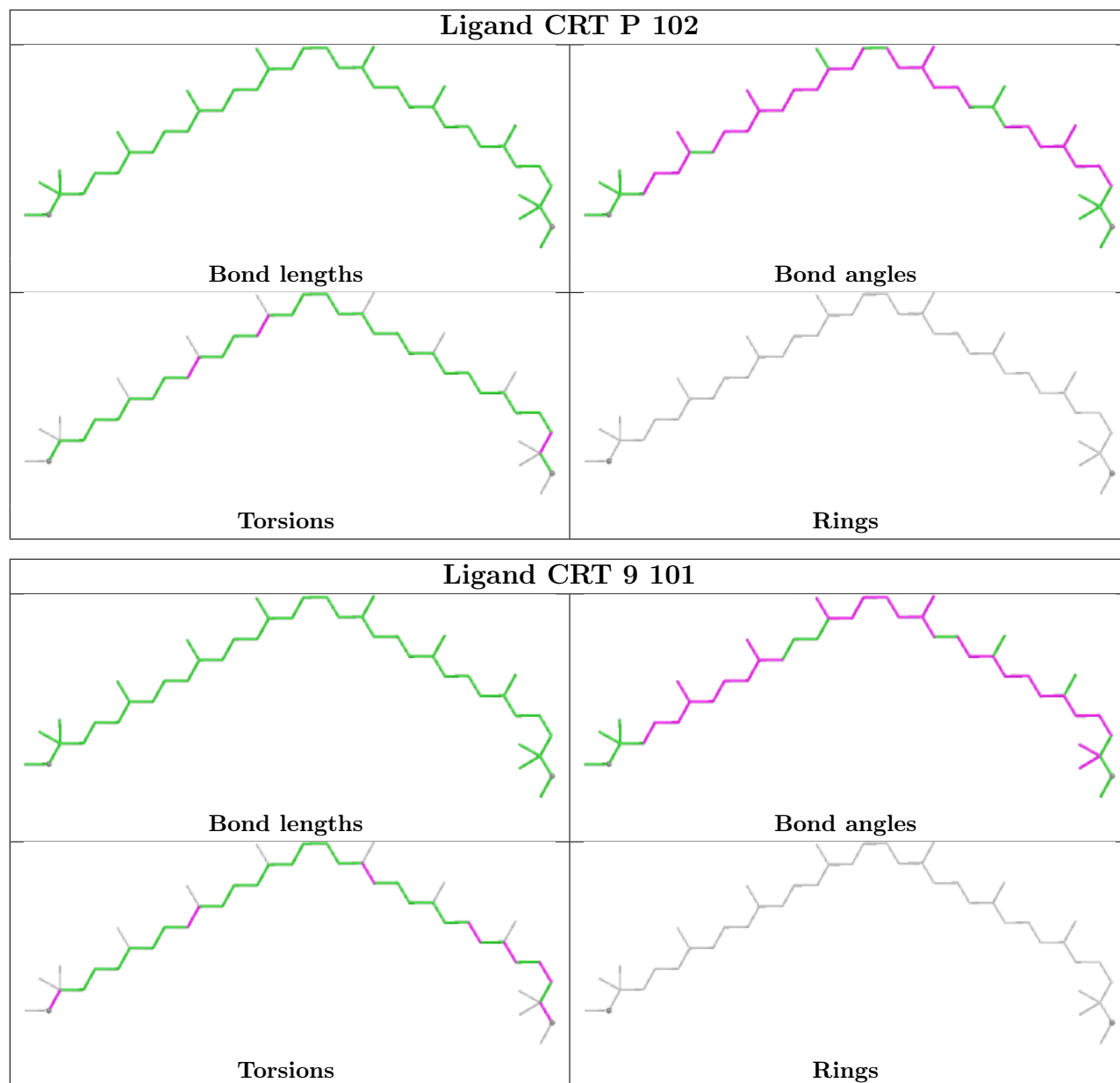


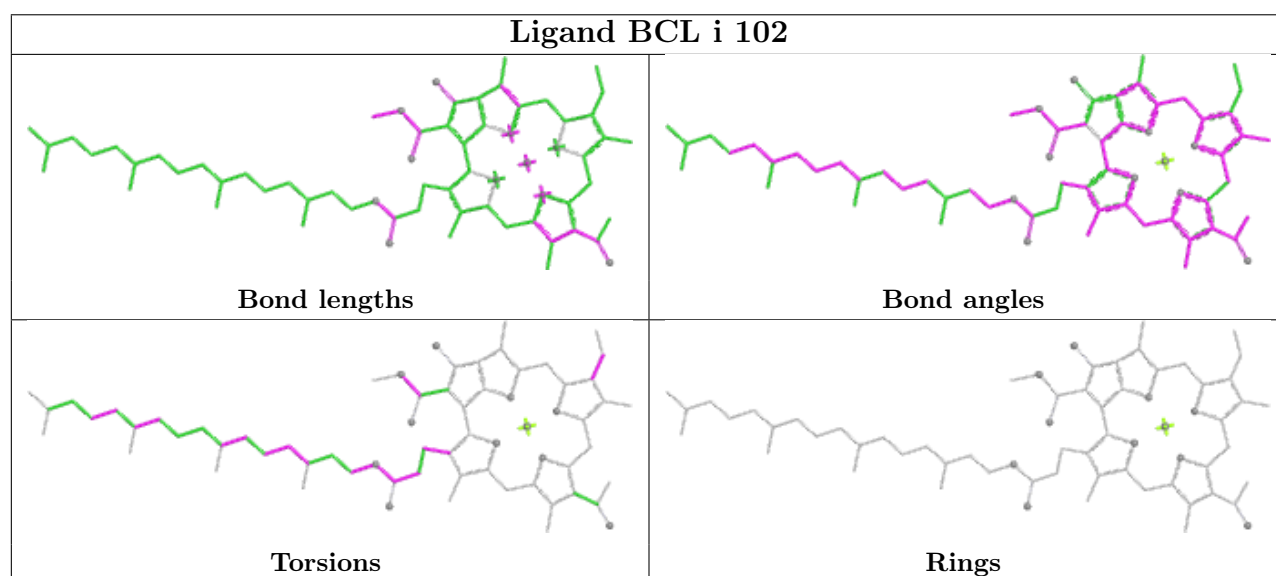
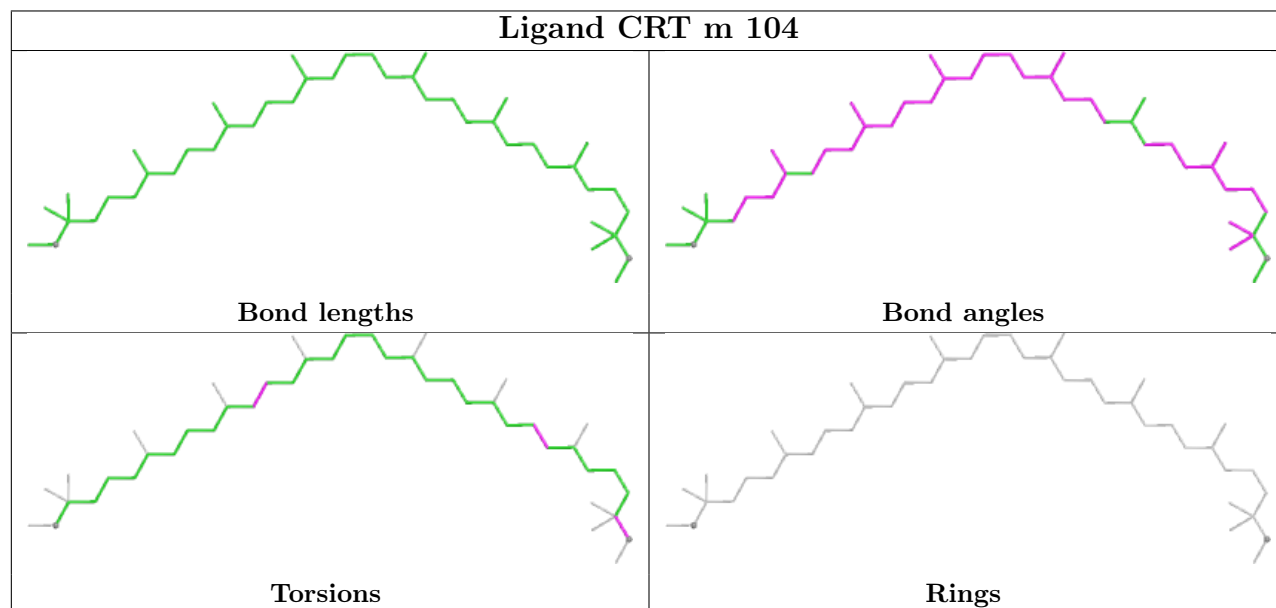
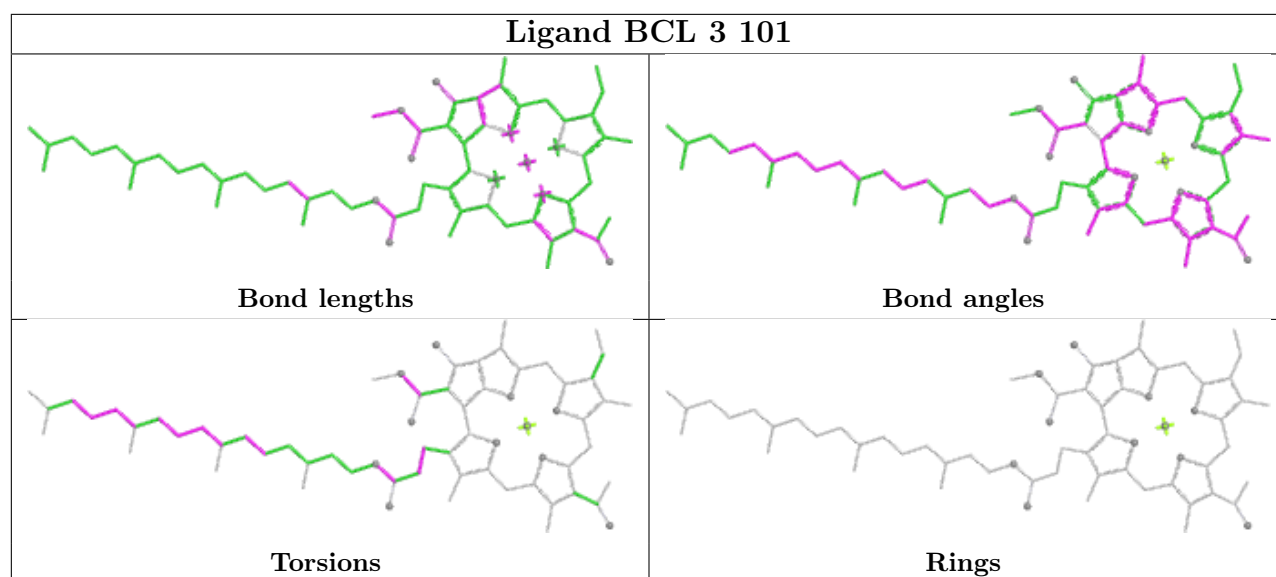
Ligand HEM C 504

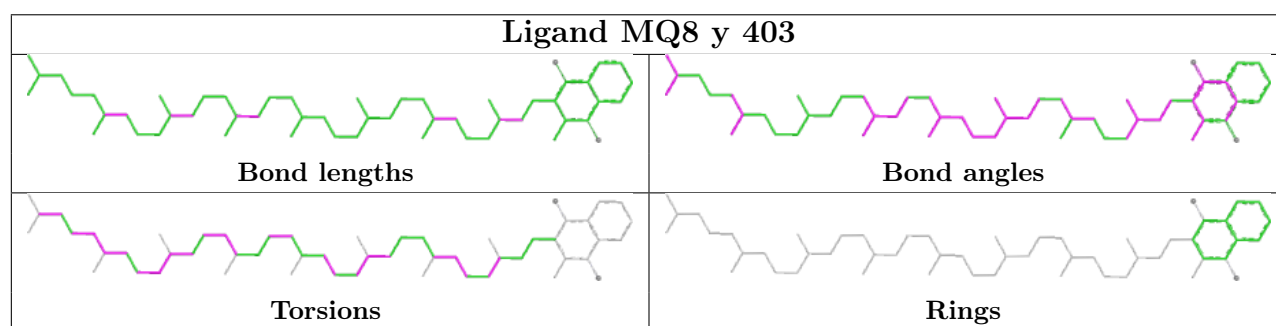
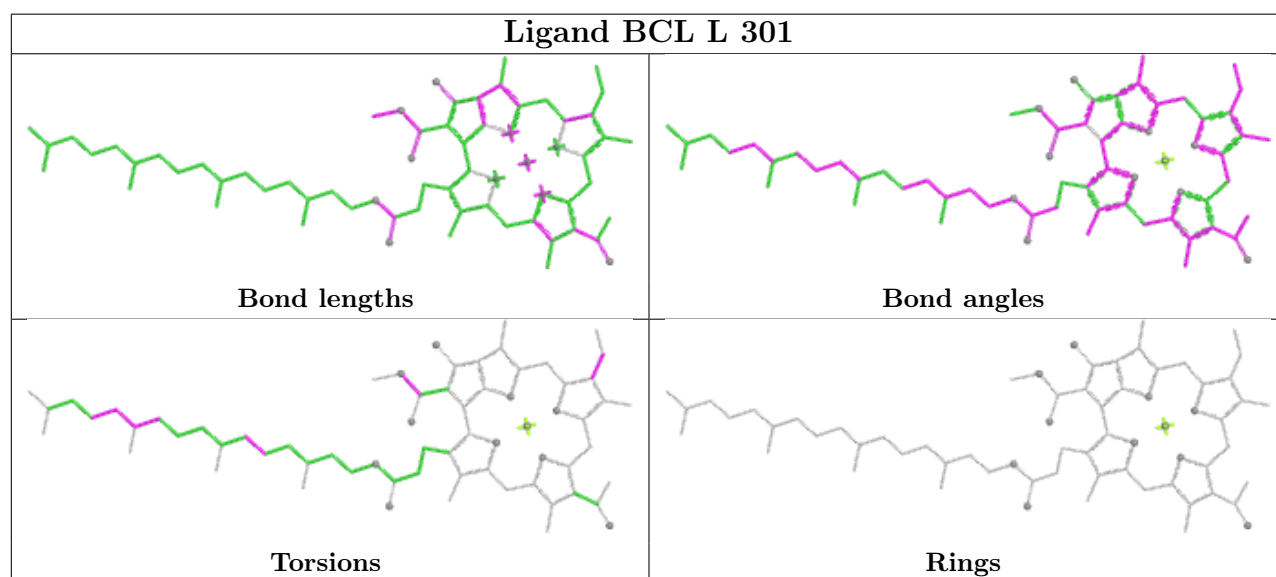
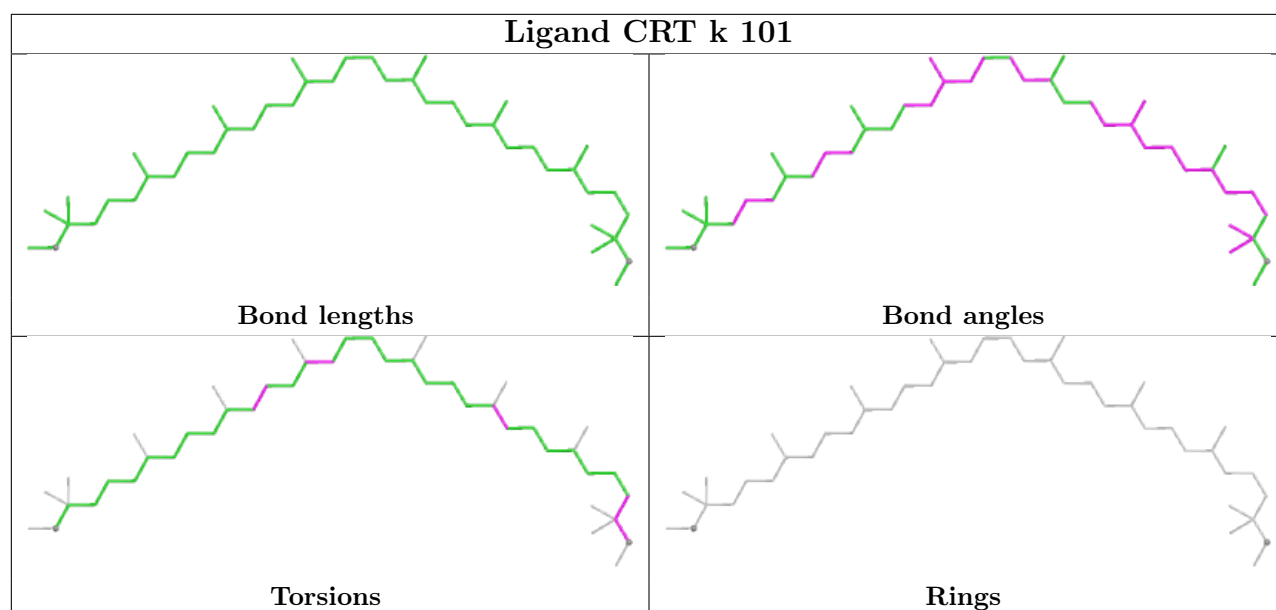


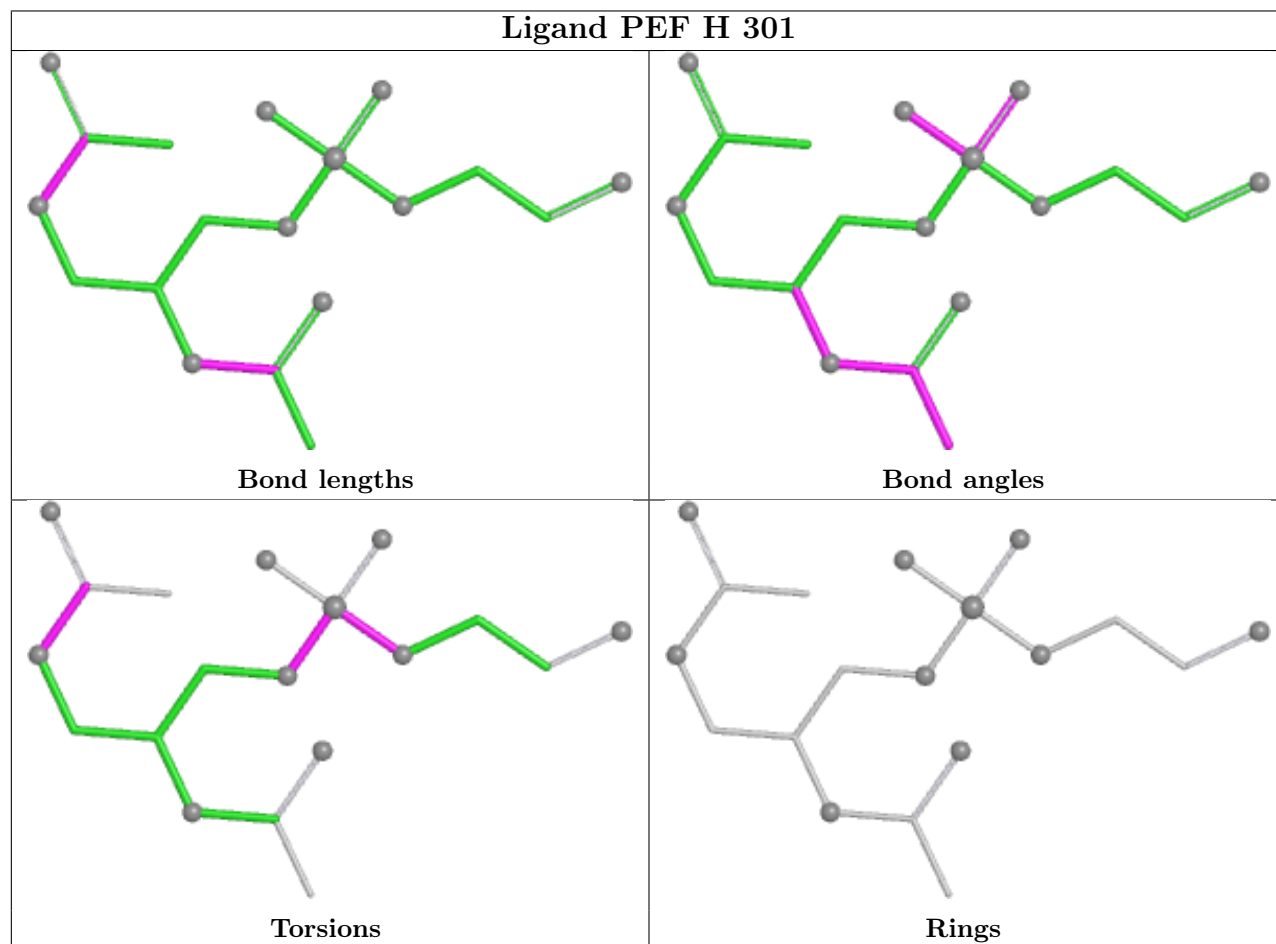
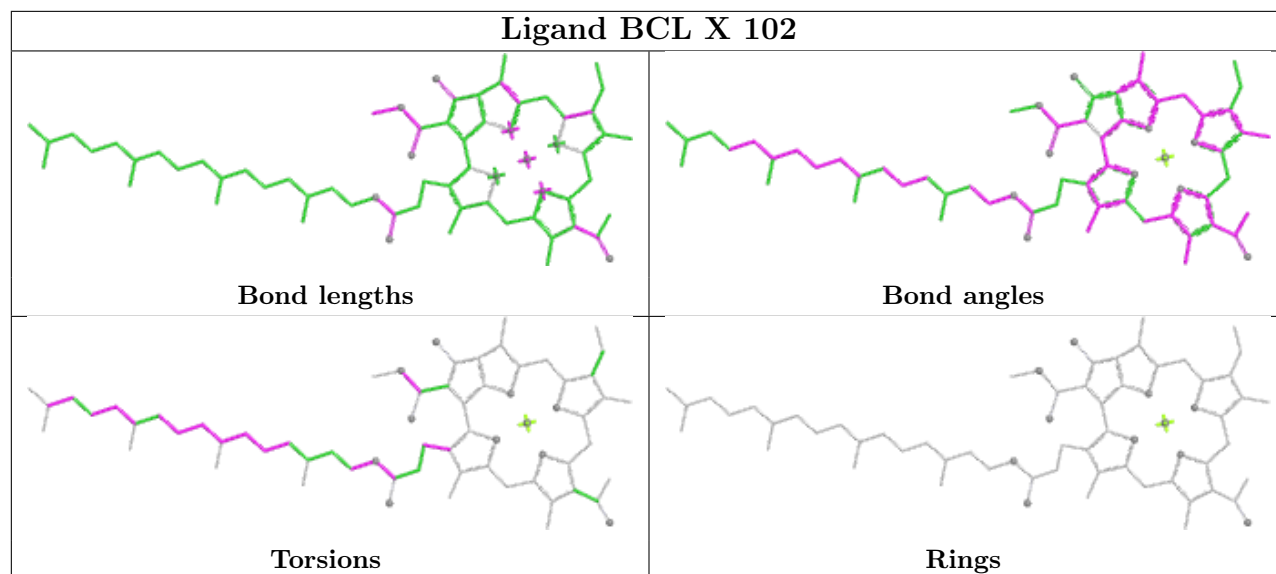


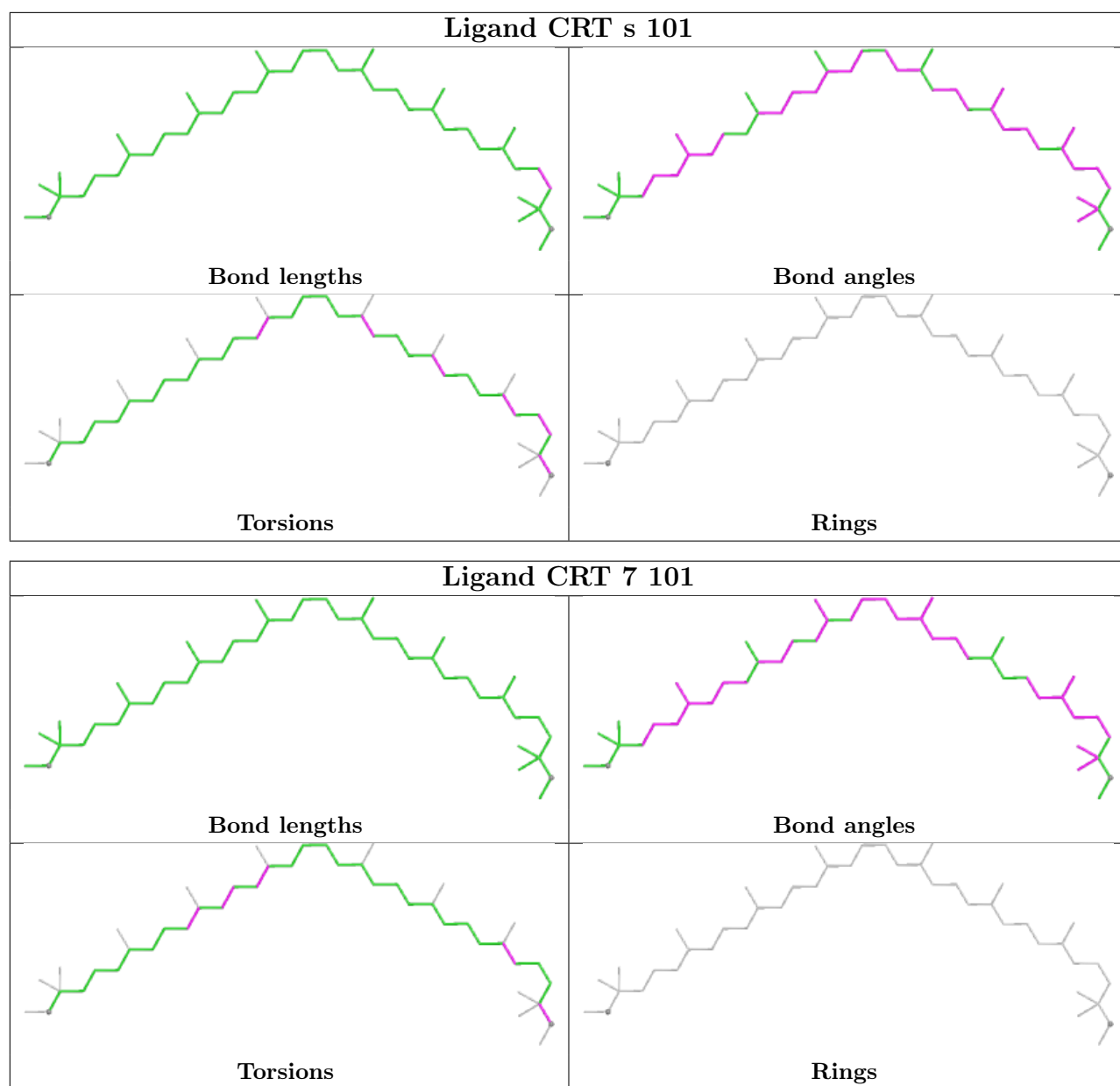


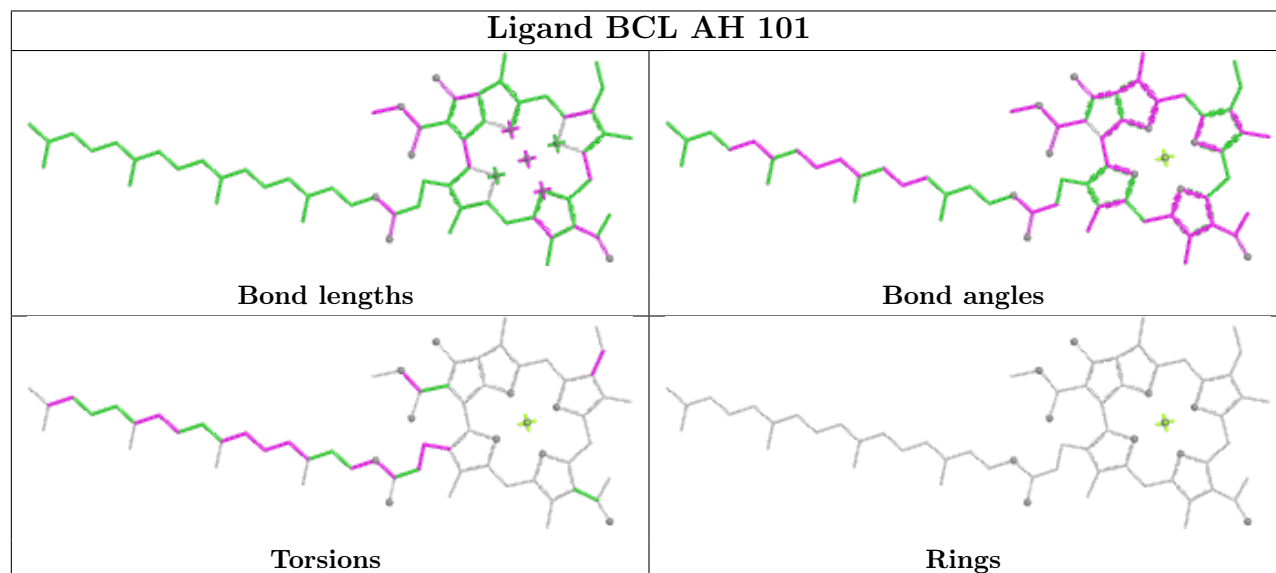
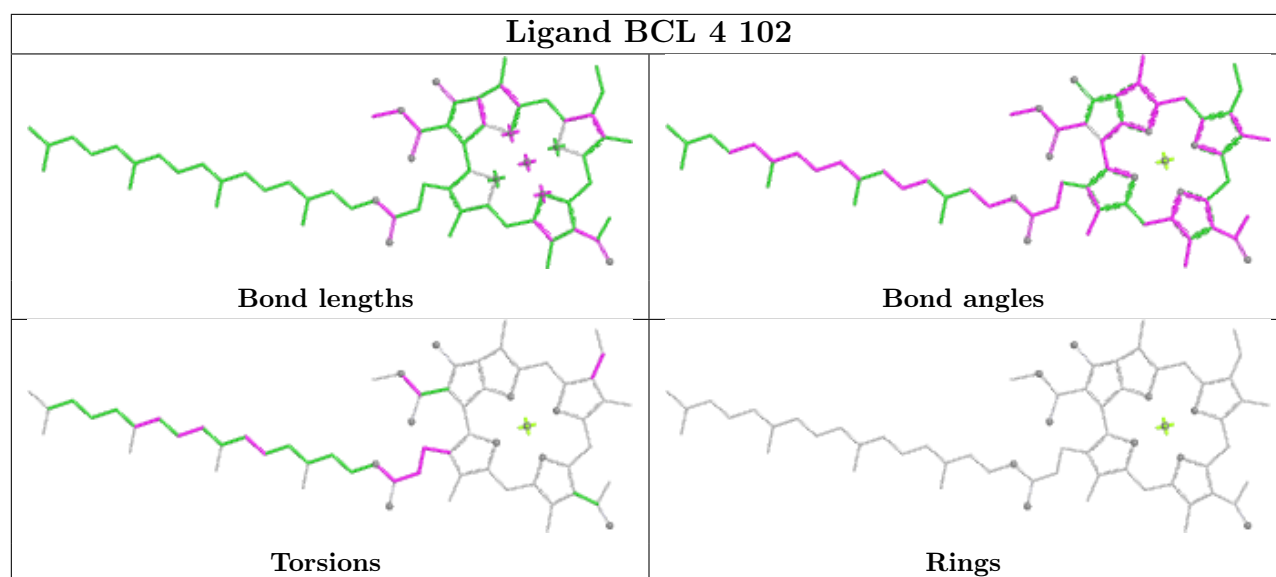


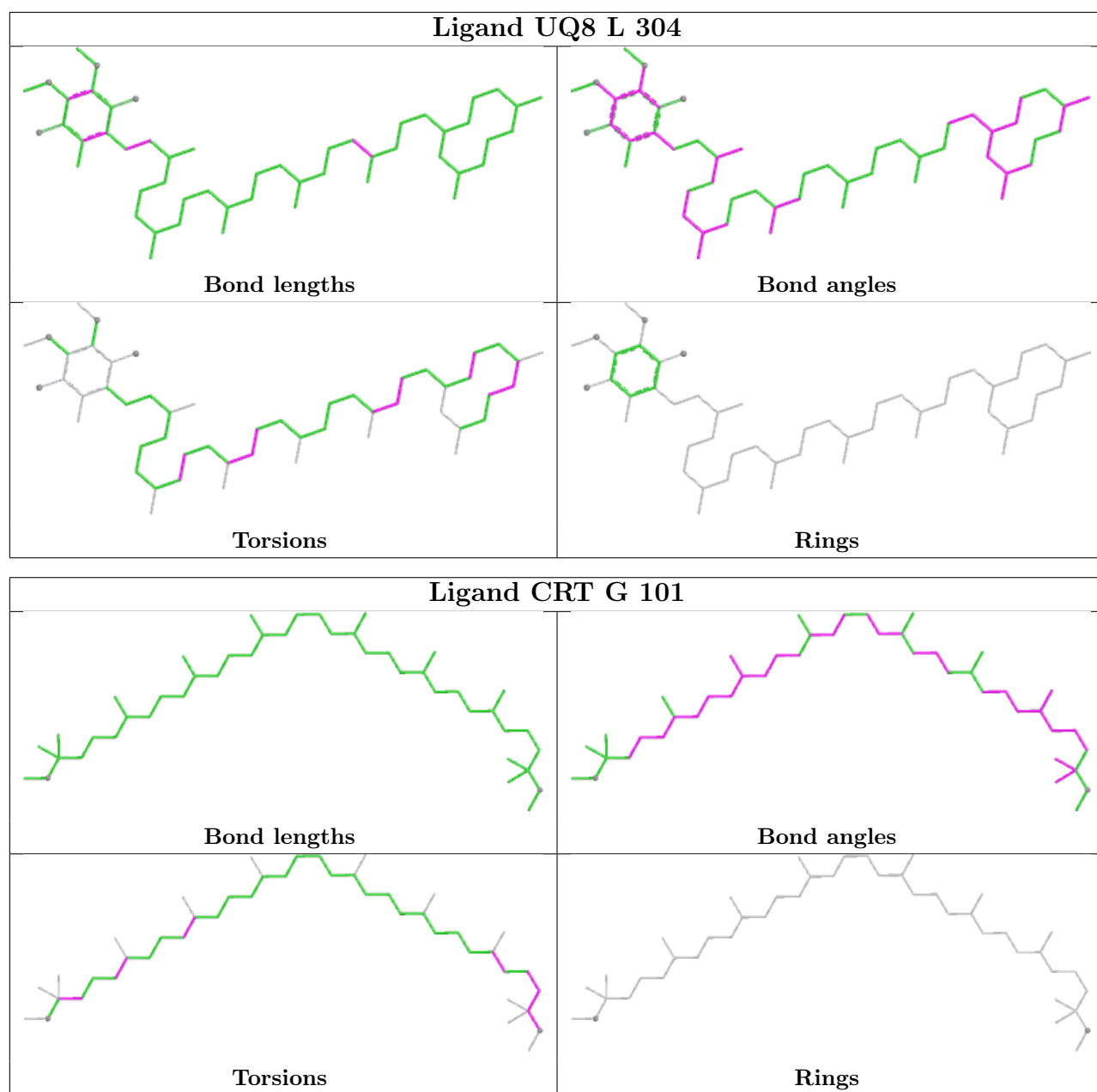


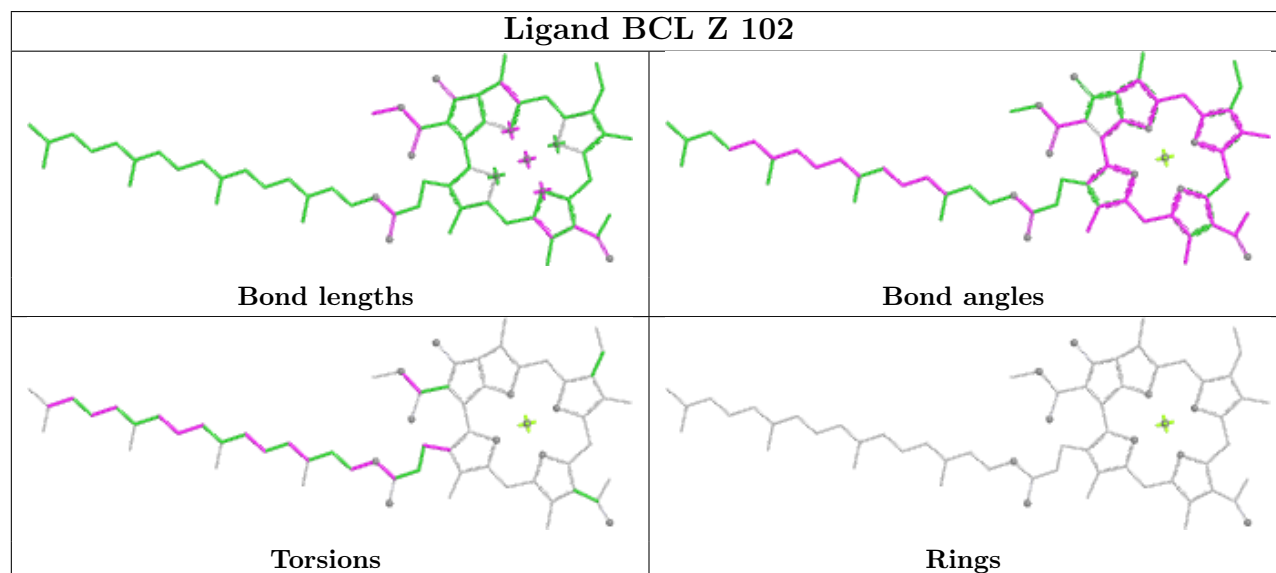
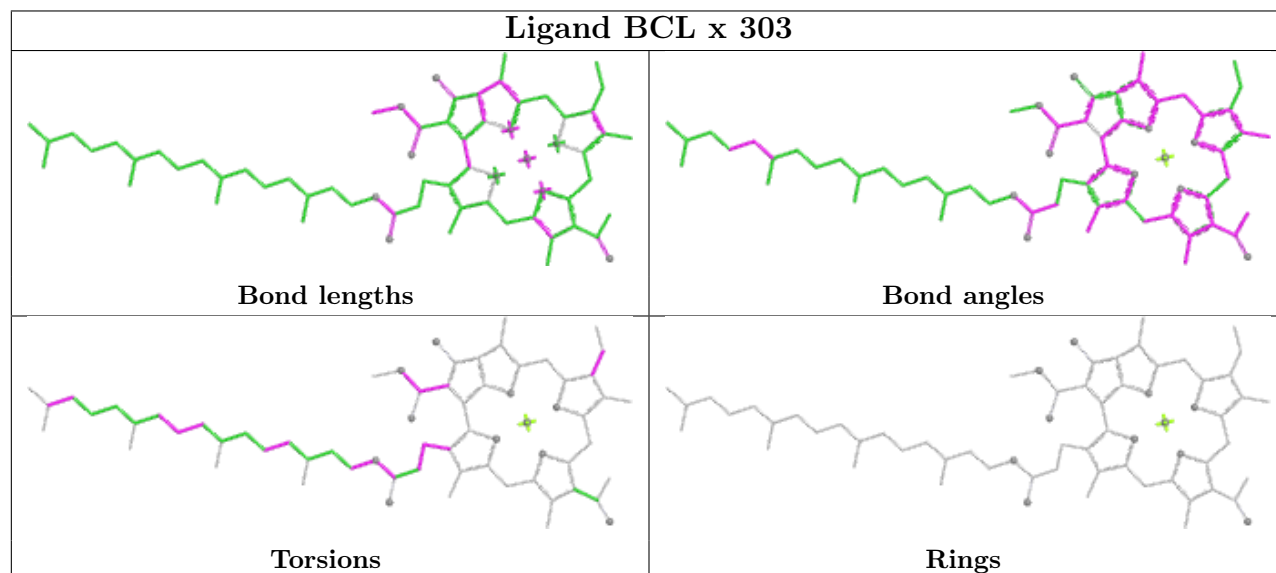
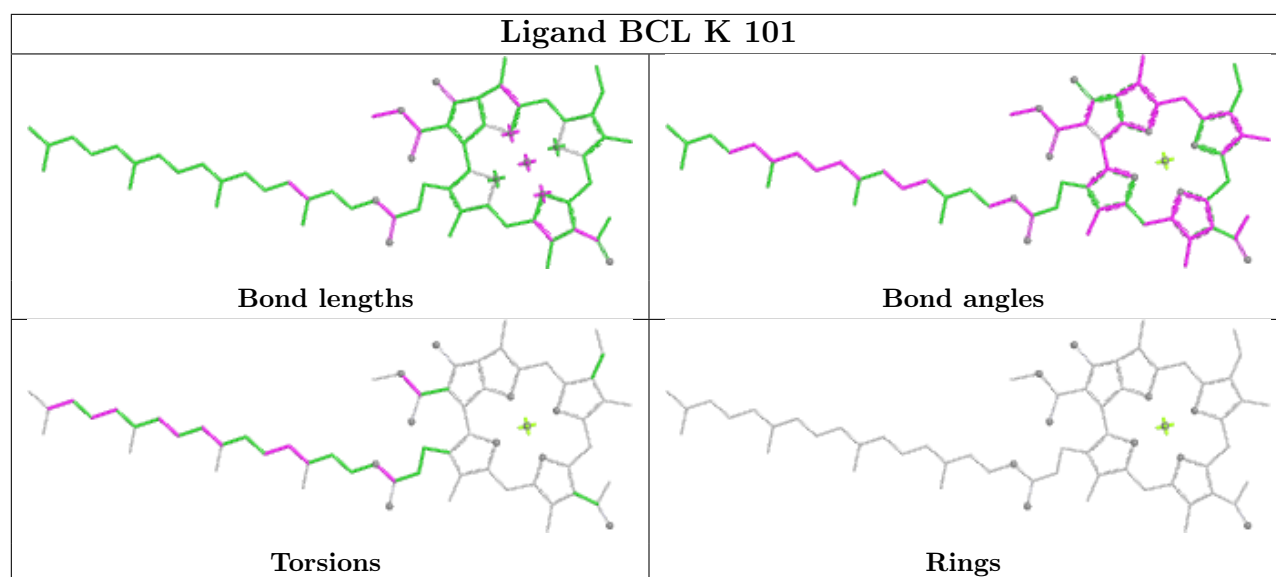


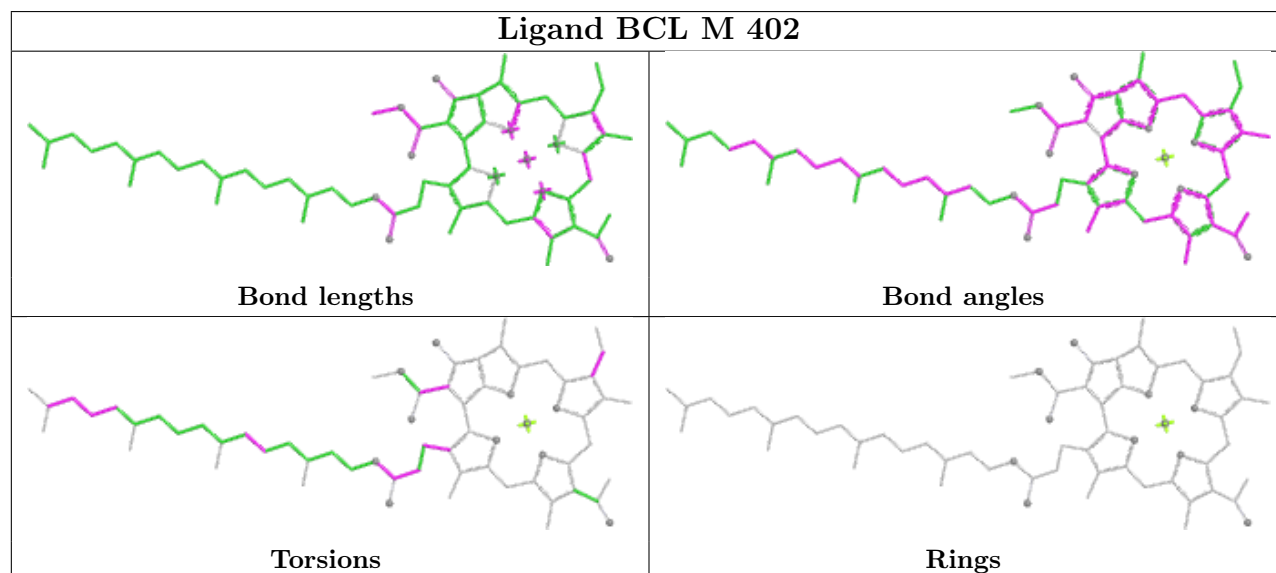
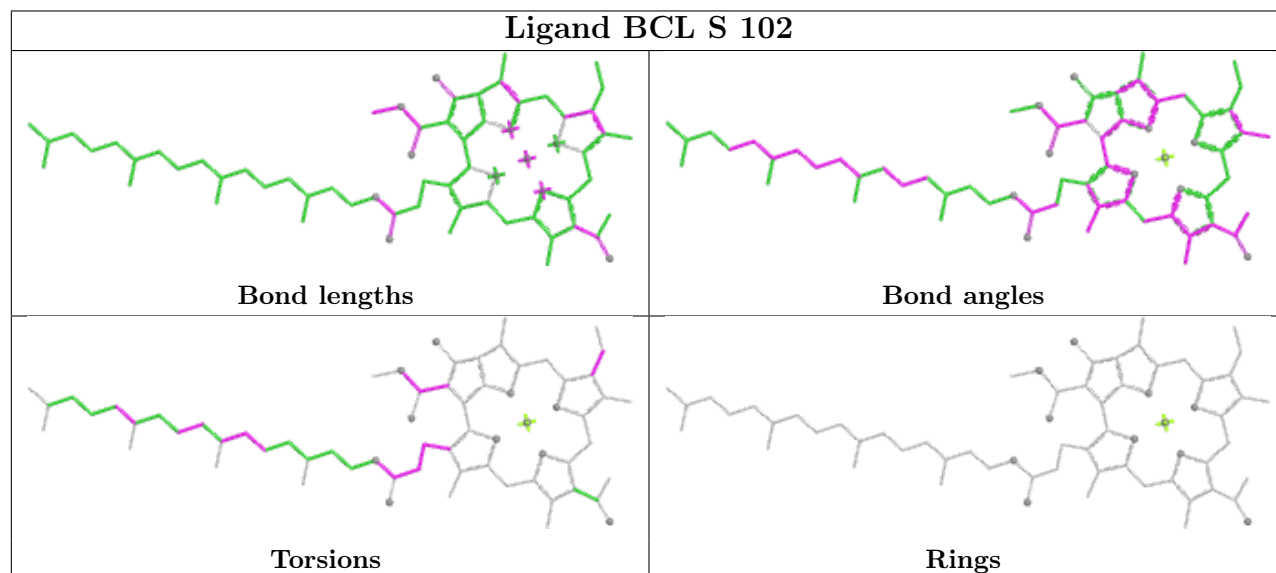
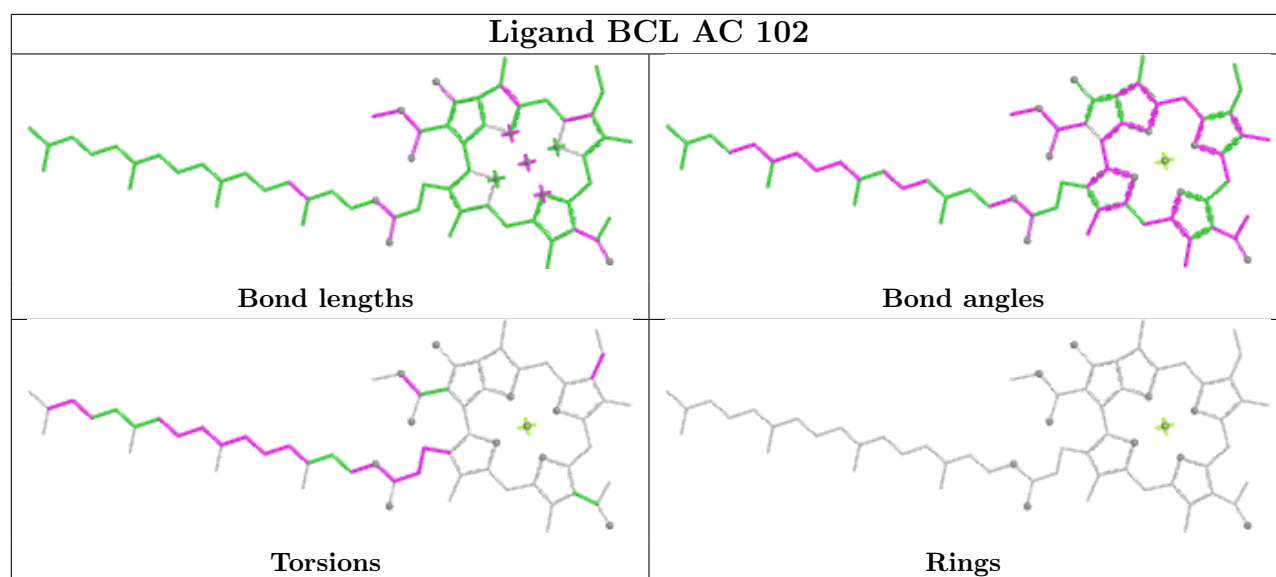


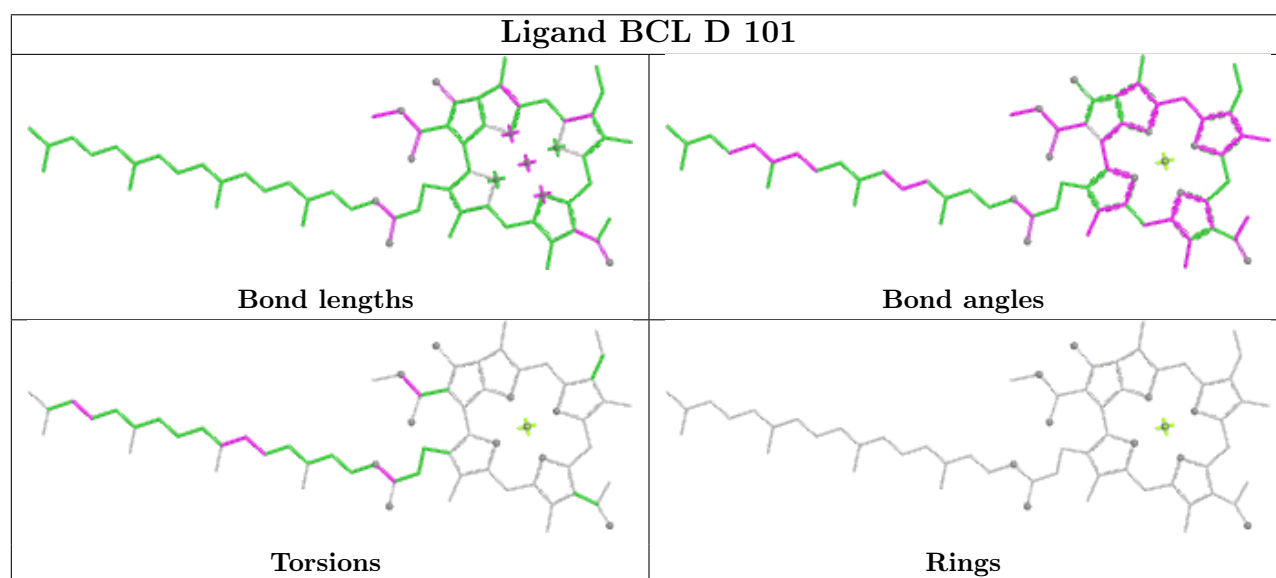
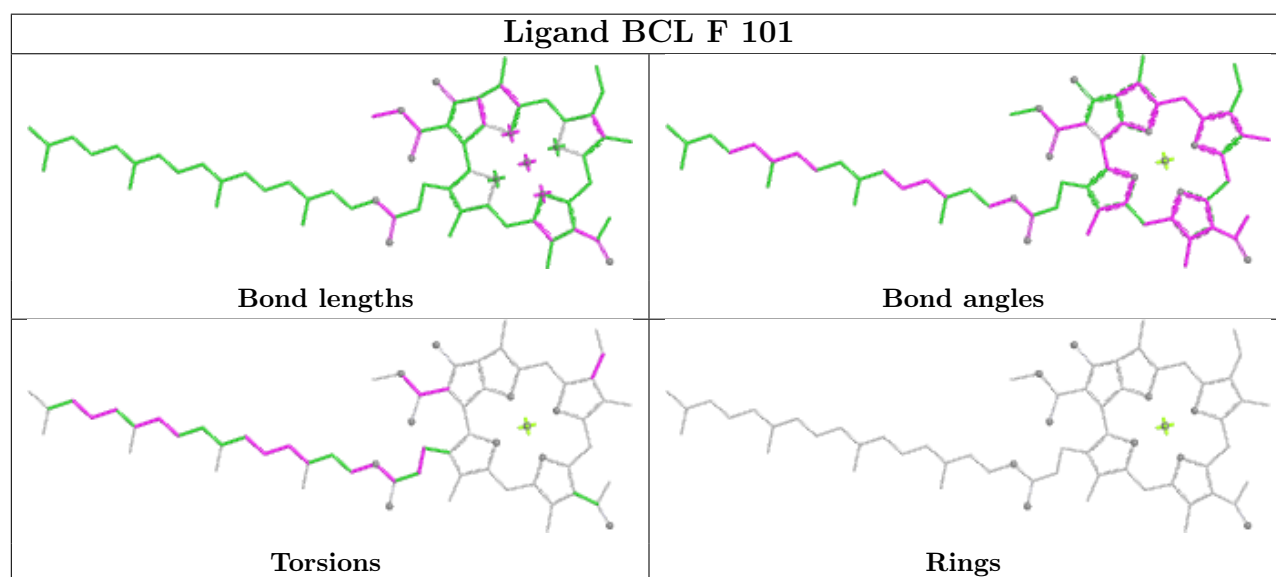
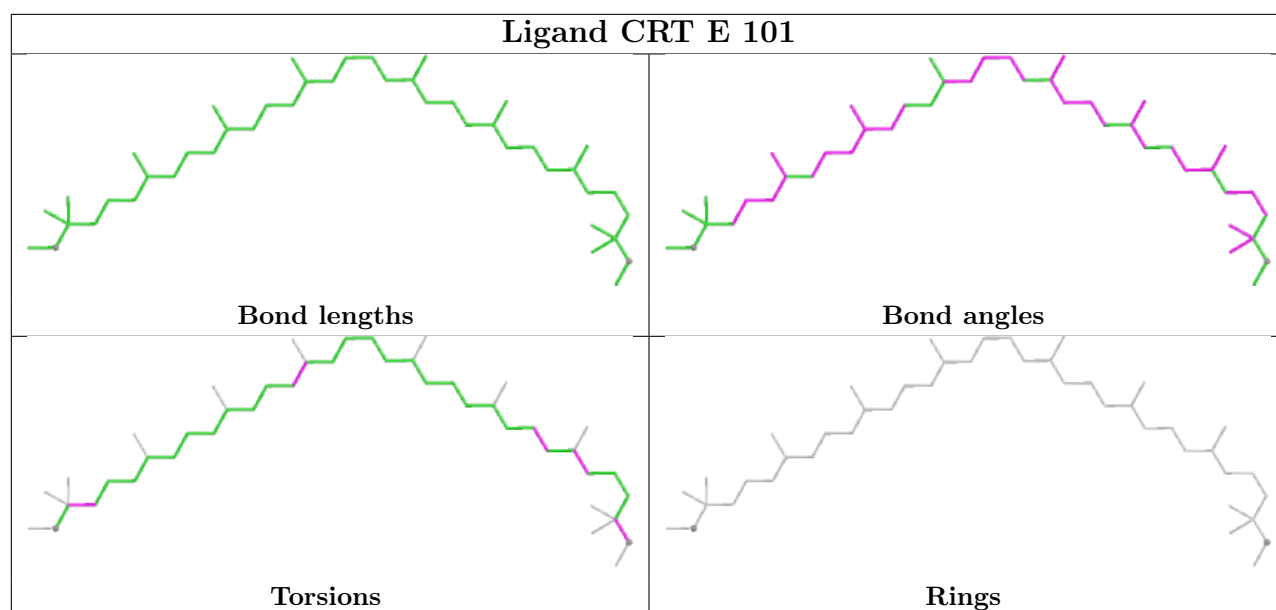


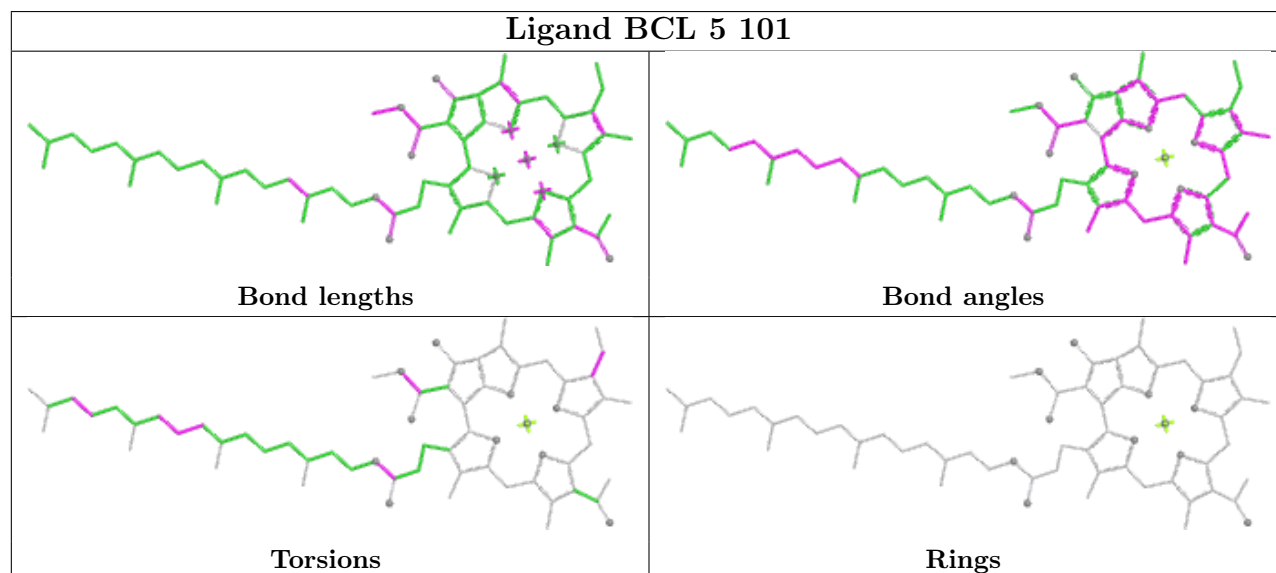
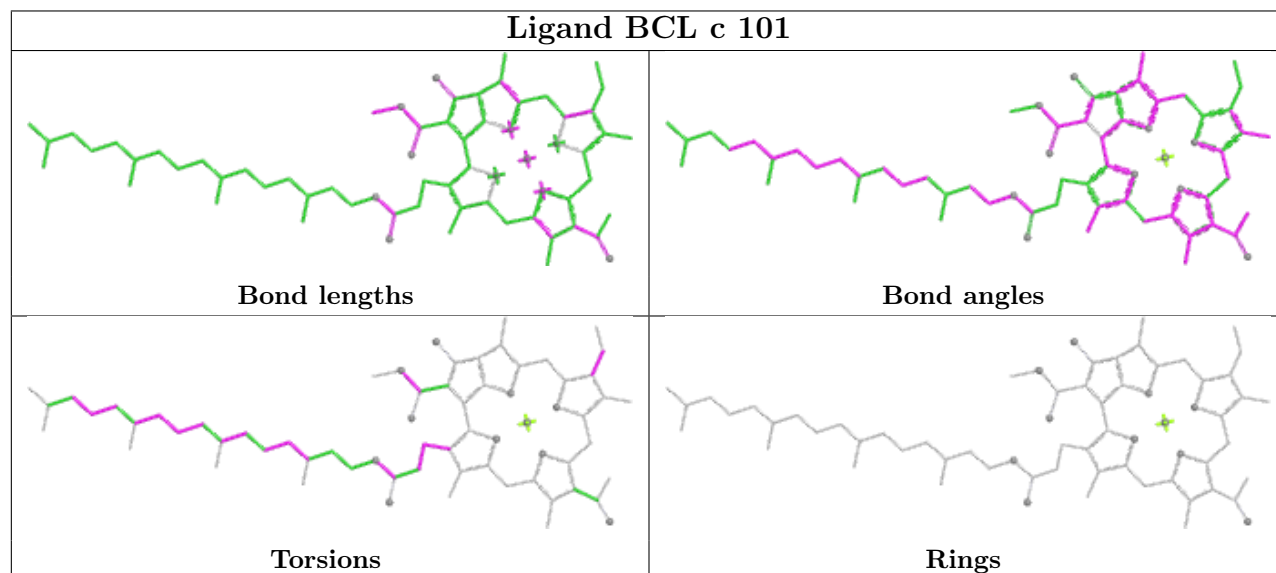
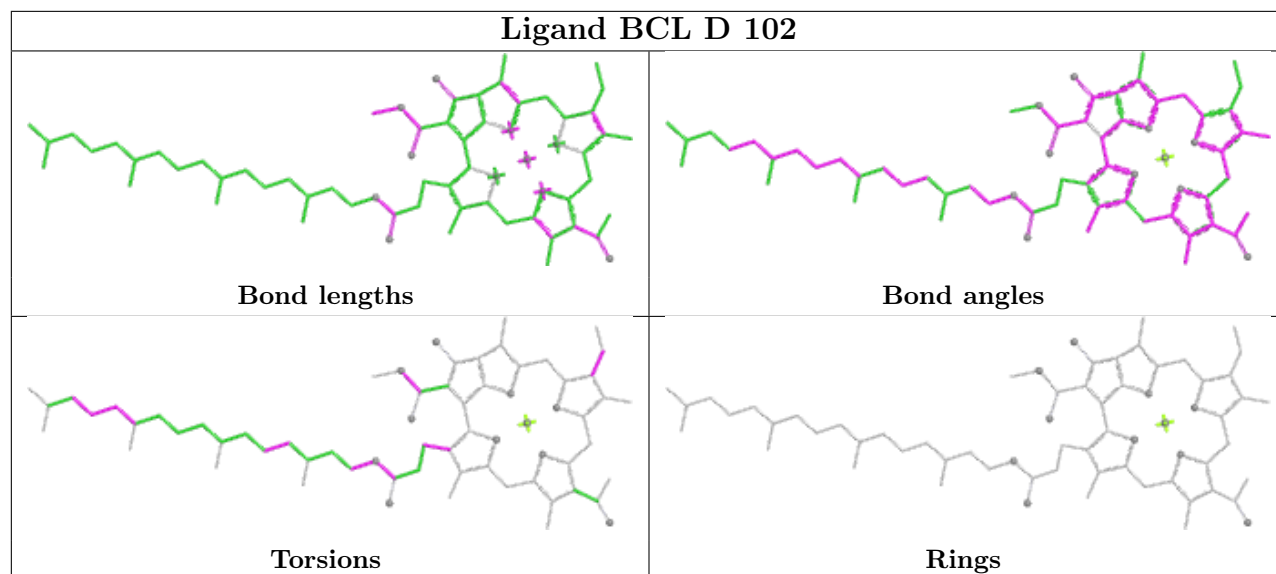


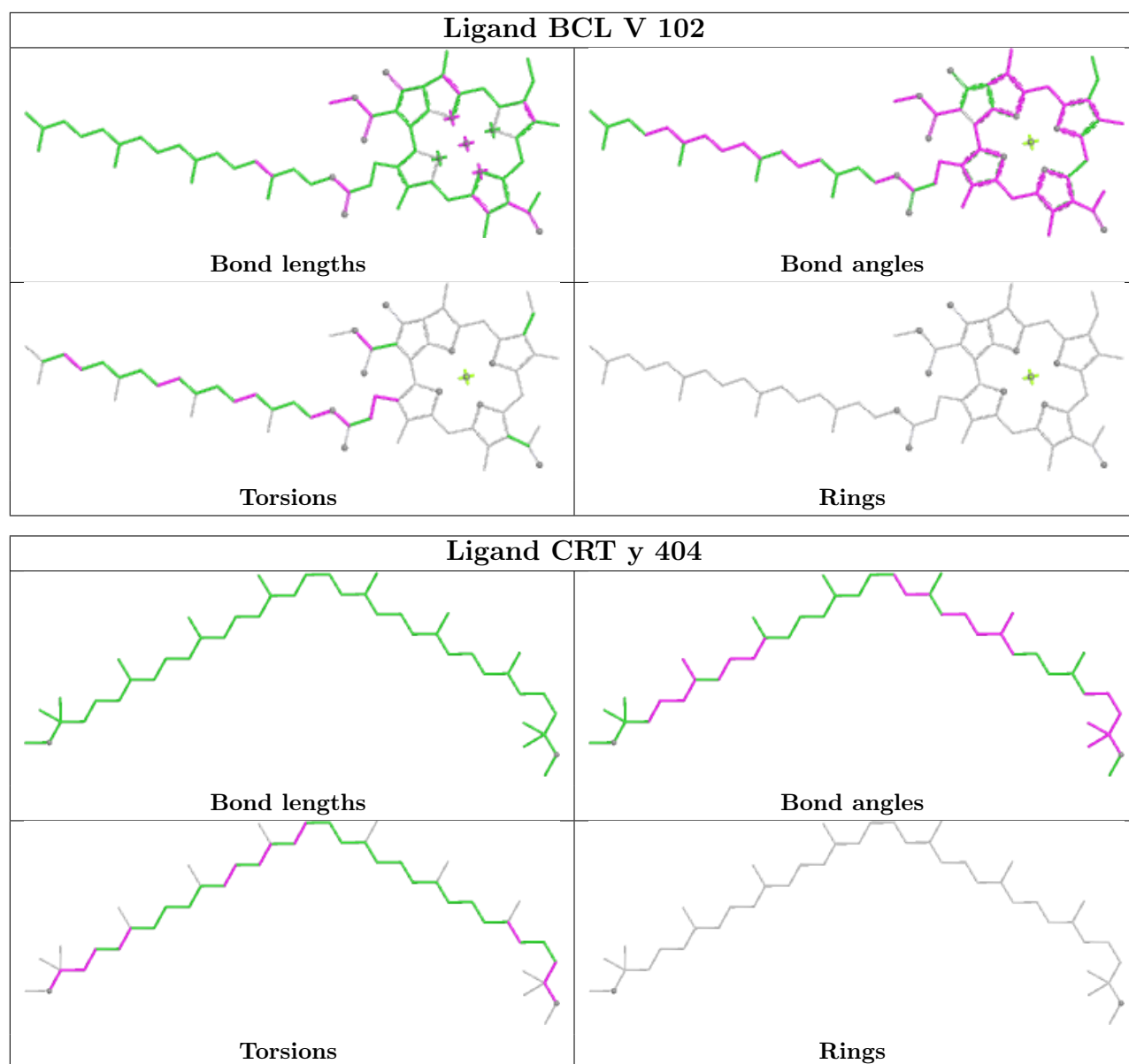


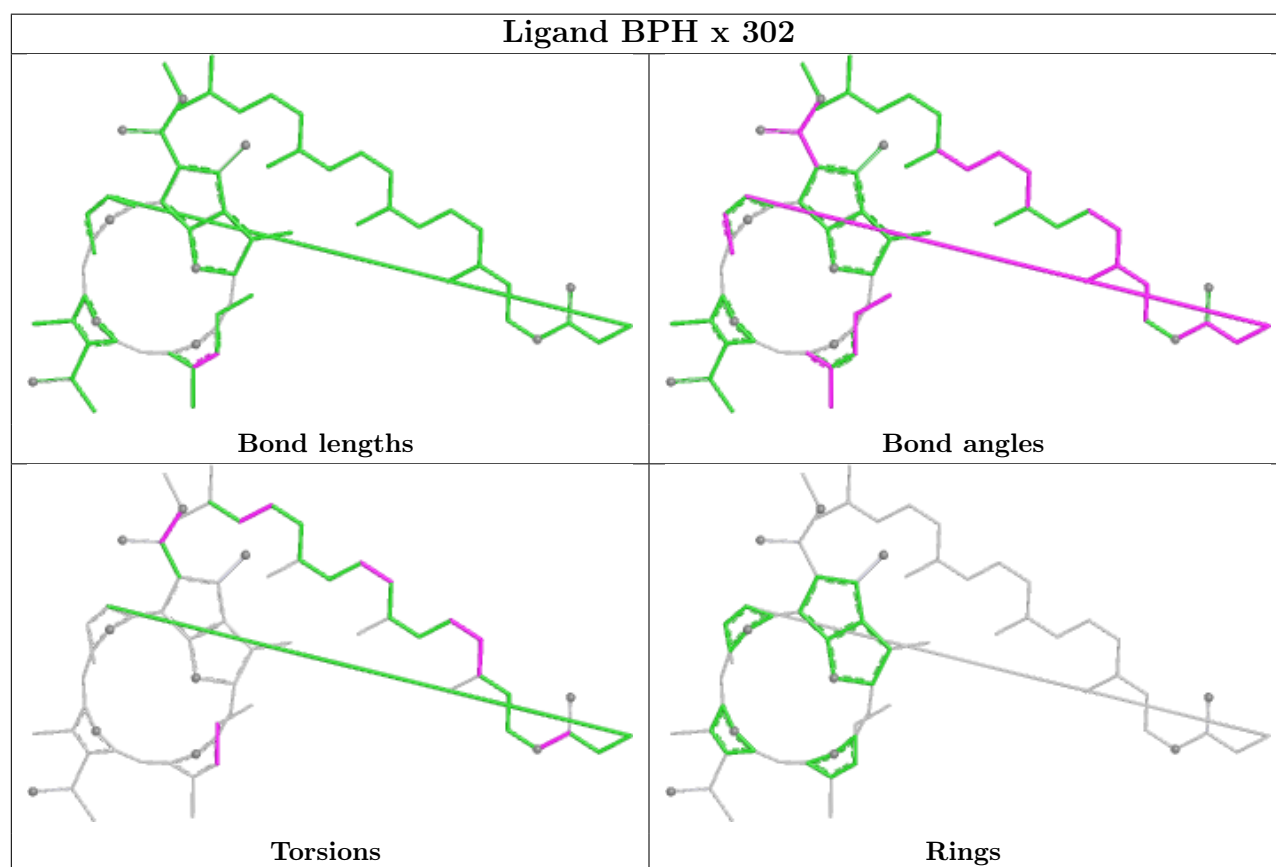
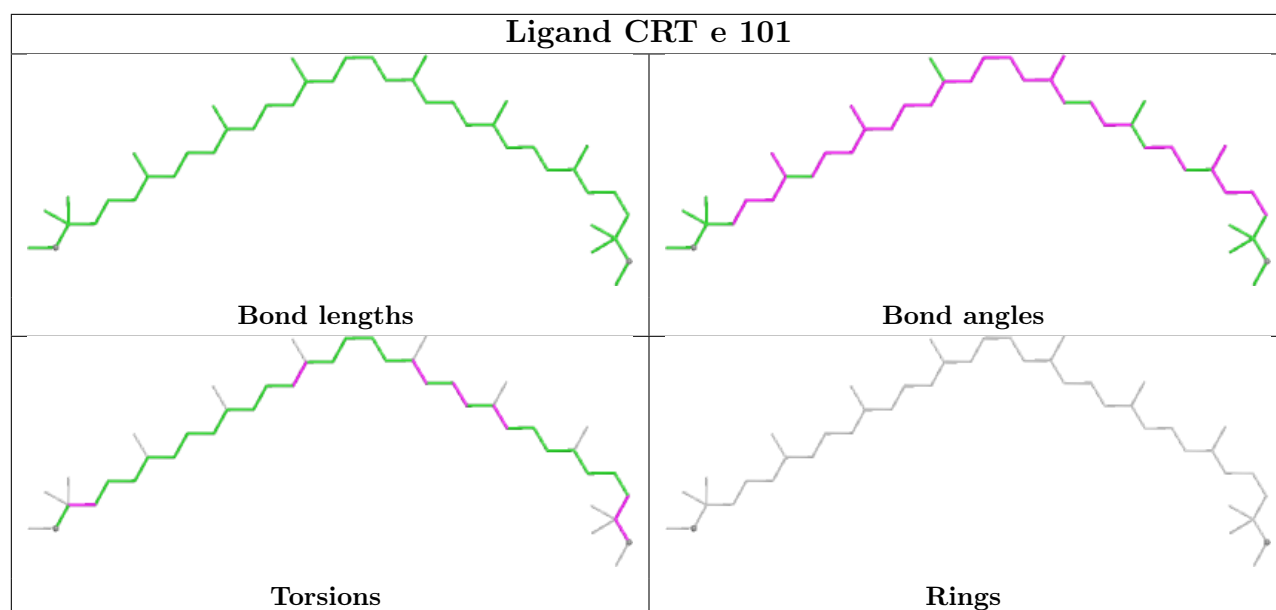




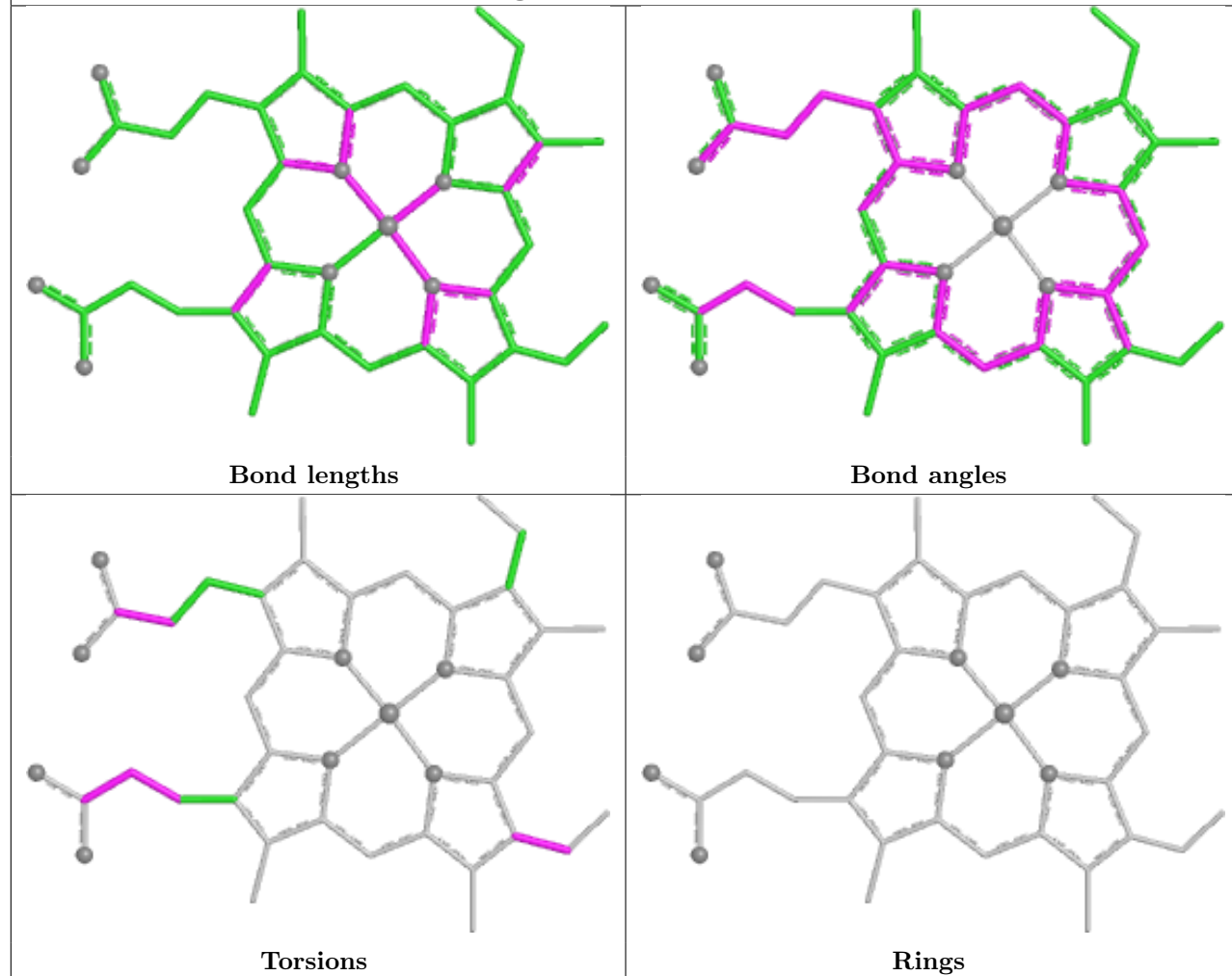


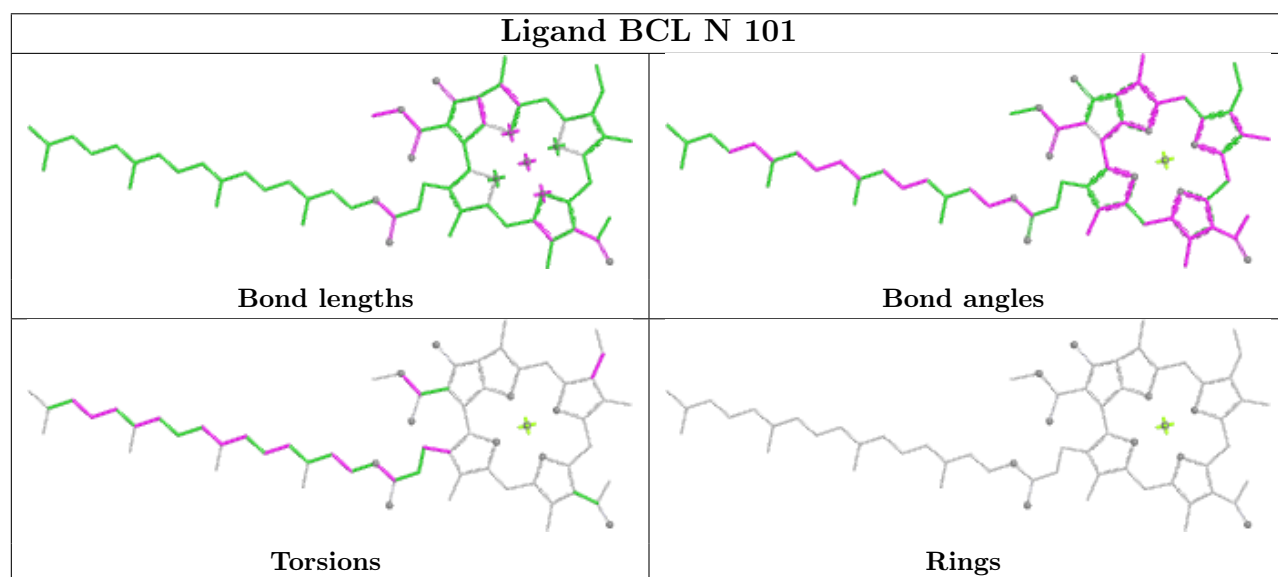
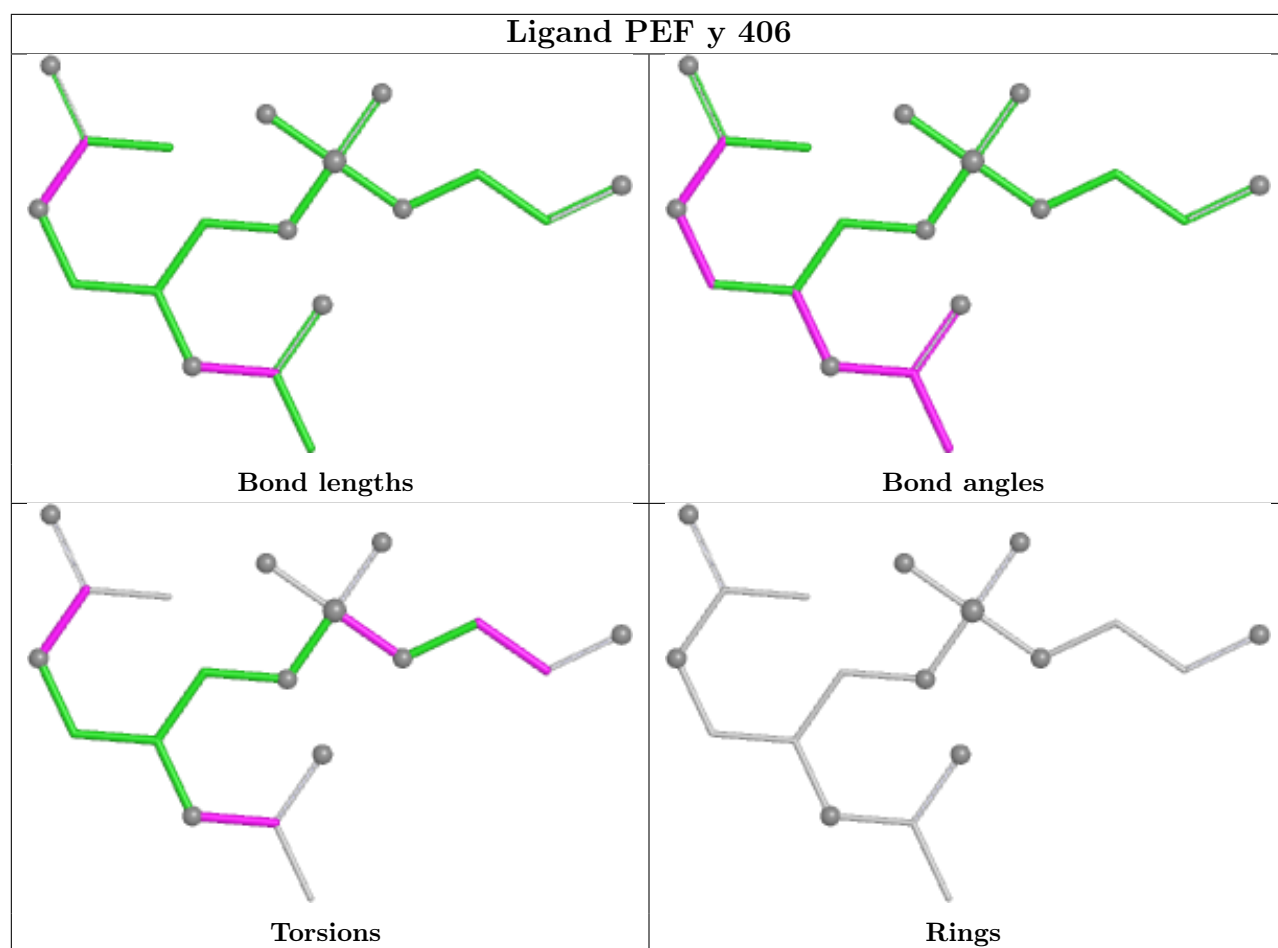


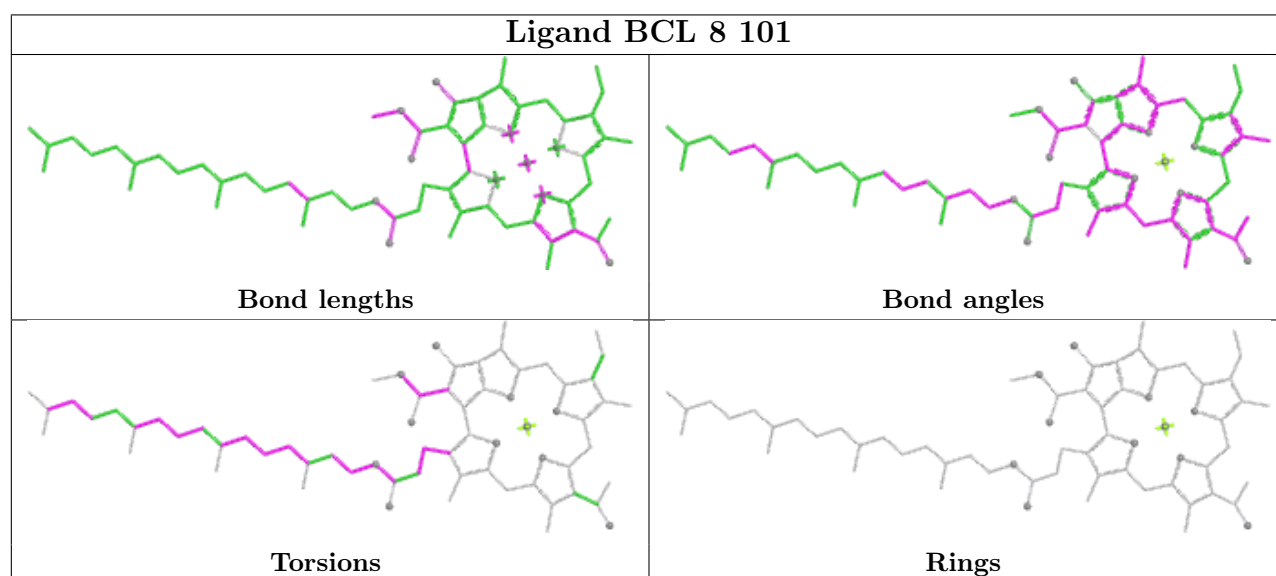
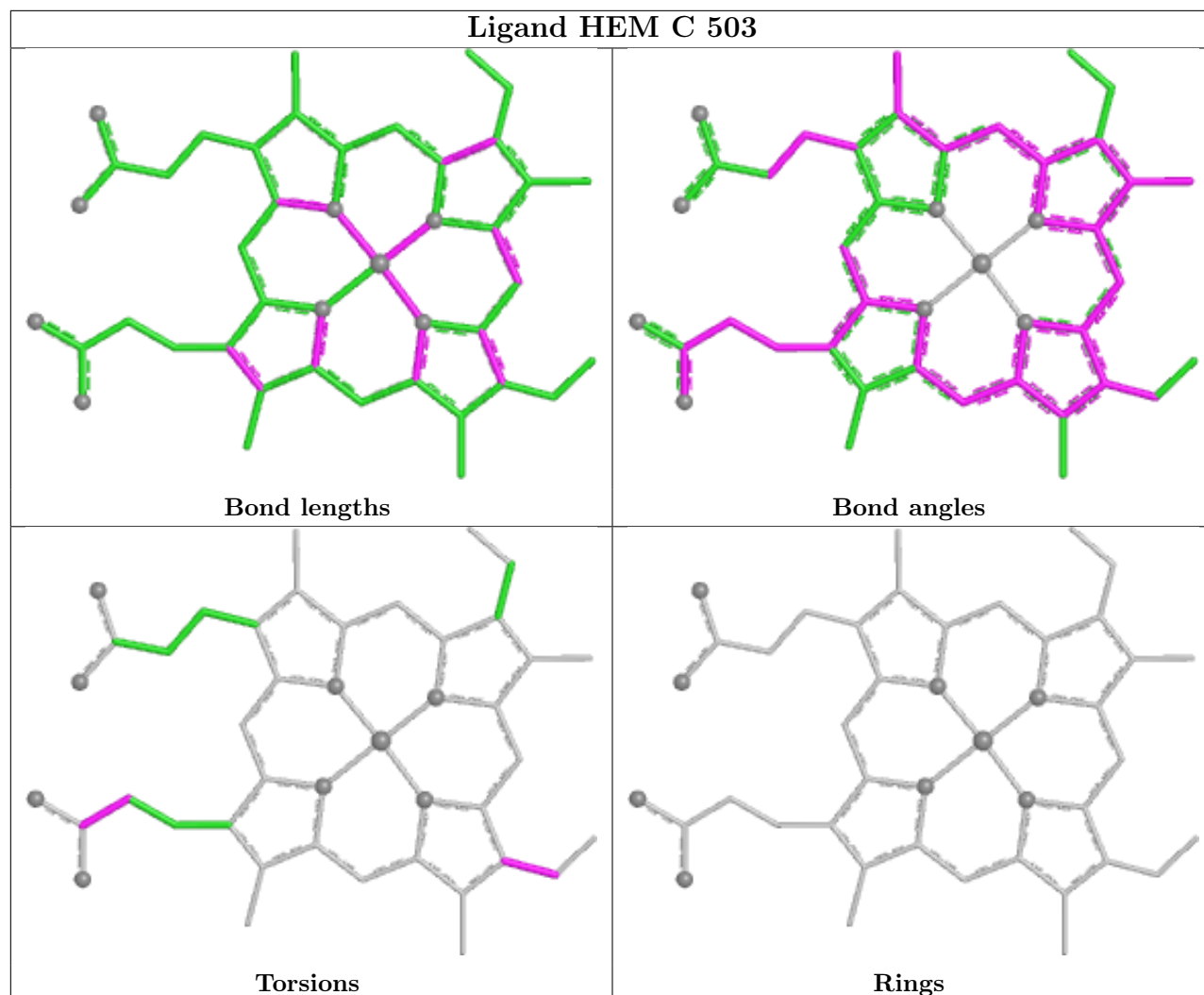


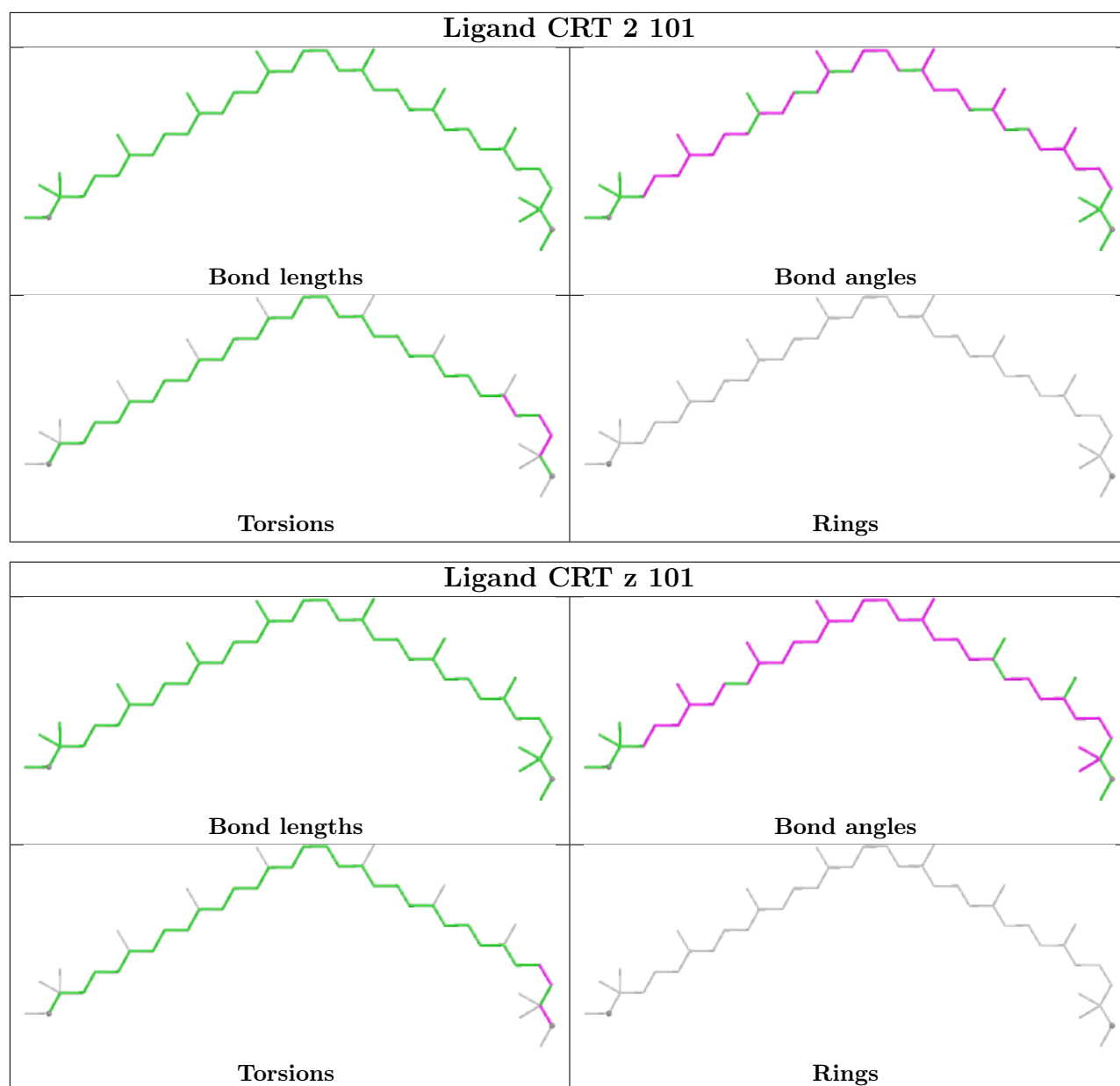


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5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	C	317/333 (95%)	0.34	20 (6%)	26	17	89, 118, 143, 160	0
1	o	317/333 (95%)	0.36	18 (5%)	29	20	97, 126, 153, 166	0
2	L	280/281 (99%)	0.26	15 (5%)	31	21	73, 99, 149, 173	0
2	x	280/281 (99%)	0.26	11 (3%)	43	29	75, 98, 145, 174	0
3	M	318/319 (99%)	0.20	15 (4%)	36	24	73, 105, 141, 160	0
3	y	318/319 (99%)	0.34	16 (5%)	34	23	73, 110, 148, 173	0
4	H	258/259 (99%)	0.03	4 (1%)	70	52	78, 105, 162, 245	0
4	t	258/259 (99%)	0.06	7 (2%)	56	37	84, 107, 140, 240	0
5	1	60/61 (98%)	0.37	3 (5%)	34	23	134, 157, 202, 223	0
5	3	60/61 (98%)	0.61	7 (11%)	9	8	137, 157, 204, 216	0
5	5	60/61 (98%)	0.70	7 (11%)	9	8	142, 169, 243, 251	0
5	7	60/61 (98%)	0.52	2 (3%)	49	33	155, 180, 257, 271	0
5	9	60/61 (98%)	0.19	2 (3%)	49	33	156, 191, 228, 241	0
5	A	60/61 (98%)	0.37	3 (5%)	34	23	165, 198, 248, 252	0
5	AA	60/61 (98%)	0.52	4 (6%)	24	16	157, 202, 261, 269	0
5	AC	60/61 (98%)	0.65	6 (10%)	12	10	161, 205, 258, 265	0
5	AE	60/61 (98%)	0.56	4 (6%)	24	16	88, 207, 255, 264	1 (1%)
5	AG	60/61 (98%)	0.36	3 (5%)	34	23	161, 192, 245, 246	0
5	AI	60/61 (98%)	0.35	6 (10%)	12	10	145, 177, 226, 231	0
5	AK	60/61 (98%)	0.36	7 (11%)	9	8	139, 163, 219, 236	0
5	D	60/61 (98%)	0.37	2 (3%)	49	33	161, 206, 256, 265	0
5	F	60/61 (98%)	0.42	3 (5%)	34	23	169, 210, 255, 258	0
5	I	60/61 (98%)	0.31	2 (3%)	49	33	178, 209, 255, 264	0
5	K	60/61 (98%)	0.50	6 (10%)	12	10	162, 203, 269, 278	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
5	O	60/61 (98%)	0.27	4 (6%)	24 16	140, 193, 265, 272	0
5	Q	60/61 (98%)	0.53	7 (11%)	9 8	142, 180, 254, 258	0
5	S	60/61 (98%)	0.34	1 (1%)	69 50	81, 189, 247, 254	1 (1%)
5	U	60/61 (98%)	0.60	7 (11%)	9 8	145, 178, 238, 244	0
5	W	60/61 (98%)	0.39	3 (5%)	34 23	131, 159, 215, 220	0
5	Y	60/61 (98%)	0.42	5 (8%)	17 13	128, 156, 220, 249	0
5	d	60/61 (98%)	0.38	3 (5%)	34 23	134, 165, 216, 223	0
5	f	60/61 (98%)	0.37	5 (8%)	17 13	143, 161, 217, 229	0
5	h	60/61 (98%)	0.48	5 (8%)	17 13	140, 170, 234, 249	0
5	j	60/61 (98%)	0.09	1 (1%)	69 50	149, 179, 230, 245	0
5	l	60/61 (98%)	0.60	7 (11%)	9 8	141, 174, 222, 231	0
5	m	60/61 (98%)	0.45	5 (8%)	17 13	142, 178, 239, 244	0
5	p	60/61 (98%)	0.66	6 (10%)	12 10	136, 182, 239, 240	0
5	r	60/61 (98%)	0.20	5 (8%)	17 13	143, 184, 248, 251	0
5	u	60/61 (98%)	0.59	7 (11%)	9 8	162, 195, 251, 260	0
5	w	60/61 (98%)	0.24	1 (1%)	69 50	165, 204, 259, 265	0
6	0	40/47 (85%)	0.09	1 (2%)	58 39	166, 222, 247, 250	0
6	2	40/47 (85%)	-0.10	0	100 100	164, 179, 206, 212	0
6	4	40/47 (85%)	-0.31	1 (2%)	58 39	162, 176, 195, 200	0
6	6	40/47 (85%)	-0.14	0	100 100	174, 192, 206, 209	0
6	8	40/47 (85%)	0.15	2 (5%)	34 23	186, 217, 229, 232	0
6	AB	40/47 (85%)	0.25	3 (7%)	20 15	177, 217, 249, 252	0
6	AD	40/47 (85%)	0.21	1 (2%)	58 39	196, 226, 250, 256	0
6	AF	40/47 (85%)	0.15	1 (2%)	58 39	211, 233, 245, 251	0
6	AH	40/47 (85%)	0.21	4 (10%)	12 10	201, 219, 238, 242	0
6	AJ	40/47 (85%)	0.03	1 (2%)	58 39	180, 200, 220, 224	0
6	AL	40/47 (85%)	0.17	2 (5%)	34 23	169, 183, 204, 214	0
6	B	40/47 (85%)	0.07	2 (5%)	34 23	180, 225, 250, 252	0
6	E	40/47 (85%)	0.32	3 (7%)	20 15	186, 222, 253, 255	0
6	G	40/47 (85%)	0.13	2 (5%)	34 23	182, 227, 257, 259	0
6	J	40/47 (85%)	0.30	2 (5%)	34 23	187, 227, 259, 261	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	N	40/47 (85%)	0.28	2 (5%) 34 23	167, 212, 250, 252	0
6	P	40/47 (85%)	0.14	3 (7%) 20 15	166, 212, 248, 255	0
6	R	40/47 (85%)	0.15	3 (7%) 20 15	164, 208, 240, 243	0
6	T	40/47 (85%)	-0.06	2 (5%) 34 23	178, 211, 230, 241	0
6	V	40/47 (85%)	-0.34	0 100 100	172, 198, 213, 222	0
6	X	40/47 (85%)	0.00	0 100 100	162, 182, 195, 198	0
6	Z	40/47 (85%)	-0.13	0 100 100	161, 175, 196, 201	0
6	c	40/47 (85%)	0.23	3 (7%) 20 15	151, 202, 239, 250	0
6	e	40/47 (85%)	-0.04	1 (2%) 58 39	172, 185, 215, 220	0
6	g	40/47 (85%)	-0.15	1 (2%) 58 39	180, 190, 212, 218	0
6	i	40/47 (85%)	-0.07	1 (2%) 58 39	182, 201, 214, 214	0
6	k	40/47 (85%)	-0.14	1 (2%) 58 39	175, 212, 229, 243	0
6	n	40/47 (85%)	0.23	1 (2%) 58 39	146, 196, 239, 246	0
6	q	40/47 (85%)	-0.07	2 (5%) 34 23	152, 190, 235, 243	0
6	s	40/47 (85%)	-0.01	1 (2%) 58 39	156, 194, 238, 243	0
6	v	40/47 (85%)	0.19	1 (2%) 58 39	175, 201, 247, 250	0
6	z	40/47 (85%)	0.05	0 100 100	176, 210, 255, 256	0
All	All	5546/5840 (94%)	0.26	292 (5%) 32 22	73, 162, 243, 278	2 (0%)

The worst 5 of 292 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	f	54	SER	10.3
5	3	46	TRP	6.9
1	o	321	ALA	6.6
4	t	56	VAL	6.5
5	m	37	MET	6.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	PGW	AE	101	21/51	0.60	0.13	141,155,167,171	0
12	PEF	y	406	19/47	0.61	0.12	116,122,128,131	0
17	PGW	S	101	21/51	0.62	0.14	122,133,142,147	0
12	PEF	H	304	19/47	0.65	0.14	160,166,175,180	0
16	PO4	y	405	5/5	0.66	0.12	134,136,141,141	0
12	PEF	m	101	19/47	0.68	0.19	119,125,133,136	0
12	PEF	A	101	19/47	0.68	0.17	142,147,157,161	0
12	PEF	x	306	19/47	0.69	0.11	97,102,107,107	0
16	PO4	H	303	5/5	0.72	0.09	158,160,164,166	0
12	PEF	y	408	19/47	0.75	0.11	102,108,116,118	0
16	PO4	t	302	5/5	0.78	0.13	142,142,144,149	0
12	PEF	M	408	19/47	0.78	0.11	95,99,103,105	0
12	PEF	y	407	19/47	0.78	0.12	97,101,106,108	0
12	PEF	L	305	12/47	0.79	0.12	113,118,123,123	0
9	BCL	I	103	66/66	0.82	0.16	200,223,264,273	0
15	CRT	T	101	44/44	0.82	0.20	154,186,198,199	0
15	CRT	7	103	44/44	0.82	0.22	171,193,205,208	0
12	PEF	H	301	19/47	0.82	0.10	108,115,119,121	0
15	CRT	m	104	44/44	0.83	0.18	171,183,189,191	0
15	CRT	v	101	44/44	0.83	0.18	170,189,194,196	0
15	CRT	AC	101	44/44	0.83	0.18	180,197,200,202	0
15	CRT	AL	101	44/44	0.83	0.24	130,168,200,203	0
9	BCL	D	102	66/66	0.83	0.15	194,218,258,259	0
9	BCL	AC	103	66/66	0.83	0.18	188,211,257,265	0
15	CRT	O	101	44/44	0.83	0.18	179,194,202,205	0
9	BCL	AG	101	66/66	0.83	0.20	179,190,215,226	0
9	BCL	d	101	66/66	0.83	0.15	131,157,168,173	0
12	PEF	H	302	19/47	0.84	0.13	139,156,167,170	0
9	BCL	p	102	66/66	0.84	0.16	128,189,203,208	0
12	PEF	p	101	16/47	0.84	0.15	131,142,148,151	0
15	CRT	I	102	44/44	0.84	0.20	194,205,211,214	0
9	BCL	u	102	66/66	0.85	0.15	181,205,248,268	0
15	CRT	e	101	44/44	0.85	0.25	140,173,206,210	0
12	PEF	M	407	16/47	0.85	0.10	86,89,91,92	0
9	BCL	l	101	66/66	0.85	0.12	123,149,159,163	0
9	BCL	m	103	66/66	0.85	0.13	173,198,219,230	0
9	BCL	D	101	66/66	0.85	0.15	153,209,226,231	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CRT	AH	102	44/44	0.85	0.17	155,198,229,231	0
9	BCL	AB	102	66/66	0.86	0.14	187,214,258,267	0
9	BCL	f	101	66/66	0.86	0.15	144,163,174,180	0
9	BCL	w	101	66/66	0.86	0.16	176,199,217,222	0
15	CRT	i	101	44/44	0.86	0.19	156,180,197,201	0
12	PEF	t	303	19/47	0.86	0.10	94,97,104,104	0
15	CRT	0	101	44/44	0.86	0.19	175,197,206,206	0
9	BCL	AE	102	66/66	0.86	0.11	188,207,244,262	0
9	BCL	z	102	66/66	0.86	0.13	183,211,253,269	0
15	CRT	G	101	44/44	0.86	0.19	187,209,215,218	0
9	BCL	AC	102	66/66	0.87	0.13	181,205,218,228	0
9	BCL	N	101	66/66	0.87	0.14	189,213,255,262	0
15	CRT	AJ	101	44/44	0.87	0.17	139,182,214,217	0
15	CRT	R	101	44/44	0.87	0.19	159,181,189,191	0
9	BCL	k	102	66/66	0.87	0.15	171,195,223,234	0
15	CRT	4	101	44/44	0.87	0.19	141,166,185,190	0
15	CRT	k	101	44/44	0.87	0.17	166,186,199,202	0
11	UQ8	x	304	53/53	0.87	0.14	80,87,90,91	0
12	PEF	H	305	19/47	0.87	0.11	93,97,104,105	0
9	BCL	P	101	66/66	0.87	0.14	173,201,216,221	0
15	CRT	n	101	44/44	0.87	0.19	166,179,185,189	0
9	BCL	G	102	66/66	0.87	0.13	197,220,264,265	0
9	BCL	u	101	66/66	0.88	0.14	133,196,212,216	0
15	CRT	M	405	44/44	0.88	0.15	90,108,139,148	0
15	CRT	g	101	44/44	0.88	0.19	145,172,198,202	0
9	BCL	m	102	66/66	0.88	0.16	157,190,207,214	0
9	BCL	V	102	66/66	0.88	0.14	162,177,208,223	0
15	CRT	q	101	44/44	0.88	0.15	159,174,179,182	0
9	BCL	g	102	66/66	0.88	0.17	153,171,206,215	0
8	BA	A	105	1/1	0.88	0.17	243,243,243,243	0
11	UQ8	L	304	53/53	0.88	0.13	81,86,88,89	0
9	BCL	AF	101	66/66	0.88	0.15	161,205,215,225	0
9	BCL	c	101	66/66	0.89	0.12	173,199,243,258	0
15	CRT	AF	102	44/44	0.89	0.15	170,212,229,231	0
9	BCL	U	101	66/66	0.89	0.16	153,176,186,191	0
8	BA	7	104	1/1	0.89	0.19	215,215,215,215	0
7	HEM	o	501	43/43	0.89	0.17	129,137,145,148	0
9	BCL	2	102	66/66	0.89	0.13	145,156,185,195	0
12	PEF	t	301	19/47	0.89	0.10	100,104,107,108	0
9	BCL	e	102	66/66	0.89	0.14	152,164,191,197	0
15	CRT	y	404	44/44	0.89	0.16	99,115,146,154	0
9	BCL	O	102	66/66	0.89	0.14	179,206,250,251	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	BCL	I	101	66/66	0.89	0.12	149,216,231,234	0
9	BCL	h	101	66/66	0.89	0.14	155,171,185,187	0
9	BCL	T	102	66/66	0.89	0.14	166,185,223,243	0
15	CRT	z	101	44/44	0.89	0.20	176,193,197,198	0
15	CRT	s	101	44/44	0.90	0.14	163,178,182,183	0
9	BCL	AI	102	66/66	0.90	0.13	163,172,197,203	0
9	BCL	AL	102	66/66	0.90	0.16	152,161,183,190	0
15	CRT	P	102	44/44	0.90	0.15	170,186,189,190	0
15	CRT	AD	101	44/44	0.90	0.19	175,204,211,213	0
9	BCL	K	101	66/66	0.90	0.16	183,209,225,229	0
9	BCL	Q	101	66/66	0.90	0.15	166,193,205,211	0
15	CRT	V	101	44/44	0.90	0.16	140,179,197,198	0
15	CRT	2	101	44/44	0.90	0.16	136,165,190,194	0
9	BCL	6	101	66/66	0.90	0.17	154,174,210,221	0
15	CRT	7	101	44/44	0.90	0.19	155,177,191,193	0
9	BCL	7	102	66/66	0.90	0.15	163,180,195,200	0
15	CRT	9	101	44/44	0.90	0.15	181,205,211,215	0
9	BCL	0	102	66/66	0.90	0.12	183,208,254,257	0
9	BCL	j	101	66/66	0.90	0.13	166,183,198,203	0
9	BCL	S	102	66/66	0.90	0.16	136,186,197,205	0
15	CRT	E	101	44/44	0.90	0.13	179,205,211,213	0
9	BCL	AI	101	66/66	0.90	0.14	167,179,190,196	0
9	BCL	s	102	66/66	0.91	0.12	174,198,247,260	0
15	CRT	Z	101	44/44	0.91	0.14	127,160,186,189	0
9	BCL	8	101	66/66	0.91	0.11	173,196,221,230	0
9	BCL	9	102	66/66	0.91	0.12	165,191,211,216	0
9	BCL	X	102	66/66	0.91	0.11	148,159,180,192	0
14	MQ8	M	404	53/53	0.91	0.13	82,100,144,151	0
14	MQ8	y	403	53/53	0.91	0.15	79,93,131,138	0
9	BCL	AH	101	66/66	0.91	0.13	182,196,206,212	0
9	BCL	3	101	66/66	0.91	0.13	138,153,165,168	0
9	BCL	l	101	66/66	0.91	0.11	157,189,205,210	0
16	PO4	M	406	5/5	0.91	0.09	121,126,127,128	0
9	BCL	AB	101	66/66	0.91	0.12	176,202,220,226	0
10	BPH	M	403	65/65	0.91	0.13	84,88,117,126	0
10	BPH	y	402	65/65	0.91	0.15	87,95,132,142	0
9	BCL	Z	102	66/66	0.91	0.13	143,151,174,182	0
9	BCL	R	102	66/66	0.91	0.11	170,194,236,245	0
9	BCL	x	305	66/66	0.92	0.14	83,90,98,105	0
9	BCL	y	401	66/66	0.92	0.16	86,93,102,106	0
9	BCL	A	102	66/66	0.92	0.12	182,205,221,225	0
15	CRT	X	101	44/44	0.92	0.15	129,166,188,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	BA	I	104	1/1	0.92	0.14	276,276,276,276	0
8	BA	U	102	1/1	0.92	0.22	224,224,224,224	0
9	BCL	q	102	66/66	0.92	0.15	170,194,226,241	0
9	BCL	r	101	66/66	0.92	0.12	160,190,204,208	0
9	BCL	F	101	66/66	0.92	0.14	183,211,226,232	0
9	BCL	AK	101	66/66	0.92	0.14	152,162,177,193	0
8	BA	3	102	1/1	0.92	0.16	191,191,191,191	0
7	HEM	C	501	43/43	0.92	0.14	118,126,133,136	0
8	BA	u	103	1/1	0.92	0.17	264,264,264,264	0
8	BA	w	102	1/1	0.92	0.09	271,271,271,271	0
8	BA	AE	103	1/1	0.92	0.10	248,248,248,248	0
9	BCL	x	301	66/66	0.92	0.18	81,86,92,97	0
9	BCL	i	102	66/66	0.92	0.12	161,181,218,232	0
9	BCL	M	401	66/66	0.93	0.13	86,94,107,114	0
9	BCL	W	101	66/66	0.93	0.14	152,165,171,179	0
9	BCL	L	303	66/66	0.93	0.16	79,86,91,96	0
9	BCL	Y	101	66/66	0.93	0.13	142,152,162,174	0
9	BCL	A	103	66/66	0.93	0.12	190,213,242,251	0
9	BCL	5	101	66/66	0.94	0.14	147,166,178,183	0
8	BA	x	308	1/1	0.94	0.07	175,175,175,175	0
9	BCL	M	402	66/66	0.94	0.12	83,90,96,99	0
9	BCL	x	303	66/66	0.94	0.14	82,89,97,98	0
10	BPH	x	302	65/65	0.94	0.15	78,84,104,106	0
8	BA	m	106	1/1	0.94	0.06	242,242,242,242	0
7	HEM	o	503	43/43	0.95	0.16	98,109,122,124	0
8	BA	O	103	1/1	0.95	0.14	244,244,244,244	0
10	BPH	L	302	65/65	0.95	0.11	79,88,109,114	0
7	HEM	o	504	43/43	0.95	0.16	111,114,119,122	0
8	BA	W	102	1/1	0.95	0.12	209,209,209,209	0
8	BA	A	104	1/1	0.95	0.11	247,247,247,247	0
8	BA	AI	103	1/1	0.95	0.13	210,210,210,210	0
8	BA	f	102	1/1	0.95	0.08	205,205,205,205	0
9	BCL	L	301	66/66	0.95	0.13	79,84,98,103	0
7	HEM	C	502	43/43	0.95	0.18	108,114,120,121	0
9	BCL	4	102	66/66	0.95	0.10	144,159,189,198	0
8	BA	D	103	1/1	0.96	0.16	252,252,252,252	0
8	BA	F	102	1/1	0.96	0.11	271,271,271,271	0
8	BA	AK	102	1/1	0.96	0.09	186,186,186,186	0
8	BA	L	306	1/1	0.96	0.05	185,185,185,185	0
8	BA	K	102	1/1	0.96	0.14	265,265,265,265	0
7	HEM	C	504	43/43	0.96	0.16	105,106,110,111	0
8	BA	p	103	1/1	0.96	0.11	257,257,257,257	0

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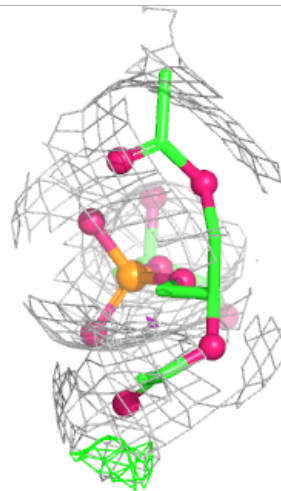
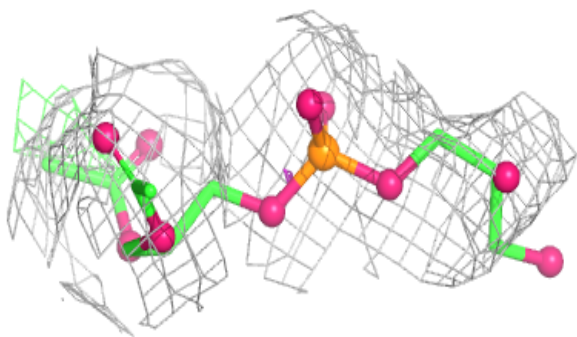
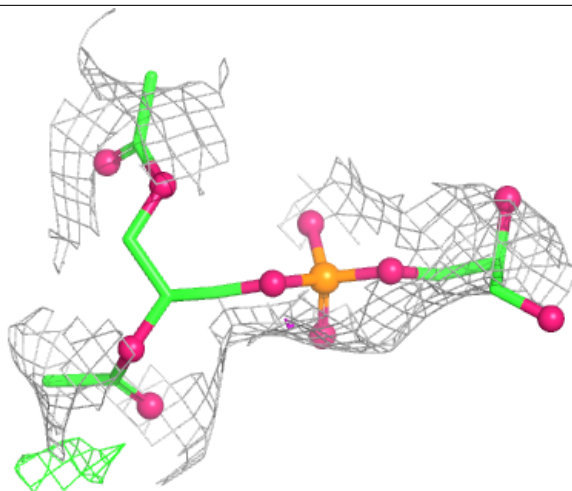
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	BA	Q	102	1/1	0.96	0.12	245,245,245,245	0
7	HEM	o	502	43/43	0.96	0.15	119,124,128,129	0
8	BA	AC	104	1/1	0.96	0.10	257,257,257,257	0
8	BA	d	102	1/1	0.97	0.07	174,174,174,174	0
8	BA	5	102	1/1	0.97	0.16	212,212,212,212	0
8	BA	m	105	1/1	0.97	0.08	226,226,226,226	0
8	BA	AG	102	1/1	0.97	0.08	225,225,225,225	0
7	HEM	C	503	43/43	0.97	0.17	96,107,121,123	0
8	BA	AA	101	1/1	0.97	0.06	260,260,260,260	0
8	BA	r	102	1/1	0.98	0.08	250,250,250,250	0
8	BA	j	102	1/1	0.98	0.04	228,228,228,228	0
8	BA	C	505	1/1	0.98	0.09	93,93,93,93	0
8	BA	L	307	1/1	0.98	0.03	160,160,160,160	0
8	BA	l	102	1/1	0.98	0.09	177,177,177,177	0
8	BA	x	307	1/1	0.98	0.04	186,186,186,186	0
8	BA	o	505	1/1	0.99	0.10	100,100,100,100	0
8	BA	S	103	1/1	0.99	0.10	227,227,227,227	0
13	FE	x	309	1/1	0.99	0.07	76,76,76,76	0
8	BA	h	102	1/1	0.99	0.13	210,210,210,210	0
8	BA	Y	102	1/1	0.99	0.14	181,181,181,181	0
13	FE	L	308	1/1	1.00	0.06	76,76,76,76	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.

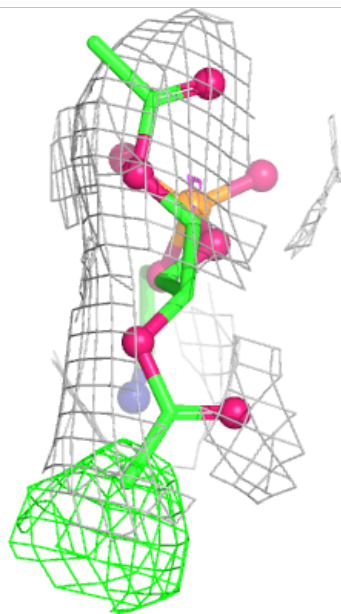
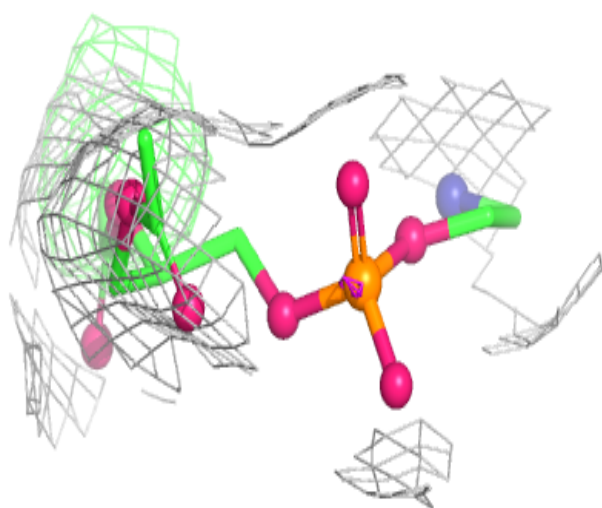
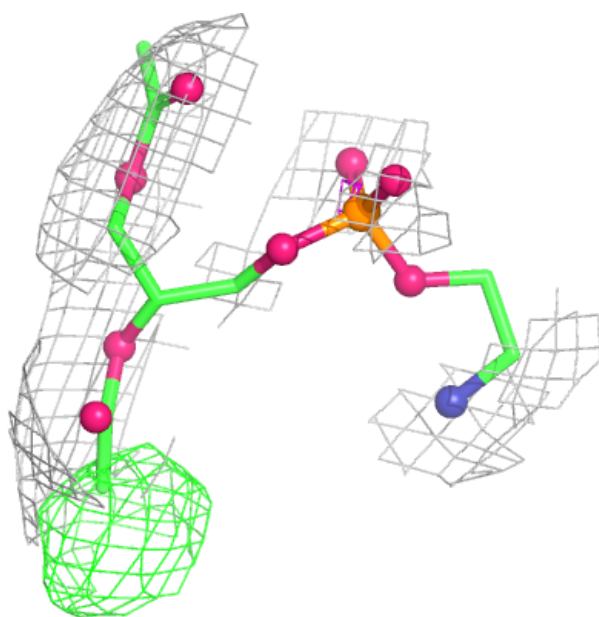
Electron density around PGW AE 101:

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



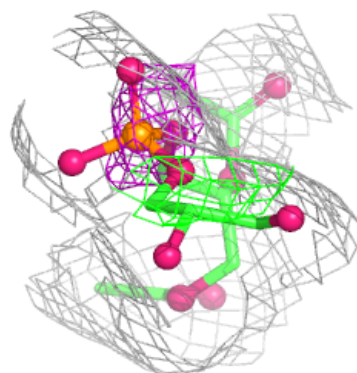
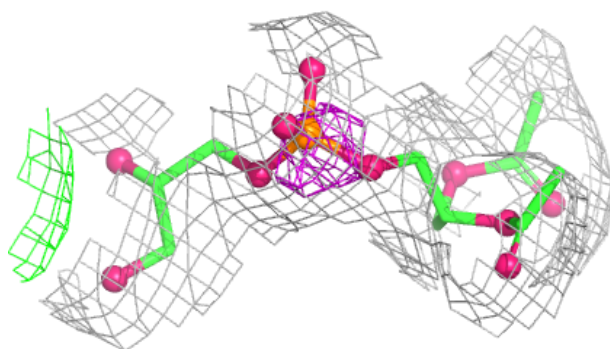
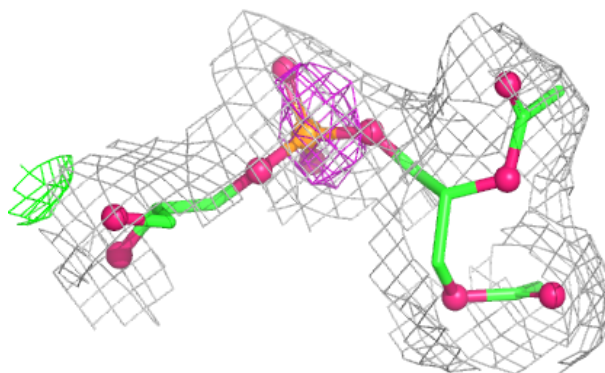
Electron density around PEF y 406:

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

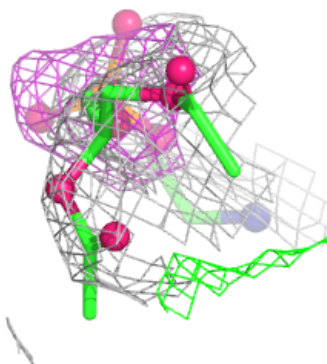
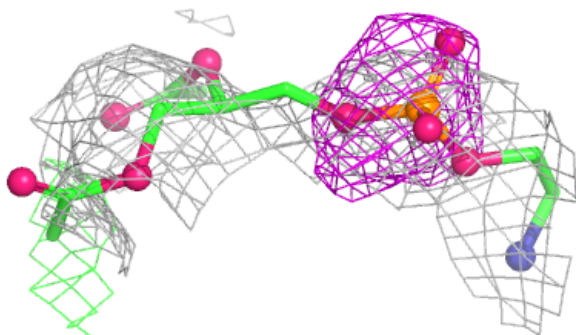
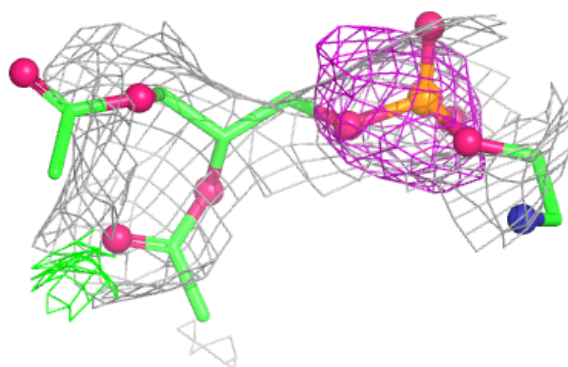


Electron density around PGW S 101:

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

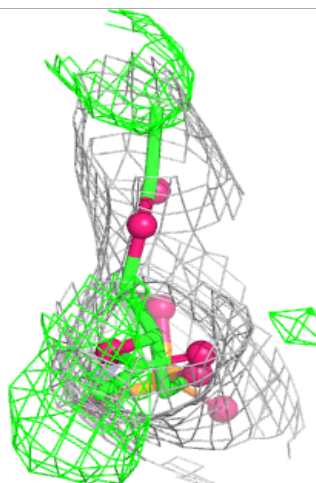
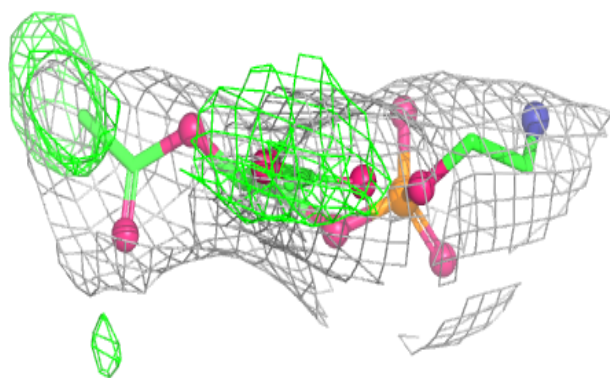
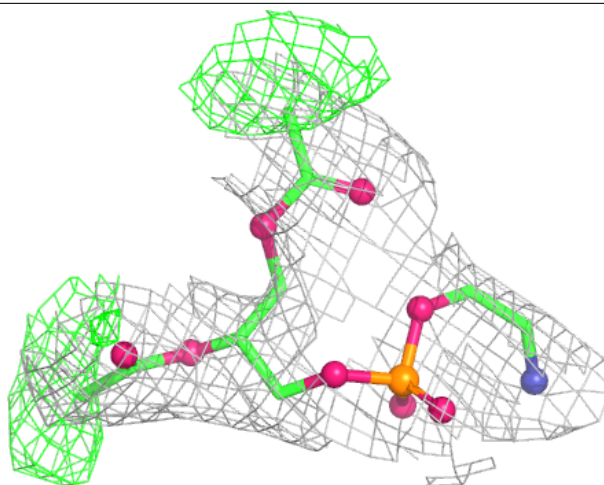
**Electron density around PEF H 304:**

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



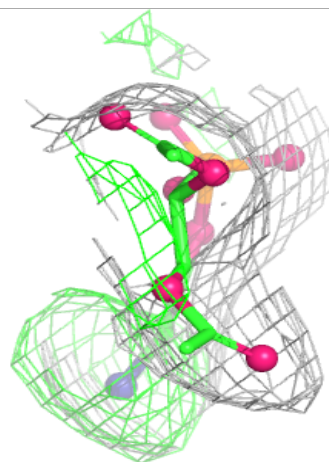
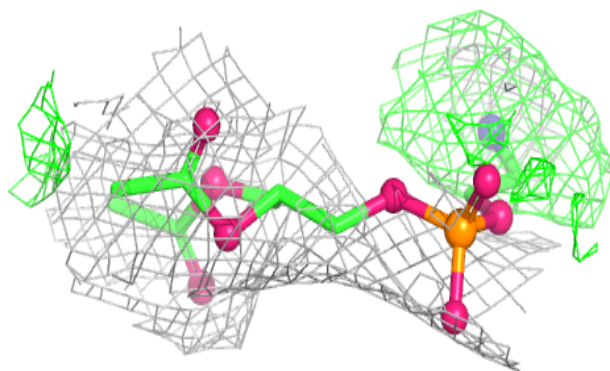
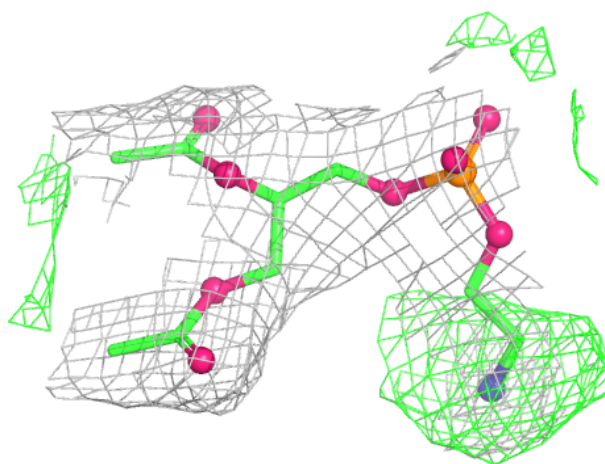
Electron density around PEF m 101:

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



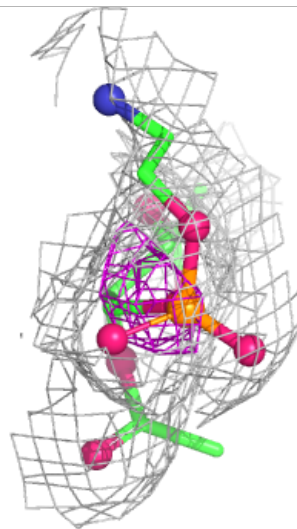
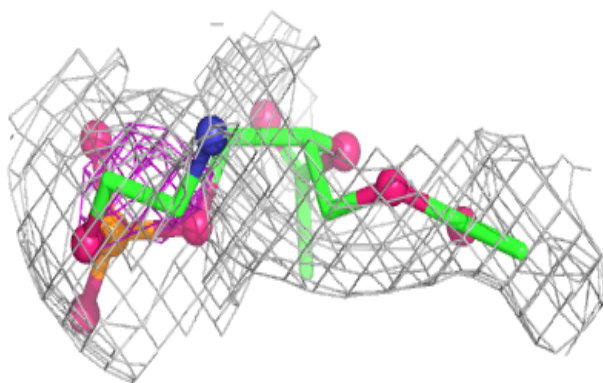
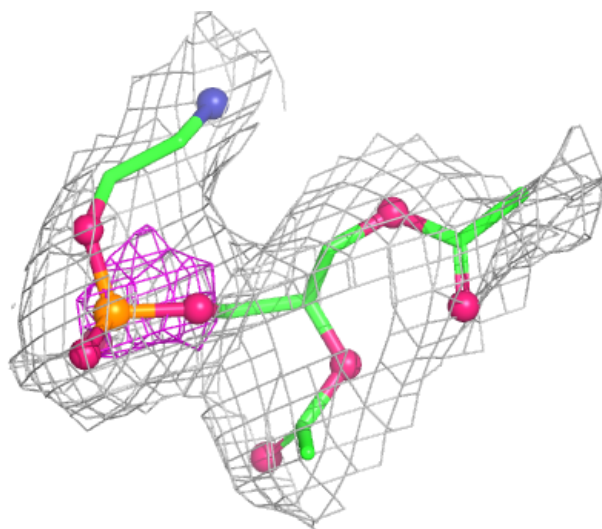
Electron density around PEF A 101:

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



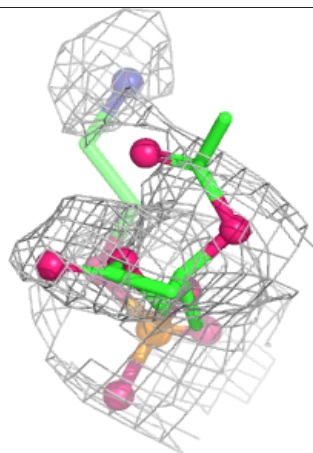
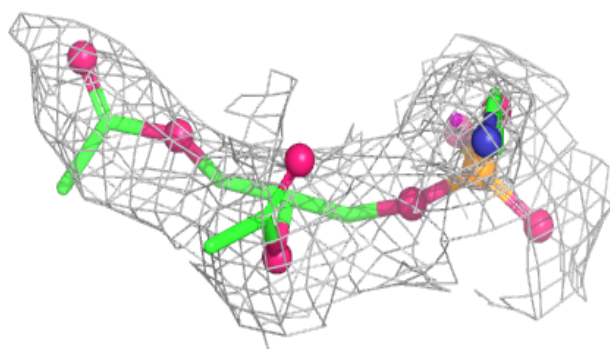
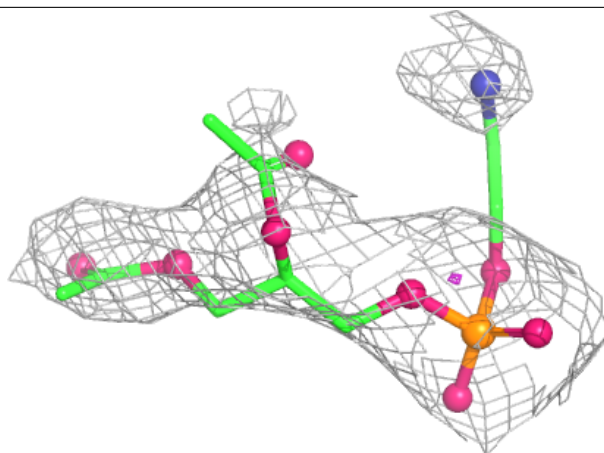
Electron density around PEF x 306:

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



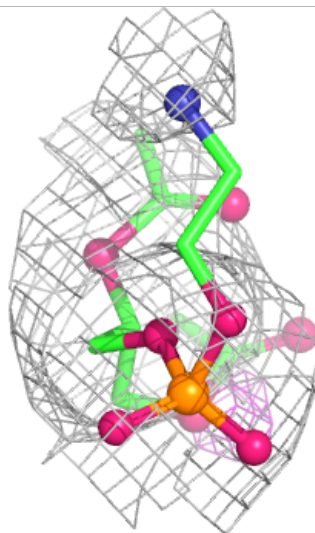
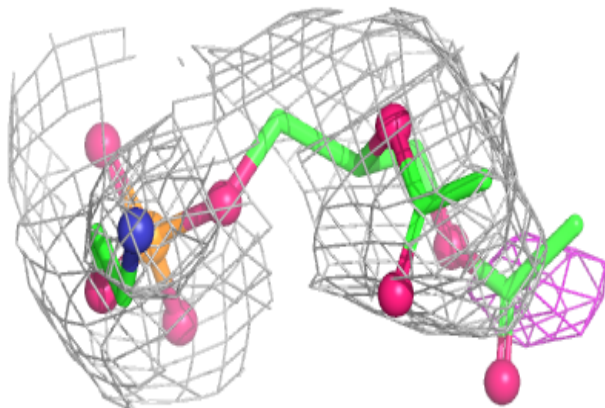
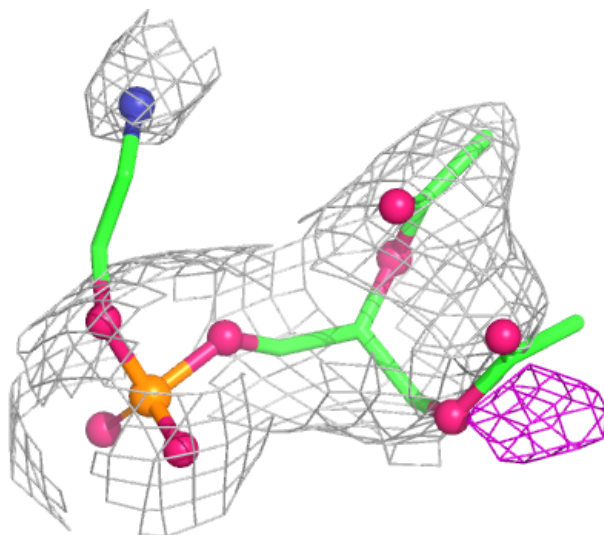
Electron density around PEF y 408:

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



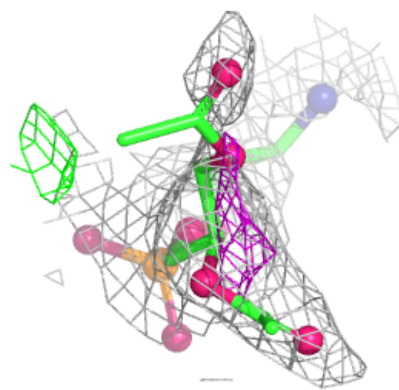
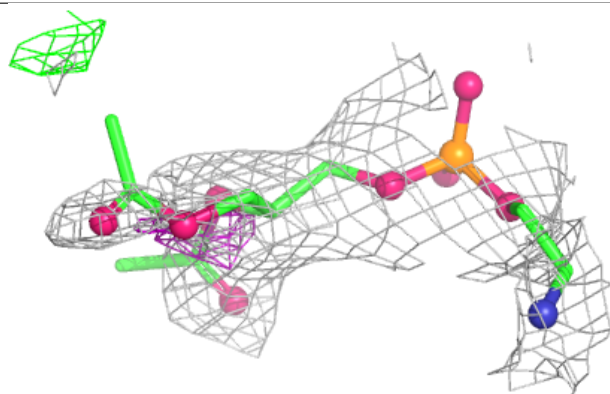
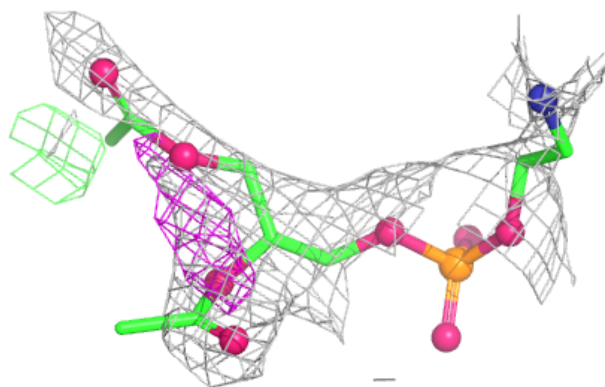
Electron density around PEF M 408:

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and green (positive)

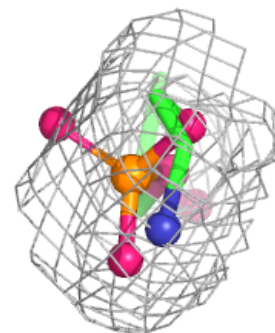
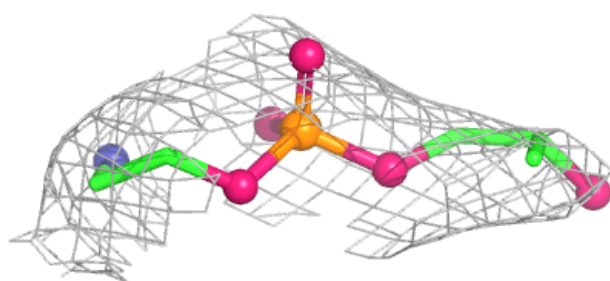
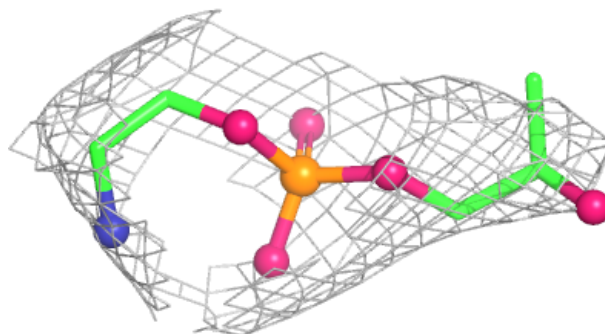


Electron density around PEF y 407:

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

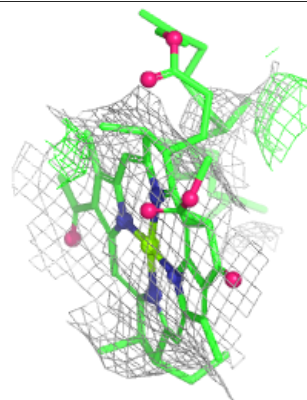
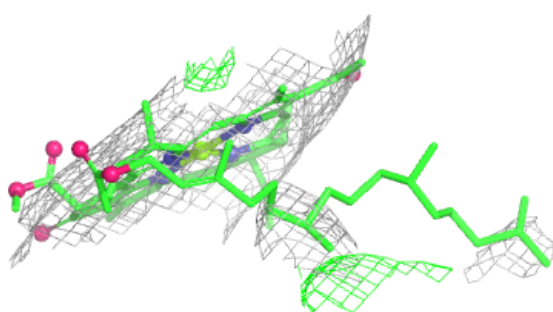
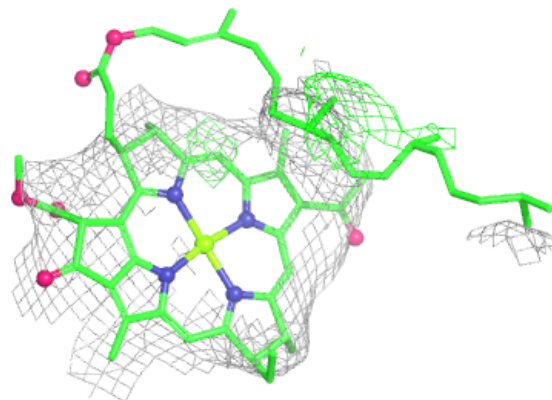
**Electron density around PEF L 305:**

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

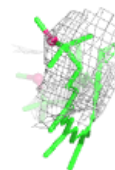
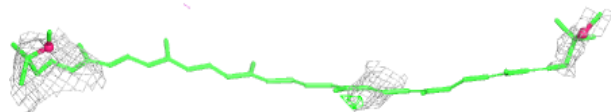
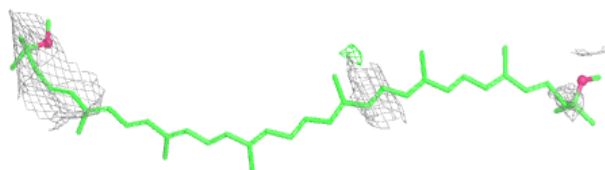


Electron density around BCL I 103:

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

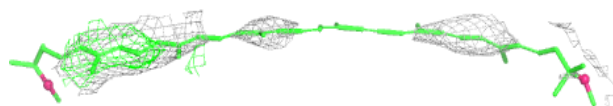
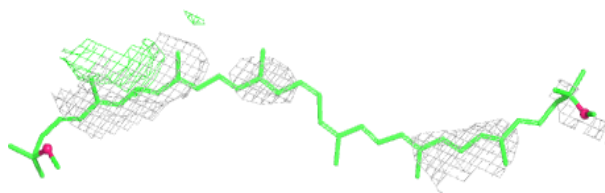
**Electron density around CRT T 101:**

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

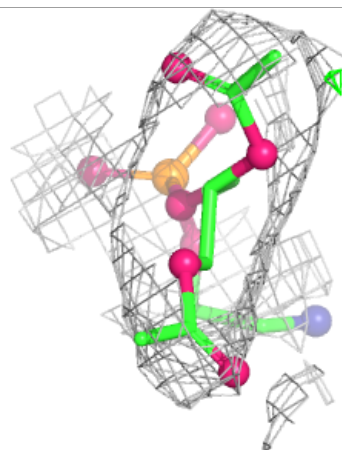
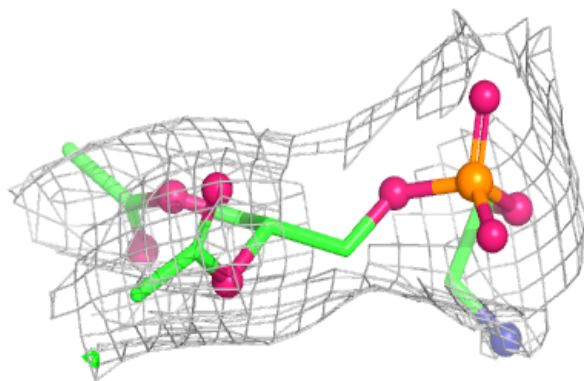
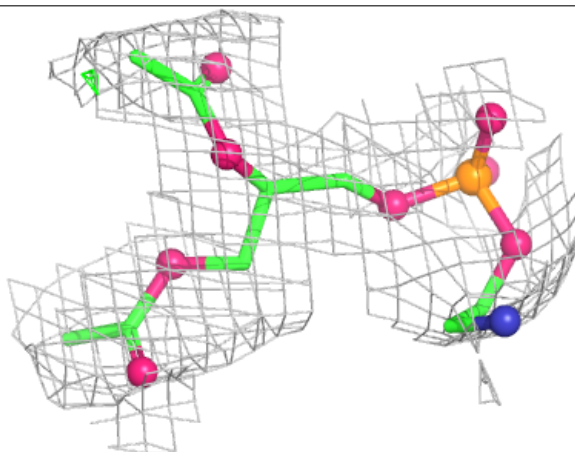


Electron density around CRT 7 103:

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

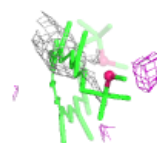
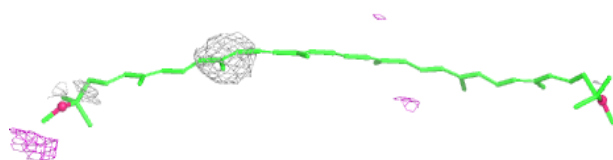
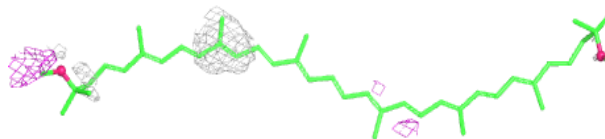
**Electron density around PEF H 301:**

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

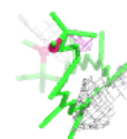
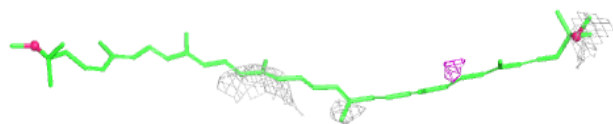
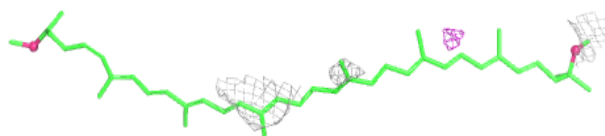


Electron density around CRT m 104:

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

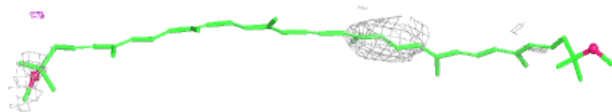
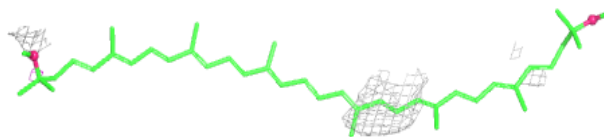
**Electron density around CRT v 101:**

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

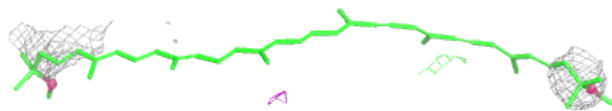
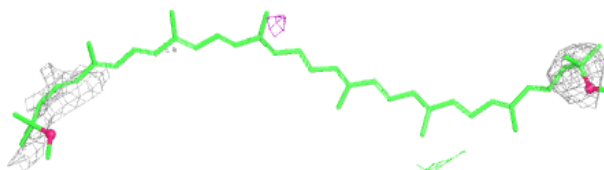


Electron density around CRT AC 101:

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

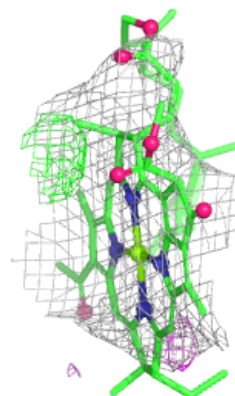
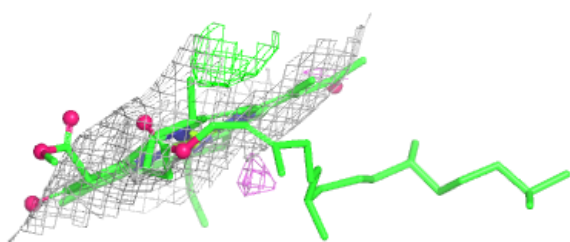
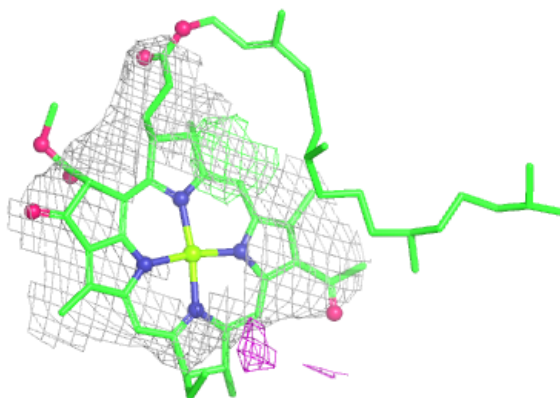
**Electron density around CRT AL 101:**

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



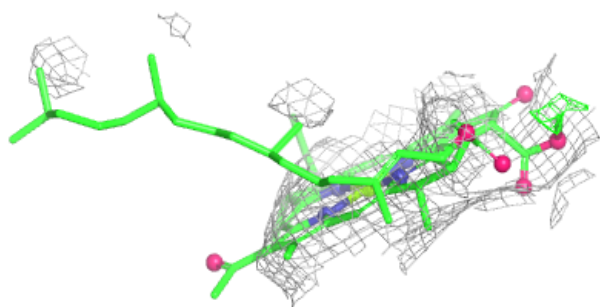
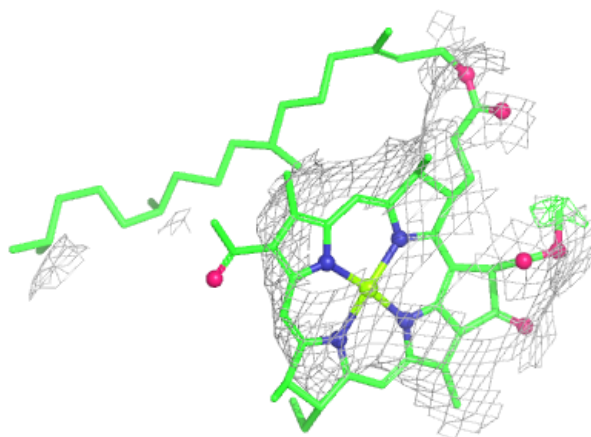
Electron density around BCL D 102:

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

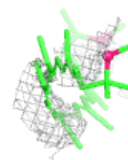
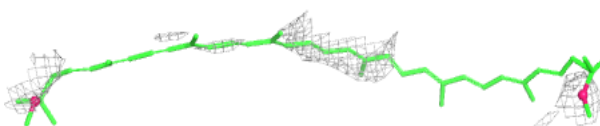
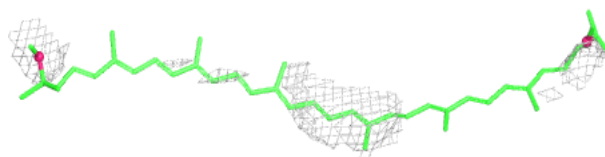


Electron density around BCL AC 103:

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

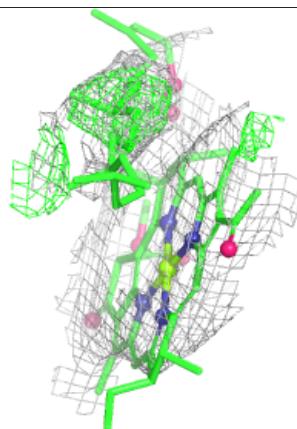
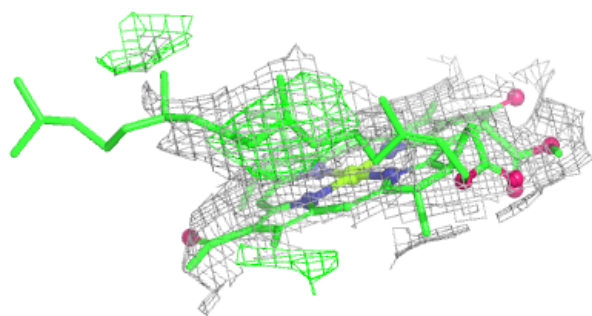
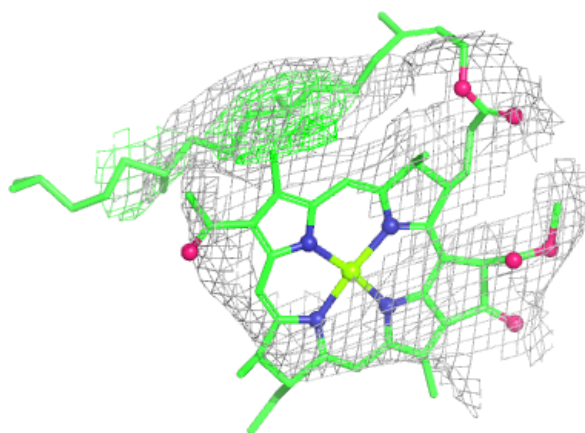
**Electron density around CRT O 101:**

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

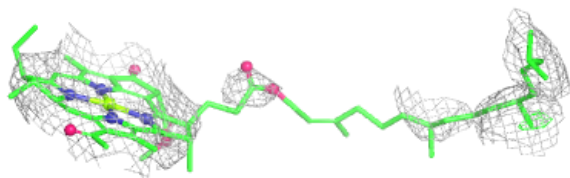
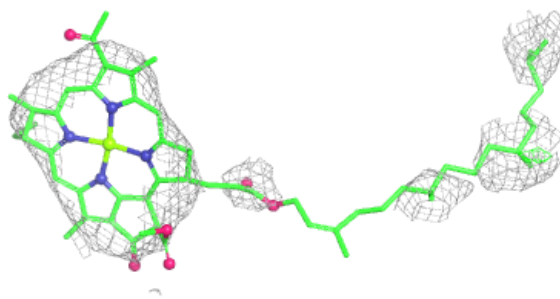


Electron density around BCL AG 101:

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

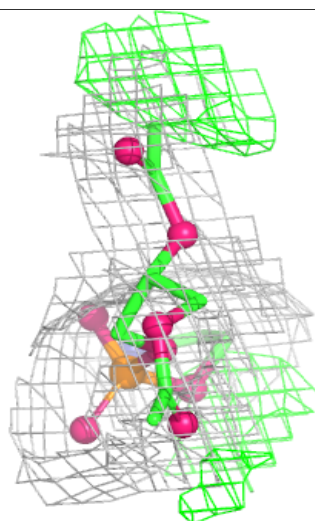
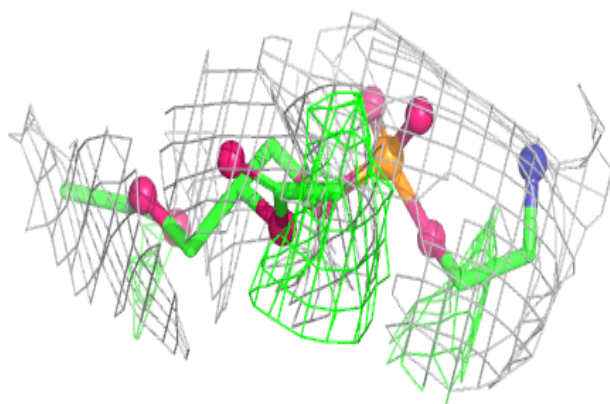
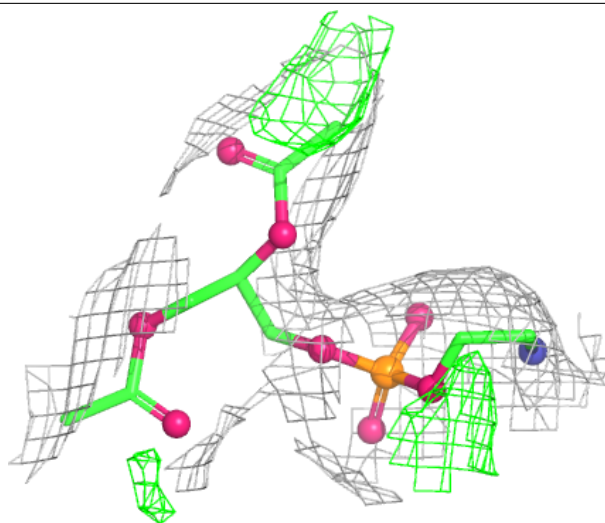
**Electron density around BCL d 101:**

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



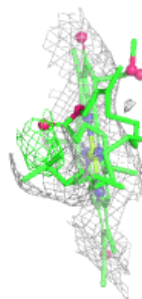
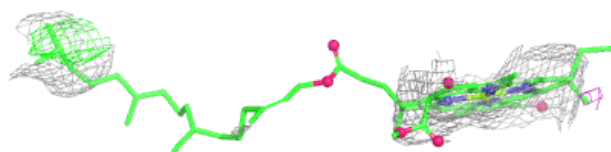
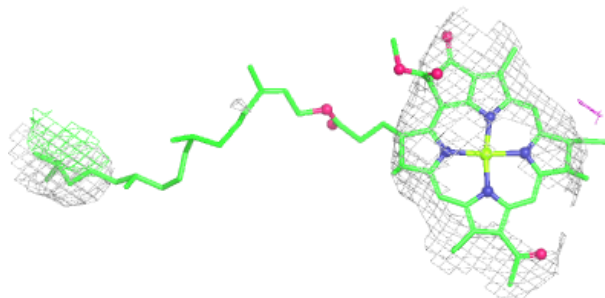
Electron density around PEF H 302:

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



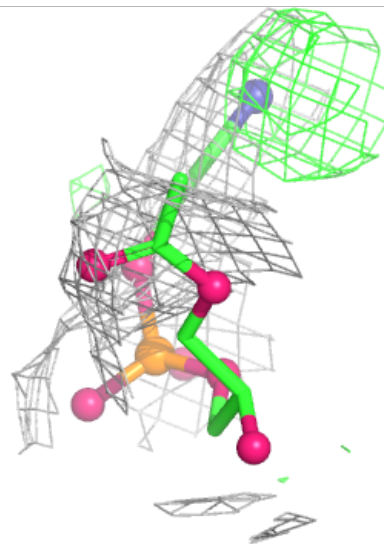
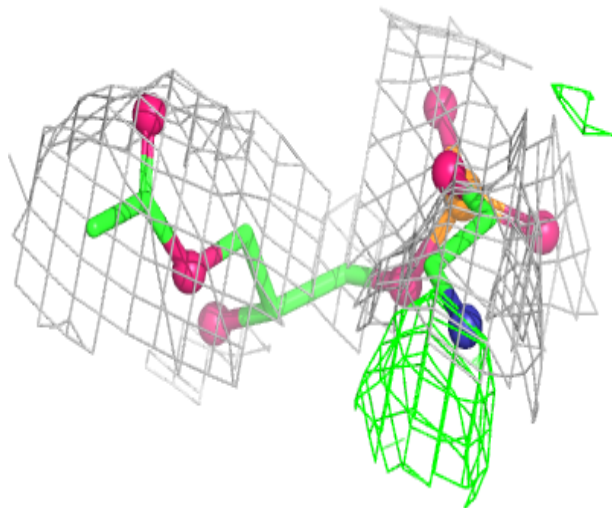
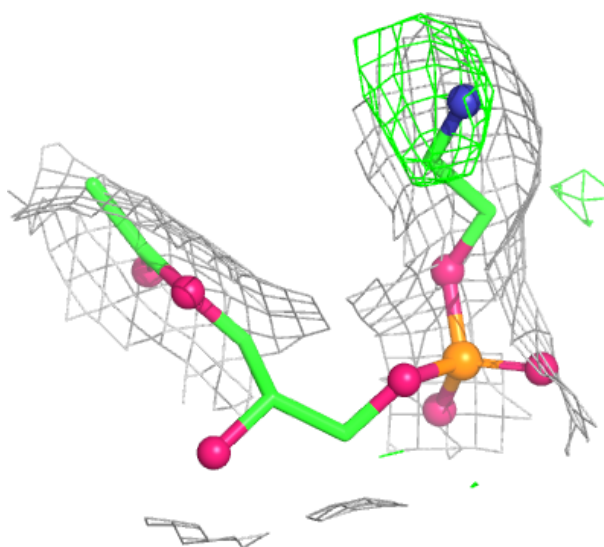
Electron density around BCL p 102:

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



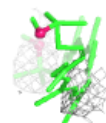
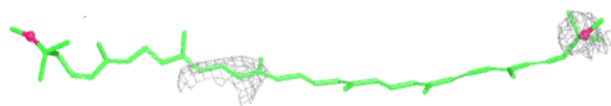
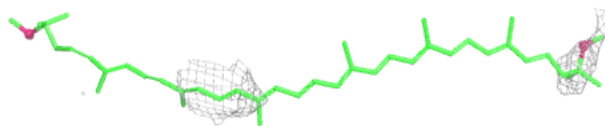
Electron density around PEF p 101:

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

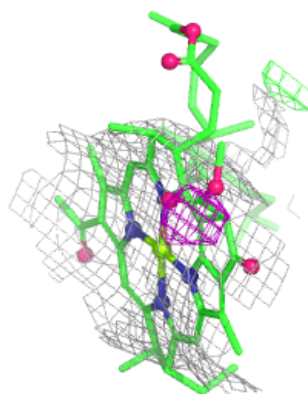
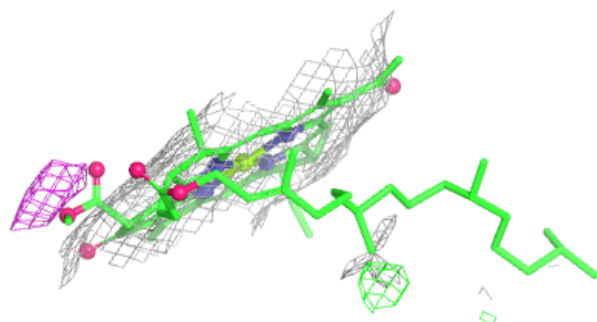
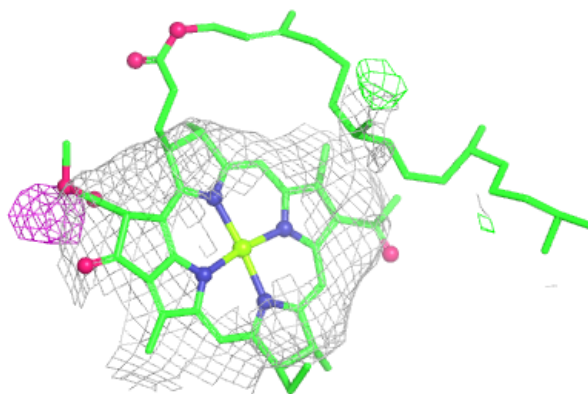


Electron density around CRT I 102:

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

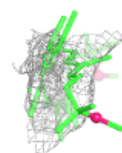
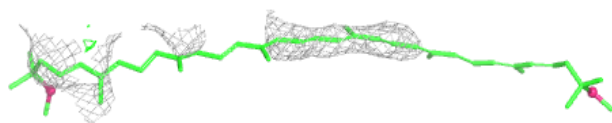
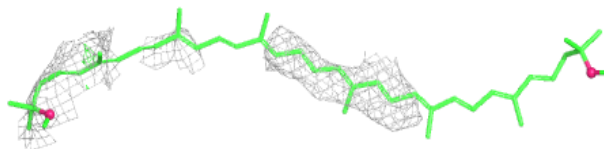
**Electron density around BCL u 102:**

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

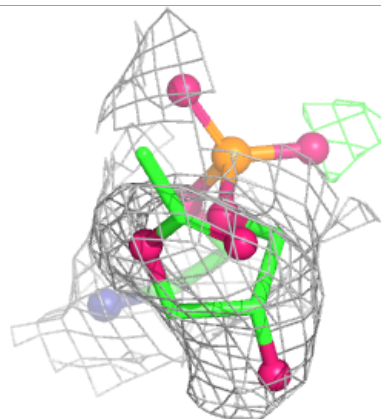
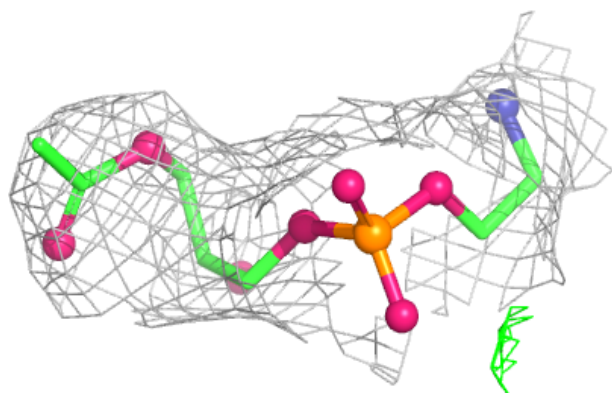
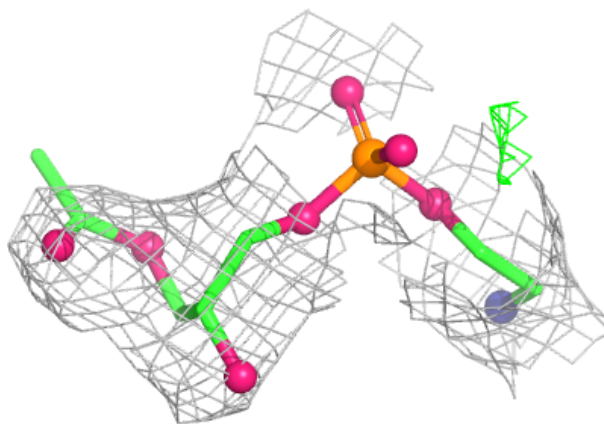


Electron density around CRT e 101:

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

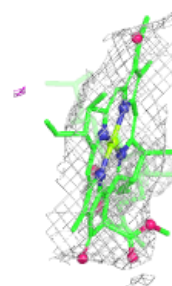
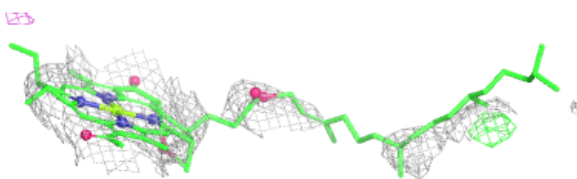
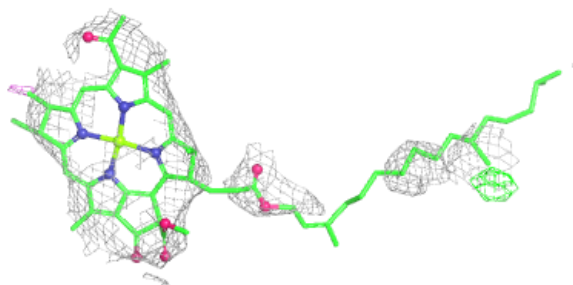
**Electron density around PEF M 407:**

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



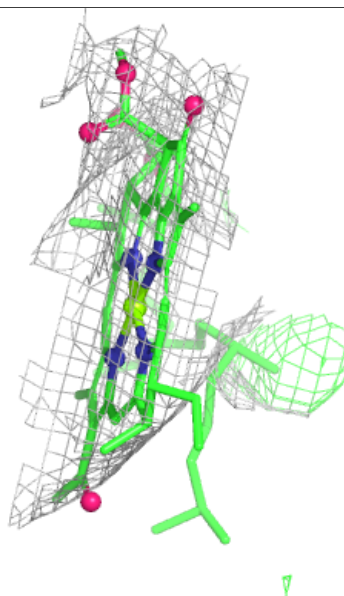
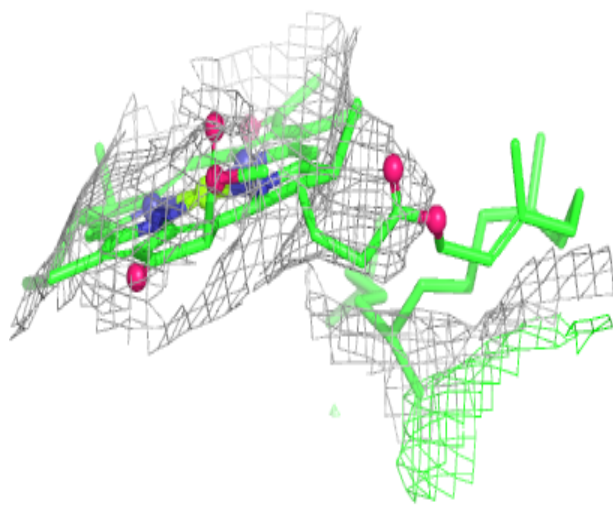
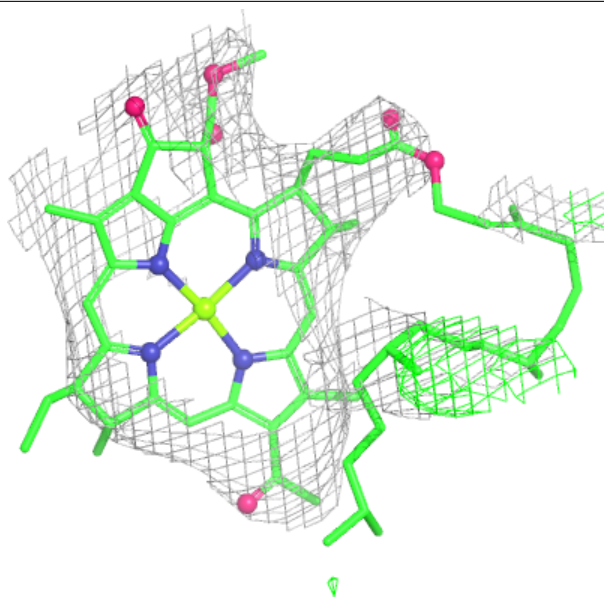
Electron density around BCL 1 101:

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



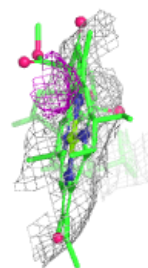
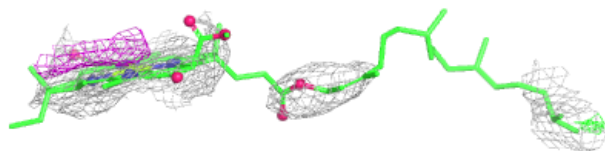
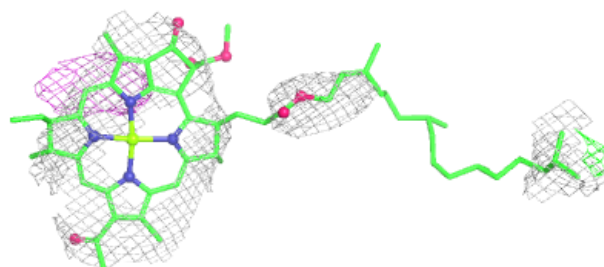
Electron density around BCL m 103:

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

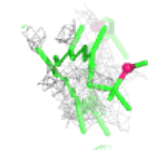
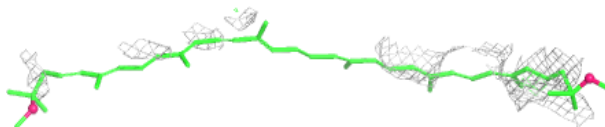
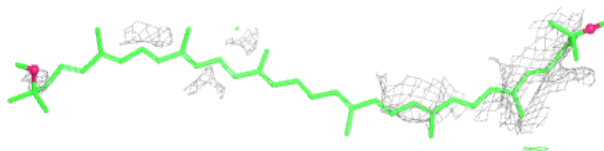


Electron density around BCL D 101:

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

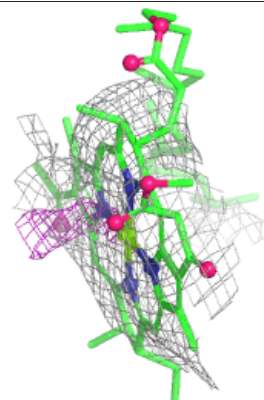
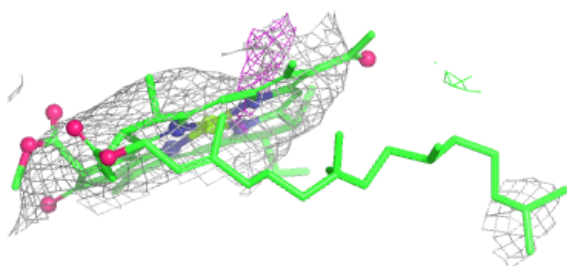
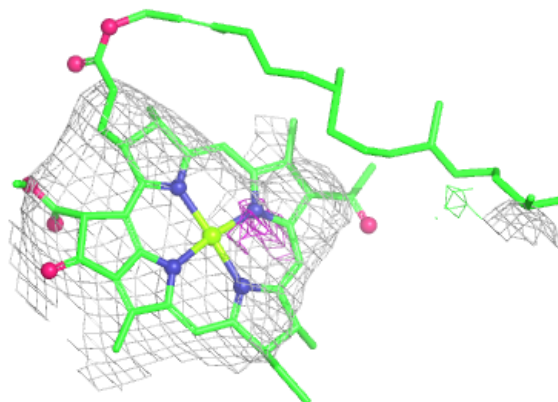
**Electron density around CRT AH 102:**

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

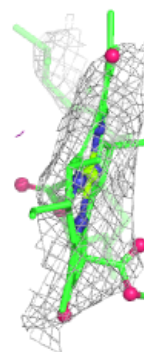
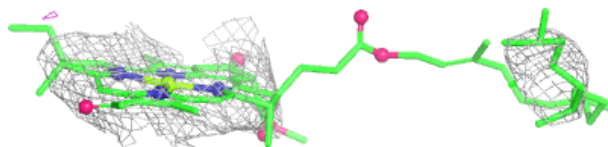
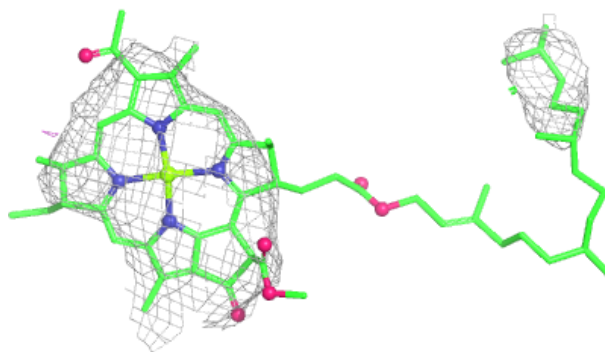


Electron density around BCL AB 102:

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

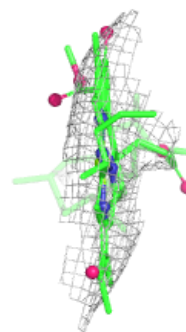
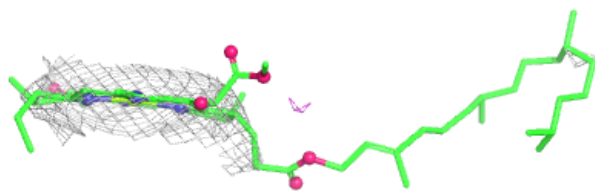
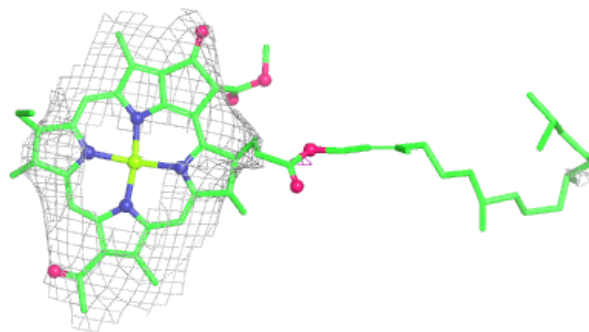
**Electron density around BCL f 101:**

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

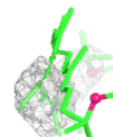
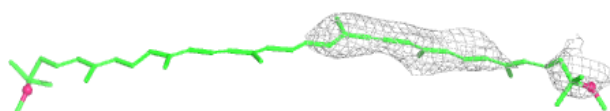
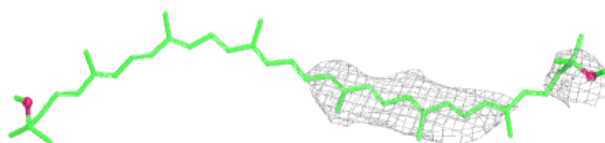


Electron density around BCL w 101:

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

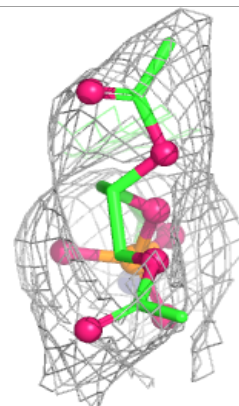
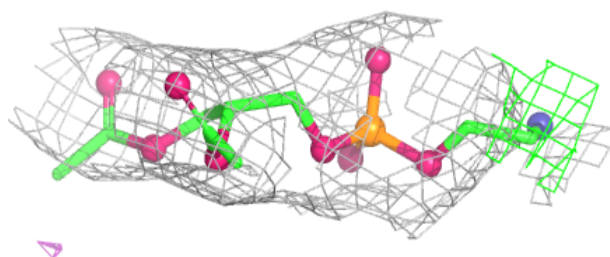
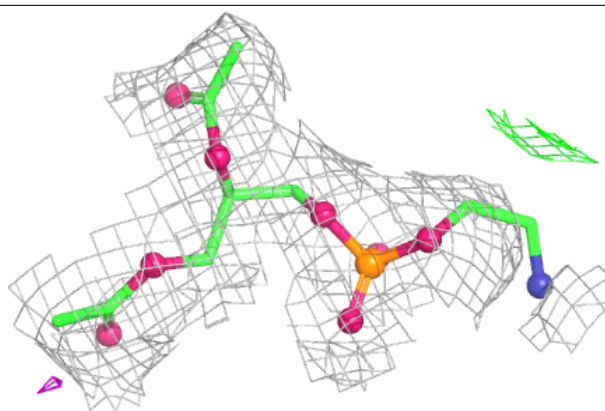
**Electron density around CRT i 101:**

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

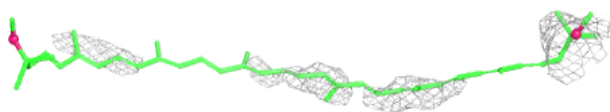
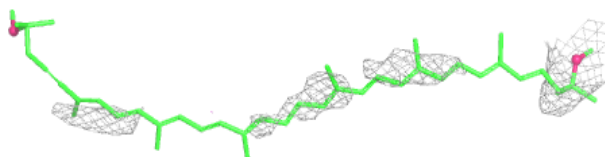


Electron density around PEF t 303:

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

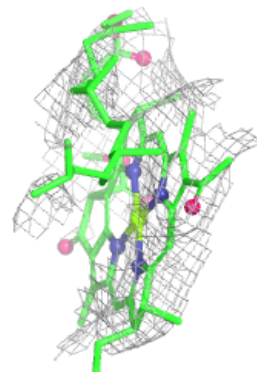
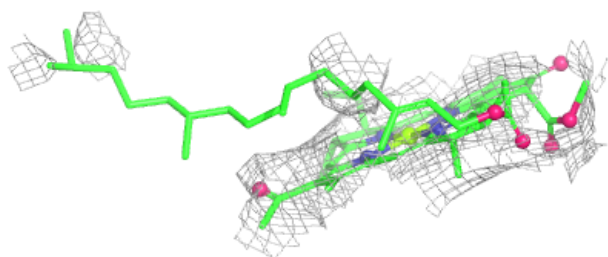
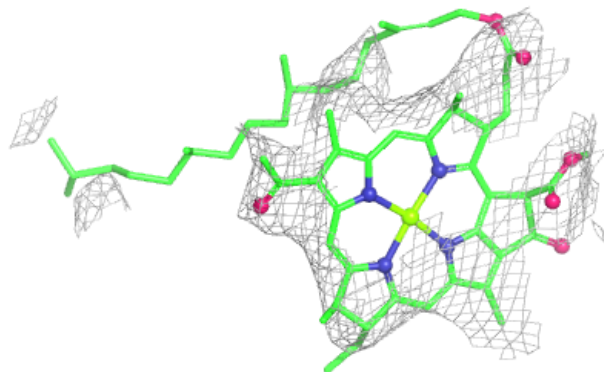
**Electron density around CRT 0 101:**

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



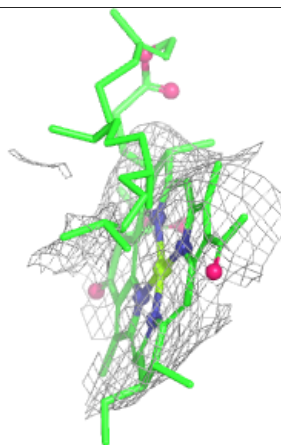
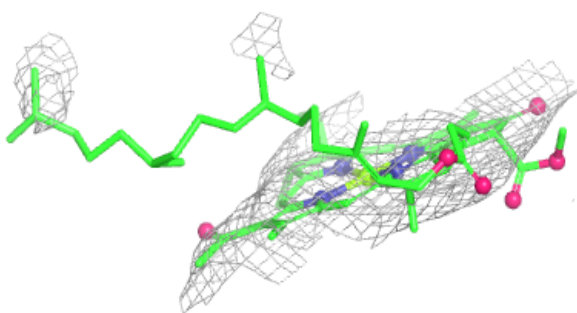
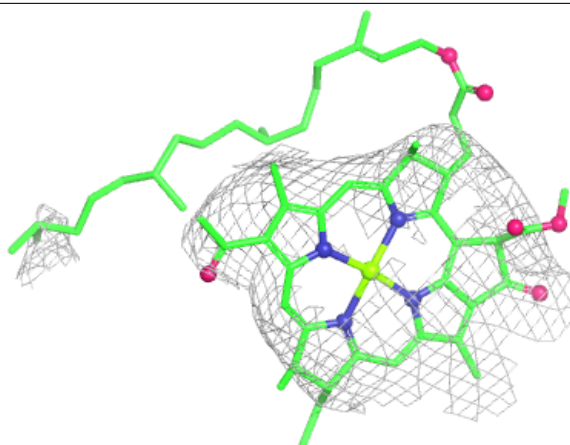
Electron density around BCL AE 102:

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

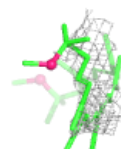
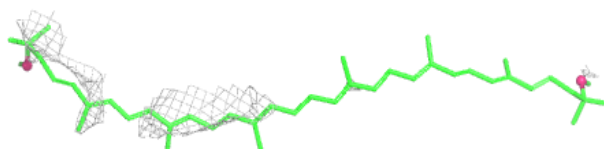


Electron density around BCL z 102:

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

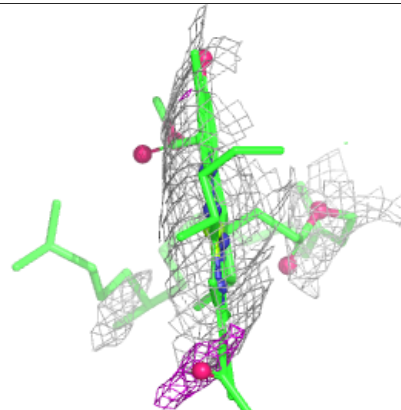
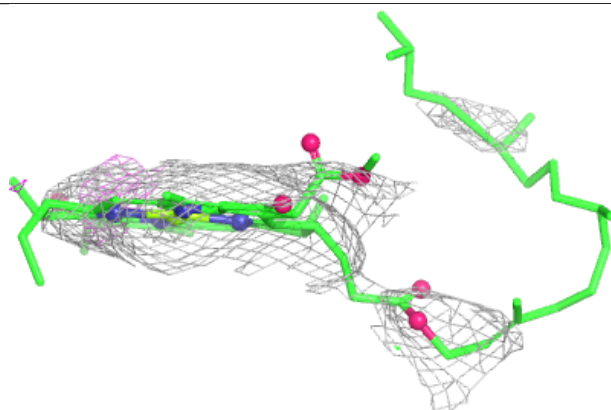
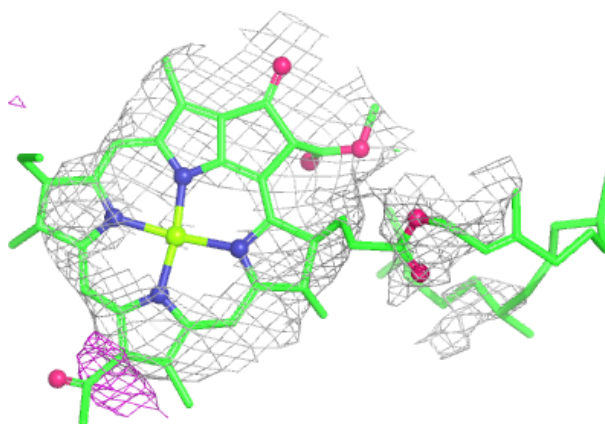
**Electron density around CRT G 101:**

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

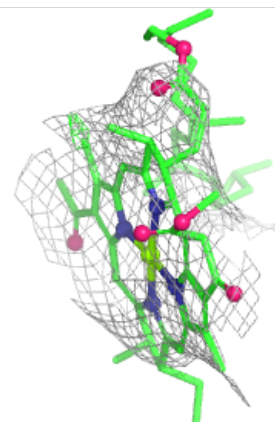
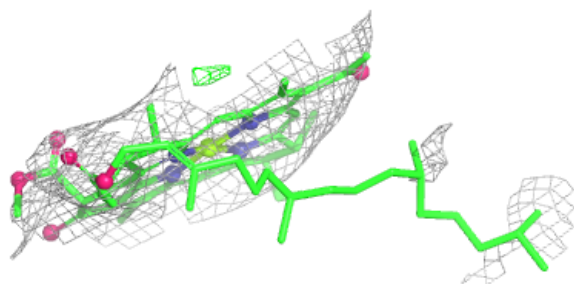
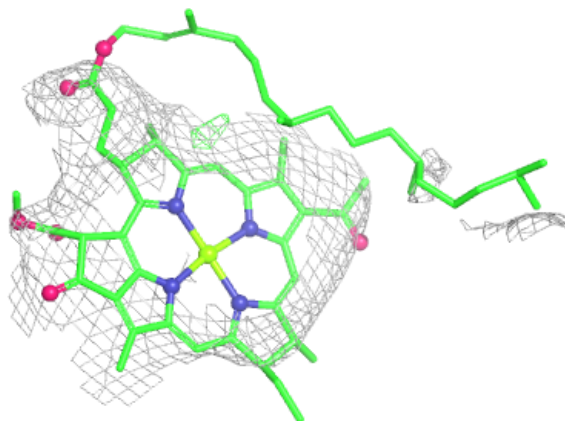


Electron density around BCL AC 102:

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

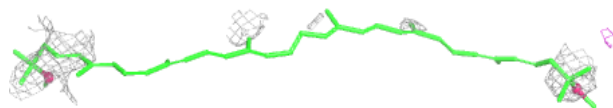
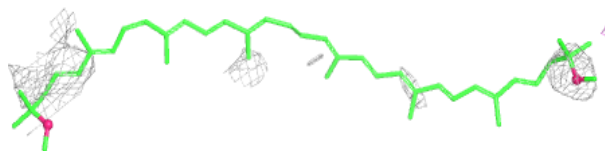
**Electron density around BCL N 101:**

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

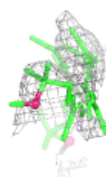
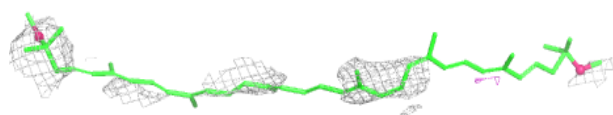
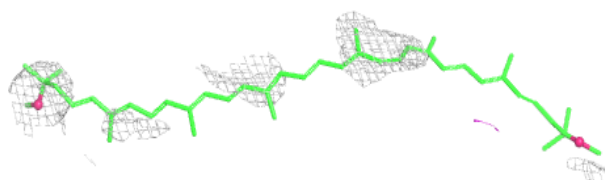


Electron density around CRT AJ 101:

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

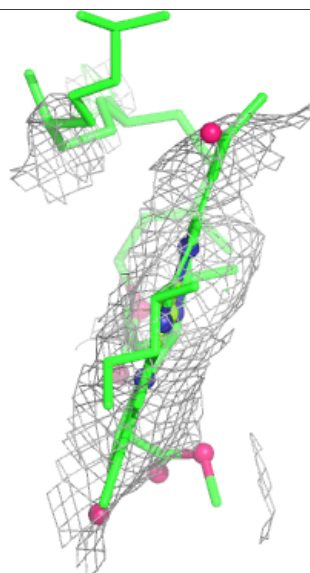
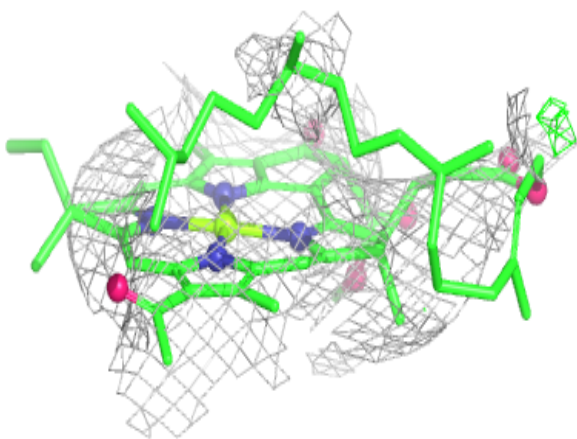
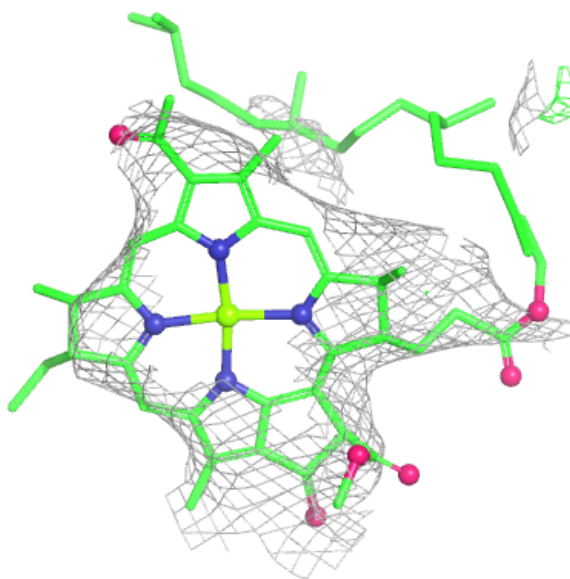
**Electron density around CRT R 101:**

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



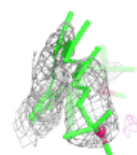
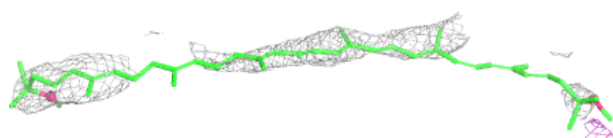
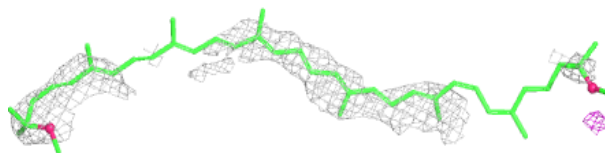
Electron density around BCL k 102:

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

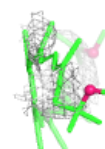
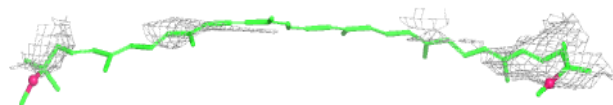
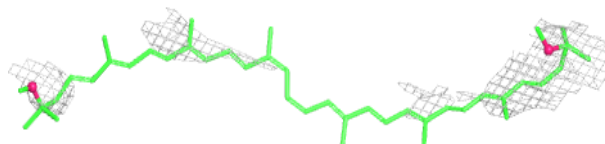


Electron density around CRT 4 101:

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

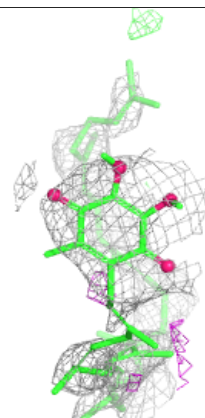
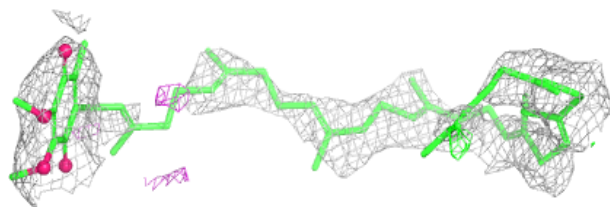
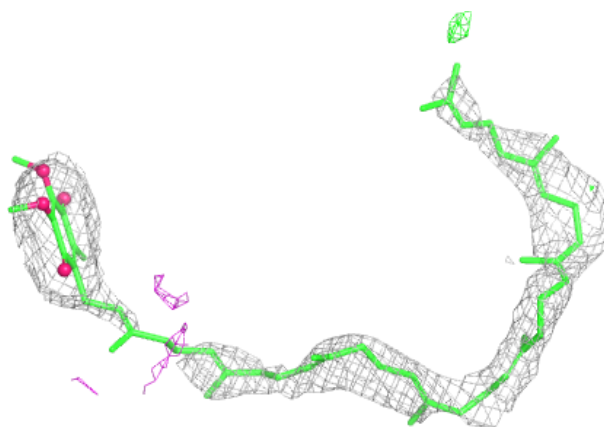
**Electron density around CRT k 101:**

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



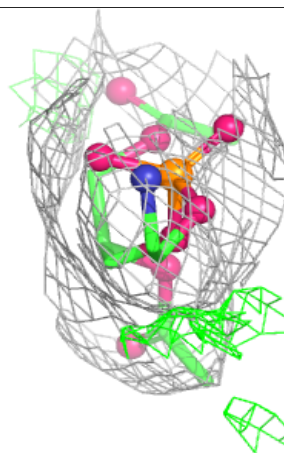
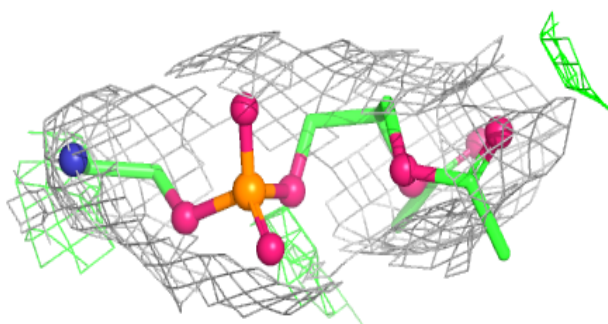
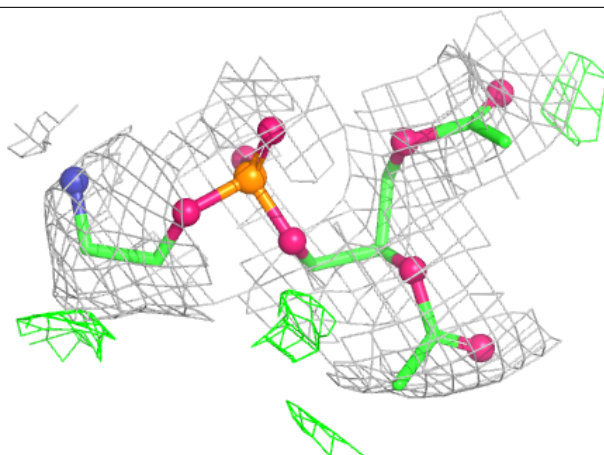
Electron density around UQ8 x 304:

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

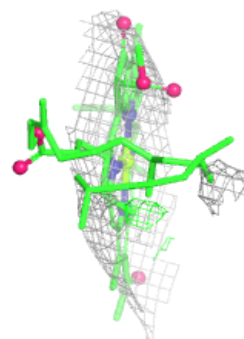
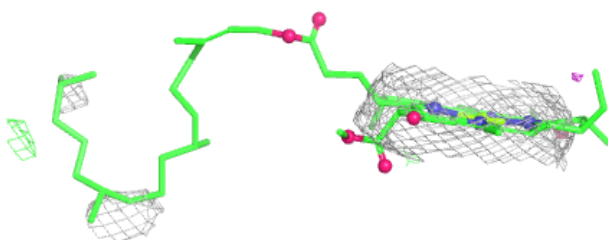
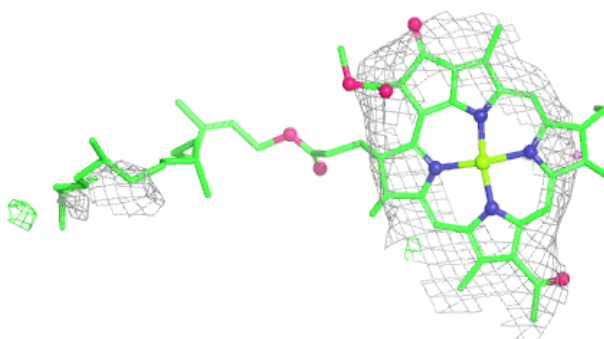


Electron density around PEF H 305:

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

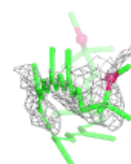
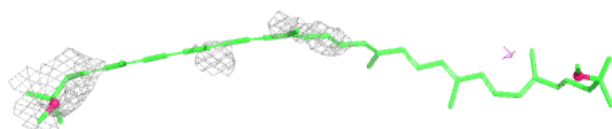
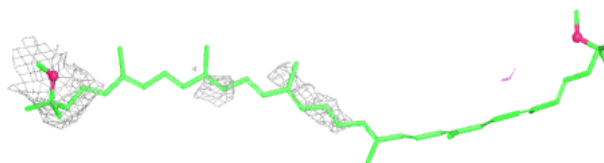
**Electron density around BCL P 101:**

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

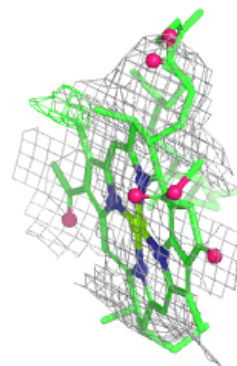
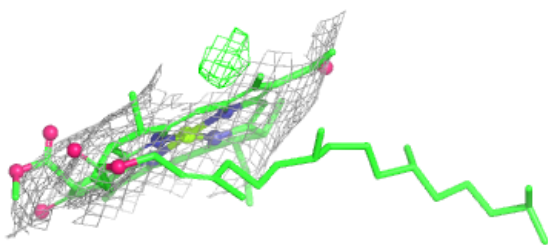
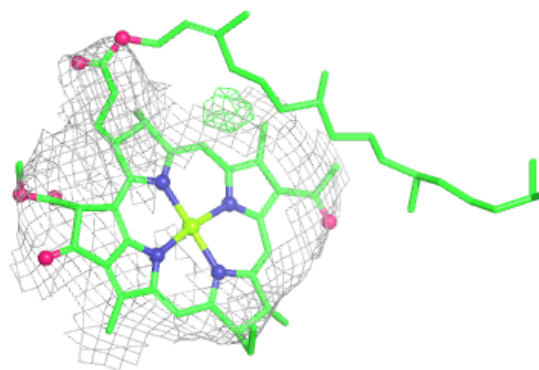


Electron density around CRT n 101:

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

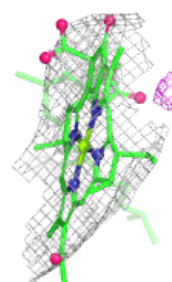
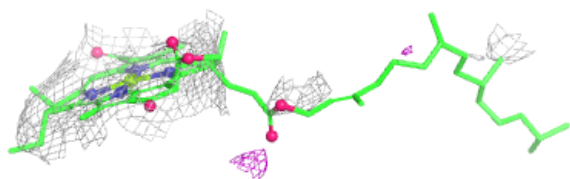
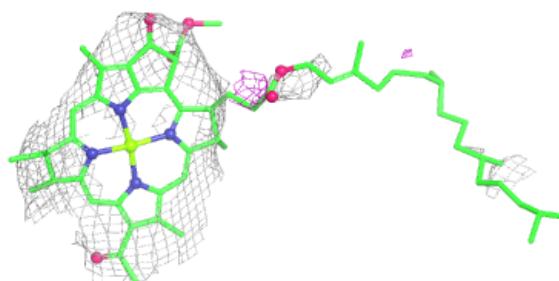
**Electron density around BCL G 102:**

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

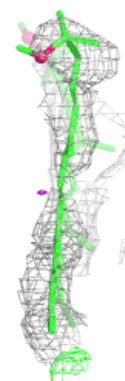
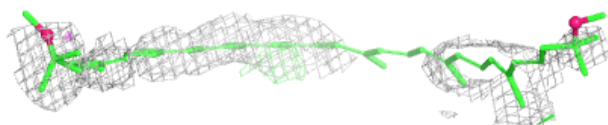
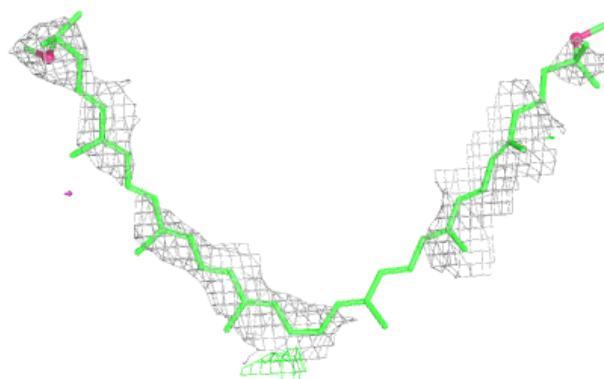


Electron density around BCL u 101:

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

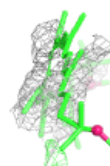
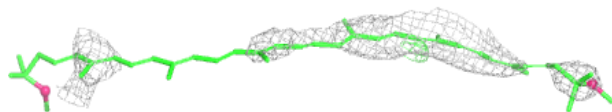
**Electron density around CRT M 405:**

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

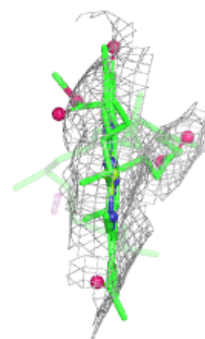
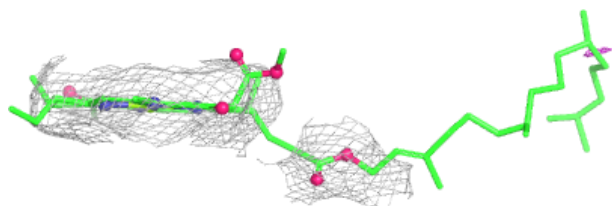
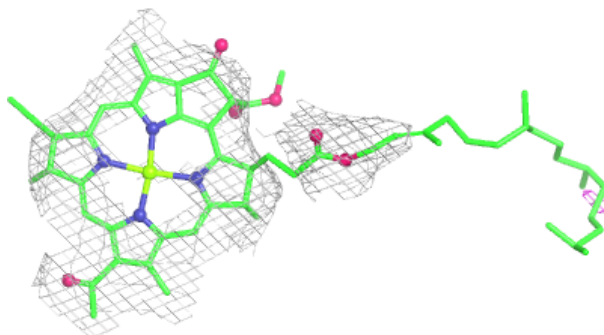


Electron density around CRT g 101:

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

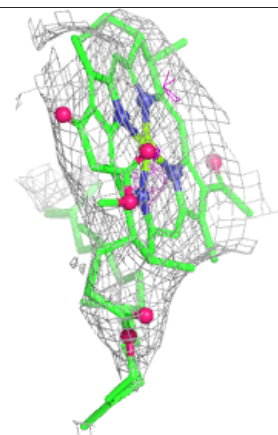
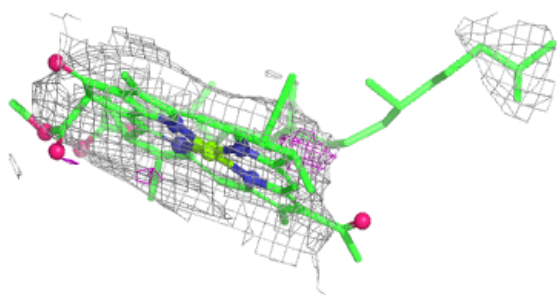
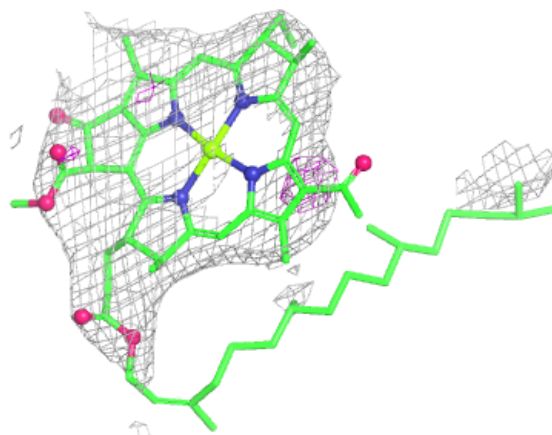
**Electron density around BCL m 102:**

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

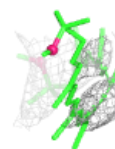
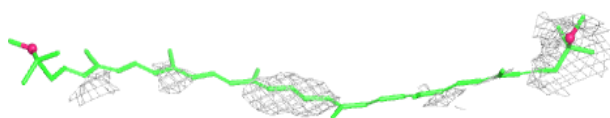
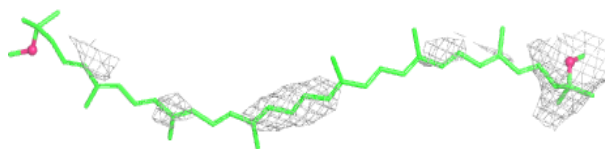


Electron density around BCL V 102:

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

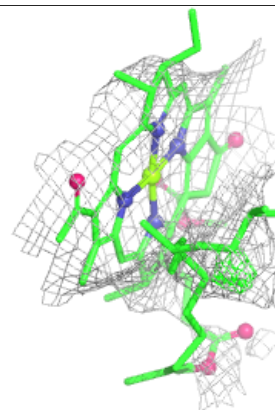
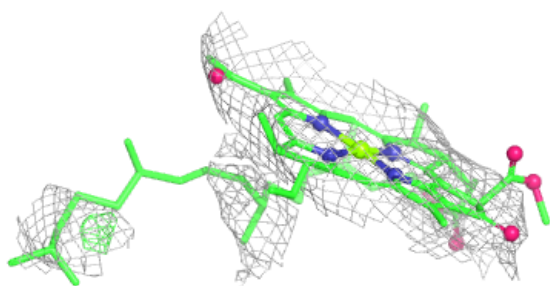
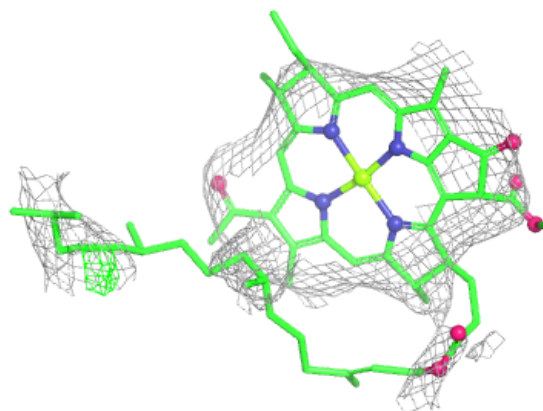
**Electron density around CRT q 101:**

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



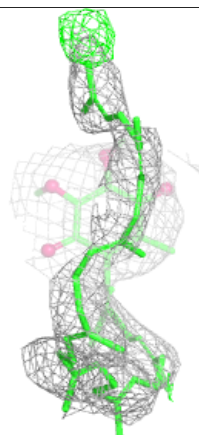
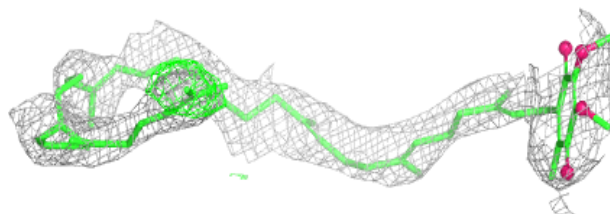
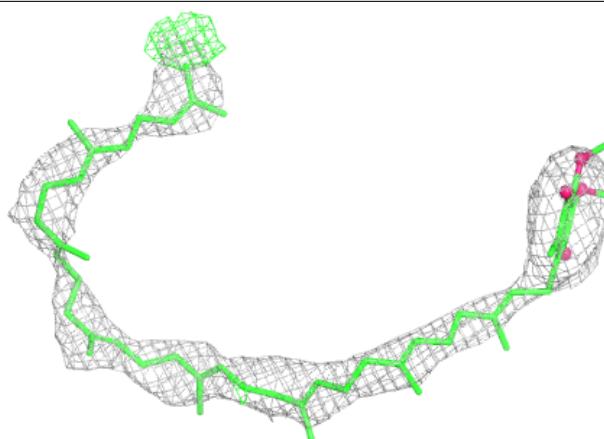
Electron density around BCL g 102:

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

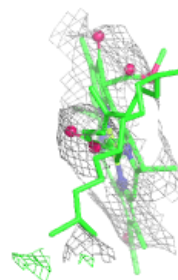
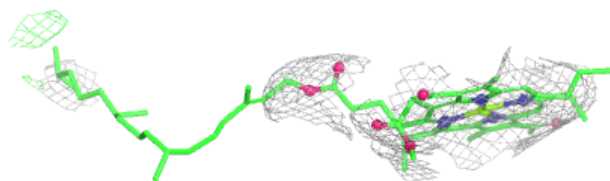
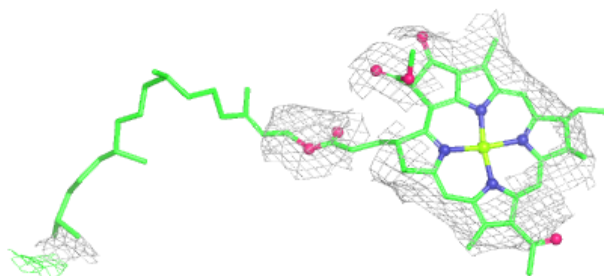


Electron density around UQ8 L 304:

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

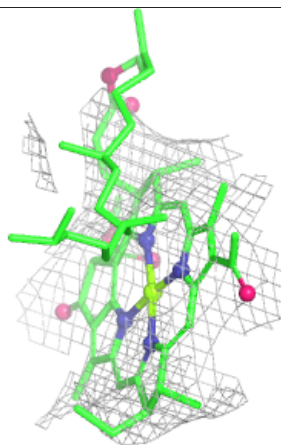
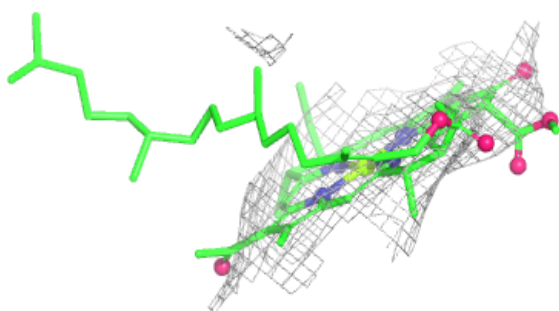
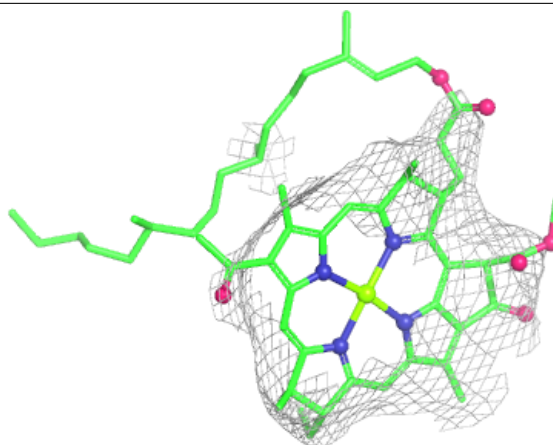
**Electron density around BCL AF 101:**

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

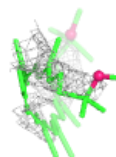
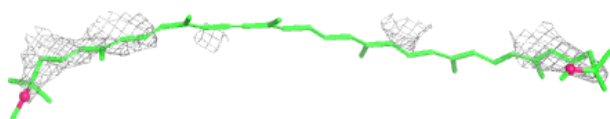
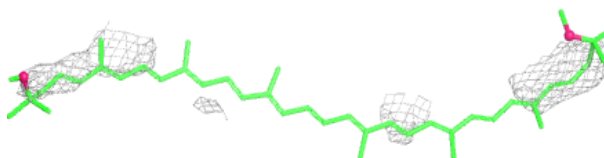


Electron density around BCL c 101:

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

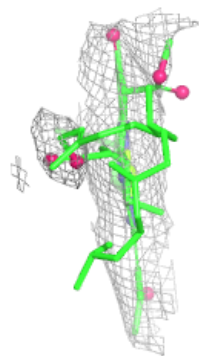
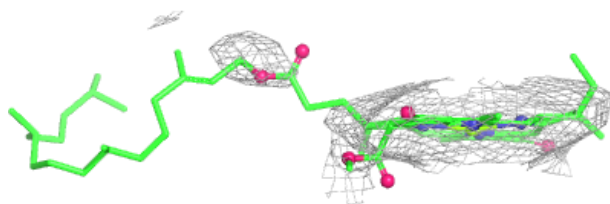
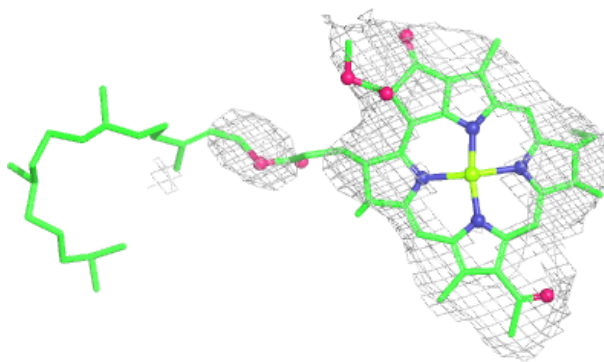
**Electron density around CRT AF 102:**

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



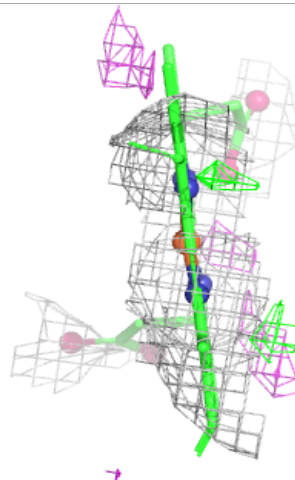
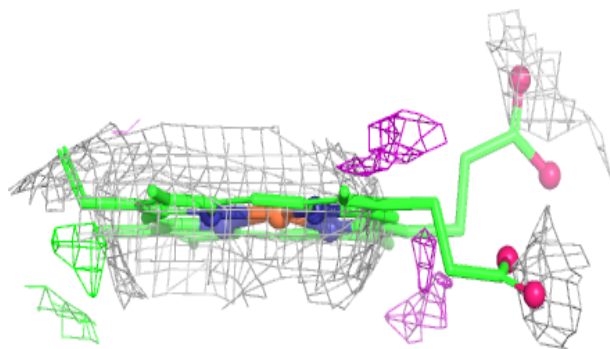
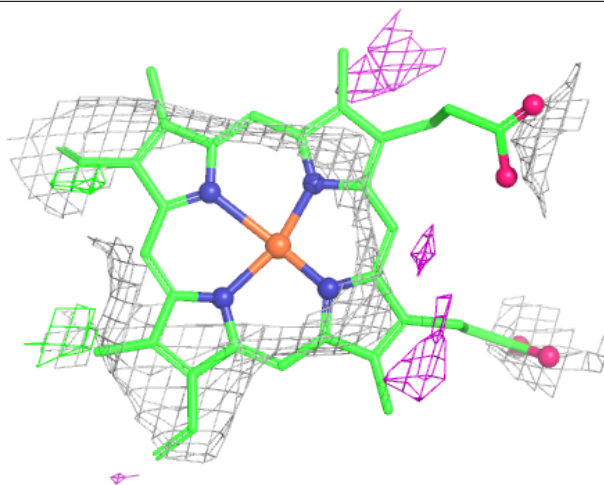
Electron density around BCL U 101:

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



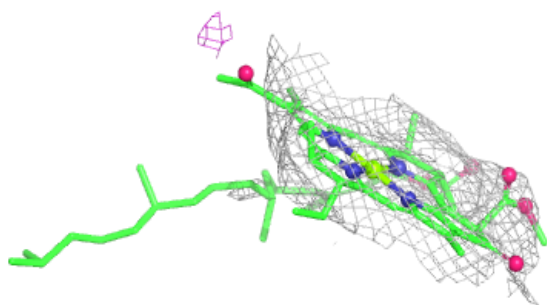
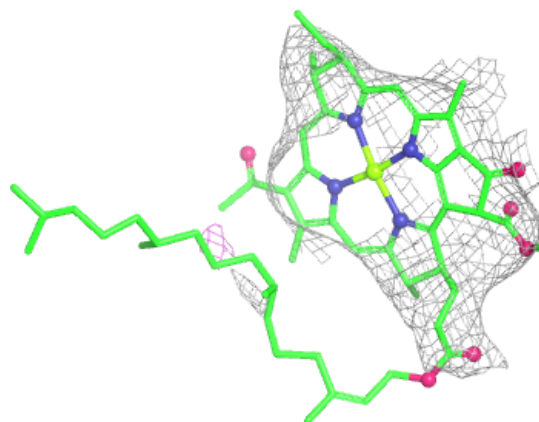
Electron density around HEM o 501:

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



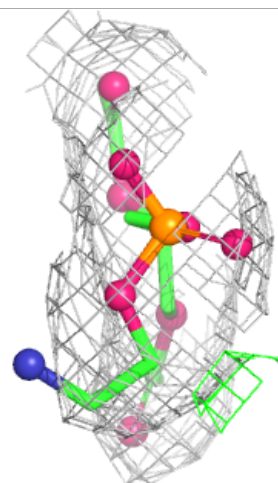
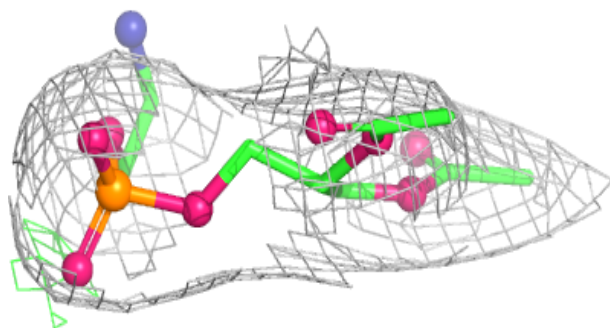
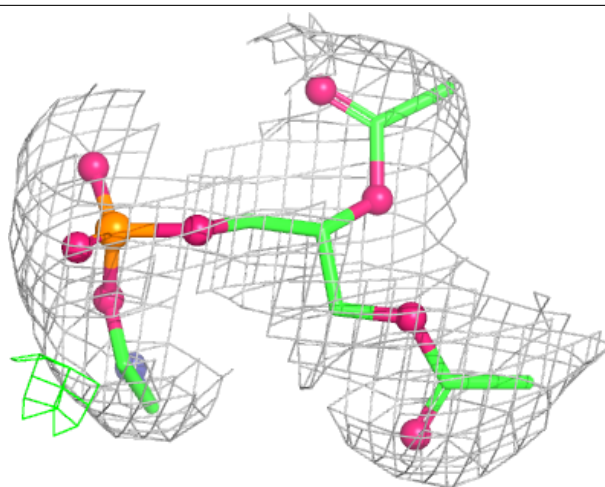
Electron density around BCL 2 102:

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



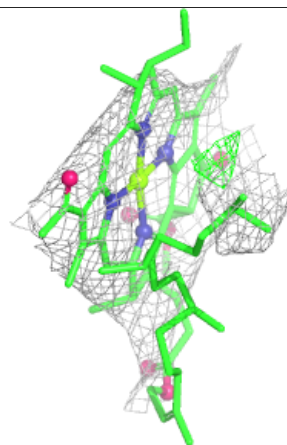
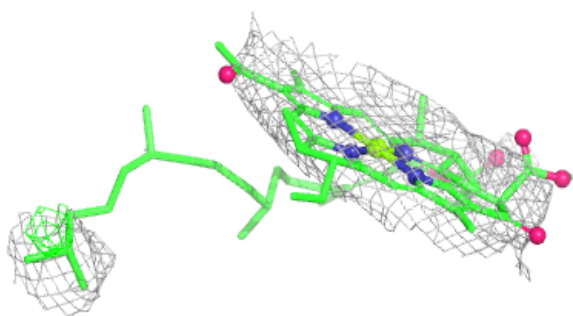
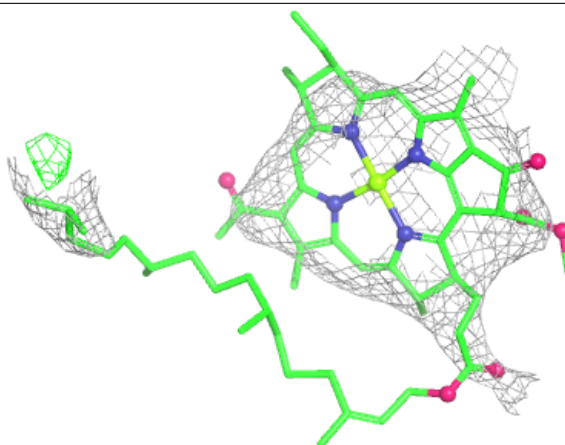
Electron density around PEF t 301:

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

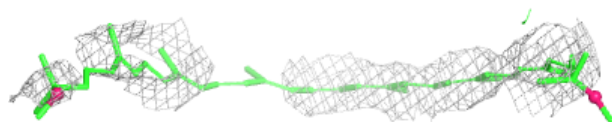
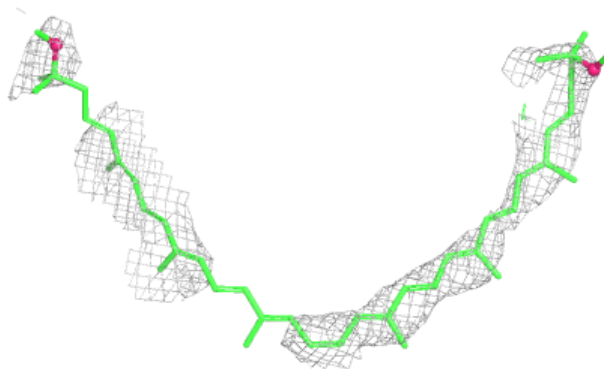


Electron density around BCL e 102:

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

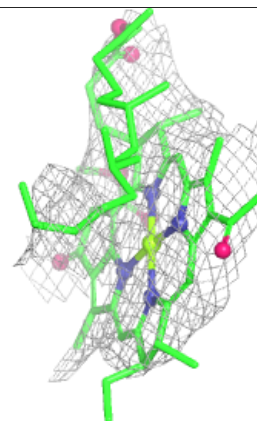
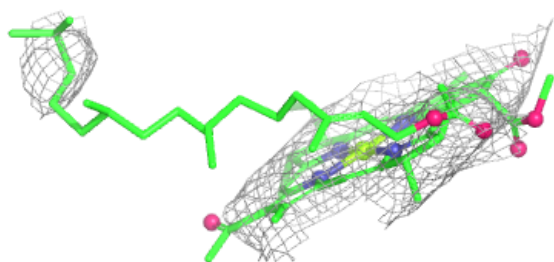
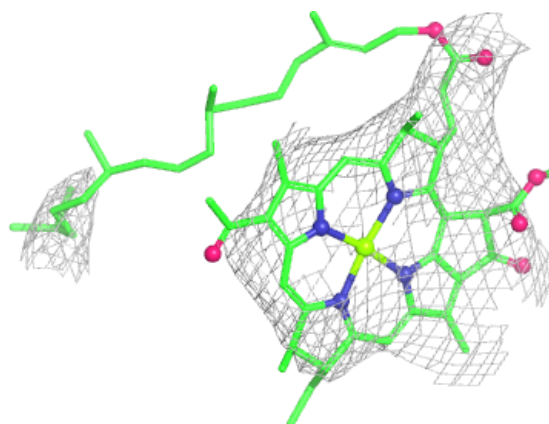
**Electron density around CRT y 404:**

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

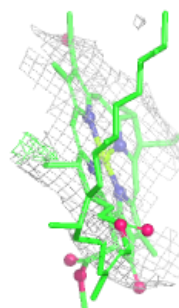
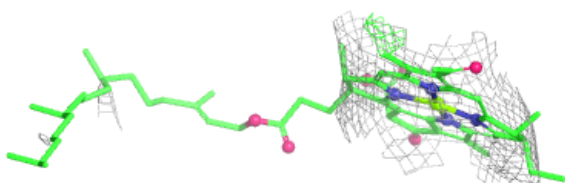
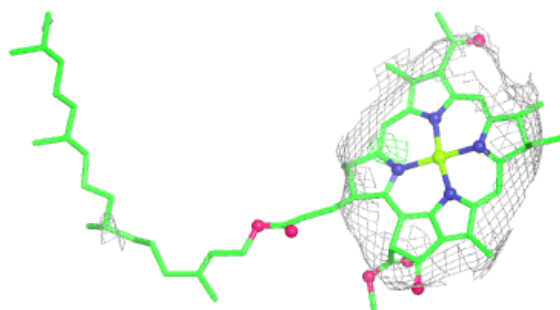


Electron density around BCL O 102:

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

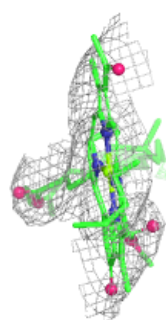
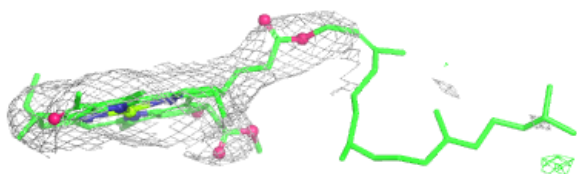
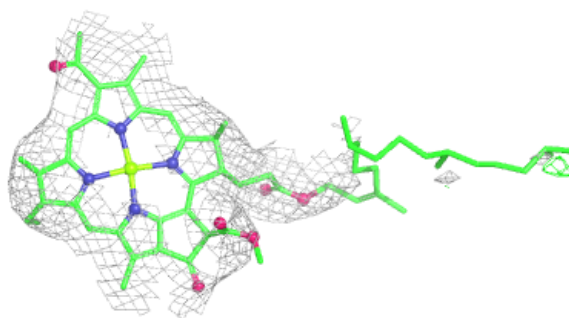
**Electron density around BCL I 101:**

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

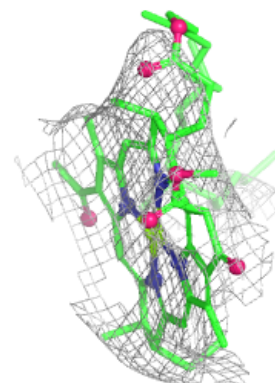
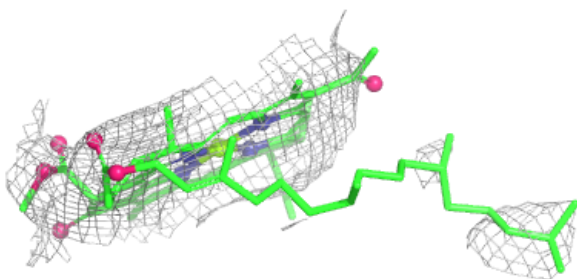
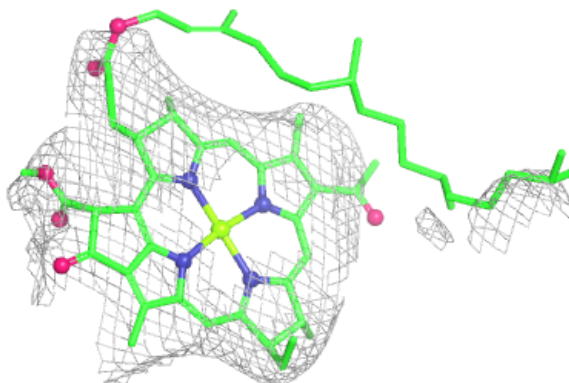


Electron density around BCL h 101:

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

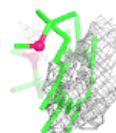
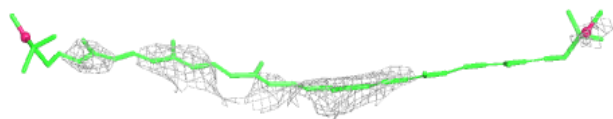
**Electron density around BCL T 102:**

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

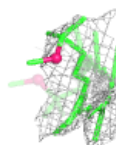
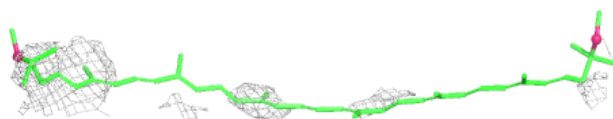
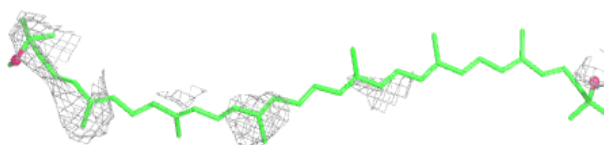


Electron density around CRT z 101:

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

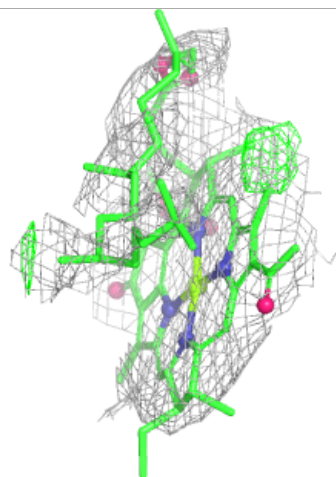
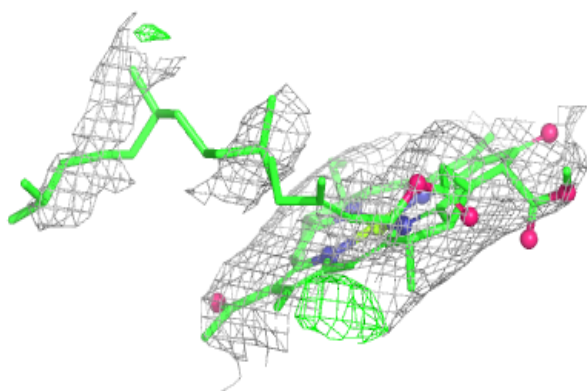
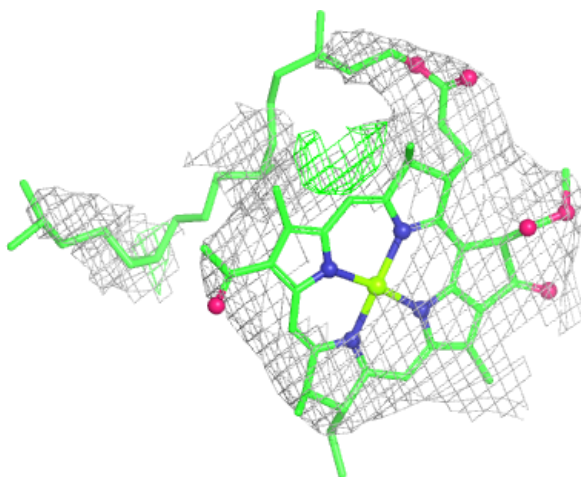
**Electron density around CRT s 101:**

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



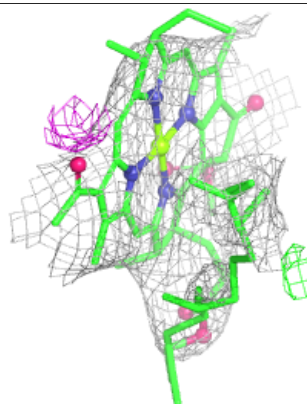
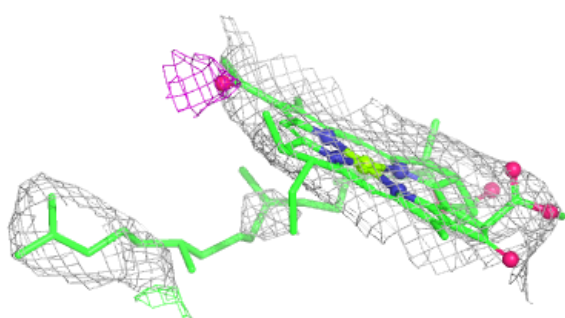
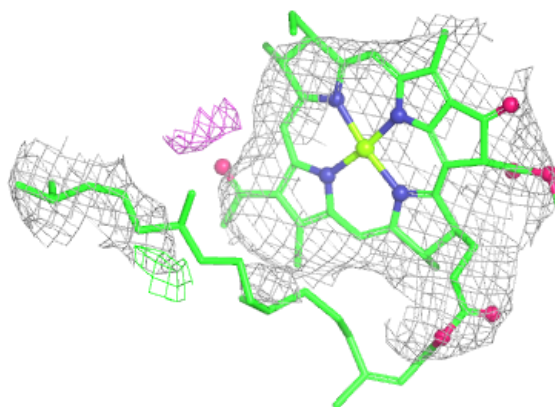
Electron density around BCL AI 102:

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

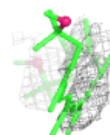
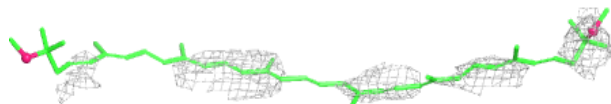
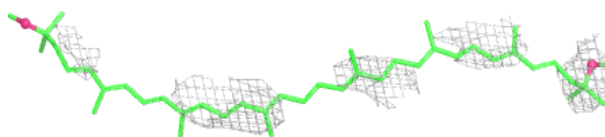


Electron density around BCL AL 102:

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

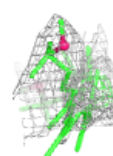
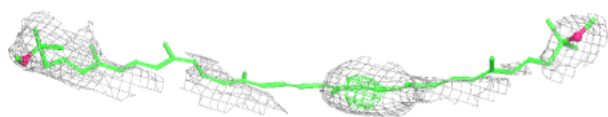
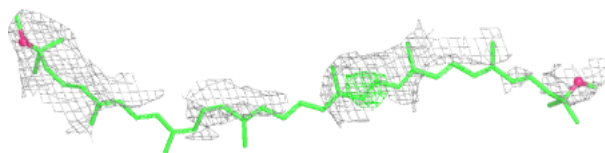
**Electron density around CRT P 102:**

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

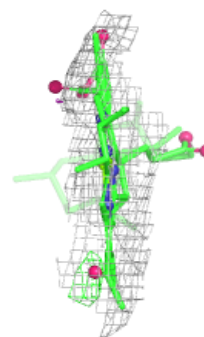
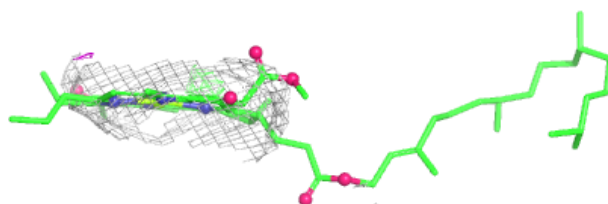
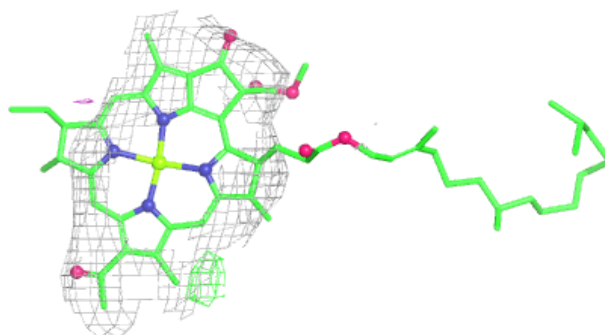


Electron density around CRT AD 101:

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

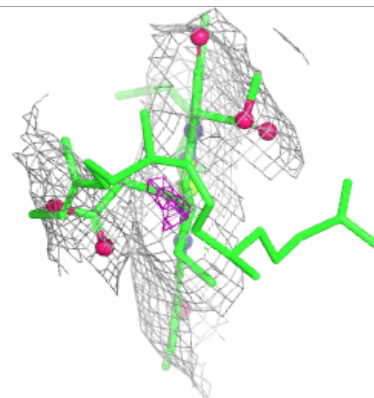
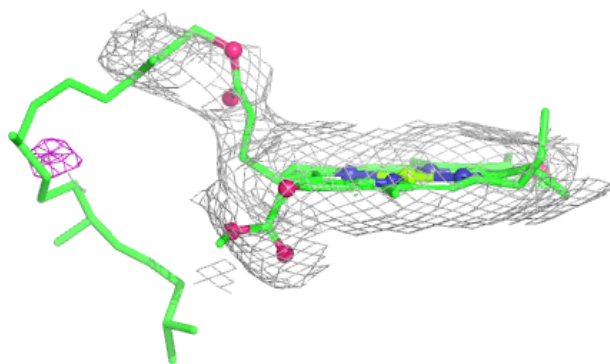
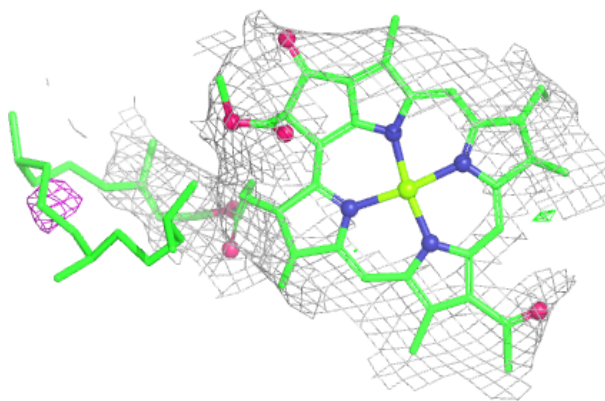
**Electron density around BCL K 101:**

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

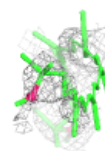
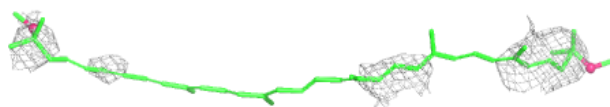
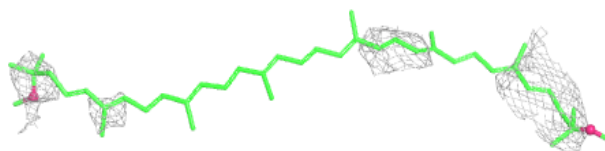


Electron density around BCL Q 101:

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

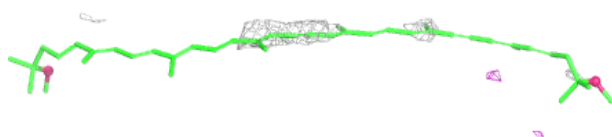
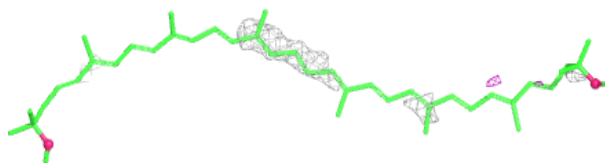
**Electron density around CRT V 101:**

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

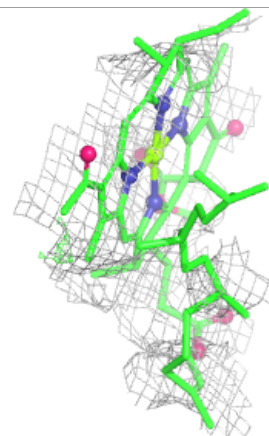
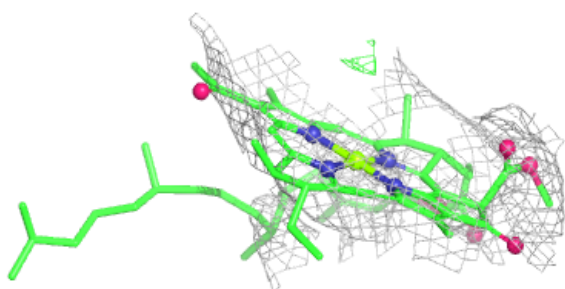
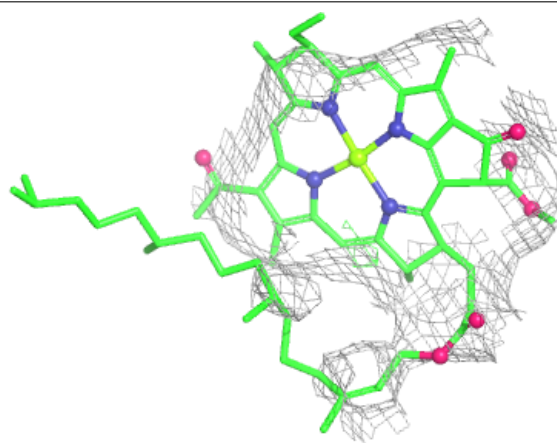


Electron density around CRT 2 101:

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

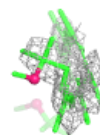
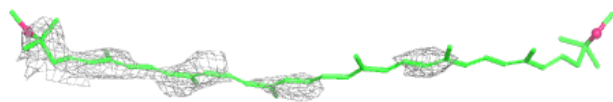
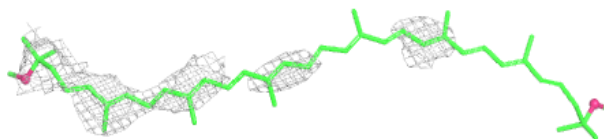
**Electron density around BCL 6 101:**

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

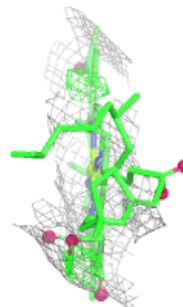
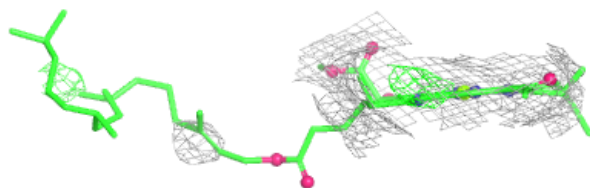
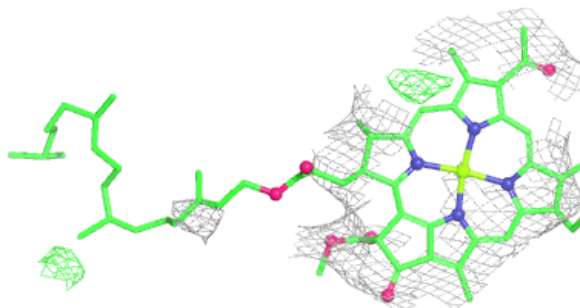


Electron density around CRT 7 101:

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

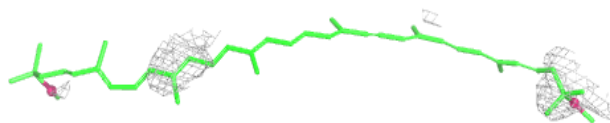
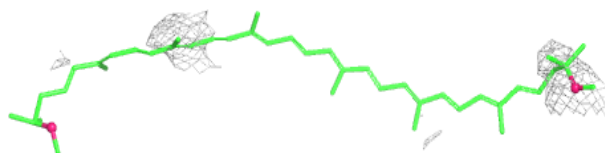
**Electron density around BCL 7 102:**

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

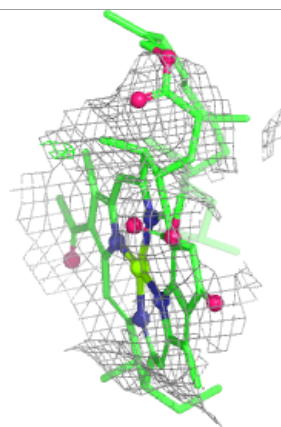
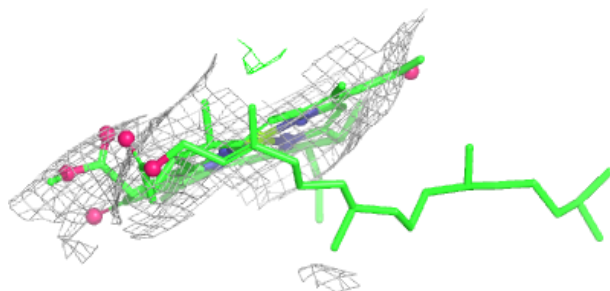
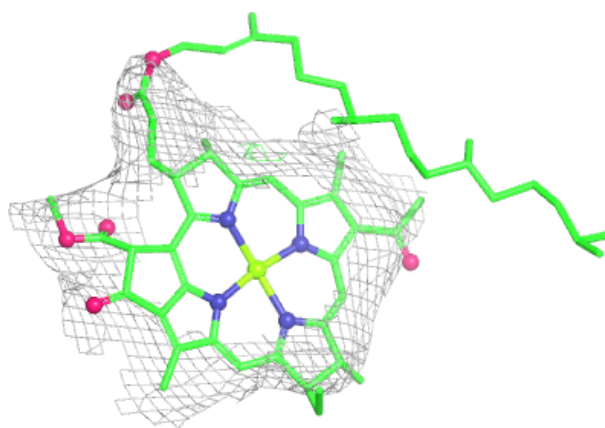


Electron density around CRT 9 101:

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

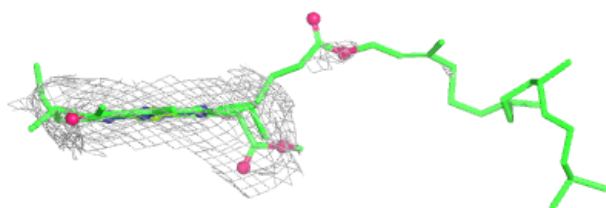
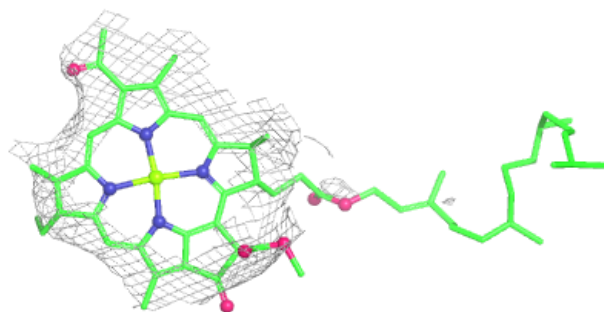
**Electron density around BCL 0 102:**

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

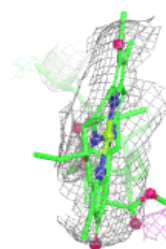
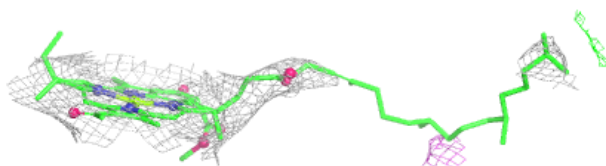
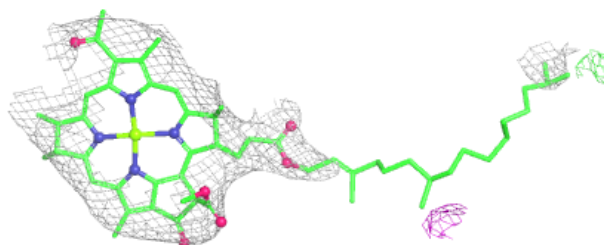


Electron density around BCL j 101:

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

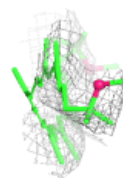
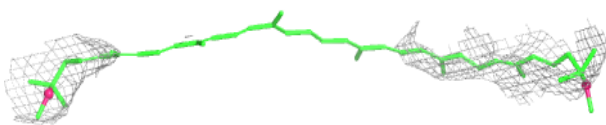
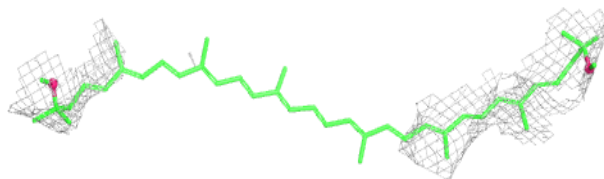
**Electron density around BCL S 102:**

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

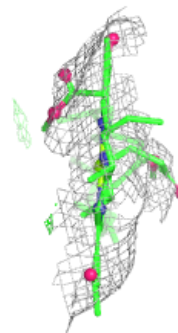
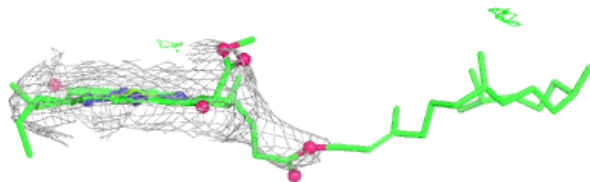
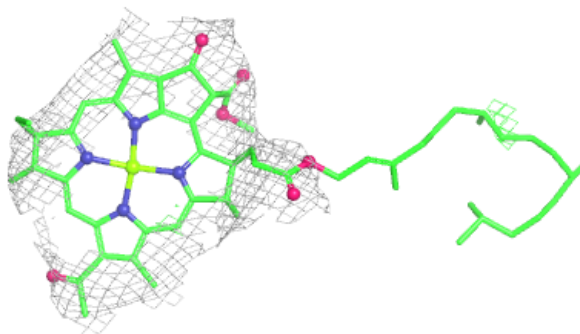


Electron density around CRT E 101:

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

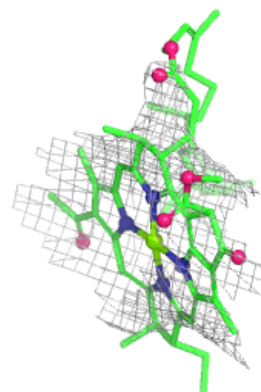
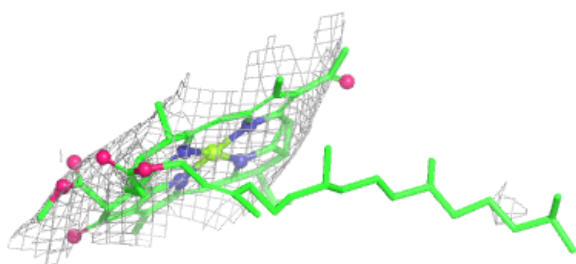
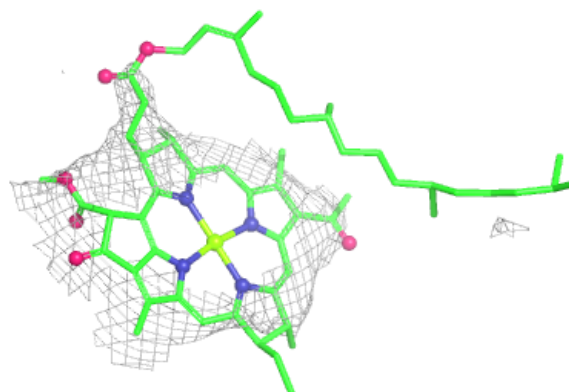
**Electron density around BCL AI 101:**

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

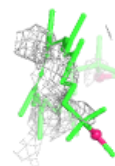
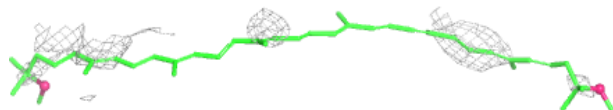
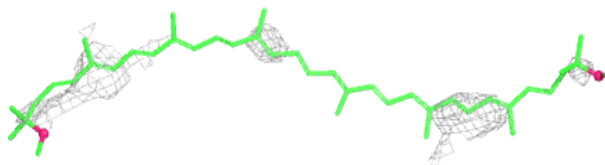


Electron density around BCL s 102:

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

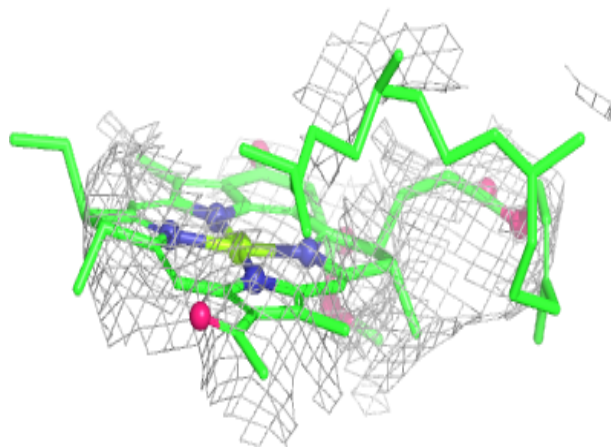
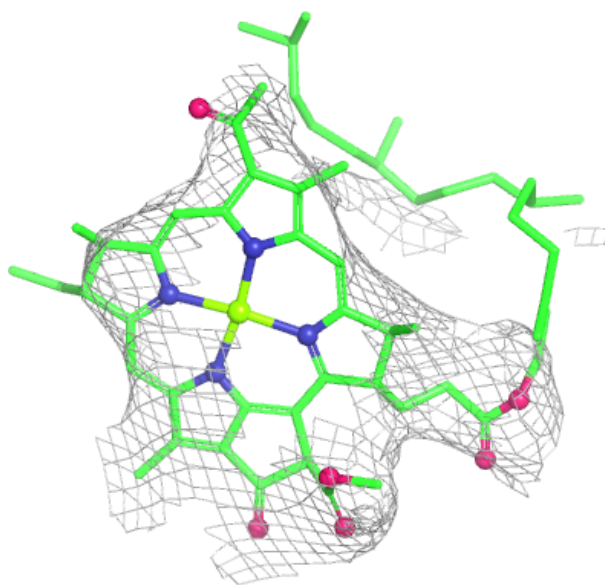
**Electron density around CRT Z 101:**

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



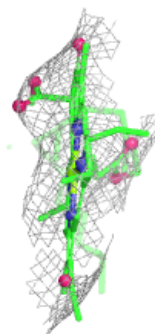
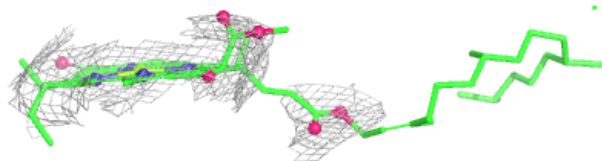
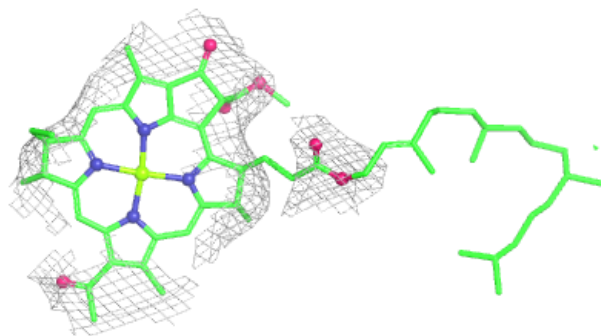
Electron density around BCL 8 101:

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



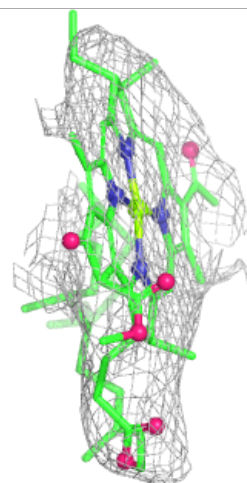
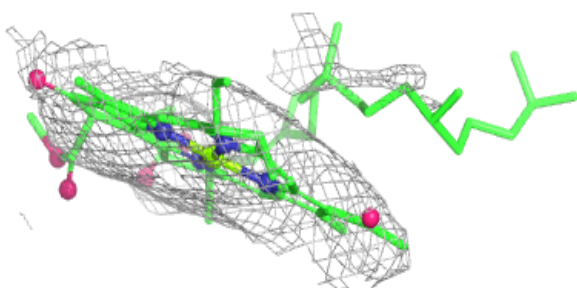
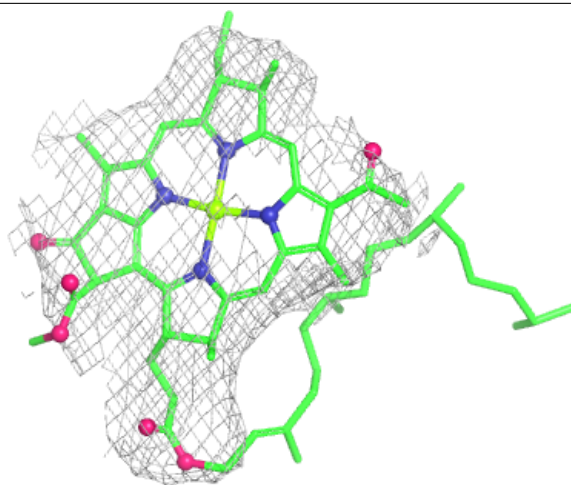
Electron density around BCL 9 102:

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



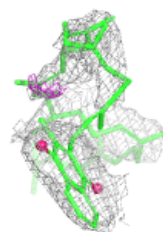
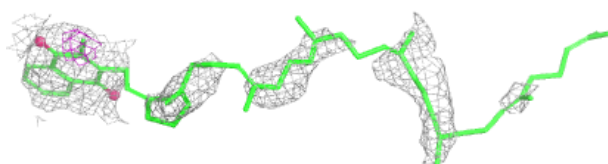
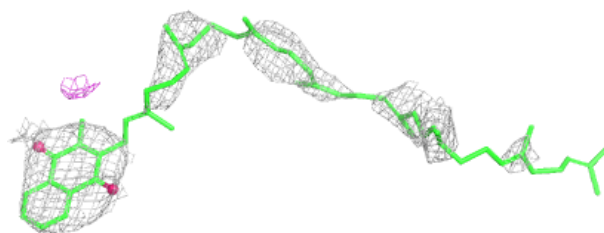
Electron density around BCL X 102:

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

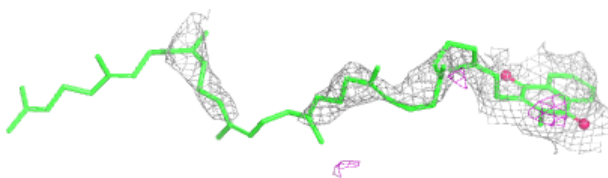
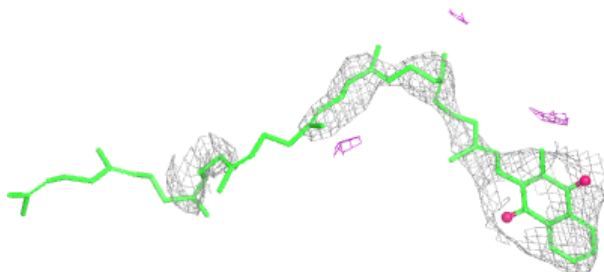


Electron density around MQ8 M 404:

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

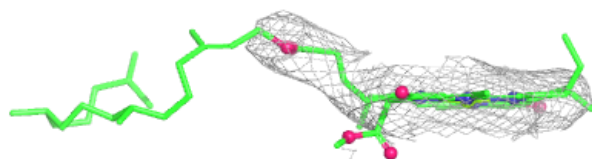
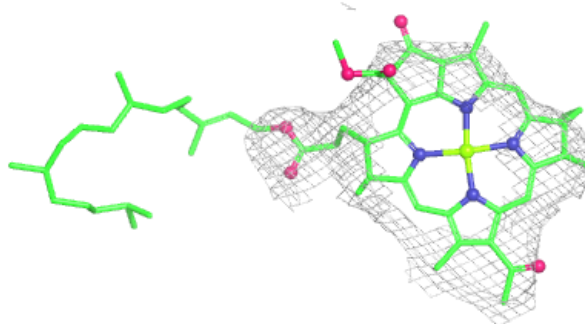
**Electron density around MQ8 y 403:**

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

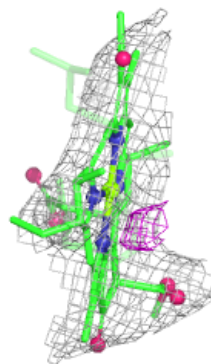
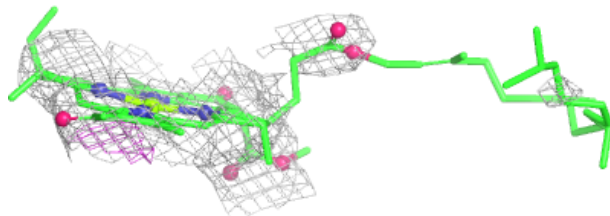
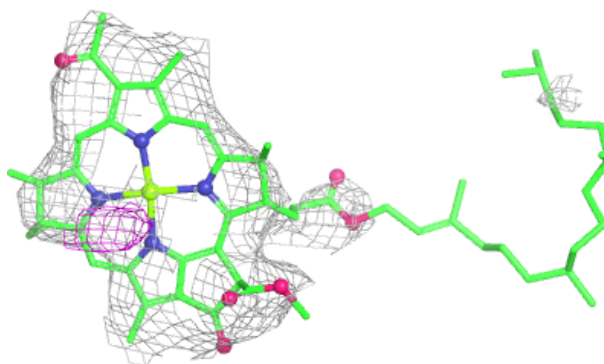


Electron density around BCL AH 101:

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

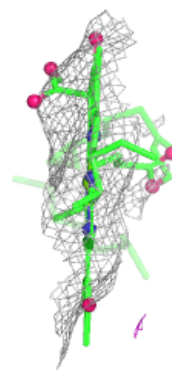
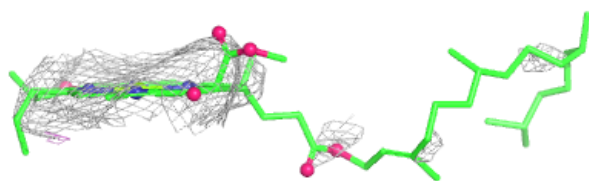
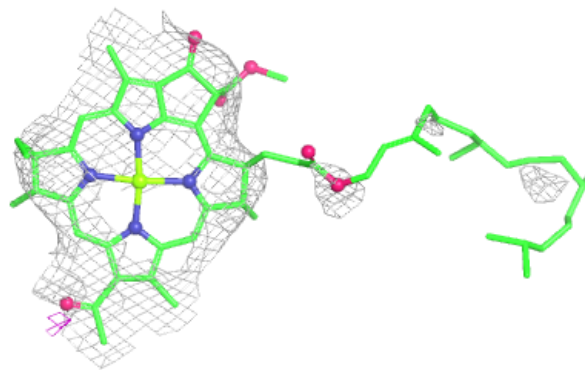
**Electron density around BCL 3 101:**

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

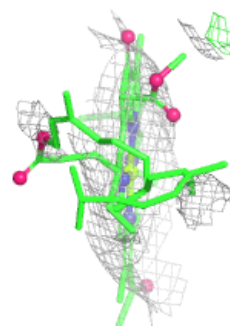
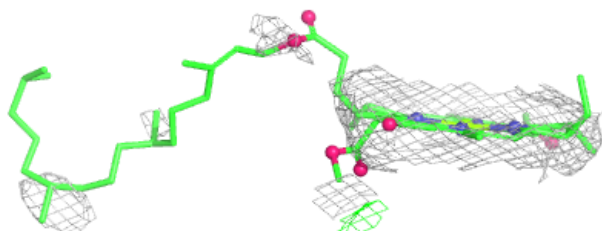
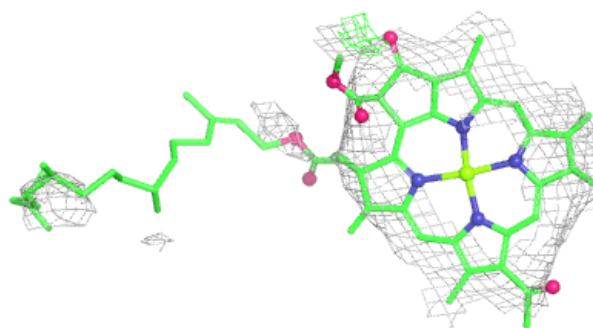


Electron density around BCL 1 101:

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

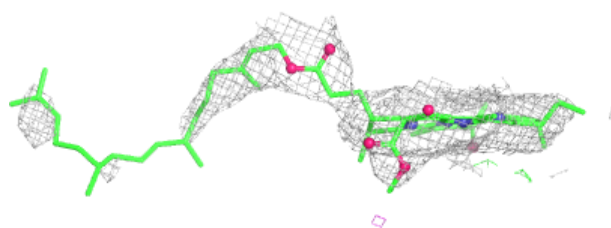
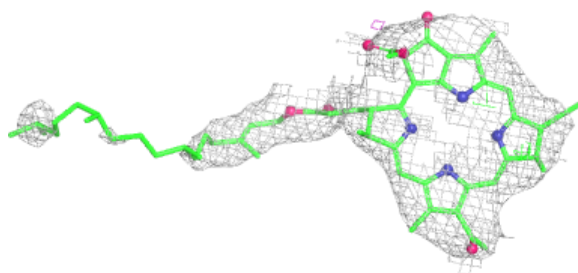
**Electron density around BCL AB 101:**

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

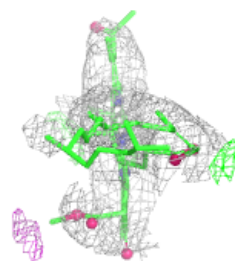
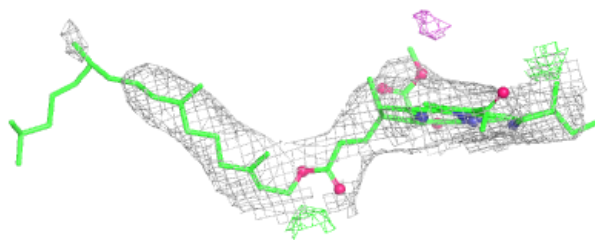
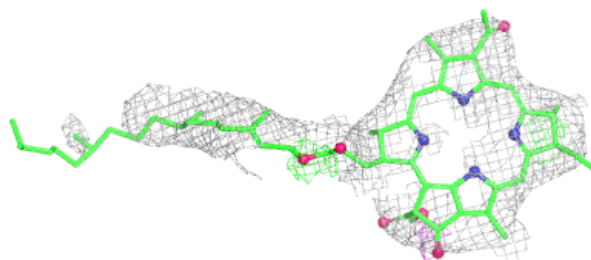


Electron density around BPH M 403:

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

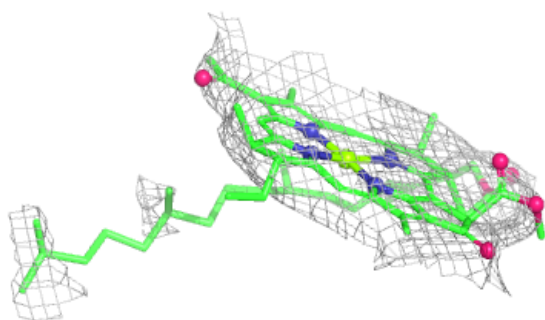
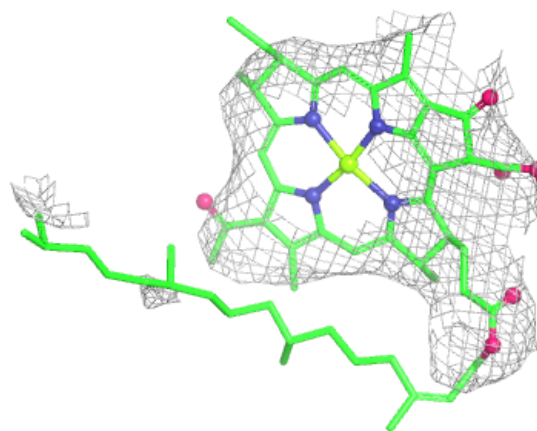
**Electron density around BPH y 402:**

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



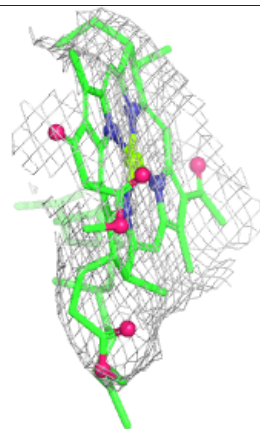
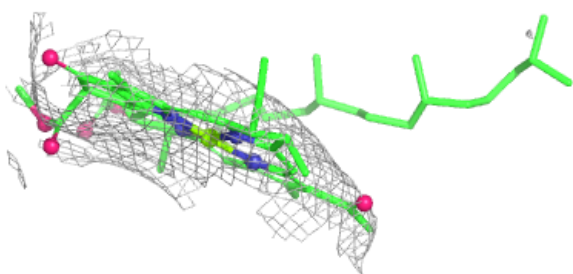
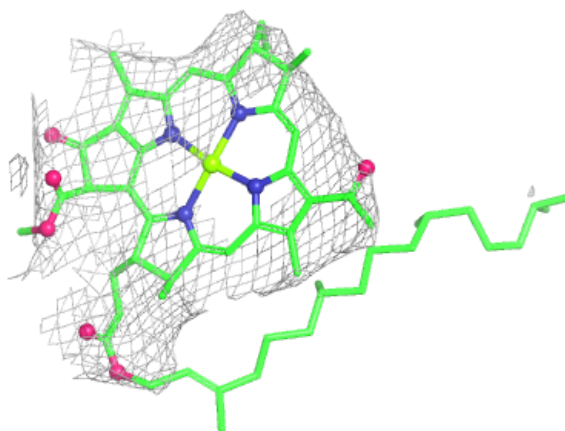
Electron density around BCL Z 102:

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



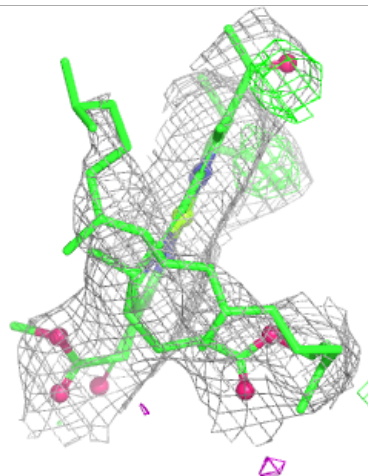
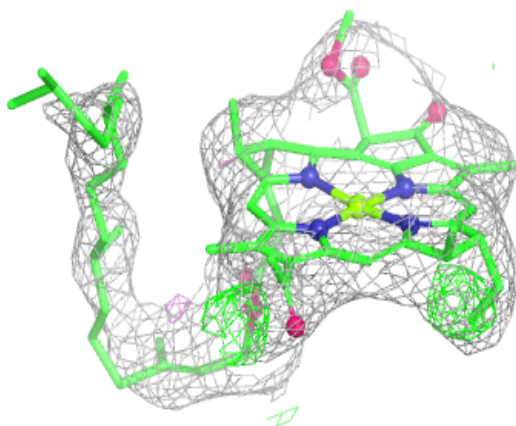
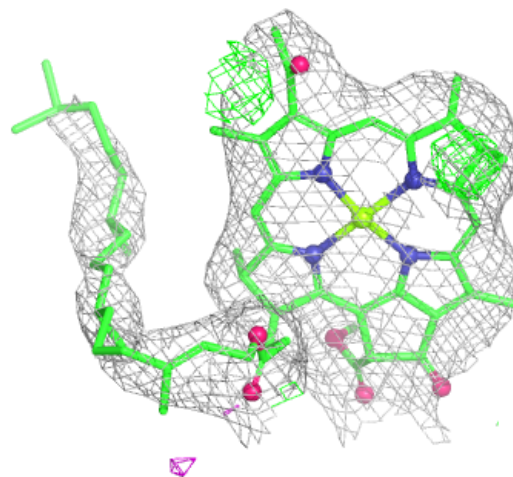
Electron density around BCL R 102:

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



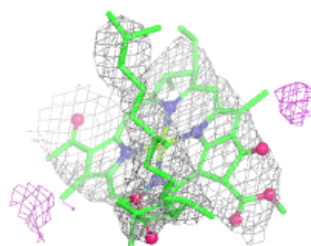
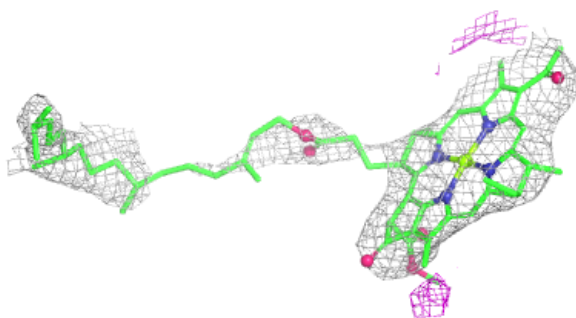
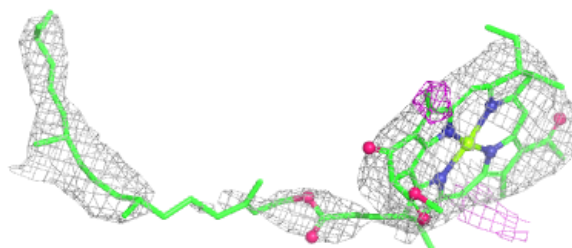
Electron density around BCL x 305:

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

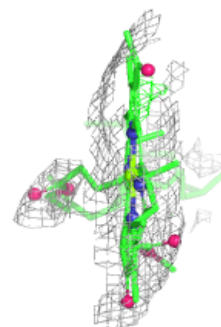
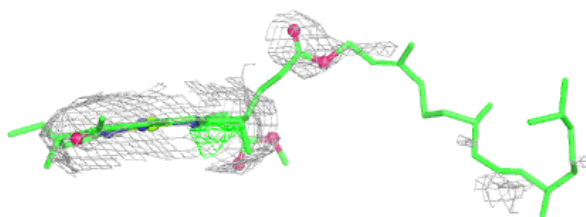
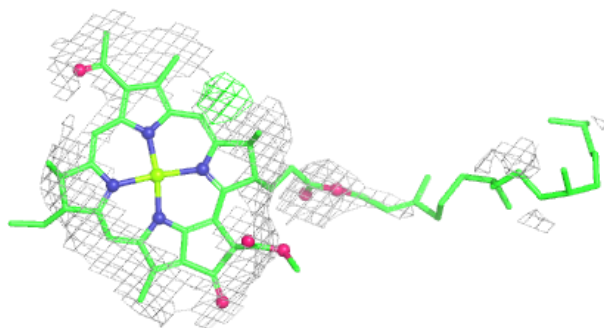


Electron density around BCL y 401:

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

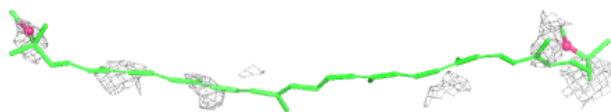
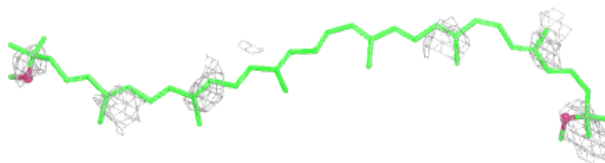
**Electron density around BCL A 102:**

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



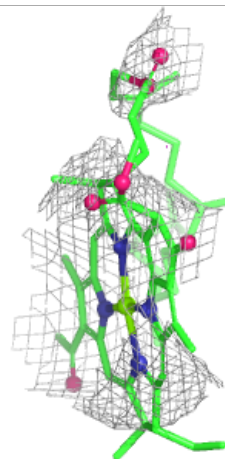
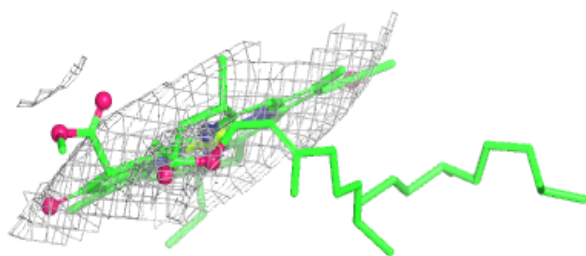
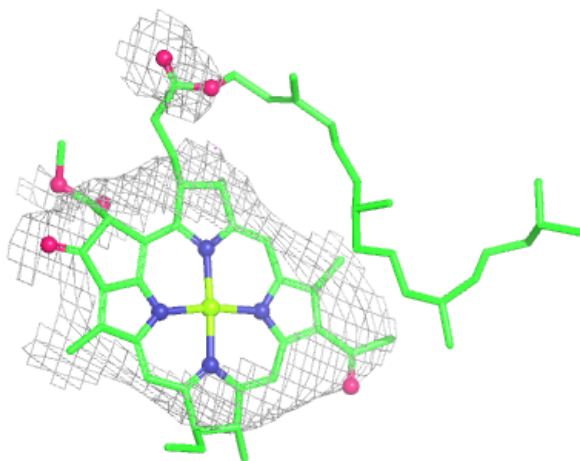
Electron density around CRT X 101:

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



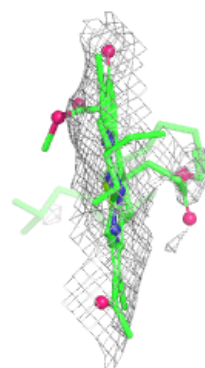
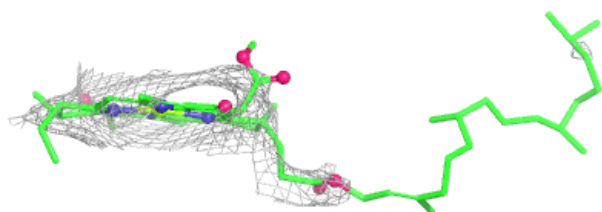
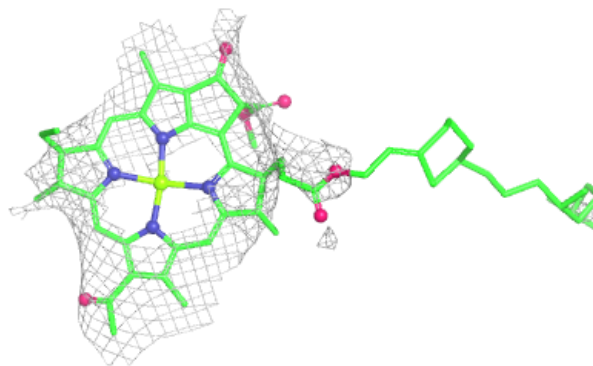
Electron density around BCL q 102:

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

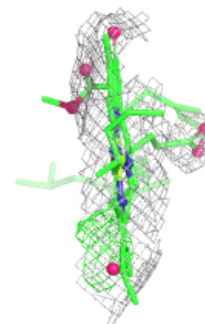
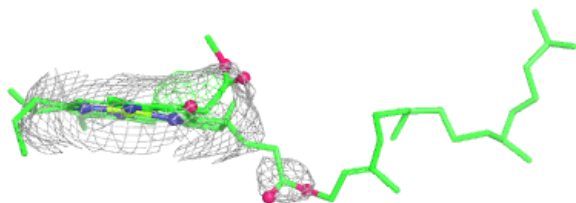
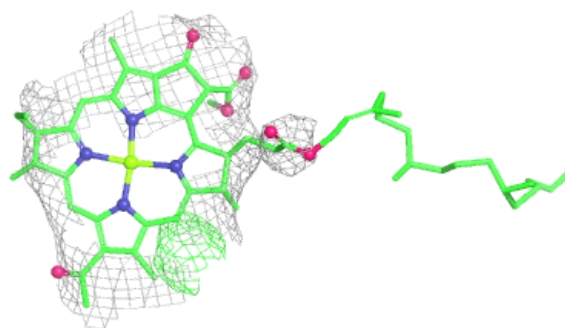


Electron density around BCL r 101:

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

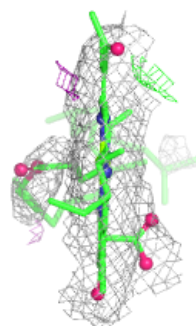
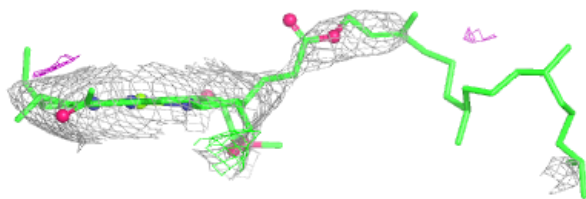
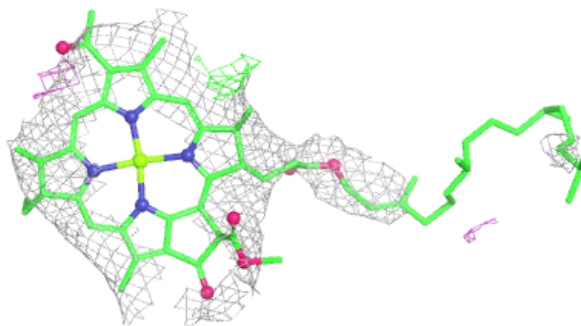
**Electron density around BCL F 101:**

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



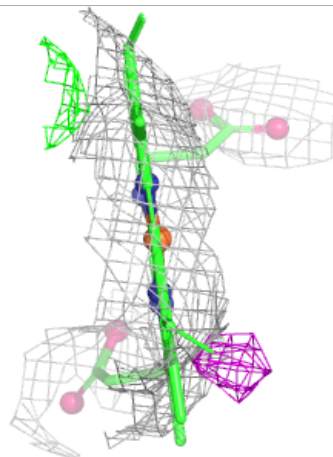
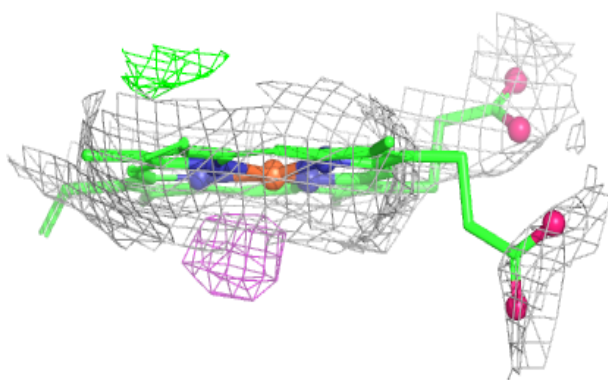
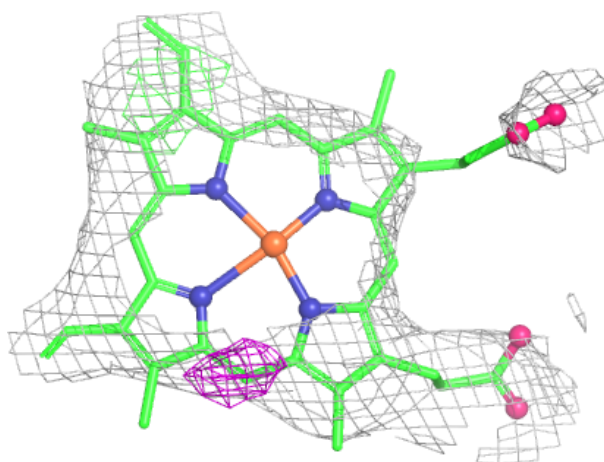
Electron density around BCL AK 101:

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



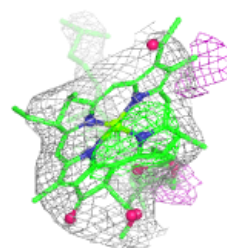
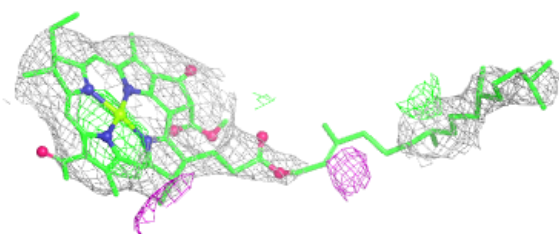
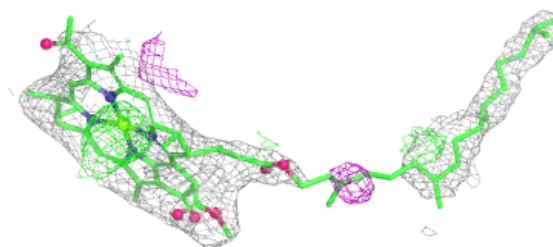
Electron density around HEM C 501:

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



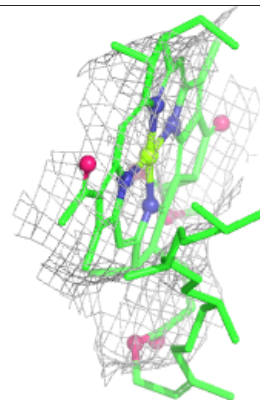
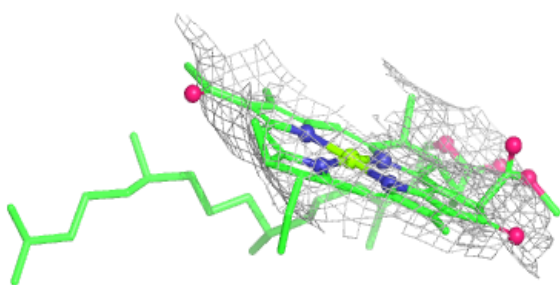
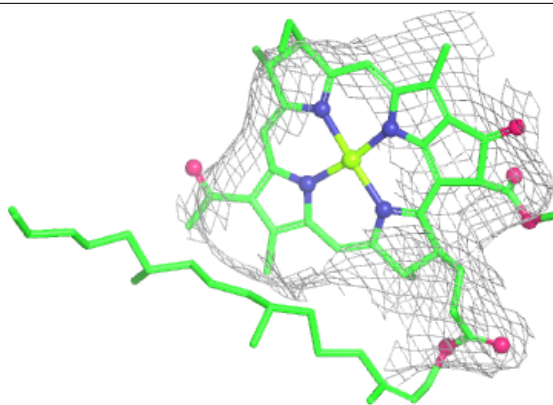
Electron density around BCL x 301:

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



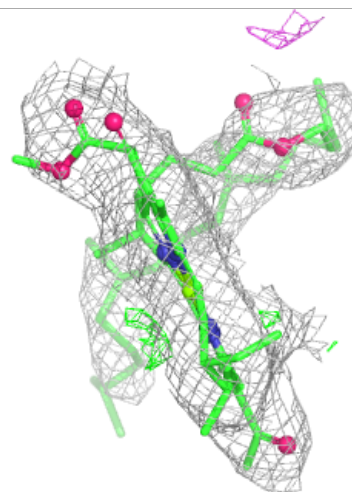
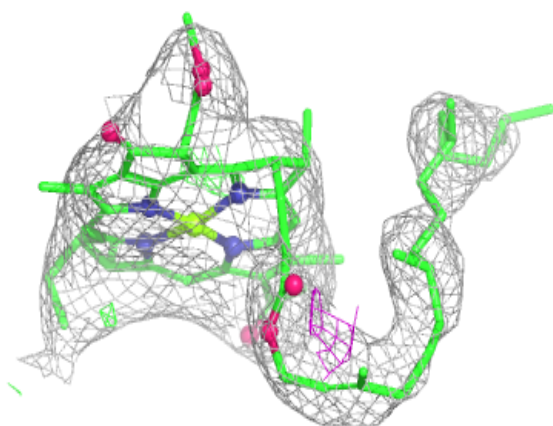
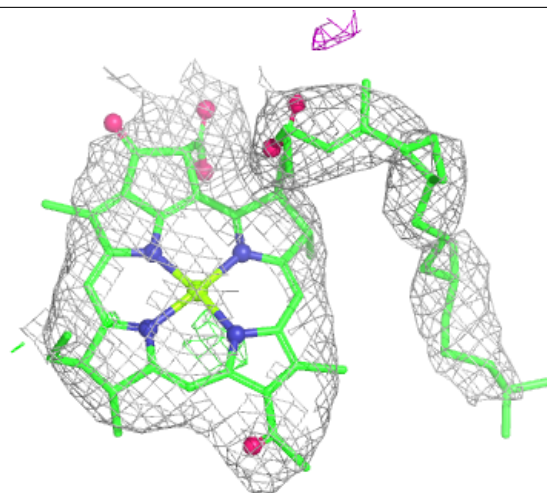
Electron density around BCL i 102:

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



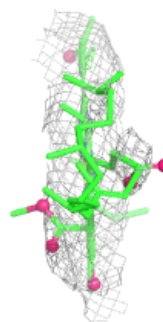
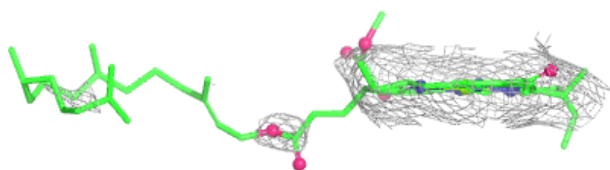
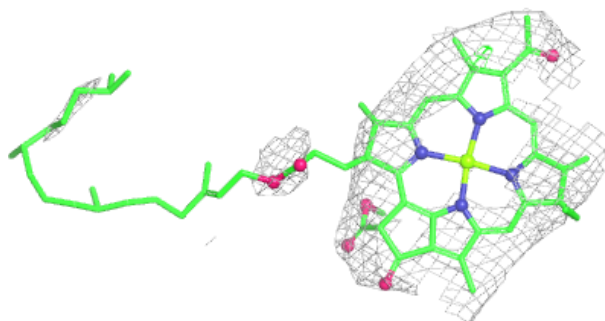
Electron density around BCL M 401:

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

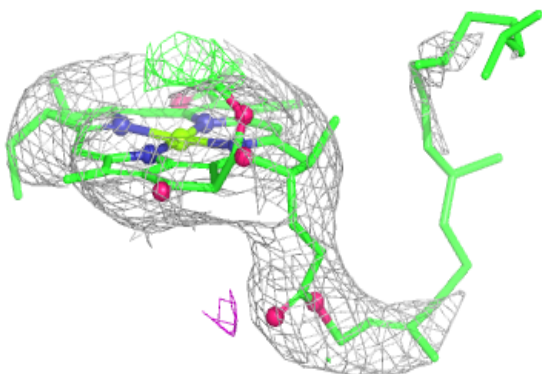
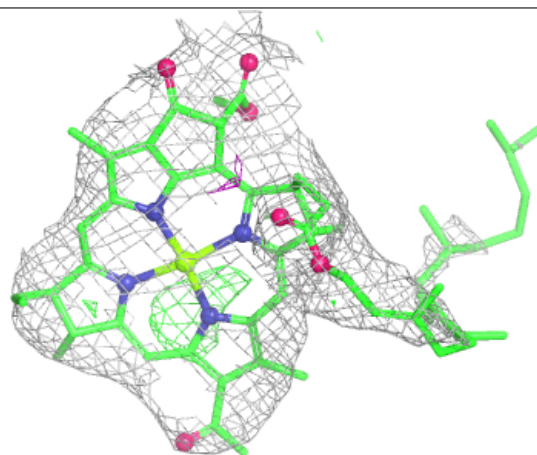


Electron density around BCL W 101:

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

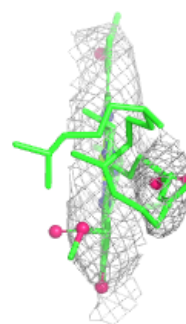
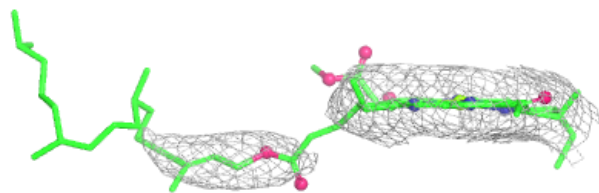
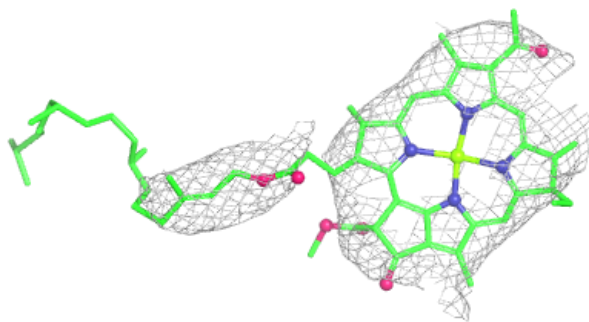
**Electron density around BCL L 303:**

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



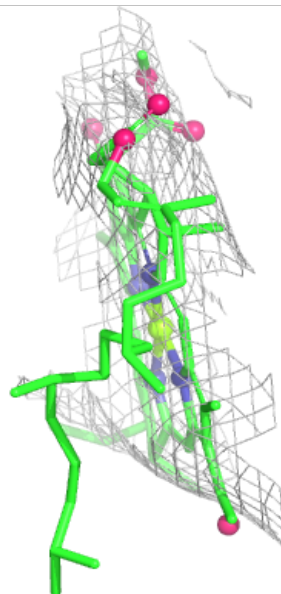
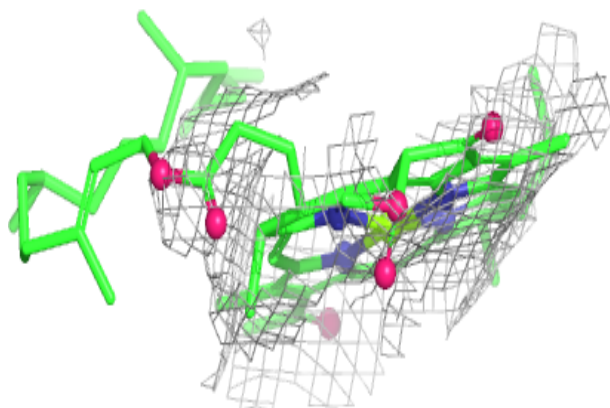
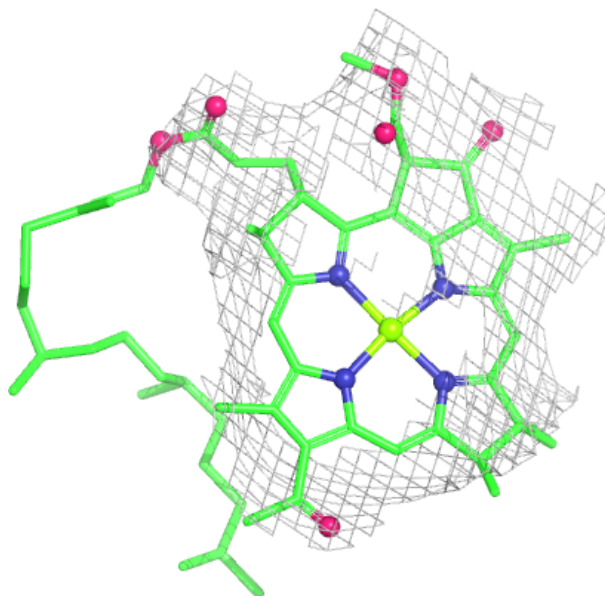
Electron density around BCL Y 101:

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



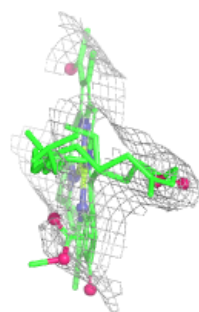
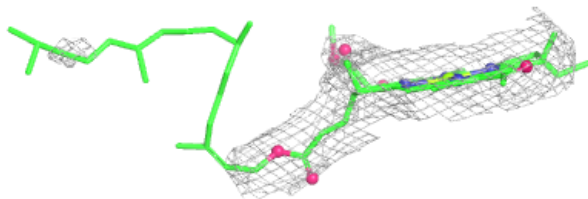
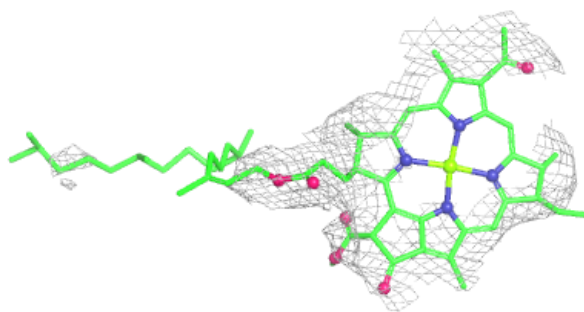
Electron density around BCL A 103:

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

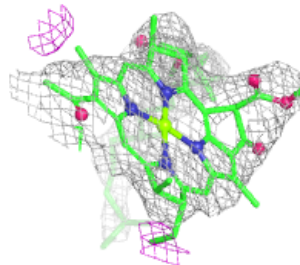
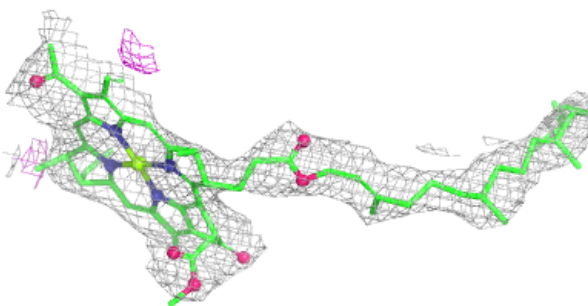
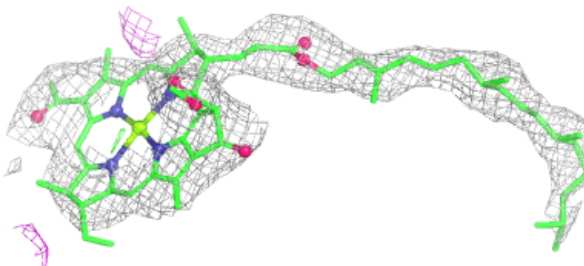


Electron density around BCL 5 101:

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

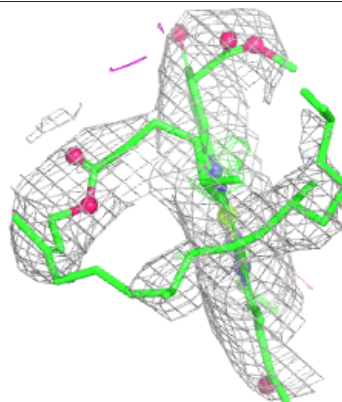
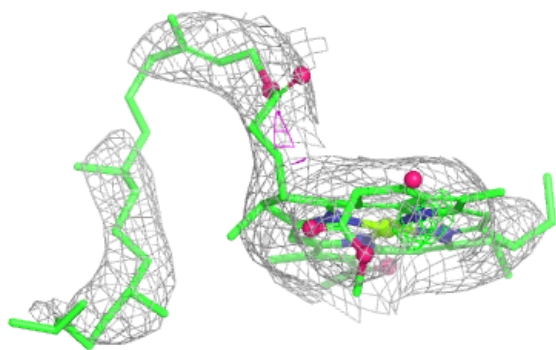
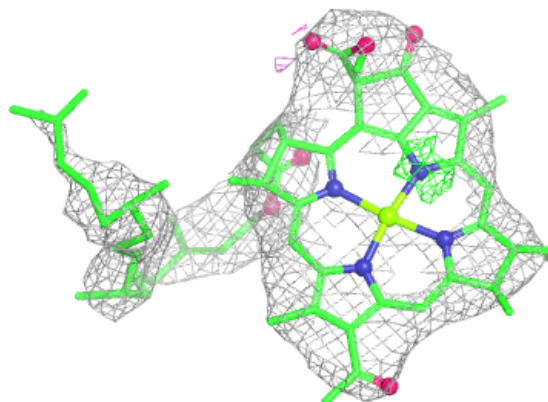
**Electron density around BCL M 402:**

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



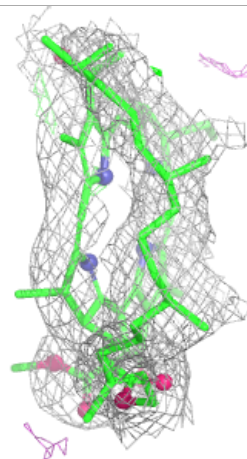
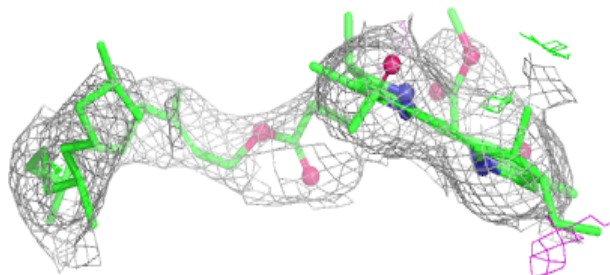
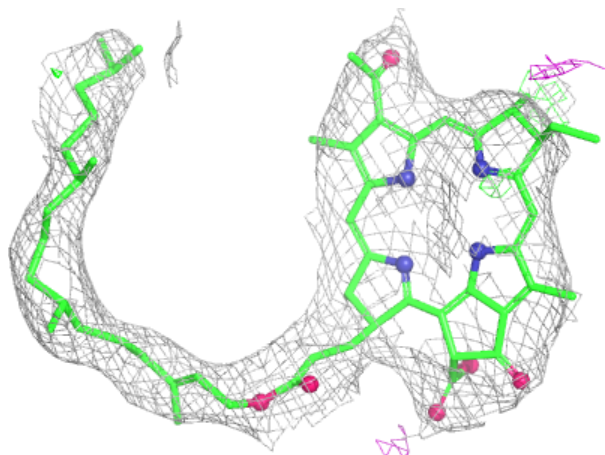
Electron density around BCL x 303:

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



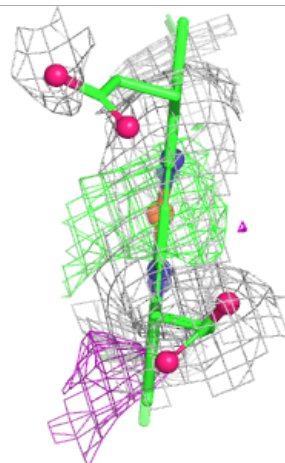
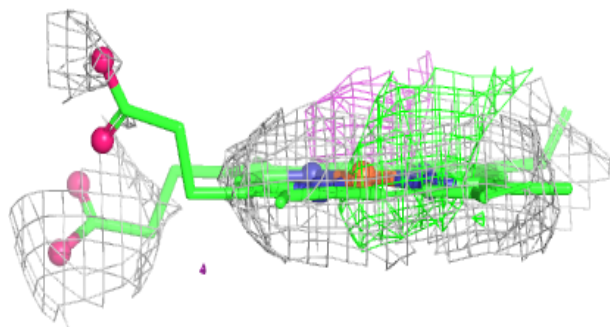
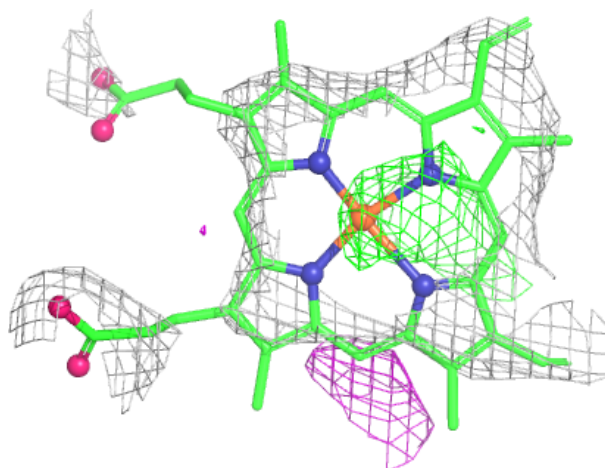
Electron density around BPH x 302:

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



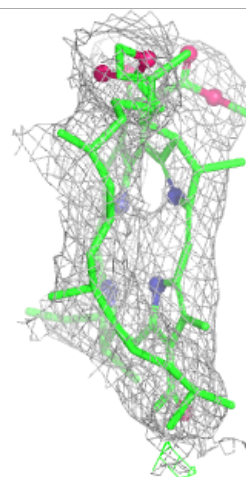
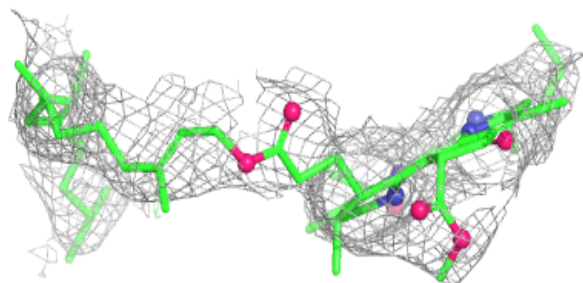
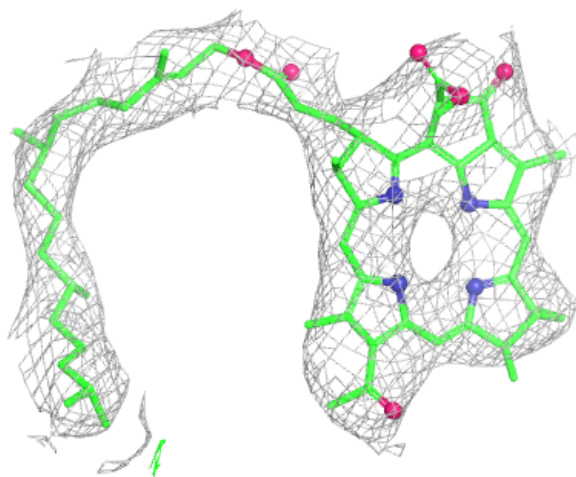
Electron density around HEM o 503:

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



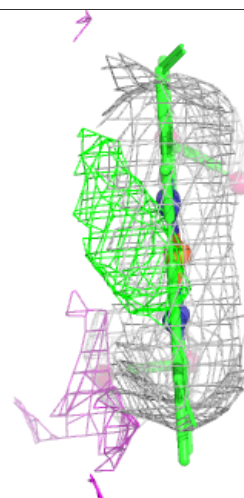
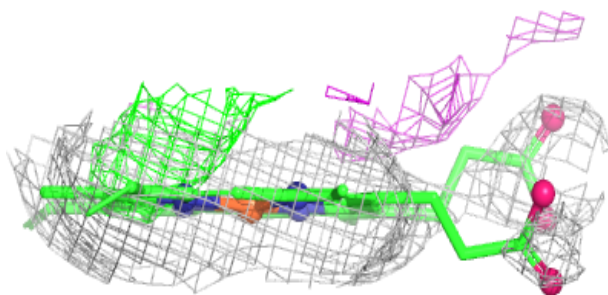
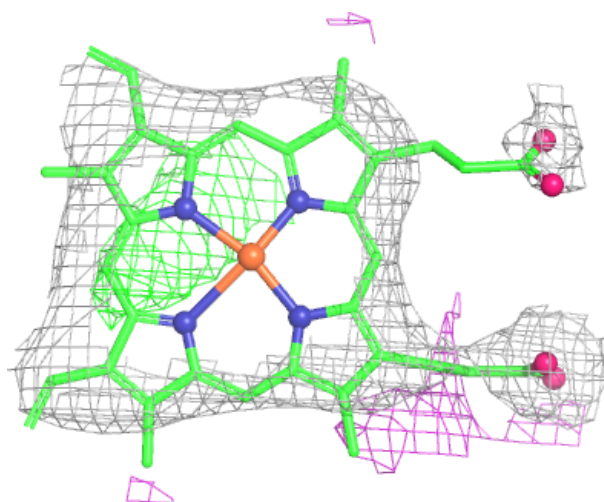
Electron density around BPH L 302:

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



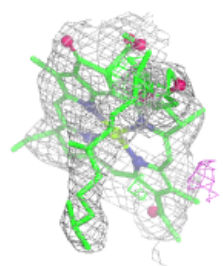
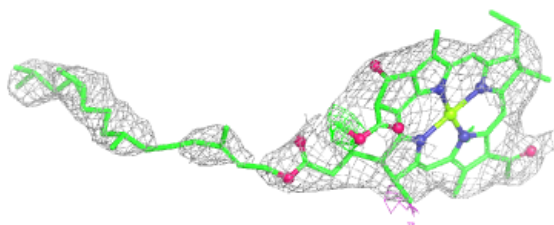
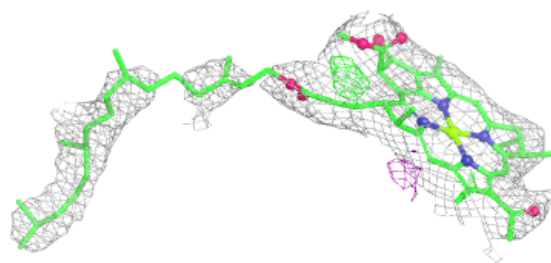
Electron density around HEM o 504:

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



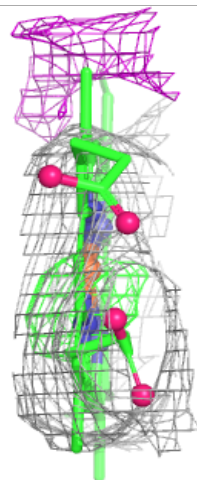
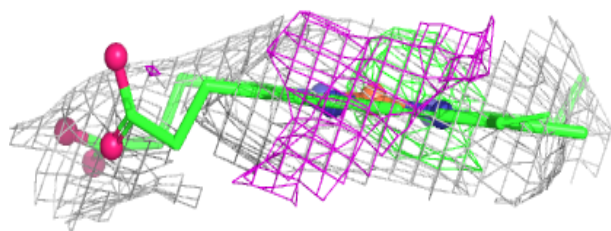
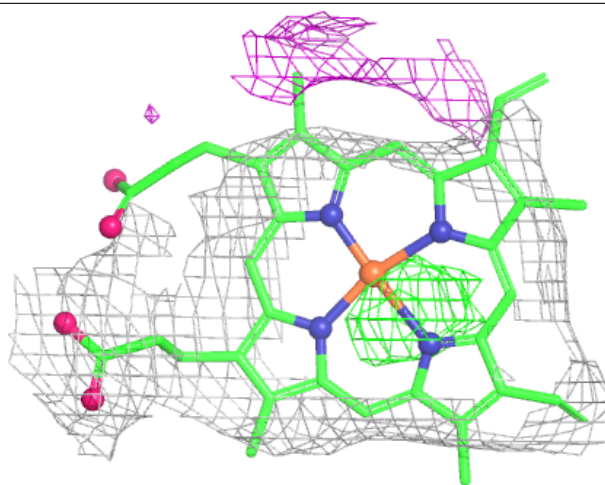
Electron density around BCL L 301:

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



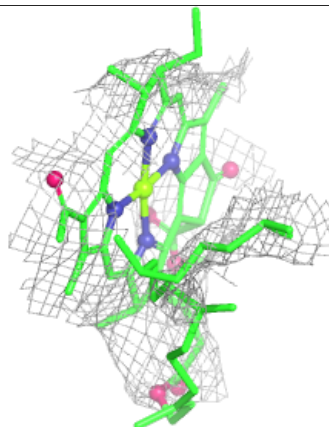
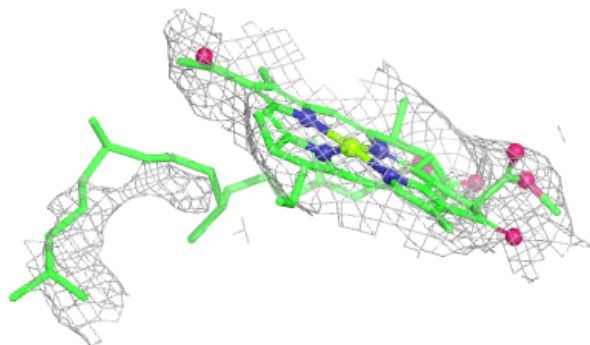
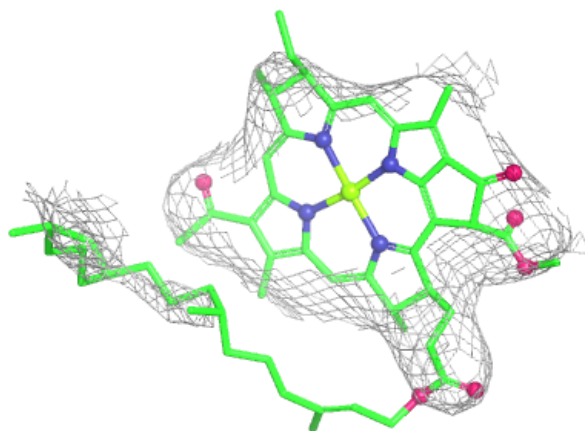
Electron density around HEM C 502:

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



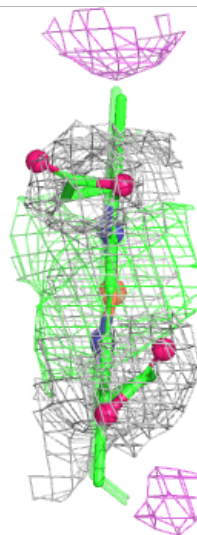
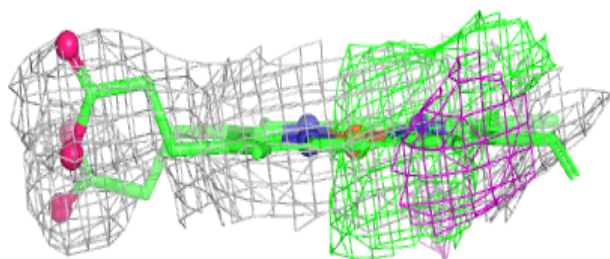
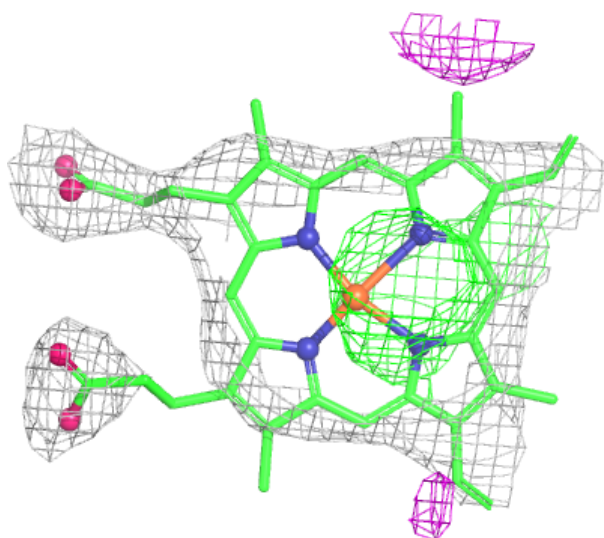
Electron density around BCL 4 102:

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



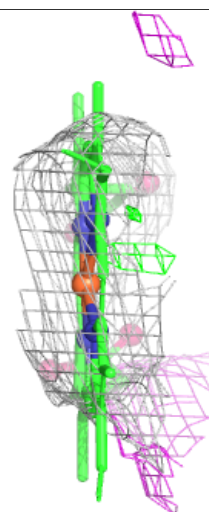
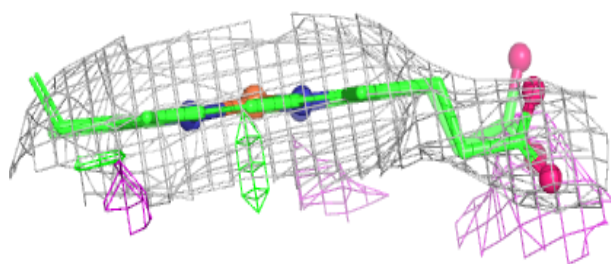
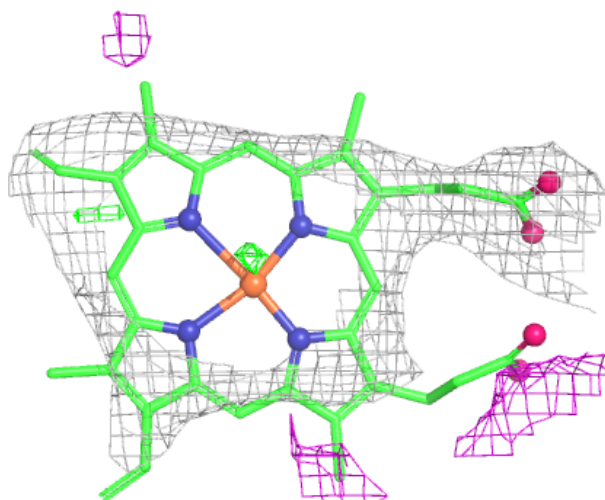
Electron density around HEM C 504:

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



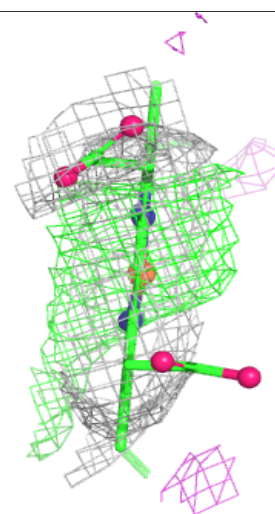
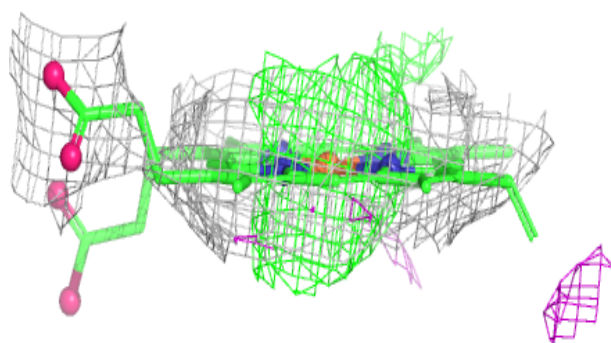
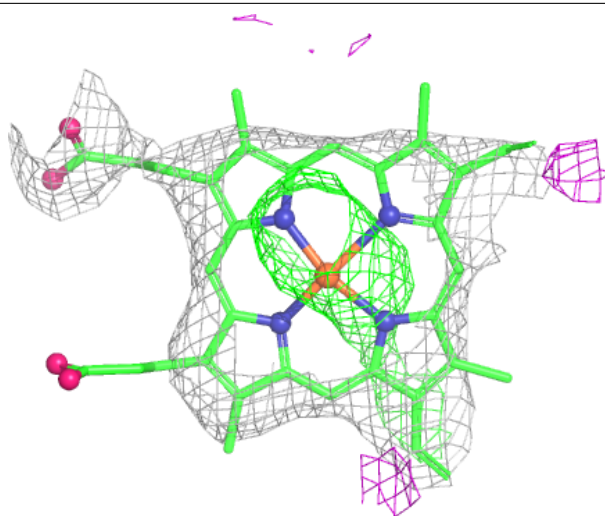
Electron density around HEM o 502:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.