



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 06:29 AM JST

PDB ID : 5B5M / pdb_00005b5m
Title : Crystal structure of the Sr-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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

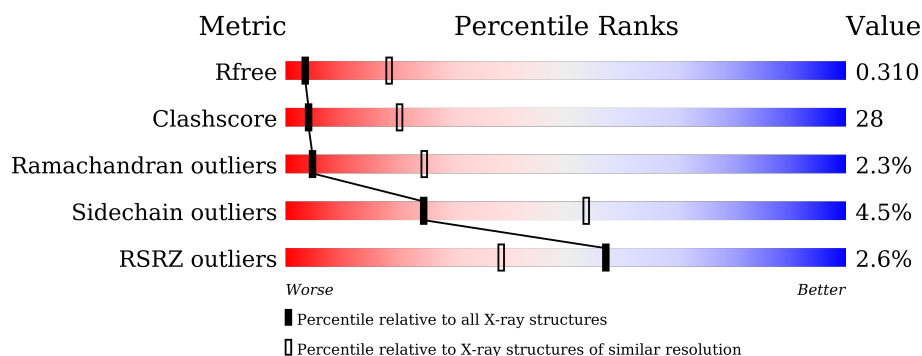
1 Overall quality at a glance

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	2% 44% 41% 9% 5%
1	o	333	3% 47% 35% 11% 5%
2	L	281	4% 41% 44% 14%
2	x	281	4% 41% 47% 11%
3	M	319	3% 37% 49% 13%
3	y	319	2% 38% 49% 13%

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Mol	Chain	Length	Quality of chain
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	
5	d	61	

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Mol	Chain	Length	Quality of chain
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	
6	N	47	

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Mol	Chain	Length	Quality of chain
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	

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 475	C 315	N 77	O 81	S 2	0	0	0
5	AE	60	Total 481	C 318	N 78	O 83	S 2	0	1	0
5	AG	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	AI	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	AK	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	h	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	j	60	Total 475	C 315	N 77	O 81	S 2	0	0	0
5	l	60	Total 475	C 315	N 77	O 81	S 2	0	0	0

- Molecule 6 is a protein called LH1 beta polypeptide.

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

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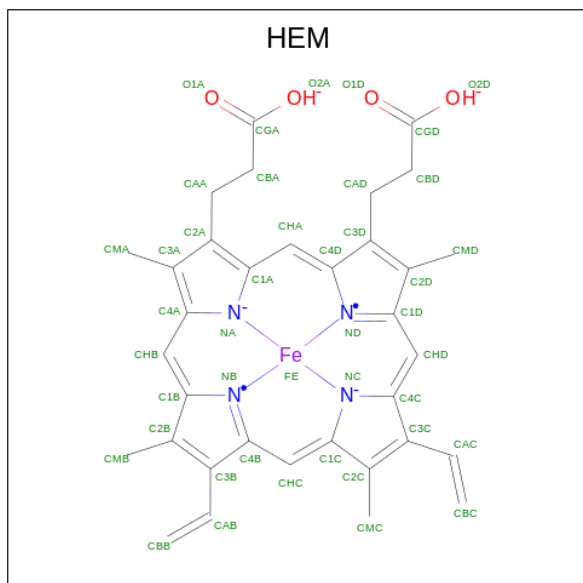
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	X	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	Z	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	2	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	4	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	6	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	8	40	Total 337	C 228	N 52	O 55	S 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	C	N	O	S	0	0	0
			337	228	52	55	2			
6	c	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 8 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

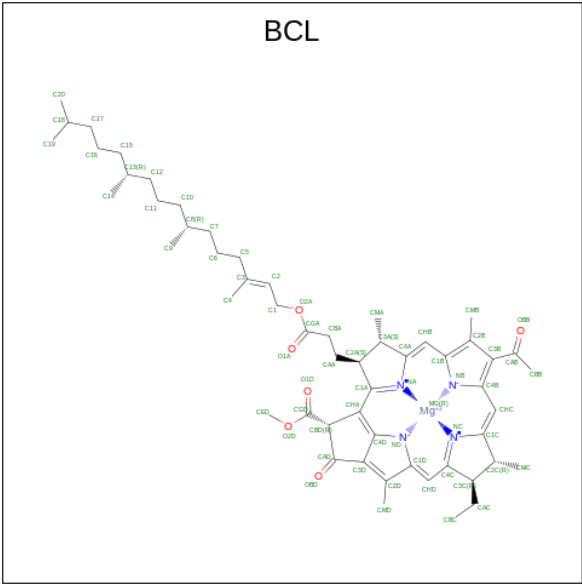
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total 1 Sr 1	0	0
8	L	2	Total 2 Sr 2	0	0
8	A	1	Total 1 Sr 1	0	0
8	D	1	Total 1 Sr 1	0	0
8	F	1	Total 1 Sr 1	0	0
8	I	1	Total 1 Sr 1	0	0
8	K	1	Total 1 Sr 1	0	0
8	O	1	Total 1 Sr 1	0	0
8	Q	1	Total 1 Sr 1	0	0
8	S	1	Total 1 Sr 1	0	0
8	U	1	Total 1 Sr 1	0	0
8	W	1	Total 1 Sr 1	0	0
8	Y	1	Total 1 Sr 1	0	0
8	1	1	Total 1 Sr 1	0	0
8	5	2	Total 2 Sr 2	0	0
8	7	1	Total 1 Sr 1	0	0
8	9	1	Total 1 Sr 1	0	0
8	o	1	Total 1 Sr 1	0	0
8	x	2	Total 2 Sr 2	0	0
8	m	1	Total 1 Sr 1	0	0
8	p	1	Total 1 Sr 1	0	0
8	r	1	Total 1 Sr 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	w	2	Total 2	Sr 2	0	0
8	AA	1	Total 1	Sr 1	0	0
8	AC	1	Total 1	Sr 1	0	0
8	AE	1	Total 1	Sr 1	0	0
8	AI	2	Total 2	Sr 2	0	0
8	AK	1	Total 1	Sr 1	0	0
8	d	1	Total 1	Sr 1	0	0
8	f	1	Total 1	Sr 1	0	0
8	h	1	Total 1	Sr 1	0	0
8	j	1	Total 1	Sr 1	0	0
8	l	1	Total 1	Sr 1	0	0

- 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	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	A	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	B	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	J	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	1	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	5	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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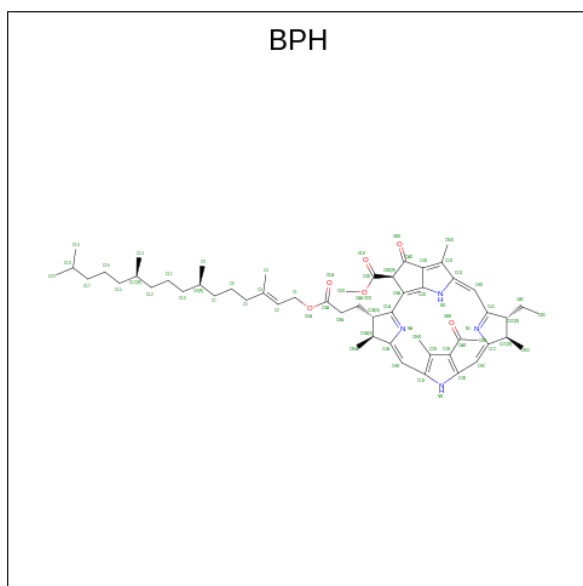
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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9	r	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	s	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	u	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	v	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	w	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	z	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AA	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	AD	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	AE	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	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	AJ	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: $C_{55}H_{76}N_4O_6$).



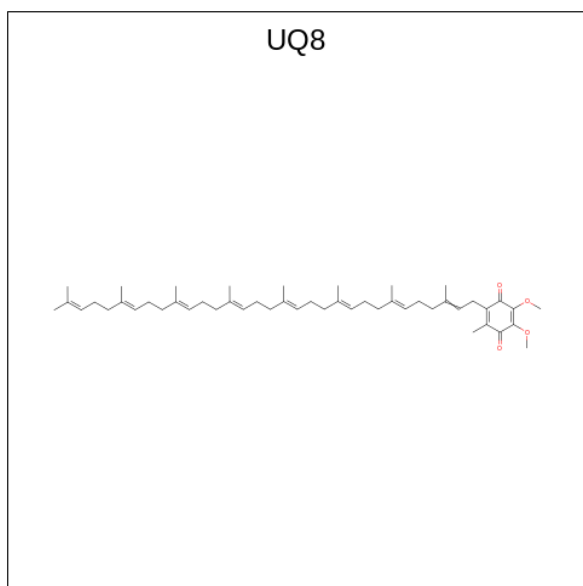
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		
10	x	1	Total	C	N	O	0	0
			65	55	4	6		

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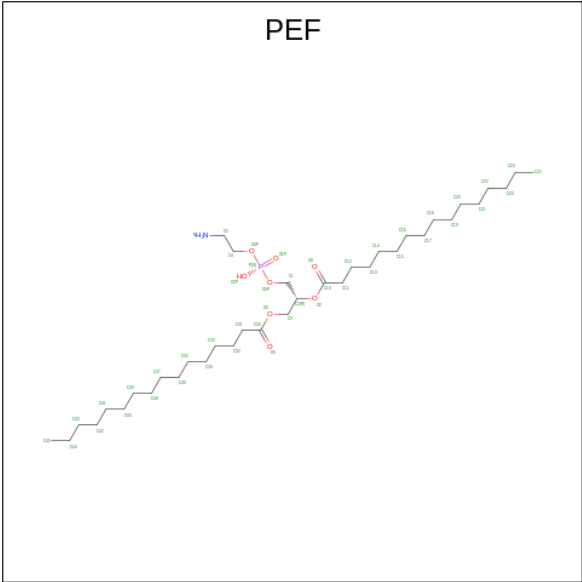
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	y	1	Total	C	N	O	0	0
			65	55	4	6		

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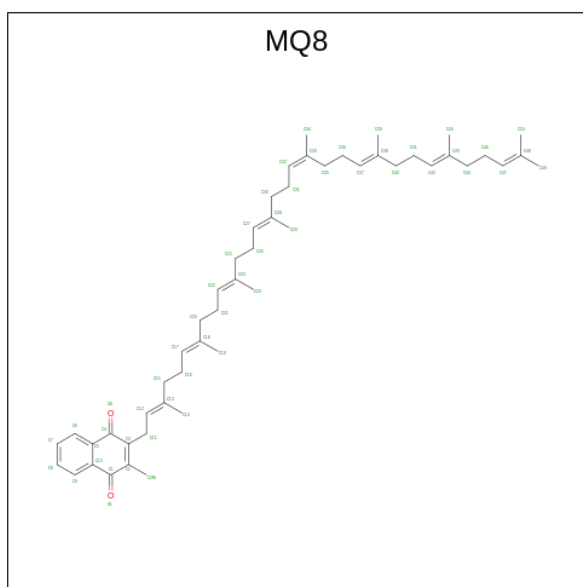
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	m	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	p	1	Total	C	N	O	P	0	0
			16	7	1	7	1		

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

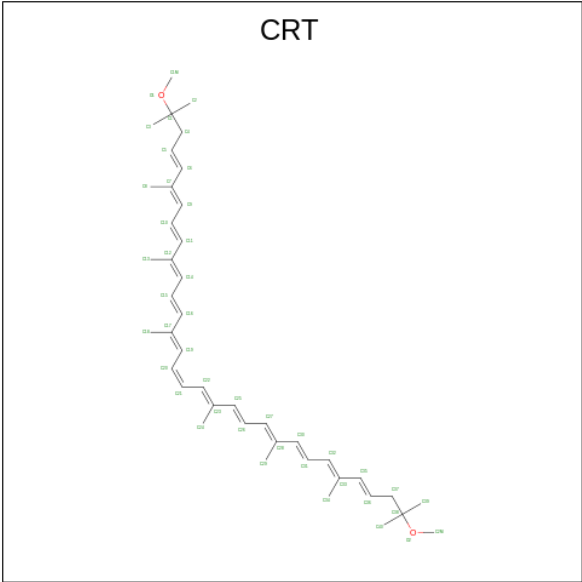
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	1	Total	Fe	0	0
			1	1		
13	x	1	Total	Fe	0	0
			1	1		

- 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).



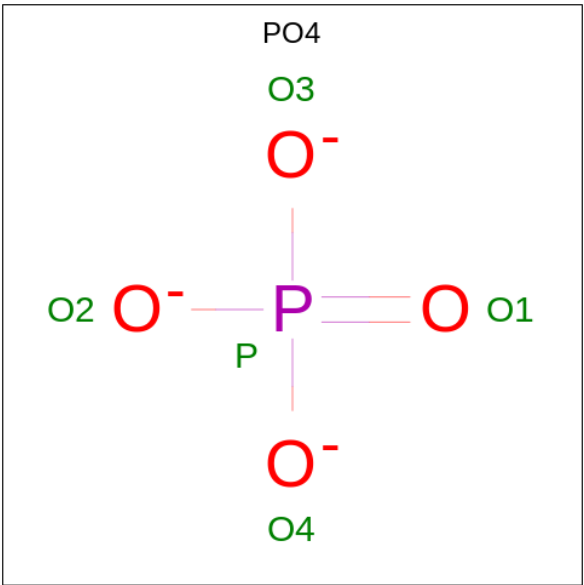
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			44	42	2		
15	A	1	Total	C	O	0	0
			44	42	2		
15	E	1	Total	C	O	0	0
			44	42	2		
15	G	1	Total	C	O	0	0
			44	42	2		
15	J	1	Total	C	O	0	0
			44	42	2		
15	N	1	Total	C	O	0	0
			44	42	2		
15	P	1	Total	C	O	0	0
			44	42	2		
15	R	1	Total	C	O	0	0
			44	42	2		
15	T	1	Total	C	O	0	0
			44	42	2		
15	U	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		

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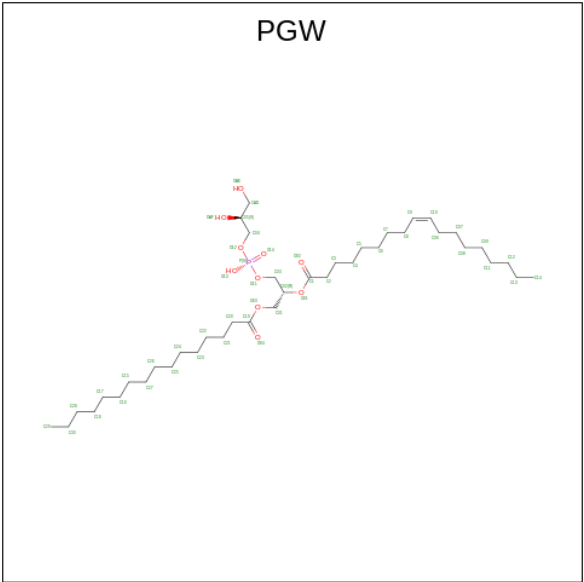
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	6	1	Total	C	O	0	0
			44	42	2		
15	8	1	Total	C	O	0	0
			44	42	2		
15	9	1	Total	C	O	0	0
			44	42	2		
15	y	1	Total	C	O	0	0
			44	42	2		
15	n	1	Total	C	O	0	0
			44	42	2		
15	p	1	Total	C	O	0	0
			44	42	2		
15	s	1	Total	C	O	0	0
			44	42	2		
15	v	1	Total	C	O	0	0
			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	AE	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	f	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		
15	c	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		

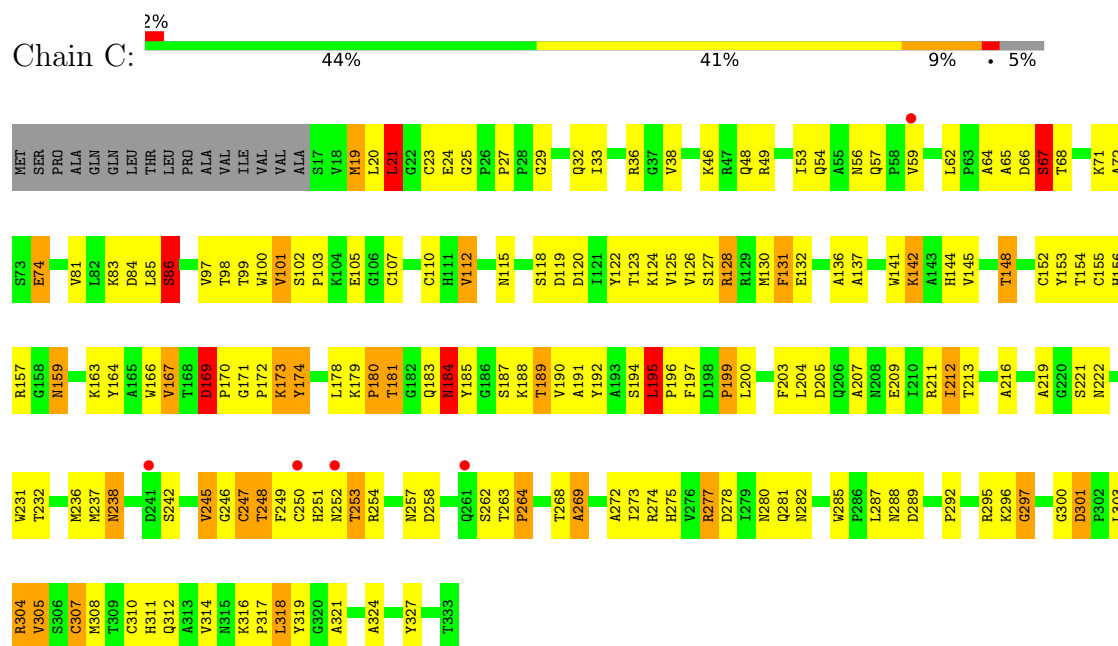
- Molecule 18 is water.

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

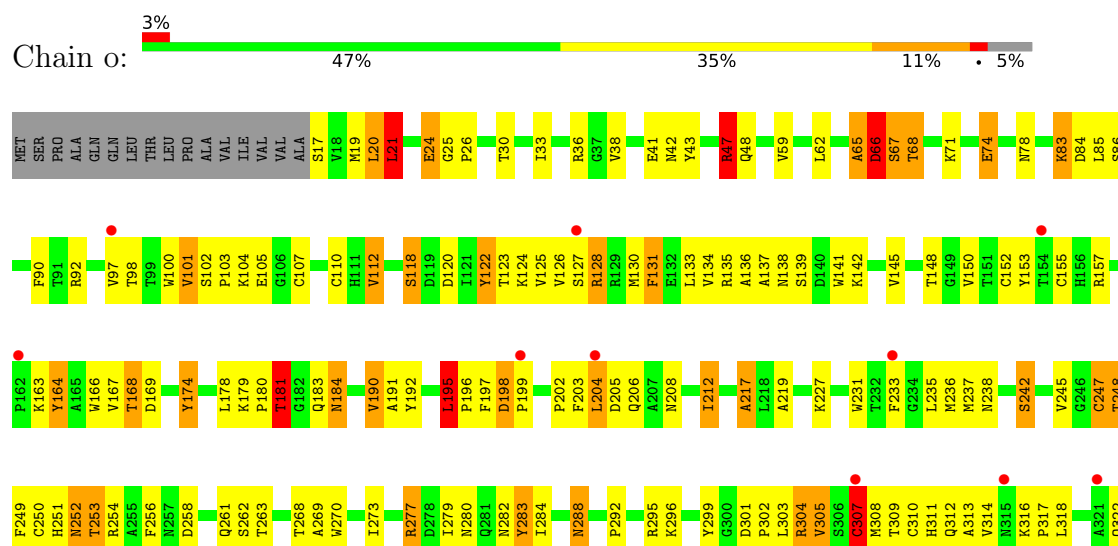
3 Residue-property plots

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

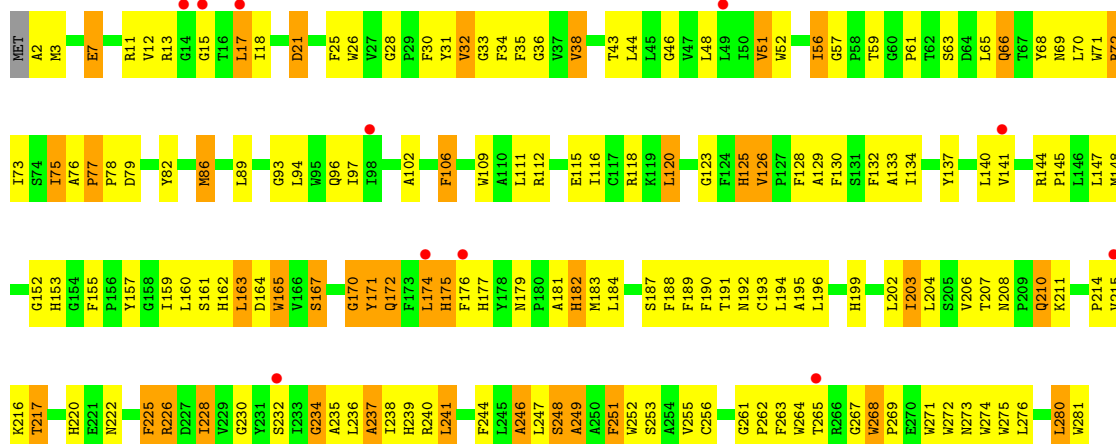


• Molecule 1: Photosynthetic reaction center cytochrome c subunit

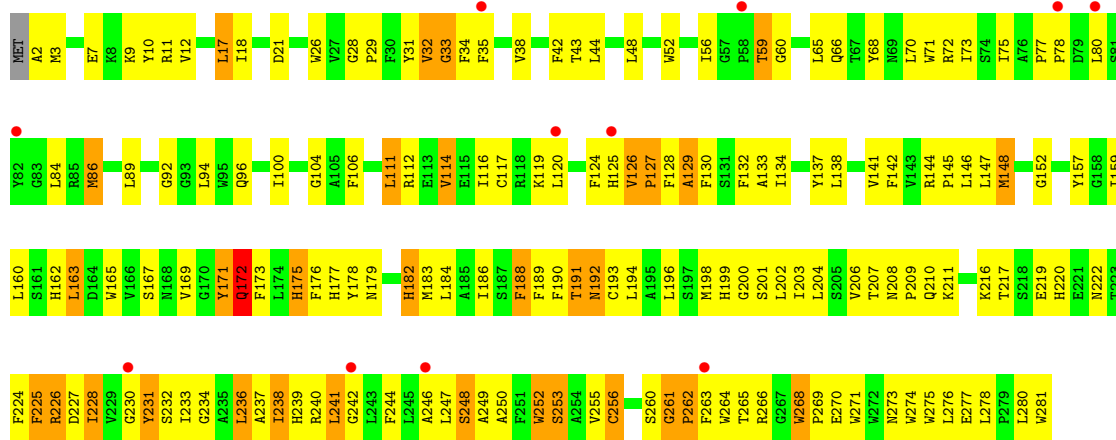




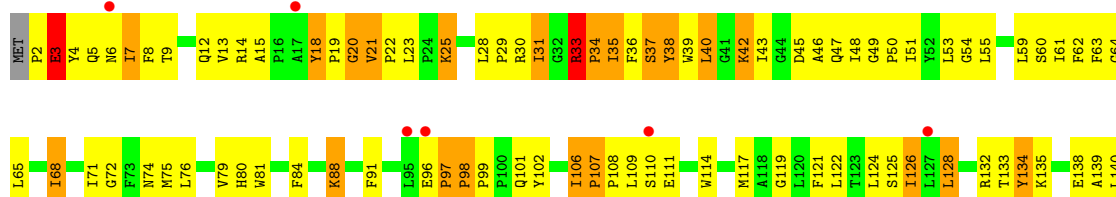
• Molecule 2: Photosynthetic reaction center L subunit

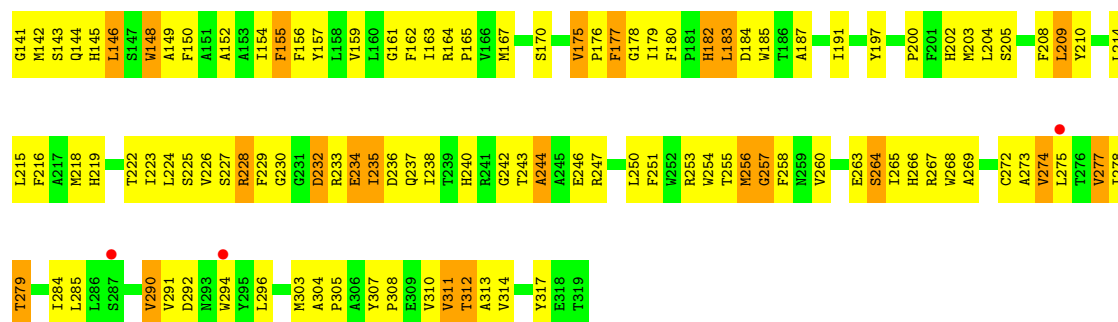


• Molecule 2: Photosynthetic reaction center L subunit

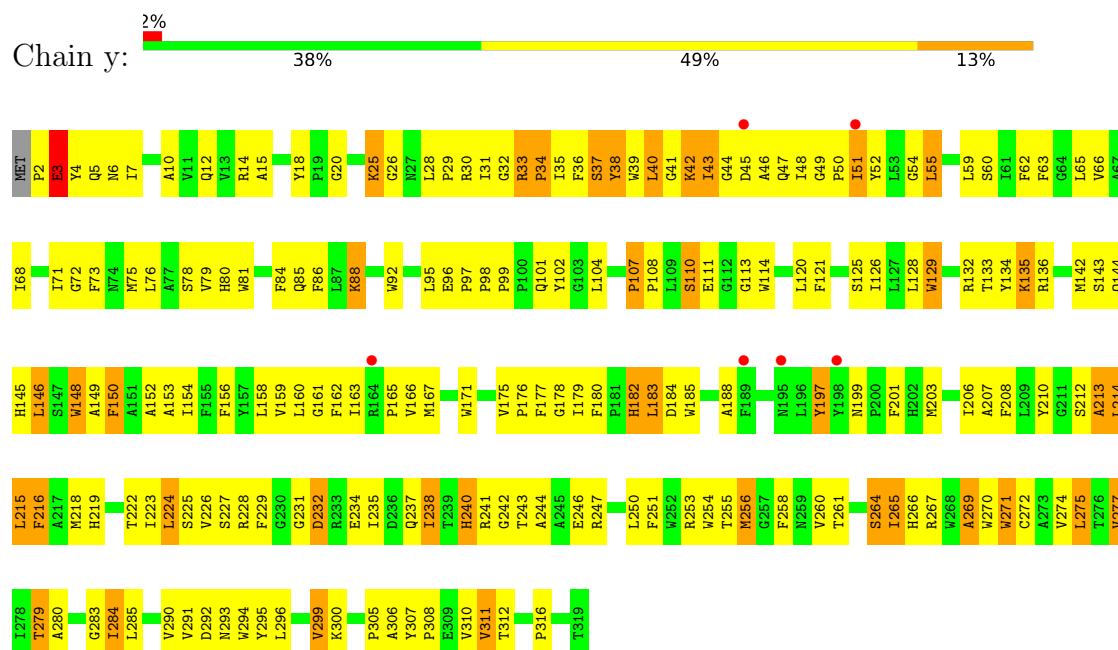


• Molecule 3: Photosynthetic reaction center M subunit





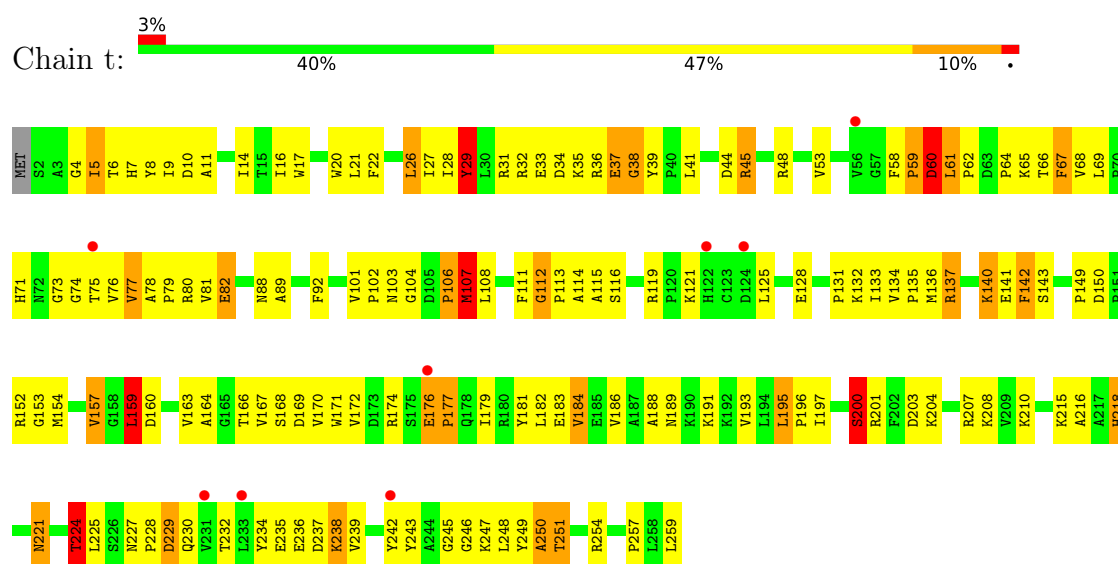
• Molecule 3: Photosynthetic reaction center M subunit



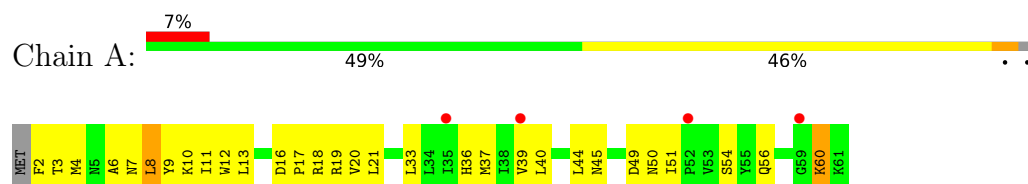
• Molecule 4: Photosynthetic reaction center H subunit



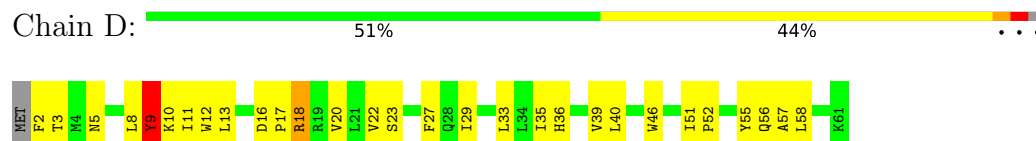
• Molecule 4: Photosynthetic reaction center H subunit



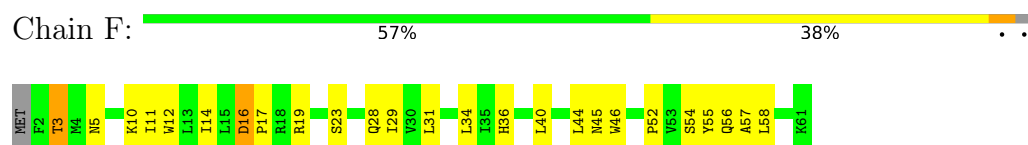
- Molecule 5: LH1 alpha polypeptide



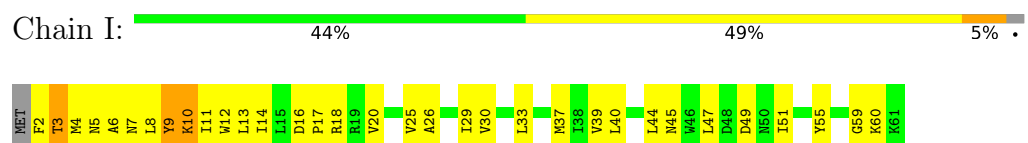
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide

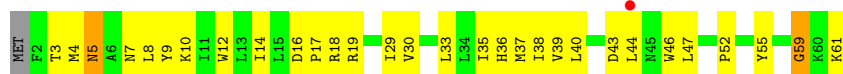


- Molecule 5: LH1 alpha polypeptide

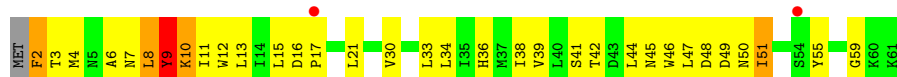
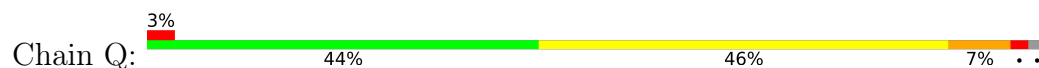




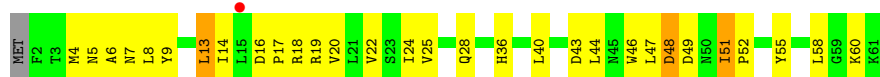
- Molecule 5: LH1 alpha polypeptide



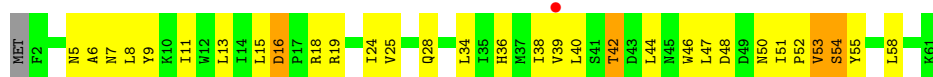
- Molecule 5: LH1 alpha polypeptide



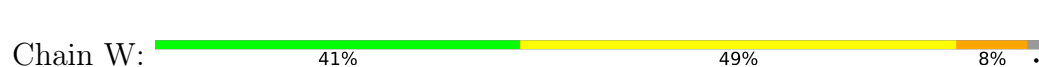
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



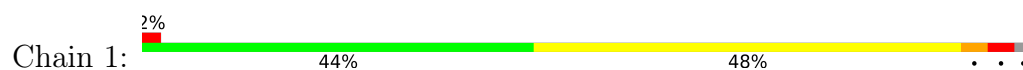
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



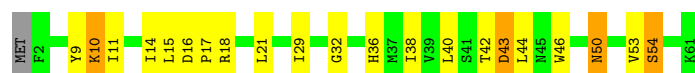
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



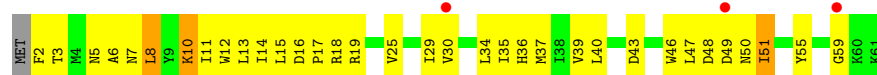
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



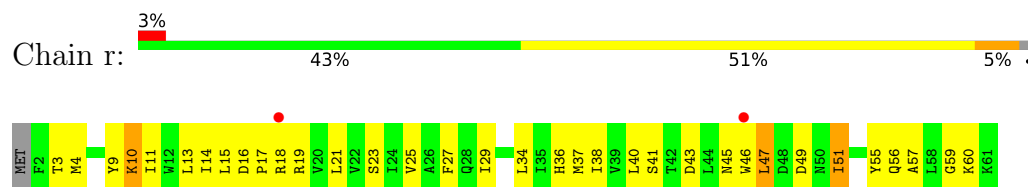
- Molecule 5: LH1 alpha polypeptide



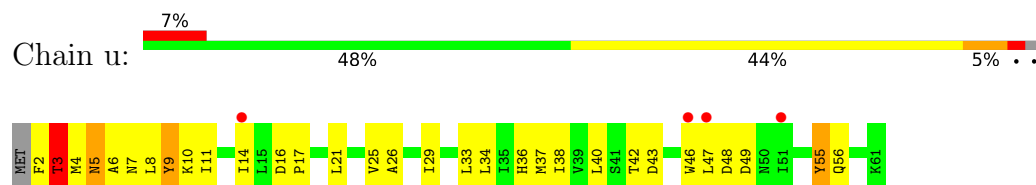
- Molecule 5: LH1 alpha polypeptide



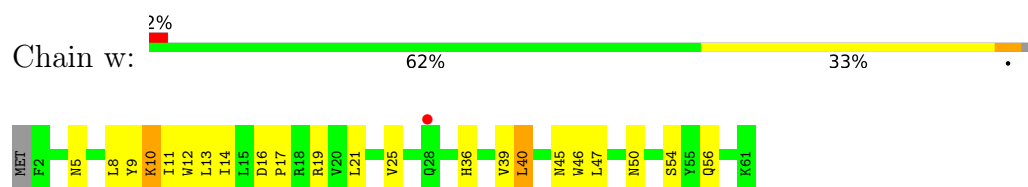
- Molecule 5: LH1 alpha polypeptide



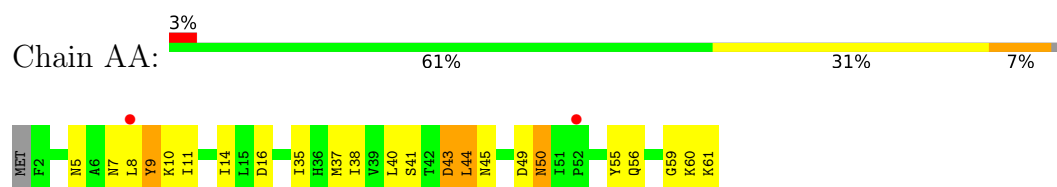
- Molecule 5: LH1 alpha polypeptide



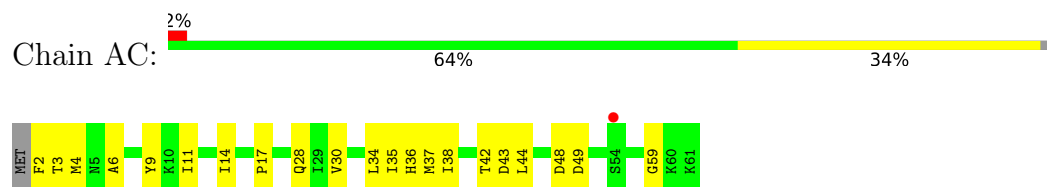
- Molecule 5: LH1 alpha polypeptide



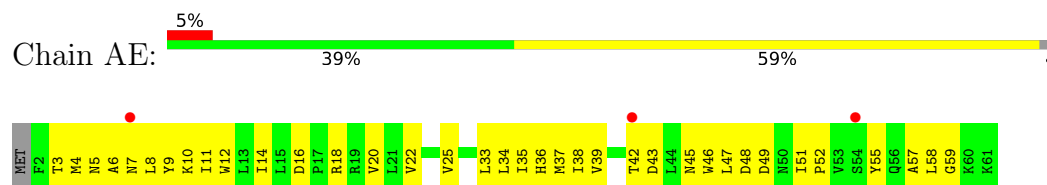
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



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- Molecule 5: LH1 alpha polypeptide



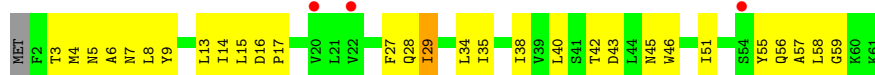
- Molecule 5: LH1 alpha polypeptide



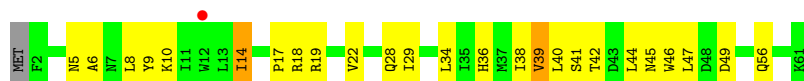
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



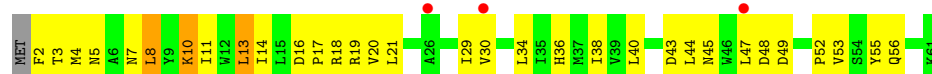
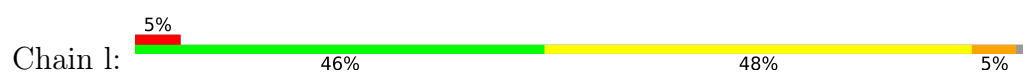
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



• Molecule 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



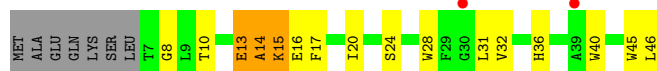
- Molecule 6: LH1 beta polypeptide



- 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:  60% 26% 15%



• Molecule 6: LH1 beta polypeptide

Chain 8:  2% 64% 21% 15%



• Molecule 6: LH1 beta polypeptide

Chain 0:  53% 30% 15%



• Molecule 6: LH1 beta polypeptide

Chain n:  2% 60% 26% 15%



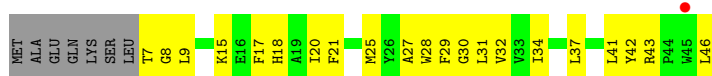
• Molecule 6: LH1 beta polypeptide

Chain q:  2% 57% 28% 15%



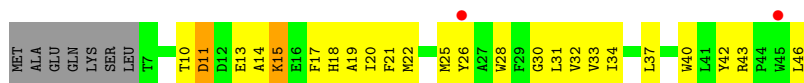
• Molecule 6: LH1 beta polypeptide

Chain s:  2% 40% 45% 15%



• Molecule 6: LH1 beta polypeptide

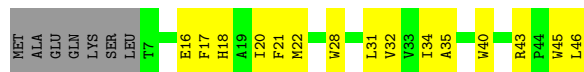
Chain v:  4% 34% 47% 15%



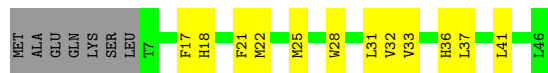
• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide



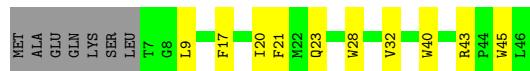
• Molecule 6: LH1 beta polypeptide



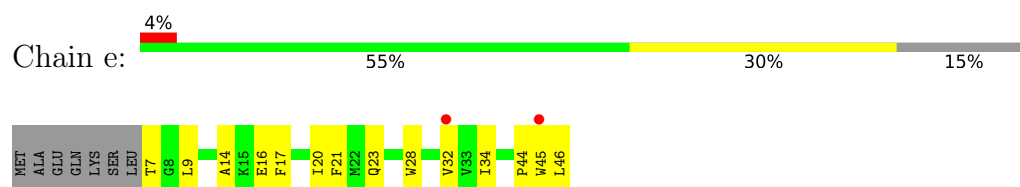
• Molecule 6: LH1 beta polypeptide



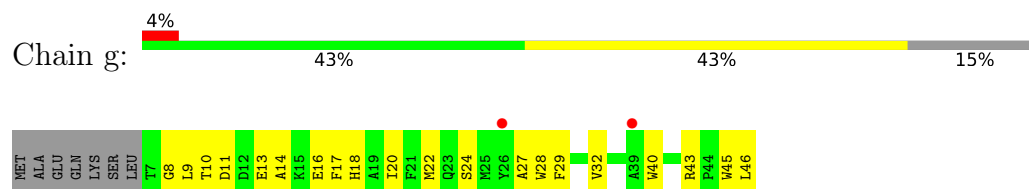
• Molecule 6: LH1 beta polypeptide



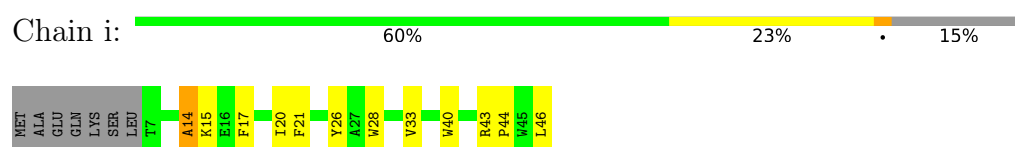
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



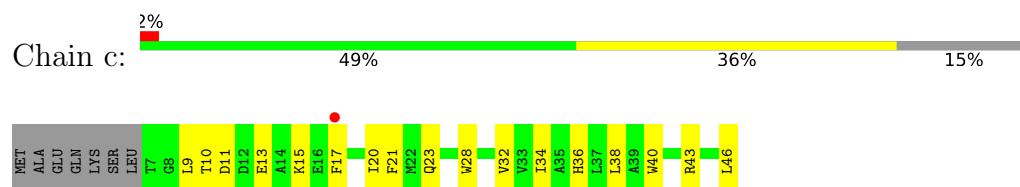
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	164.89Å 148.95Å 210.23Å 90.00° 108.18° 90.00°	Depositor
Resolution (Å)	48.18 – 3.30 48.18 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.18-3.30) 98.3 (48.18-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.271 , 0.309 0.272 , 0.310	Depositor DCC
R_{free} test set	7034 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	107.8	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 107.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	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)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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: BPH, PO4, PGW, FE, PEF, CRT, BCL, MQ8, UQ8, HEM, SR

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	1.07	2/2528 (0.1%)	1.72	69/3451 (2.0%)
1	o	1.04	2/2528 (0.1%)	1.59	48/3451 (1.4%)
2	L	1.12	7/2318 (0.3%)	1.61	56/3167 (1.8%)
2	x	1.14	9/2318 (0.4%)	1.55	40/3167 (1.3%)
3	M	1.03	1/2646 (0.0%)	1.59	54/3621 (1.5%)
3	y	1.05	4/2646 (0.2%)	1.50	39/3621 (1.1%)
4	H	1.03	3/2037 (0.1%)	1.61	38/2776 (1.4%)
4	t	1.12	1/2037 (0.0%)	1.67	40/2776 (1.4%)
5	1	0.77	0/485	1.31	4/664 (0.6%)
5	3	0.71	0/485	1.20	2/664 (0.3%)
5	5	0.69	0/485	1.18	4/664 (0.6%)
5	7	0.63	0/485	1.10	3/664 (0.5%)
5	9	0.64	0/485	1.12	3/664 (0.5%)
5	A	0.66	0/485	1.17	3/664 (0.5%)
5	AA	0.60	0/485	1.17	4/664 (0.6%)
5	AC	0.60	0/485	1.02	0/664
5	AE	0.52	0/491	1.07	2/672 (0.3%)
5	AG	0.56	0/485	1.11	2/664 (0.3%)
5	AI	0.71	0/485	1.21	4/664 (0.6%)
5	AK	0.69	0/485	1.18	1/664 (0.2%)
5	D	0.61	0/485	1.19	4/664 (0.6%)
5	F	0.67	0/485	1.19	4/664 (0.6%)
5	I	0.70	0/485	1.21	6/664 (0.9%)
5	K	0.62	0/485	1.14	5/664 (0.8%)
5	O	0.64	0/485	1.25	3/664 (0.5%)
5	Q	0.65	0/485	1.23	6/664 (0.9%)
5	S	0.68	0/491	1.02	2/672 (0.3%)
5	U	0.77	0/485	1.26	4/664 (0.6%)
5	W	0.81	0/485	1.26	3/664 (0.5%)
5	Y	0.86	0/485	1.20	1/664 (0.2%)
5	d	0.63	0/485	1.15	3/664 (0.5%)
5	f	0.71	1/485 (0.2%)	1.19	7/664 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	h	0.71	0/485	1.04	2/664 (0.3%)
5	j	0.61	0/485	1.09	3/664 (0.5%)
5	l	0.64	0/485	1.09	2/664 (0.3%)
5	m	0.65	0/485	1.14	3/664 (0.5%)
5	p	0.66	0/485	1.15	2/664 (0.3%)
5	r	0.79	1/485 (0.2%)	1.11	1/664 (0.2%)
5	u	0.73	0/485	1.22	8/664 (1.2%)
5	w	0.59	0/485	1.09	2/664 (0.3%)
6	0	0.53	0/350	1.07	1/476 (0.2%)
6	2	0.68	0/350	1.17	5/476 (1.1%)
6	4	0.64	0/350	1.01	2/476 (0.4%)
6	6	0.53	0/350	0.89	0/476
6	8	0.54	0/350	0.98	0/476
6	AB	0.53	0/350	0.99	0/476
6	AD	0.47	0/350	0.90	0/476
6	AF	0.50	0/350	0.94	0/476
6	AH	0.56	0/350	1.05	2/476 (0.4%)
6	AJ	0.62	0/350	0.96	0/476
6	AL	0.58	0/350	0.95	0/476
6	B	0.54	0/350	1.01	1/476 (0.2%)
6	E	0.65	0/350	1.18	4/476 (0.8%)
6	G	0.55	0/350	1.00	1/476 (0.2%)
6	J	0.64	0/350	1.05	1/476 (0.2%)
6	N	0.57	0/350	1.08	0/476
6	P	0.57	0/350	1.11	2/476 (0.4%)
6	R	0.56	0/350	1.01	1/476 (0.2%)
6	T	0.55	0/350	1.07	1/476 (0.2%)
6	V	0.59	0/350	0.92	0/476
6	X	0.63	0/350	1.10	2/476 (0.4%)
6	Z	0.62	0/350	0.92	0/476
6	c	0.46	0/350	0.95	0/476
6	e	0.58	0/350	0.88	0/476
6	g	0.57	0/350	0.96	2/476 (0.4%)
6	i	0.58	0/350	0.97	2/476 (0.4%)
6	k	0.45	0/350	0.92	0/476
6	n	0.55	0/350	0.96	0/476
6	q	0.58	0/350	1.11	2/476 (0.4%)
6	s	0.63	0/350	1.07	1/476 (0.2%)
6	v	0.60	0/350	1.06	2/476 (0.4%)
6	z	0.51	0/350	1.07	0/476
All	All	0.85	31/45790 (0.1%)	1.33	519/62526 (0.8%)

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	3
2	x	0	1
3	M	0	2
3	y	0	3
4	t	0	1
5	1	0	2
6	AJ	0	2
6	X	0	1
All	All	0	15

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	241	LEU	CA-C	-7.31	1.43	1.52
2	x	126	VAL	CA-CB	-7.01	1.50	1.54
3	y	261	THR	CA-CB	-6.52	1.42	1.54
3	y	212	SER	CA-C	-6.47	1.43	1.52
2	L	265	THR	CA-CB	-6.47	1.44	1.54

The worst 5 of 519 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	195	LEU	CA-C-N	-12.82	105.65	120.13
1	o	195	LEU	C-N-CA	-12.82	105.65	120.13
2	x	228	ILE	N-CA-C	12.27	122.06	110.53
4	H	71	HIS	N-CA-C	12.10	127.75	111.30
4	H	258	LEU	N-CA-C	-10.96	102.12	114.62

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	189	THR	Mainchain
1	C	246	GLY	Mainchain
1	C	57	GLN	Sidechain
3	M	272	CYS	Mainchain
3	M	9	THR	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	144	0
1	o	2458	0	2385	157	0
2	L	2231	0	2192	181	0
2	x	2231	0	2192	189	0
3	M	2546	0	2521	228	0
3	y	2546	0	2521	221	0
4	H	1982	0	1981	128	0
4	t	1982	0	1981	131	0
5	1	475	0	486	42	0
5	3	475	0	486	23	0
5	5	475	0	486	23	0
5	7	475	0	486	31	0
5	9	475	0	486	41	0
5	A	475	0	486	29	0
5	AA	475	0	486	20	0
5	AC	475	0	486	25	0
5	AE	481	0	490	38	0
5	AG	475	0	486	23	0
5	AI	475	0	486	26	0
5	AK	475	0	486	21	0
5	D	475	0	486	35	0
5	F	475	0	486	27	0
5	I	475	0	486	41	0
5	K	475	0	486	11	0
5	O	475	0	486	31	0
5	Q	475	0	486	35	0
5	S	481	0	490	34	0
5	U	475	0	486	29	0
5	W	475	0	486	39	0
5	Y	475	0	486	38	0
5	d	475	0	486	28	0
5	f	475	0	486	23	0
5	h	475	0	486	30	0
5	j	475	0	486	43	0
5	l	475	0	486	40	0
5	m	475	0	486	27	0
5	p	475	0	486	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	r	475	0	486	32	0
5	u	475	0	486	36	0
5	w	475	0	486	21	0
6	0	337	0	323	22	0
6	2	337	0	323	18	0
6	4	337	0	323	12	0
6	6	337	0	323	11	0
6	8	337	0	323	14	0
6	AB	337	0	323	13	0
6	AD	337	0	323	18	0
6	AF	337	0	323	15	0
6	AH	337	0	323	21	0
6	AJ	337	0	323	21	0
6	AL	337	0	323	17	0
6	B	337	0	323	31	0
6	E	337	0	323	28	0
6	G	337	0	323	25	0
6	J	337	0	323	26	0
6	N	337	0	323	16	0
6	P	337	0	323	21	0
6	R	337	0	323	24	0
6	T	337	0	323	24	0
6	V	337	0	323	16	0
6	X	337	0	323	22	0
6	Z	337	0	323	21	0
6	c	337	0	323	17	0
6	e	337	0	323	19	0
6	g	337	0	323	21	0
6	i	337	0	323	14	0
6	k	337	0	323	18	0
6	n	337	0	323	19	0
6	q	337	0	323	18	0
6	s	337	0	323	23	0
6	v	337	0	323	25	0
6	z	337	0	323	11	0
7	C	172	0	120	33	0
7	o	172	0	120	36	0
8	1	1	0	0	0	0
8	5	2	0	0	0	0
8	7	1	0	0	0	0
8	9	1	0	0	0	0
8	A	1	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	AI	2	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	l	1	0	0	0	0
8	m	1	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	w	2	0	0	0	0
8	x	2	0	0	0	0
9	0	66	0	74	8	0
9	1	132	0	148	14	0
9	3	66	0	74	11	0
9	4	66	0	74	13	0
9	5	132	0	148	14	0
9	7	66	0	74	8	0
9	8	66	0	74	14	0
9	9	66	0	74	10	0
9	A	66	0	74	9	0
9	AA	66	0	74	8	0
9	AB	66	0	74	10	0
9	AC	66	0	74	8	0
9	AD	66	0	74	12	0
9	AE	132	0	148	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AH	132	0	148	22	0
9	AI	66	0	74	11	0
9	AJ	66	0	74	5	0
9	AK	66	0	74	7	0
9	AL	66	0	74	10	0
9	B	66	0	74	9	0
9	D	132	0	148	18	0
9	F	66	0	74	10	0
9	G	66	0	74	7	0
9	I	66	0	74	9	0
9	J	66	0	74	12	0
9	K	66	0	74	5	0
9	L	198	0	222	32	0
9	M	66	0	74	12	0
9	N	66	0	74	5	0
9	O	66	0	74	8	0
9	P	66	0	74	6	0
9	Q	66	0	74	5	0
9	R	66	0	74	6	0
9	S	66	0	74	8	0
9	T	66	0	74	12	0
9	U	66	0	74	10	0
9	V	66	0	74	9	0
9	W	66	0	74	12	0
9	X	66	0	74	12	0
9	Y	66	0	74	13	0
9	Z	66	0	74	9	0
9	c	66	0	74	7	0
9	d	66	0	74	9	0
9	e	66	0	74	11	0
9	f	66	0	74	10	0
9	g	66	0	74	12	0
9	h	66	0	74	10	0
9	i	66	0	74	8	0
9	j	66	0	74	11	0
9	k	66	0	74	12	0
9	l	66	0	74	13	0
9	m	132	0	148	13	0
9	p	132	0	148	17	0
9	r	66	0	74	12	0
9	s	66	0	74	4	0
9	u	66	0	74	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	v	66	0	74	9	0
9	w	66	0	74	12	0
9	x	198	0	222	37	0
9	y	66	0	74	11	0
9	z	66	0	74	6	0
10	L	65	0	76	14	0
10	M	65	0	76	13	0
10	x	65	0	76	12	0
10	y	65	0	76	14	0
11	L	53	0	74	18	0
11	x	53	0	74	20	0
12	A	19	0	11	3	0
12	H	57	0	33	13	0
12	L	12	0	9	1	0
12	M	54	0	33	9	0
12	m	19	0	11	4	0
12	p	16	0	11	5	0
12	t	38	0	22	13	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	9	0
14	y	53	0	72	10	0
15	2	44	0	60	14	0
15	4	44	0	60	10	0
15	6	44	0	60	5	0
15	8	44	0	60	14	0
15	9	44	0	60	14	0
15	A	44	0	60	8	0
15	AC	44	0	60	7	0
15	AD	44	0	60	10	0
15	AE	44	0	60	13	0
15	AH	44	0	60	8	0
15	AJ	44	0	60	10	0
15	AL	44	0	60	11	0
15	E	44	0	60	9	0
15	G	44	0	60	10	0
15	J	44	0	60	12	0
15	M	44	0	60	11	0
15	N	44	0	60	15	0
15	P	44	0	60	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	R	44	0	60	8	0
15	T	44	0	60	13	0
15	U	44	0	60	5	0
15	X	44	0	60	12	0
15	Z	44	0	60	9	0
15	c	44	0	60	6	0
15	e	44	0	60	11	0
15	f	44	0	60	12	0
15	i	44	0	60	6	0
15	k	44	0	60	11	0
15	n	44	0	60	15	0
15	p	44	0	60	9	0
15	s	44	0	60	13	0
15	v	44	0	60	7	0
15	y	44	0	60	10	0
15	z	44	0	60	3	0
16	H	5	0	0	0	0
16	M	5	0	0	0	0
16	t	5	0	0	0	0
16	y	5	0	0	1	0
17	AE	21	0	12	1	0
17	S	21	0	12	3	0
18	AI	1	0	0	0	0
18	C	1	0	0	0	0
18	L	1	0	0	0	0
18	W	1	0	0	1	0
18	o	1	0	0	0	0
18	x	1	0	0	0	0
All	All	51893	0	52456	2877	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

The worst 5 of 2877 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:h:45:ASN:O	5:h:49:ASP:OD2	1.56	1.19
5:AA:45:ASN:O	5:AA:49:ASP:OD2	1.63	1.16
1:C:307:CYS:SG	7:C:504:HEM:HAB	1.94	1.07
5:j:45:ASN:O	5:j:49:ASP:OD2	1.74	1.04
5:Y:5:ASN:OD1	6:2:23:GLN:NE2	1.94	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	315/333 (95%)	276 (88%)	32 (10%)	7 (2%)	5	26
1	o	315/333 (95%)	277 (88%)	30 (10%)	8 (2%)	4	23
2	L	278/281 (99%)	247 (89%)	27 (10%)	4 (1%)	9	33
2	x	278/281 (99%)	248 (89%)	27 (10%)	3 (1%)	11	39
3	M	316/319 (99%)	282 (89%)	30 (10%)	4 (1%)	9	35
3	y	316/319 (99%)	284 (90%)	28 (9%)	4 (1%)	9	35
4	H	256/259 (99%)	213 (83%)	34 (13%)	9 (4%)	3	18
4	t	256/259 (99%)	214 (84%)	33 (13%)	9 (4%)	3	18
5	1	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	3	58/61 (95%)	44 (76%)	10 (17%)	4 (7%)	1	7
5	5	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	7	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	18
5	9	58/61 (95%)	49 (84%)	5 (9%)	4 (7%)	1	7
5	A	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	18
5	AA	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	30
5	AC	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	AE	59/61 (97%)	50 (85%)	6 (10%)	3 (5%)	1	11
5	AG	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	30
5	AI	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	30
5	AK	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	18
5	D	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	18
5	F	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	7
5	K	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
5	O	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	30
5	Q	58/61 (95%)	47 (81%)	6 (10%)	5 (9%)	0	4
5	S	59/61 (97%)	48 (81%)	8 (14%)	3 (5%)	1	11
5	U	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	7	30
5	W	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	18
5	Y	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	18
5	d	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	18
5	f	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	18
5	h	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	1	11
5	j	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	7	30
5	l	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	18
5	m	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	18
5	p	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	0	4
5	r	58/61 (95%)	45 (78%)	9 (16%)	4 (7%)	1	7
5	u	58/61 (95%)	47 (81%)	10 (17%)	1 (2%)	7	30
5	w	58/61 (95%)	46 (79%)	11 (19%)	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%)	38 (100%)	0	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%)	36 (95%)	2 (5%)	0	100	100
6	AJ	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	AL	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	B	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
6	E	38/47 (81%)	38 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	38/47 (81%)	38 (100%)	0	0	100	100
6	J	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	N	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
6	P	38/47 (81%)	37 (97%)	0	1 (3%)	4	23
6	R	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	T	38/47 (81%)	37 (97%)	0	1 (3%)	4	23
6	V	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	X	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	4	23
6	Z	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	c	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	e	38/47 (81%)	37 (97%)	1 (3%)	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%)	36 (95%)	2 (5%)	0	100	100
6	v	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
All	All	5404/5840 (92%)	4736 (88%)	543 (10%)	125 (2%)	5	25

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	SER
1	C	84	ASP
1	C	195	LEU
4	H	38	GLY
4	H	142	PHE

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%)	245 (92%)	20 (8%)	12	38
1	o	265/278 (95%)	246 (93%)	19 (7%)	13	40
2	L	228/229 (100%)	212 (93%)	16 (7%)	14	41
2	x	228/229 (100%)	212 (93%)	16 (7%)	14	41
3	M	256/257 (100%)	233 (91%)	23 (9%)	9	31
3	y	256/257 (100%)	234 (91%)	22 (9%)	10	33
4	H	210/211 (100%)	188 (90%)	22 (10%)	6	25
4	t	210/211 (100%)	184 (88%)	26 (12%)	4	19
5	1	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	3	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	5	52/56 (93%)	52 (100%)	0	100	100
5	7	52/56 (93%)	52 (100%)	0	100	100
5	9	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	A	52/56 (93%)	51 (98%)	1 (2%)	50	68
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%)	50 (96%)	2 (4%)	29	57
5	AI	52/56 (93%)	52 (100%)	0	100	100
5	AK	52/56 (93%)	52 (100%)	0	100	100
5	D	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	F	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	I	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	K	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	O	52/56 (93%)	50 (96%)	2 (4%)	29	57
5	Q	52/56 (93%)	49 (94%)	3 (6%)	18	47
5	S	53/56 (95%)	51 (96%)	2 (4%)	29	57
5	U	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	W	52/56 (93%)	51 (98%)	1 (2%)	50	68
5	Y	52/56 (93%)	51 (98%)	1 (2%)	50	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	d	52/56 (93%)	51 (98%)	1 (2%)	50	68
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%)	50 (96%)	2 (4%)	29	57
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%)	51 (98%)	1 (2%)	50	68
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%)	31 (94%)	2 (6%)	17	45
6	E	33/39 (85%)	33 (100%)	0	100	100
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
6	X	33/39 (85%)	32 (97%)	1 (3%)	36	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Z	33/39 (85%)	32 (97%)	1 (3%)	36	61
6	c	33/39 (85%)	33 (100%)	0	100	100
6	e	33/39 (85%)	32 (97%)	1 (3%)	36	61
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%)	4431 (96%)	209 (4%)	24	53

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	o	169	ASP
3	y	31	ILE
5	AG	51	ILE
1	o	238	ASN
2	x	148	MET

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

Mol	Chain	Res	Type
2	x	172	GLN
5	m	7	ASN
2	x	273	ASN
3	y	240	HIS
5	u	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	$\# Z > 2$
12	PEF	y	406	-	18,18,46	1.56	2 (11%)	21,23,51	1.73	3 (14%)
15	CRT	4	101	-	41,43,43	0.73	0	50,54,54	4.06	21 (42%)
9	BCL	1	101	5	69,74,74	1.78	13 (18%)	83,115,115	2.19	24 (28%)
15	CRT	9	102	-	41,43,43	0.77	0	50,54,54	3.68	17 (34%)
12	PEF	x	306	-	18,18,46	1.72	2 (11%)	21,23,51	1.41	3 (14%)
15	CRT	k	101	-	41,43,43	0.79	1 (2%)	50,54,54	3.63	15 (30%)
9	BCL	y	401	-	69,74,74	1.90	16 (23%)	83,115,115	2.38	36 (43%)
17	PGW	AE	101	-	20,20,50	1.04	1 (5%)	23,26,56	1.36	2 (8%)
9	BCL	AE	102	5	69,74,74	1.76	13 (18%)	83,115,115	2.17	29 (34%)
15	CRT	AL	101	-	41,43,43	0.76	0	50,54,54	1.55	13 (26%)
9	BCL	AC	102	6	69,74,74	1.74	14 (20%)	83,115,115	2.18	29 (34%)
9	BCL	Z	102	6	69,74,74	1.85	15 (21%)	83,115,115	2.36	28 (33%)
9	BCL	O	101	-	69,74,74	1.80	13 (18%)	83,115,115	2.33	32 (38%)
9	BCL	X	102	6	69,74,74	1.81	16 (23%)	83,115,115	2.11	31 (37%)
7	HEM	o	503	1	50,50,50	2.55	9 (18%)	66,82,82	1.95	21 (31%)
9	BCL	k	102	6	69,74,74	1.80	14 (20%)	83,115,115	2.33	30 (36%)
12	PEF	A	101	-	18,18,46	1.54	2 (11%)	21,23,51	1.74	3 (14%)
9	BCL	L	303	3	69,74,74	1.84	17 (24%)	83,115,115	2.43	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	T	102	6	69,74,74	1.79	15 (21%)	83,115,115	2.26	29 (34%)
12	PEF	M	407	-	15,15,46	1.05	1 (6%)	17,19,51	1.31	2 (11%)
9	BCL	K	101	5	69,74,74	1.79	17 (24%)	83,115,115	2.23	31 (37%)
15	CRT	G	101	-	41,43,43	0.73	0	50,54,54	3.74	17 (34%)
9	BCL	f	101	5	69,74,74	1.85	16 (23%)	83,115,115	2.21	25 (30%)
15	CRT	R	101	-	41,43,43	0.75	0	50,54,54	3.43	19 (38%)
7	HEM	o	504	1	50,50,50	2.61	12 (24%)	66,82,82	2.10	19 (28%)
12	PEF	y	407	-	18,18,46	1.82	2 (11%)	21,23,51	1.58	3 (14%)
15	CRT	AE	103	-	41,43,43	0.75	0	50,54,54	3.69	15 (30%)
15	CRT	c	101	-	41,43,43	0.78	0	50,54,54	3.47	18 (36%)
9	BCL	d	101	-	69,74,74	1.78	14 (20%)	83,115,115	2.22	29 (34%)
9	BCL	AI	101	5	69,74,74	1.81	15 (21%)	83,115,115	2.16	28 (33%)
9	BCL	AL	102	6	69,74,74	1.87	18 (26%)	83,115,115	2.24	27 (32%)
7	HEM	C	504	1	50,50,50	2.60	10 (20%)	66,82,82	2.22	19 (28%)
9	BCL	x	305	2	69,74,74	1.89	14 (20%)	83,115,115	2.49	31 (37%)
9	BCL	Q	101	5	69,74,74	1.82	15 (21%)	83,115,115	2.25	29 (34%)
9	BCL	G	102	6	69,74,74	1.83	14 (20%)	83,115,115	2.21	33 (39%)
9	BCL	l	101	-	69,74,74	1.77	15 (21%)	83,115,115	2.28	33 (39%)
9	BCL	AB	101	6	69,74,74	1.83	15 (21%)	83,115,115	2.19	30 (36%)
9	BCL	e	102	6	69,74,74	1.82	15 (21%)	83,115,115	2.19	30 (36%)
9	BCL	F	101	-	69,74,74	1.79	17 (24%)	83,115,115	2.18	33 (39%)
12	PEF	p	101	-	15,15,46	0.93	1 (6%)	17,19,51	0.84	1 (5%)
9	BCL	P	101	5	69,74,74	1.86	16 (23%)	83,115,115	2.23	32 (38%)
9	BCL	7	101	5	69,74,74	1.77	15 (21%)	83,115,115	2.13	28 (33%)
15	CRT	J	101	-	41,43,43	0.76	0	50,54,54	3.78	19 (38%)
9	BCL	L	301	-	69,74,74	1.91	19 (27%)	83,115,115	2.37	27 (32%)
7	HEM	o	501	1	50,50,50	2.45	7 (14%)	66,82,82	1.85	12 (18%)
9	BCL	s	102	6	69,74,74	1.89	15 (21%)	83,115,115	2.29	27 (32%)
9	BCL	z	102	-	69,74,74	1.79	14 (20%)	83,115,115	2.23	32 (38%)
15	CRT	6	101	-	41,43,43	0.81	0	50,54,54	3.60	18 (36%)
15	CRT	AH	102	-	41,43,43	0.75	0	50,54,54	3.44	16 (32%)
9	BCL	5	101	5	69,74,74	1.84	14 (20%)	83,115,115	2.29	28 (33%)
15	CRT	T	101	-	41,43,43	0.83	0	50,54,54	4.20	23 (46%)
9	BCL	9	103	5	69,74,74	1.81	16 (23%)	83,115,115	2.22	29 (34%)
10	BPH	L	302	-	59,70,70	0.67	1 (1%)	61,101,101	1.45	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	AD	101	5	69,74,74	1.80	13 (18%)	83,115,115	2.13	29 (34%)
9	BCL	0	101	6	69,74,74	1.82	15 (21%)	83,115,115	2.11	29 (34%)
9	BCL	W	101	5	69,74,74	1.79	15 (21%)	83,115,115	2.09	24 (28%)
16	PO4	H	302	-	4,4,4	0.75	0	6,6,6	0.54	0
15	CRT	N	101	-	41,43,43	0.81	0	50,54,54	4.01	19 (38%)
10	BPH	y	402	-	59,70,70	0.81	2 (3%)	61,101,101	1.32	7 (11%)
15	CRT	P	102	-	41,43,43	0.78	0	50,54,54	1.88	15 (30%)
15	CRT	AC	101	-	41,43,43	0.74	0	50,54,54	1.78	11 (22%)
15	CRT	AD	102	-	41,43,43	0.78	0	50,54,54	3.55	15 (30%)
14	MQ8	M	403	-	54,54,54	1.10	5 (9%)	66,69,69	1.61	14 (21%)
15	CRT	AJ	101	-	41,43,43	0.75	0	50,54,54	1.94	15 (30%)
9	BCL	AH	101	5	69,74,74	1.81	13 (18%)	83,115,115	2.23	28 (33%)
9	BCL	D	102	6	69,74,74	1.77	15 (21%)	83,115,115	2.29	32 (38%)
9	BCL	Y	101	5	69,74,74	1.89	15 (21%)	83,115,115	2.30	25 (30%)
12	PEF	t	303	-	18,18,46	1.49	2 (11%)	21,23,51	2.40	8 (38%)
9	BCL	N	102	6	69,74,74	1.79	15 (21%)	83,115,115	2.21	28 (33%)
16	PO4	y	405	-	4,4,4	0.81	0	6,6,6	0.52	0
9	BCL	V	101	6	69,74,74	1.83	16 (23%)	83,115,115	2.20	26 (31%)
7	HEM	C	503	1	50,50,50	2.57	11 (22%)	66,82,82	2.24	22 (33%)
16	PO4	M	405	-	4,4,4	0.60	0	6,6,6	1.05	0
9	BCL	c	102	-	69,74,74	1.75	14 (20%)	83,115,115	2.26	30 (36%)
15	CRT	Z	101	-	41,43,43	0.87	0	50,54,54	1.80	12 (24%)
15	CRT	U	102	-	41,43,43	0.73	0	50,54,54	3.26	19 (38%)
9	BCL	p	104	6	69,74,74	1.87	17 (24%)	83,115,115	2.28	31 (37%)
9	BCL	AE	104	6	69,74,74	1.77	15 (21%)	83,115,115	2.27	29 (34%)
14	MQ8	y	403	-	54,54,54	1.20	6 (11%)	66,69,69	1.67	16 (24%)
12	PEF	M	406	-	18,18,46	1.44	2 (11%)	21,23,51	2.24	4 (19%)
15	CRT	z	101	-	41,43,43	0.72	0	50,54,54	3.71	15 (30%)
9	BCL	L	305	2	69,74,74	1.80	13 (18%)	83,115,115	2.21	29 (34%)
15	CRT	M	404	-	41,43,43	0.85	0	50,54,54	3.73	13 (26%)
15	CRT	8	101	-	41,43,43	0.85	0	50,54,54	3.56	9 (18%)
9	BCL	B	101	5	69,74,74	1.78	14 (20%)	83,115,115	2.12	28 (33%)
12	PEF	H	303	-	18,18,46	1.51	2 (11%)	21,23,51	1.34	2 (9%)
9	BCL	M	401	-	69,74,74	1.95	19 (27%)	83,115,115	2.42	31 (37%)
9	BCL	x	301	-	69,74,74	1.88	19 (27%)	83,115,115	2.50	23 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CRT	y	404	-	41,43,43	0.94	1 (2%)	50,54,54	3.64	17 (34%)
9	BCL	AK	101	5	69,74,74	1.82	15 (21%)	83,115,115	2.23	30 (36%)
12	PEF	t	301	-	18,18,46	1.50	2 (11%)	21,23,51	1.32	4 (19%)
9	BCL	p	102	5	69,74,74	1.79	14 (20%)	83,115,115	2.23	27 (32%)
15	CRT	f	102	-	41,43,43	0.89	0	50,54,54	3.95	21 (42%)
15	CRT	v	101	-	41,43,43	0.77	0	50,54,54	3.93	18 (36%)
11	UQ8	x	304	-	53,53,53	1.52	3 (5%)	64,67,67	2.29	27 (42%)
9	BCL	AH	103	6	69,74,74	1.77	13 (18%)	83,115,115	2.29	30 (36%)
15	CRT	2	101	-	41,43,43	0.75	0	50,54,54	1.81	16 (32%)
15	CRT	p	103	-	41,43,43	0.71	0	50,54,54	3.75	16 (32%)
9	BCL	l	102	6	69,74,74	1.82	15 (21%)	83,115,115	2.15	21 (25%)
9	BCL	h	101	-	69,74,74	1.84	16 (23%)	83,115,115	2.19	28 (33%)
12	PEF	H	301	-	18,18,46	1.57	2 (11%)	21,23,51	1.74	3 (14%)
15	CRT	E	101	-	41,43,43	0.80	0	50,54,54	3.46	16 (32%)
15	CRT	i	101	-	41,43,43	0.81	0	50,54,54	3.50	14 (28%)
9	BCL	U	101	5	69,74,74	1.83	15 (21%)	83,115,115	2.16	23 (27%)
7	HEM	o	502	1	50,50,50	2.45	9 (18%)	66,82,82	2.29	24 (36%)
9	BCL	m	102	-	69,74,74	1.80	14 (20%)	83,115,115	2.24	24 (28%)
9	BCL	v	102	6	69,74,74	1.83	15 (21%)	83,115,115	2.25	29 (34%)
9	BCL	g	101	6	69,74,74	1.77	14 (20%)	83,115,115	2.20	32 (38%)
9	BCL	j	101	-	69,74,74	1.77	12 (17%)	83,115,115	2.20	28 (33%)
9	BCL	r	101	-	69,74,74	1.84	16 (23%)	83,115,115	2.11	28 (33%)
9	BCL	5	102	6	69,74,74	1.90	15 (21%)	83,115,115	2.34	33 (39%)
15	CRT	n	101	-	41,43,43	0.80	0	50,54,54	3.87	15 (30%)
12	PEF	M	408	-	18,18,46	1.65	2 (11%)	21,23,51	1.95	3 (14%)
9	BCL	AA	101	-	69,74,74	1.82	13 (18%)	83,115,115	2.15	26 (31%)
7	HEM	C	501	1	50,50,50	2.55	8 (16%)	66,82,82	2.16	18 (27%)
15	CRT	X	101	-	41,43,43	0.87	0	50,54,54	1.89	11 (22%)
12	PEF	H	304	-	18,18,46	1.59	2 (11%)	21,23,51	1.80	5 (23%)
12	PEF	m	101	-	18,18,46	1.64	2 (11%)	21,23,51	1.56	3 (14%)
9	BCL	i	102	6	69,74,74	1.80	13 (18%)	83,115,115	2.17	26 (31%)
17	PGW	S	101	-	20,20,50	1.06	1 (5%)	23,26,56	1.24	3 (13%)
12	PEF	y	408	-	18,18,46	1.75	3 (16%)	21,23,51	2.02	5 (23%)
7	HEM	C	502	1	50,50,50	2.45	9 (18%)	66,82,82	2.31	21 (31%)
9	BCL	A	102	6	69,74,74	1.82	13 (18%)	83,115,115	2.23	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	3	101	5	69,74,74	1.87	16 (23%)	83,115,115	2.24	30 (36%)
9	BCL	x	303	3	69,74,74	2.11	17 (24%)	83,115,115	2.32	28 (33%)
9	BCL	4	102	6	69,74,74	1.85	15 (21%)	83,115,115	2.35	32 (38%)
9	BCL	m	103	6	69,74,74	1.78	17 (24%)	83,115,115	2.24	28 (33%)
15	CRT	A	103	-	41,43,43	0.80	0	50,54,54	3.51	17 (34%)
15	CRT	e	101	-	41,43,43	0.78	0	50,54,54	1.78	12 (24%)
9	BCL	R	102	6	69,74,74	1.72	12 (17%)	83,115,115	2.27	28 (33%)
9	BCL	AJ	102	6	69,74,74	1.81	15 (21%)	83,115,115	2.13	25 (30%)
10	BPH	M	402	-	59,70,70	0.85	3 (5%)	61,101,101	1.62	10 (16%)
12	PEF	L	306	-	10,11,46	0.73	0	11,14,51	1.46	1 (9%)
10	BPH	x	302	-	59,70,70	0.88	1 (1%)	61,101,101	1.64	8 (13%)
9	BCL	D	101	5	69,74,74	1.85	14 (20%)	83,115,115	2.27	26 (31%)
9	BCL	J	102	6	69,74,74	1.82	16 (23%)	83,115,115	2.25	32 (38%)
15	CRT	s	101	-	41,43,43	0.71	0	50,54,54	3.49	16 (32%)
9	BCL	S	102	5	69,74,74	1.82	14 (20%)	83,115,115	2.23	32 (38%)
16	PO4	t	302	-	4,4,4	0.52	0	6,6,6	1.95	2 (33%)
11	UQ8	L	304	-	53,53,53	1.50	6 (11%)	64,67,67	1.81	19 (29%)
9	BCL	8	102	-	69,74,74	1.80	15 (21%)	83,115,115	2.17	28 (33%)
9	BCL	I	101	-	69,74,74	1.88	15 (21%)	83,115,115	2.22	28 (33%)
9	BCL	u	101	5	69,74,74	1.85	16 (23%)	83,115,115	2.11	28 (33%)
9	BCL	w	101	5	69,74,74	1.86	17 (24%)	83,115,115	2.24	30 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEF	y	406	-	-	2/20/20/50	-
15	CRT	4	101	-	-	13/51/51/51	-
9	BCL	1	101	5	-	19/41/137/137	-
15	CRT	9	102	-	-	9/51/51/51	-
12	PEF	x	306	-	-	15/20/20/50	-
15	CRT	k	101	-	-	6/51/51/51	-
9	BCL	y	401	-	-	13/41/137/137	-
17	PGW	AE	101	-	-	12/23/23/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	AE	102	5	-	13/41/137/137	-
15	CRT	AL	101	-	-	9/51/51/51	-
9	BCL	AC	102	6	-	15/41/137/137	-
9	BCL	Z	102	6	-	16/41/137/137	-
9	BCL	O	101	-	-	18/41/137/137	-
9	BCL	X	102	6	-	23/41/137/137	-
7	HEM	o	503	1	-	4/14/54/54	-
9	BCL	k	102	6	-	21/41/137/137	-
12	PEF	A	101	-	-	9/20/20/50	-
9	BCL	L	303	3	-	18/41/137/137	-
9	BCL	T	102	6	-	17/41/137/137	-
12	PEF	M	407	-	-	8/16/16/50	-
9	BCL	K	101	5	-	13/41/137/137	-
15	CRT	G	101	-	-	6/51/51/51	-
9	BCL	f	101	5	-	19/41/137/137	-
15	CRT	R	101	-	-	12/51/51/51	-
7	HEM	o	504	1	-	2/14/54/54	-
12	PEF	y	407	-	-	7/20/20/50	-
15	CRT	AE	103	-	-	5/51/51/51	-
15	CRT	c	101	-	-	8/51/51/51	-
9	BCL	d	101	-	-	16/41/137/137	-
9	BCL	AI	101	5	-	19/41/137/137	-
9	BCL	AL	102	6	-	15/41/137/137	-
7	HEM	C	504	1	-	6/14/54/54	-
9	BCL	x	305	2	-	20/41/137/137	-
9	BCL	Q	101	5	-	22/41/137/137	-
9	BCL	G	102	6	-	16/41/137/137	-
9	BCL	l	101	-	-	15/41/137/137	-
9	BCL	AB	101	6	-	19/41/137/137	-
9	BCL	e	102	6	-	18/41/137/137	-
9	BCL	F	101	-	-	20/41/137/137	-
12	PEF	p	101	-	-	6/16/16/50	-
9	BCL	P	101	5	-	17/41/137/137	-
9	BCL	7	101	5	-	17/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	J	101	-	-	10/51/51/51	-
9	BCL	L	301	-	-	12/41/137/137	-
7	HEM	o	501	1	-	6/14/54/54	-
9	BCL	s	102	6	-	17/41/137/137	-
9	BCL	z	102	-	-	17/41/137/137	-
15	CRT	6	101	-	-	8/51/51/51	-
15	CRT	AH	102	-	-	14/51/51/51	-
9	BCL	5	101	5	-	16/41/137/137	-
15	CRT	T	101	-	-	7/51/51/51	-
9	BCL	9	103	5	-	14/41/137/137	-
10	BPH	L	302	-	-	16/37/105/105	0/5/6/6
9	BCL	AD	101	5	-	21/41/137/137	-
9	BCL	0	101	6	-	12/41/137/137	-
9	BCL	W	101	5	-	19/41/137/137	-
15	CRT	N	101	-	-	10/51/51/51	-
10	BPH	y	402	-	-	15/37/105/105	0/5/6/6
15	CRT	P	102	-	-	7/51/51/51	-
15	CRT	AC	101	-	-	5/51/51/51	-
15	CRT	AD	102	-	-	11/51/51/51	-
14	MQ8	M	403	-	-	21/47/67/67	0/2/2/2
15	CRT	AJ	101	-	-	7/51/51/51	-
9	BCL	AH	101	5	-	21/41/137/137	-
9	BCL	D	102	6	-	12/41/137/137	-
9	BCL	Y	101	5	-	20/41/137/137	-
12	PEF	t	303	-	-	7/20/20/50	-
9	BCL	N	102	6	-	18/41/137/137	-
9	BCL	V	101	6	-	15/41/137/137	-
7	HEM	C	503	1	-	4/14/54/54	-
9	BCL	c	102	-	-	18/41/137/137	-
15	CRT	Z	101	-	-	11/51/51/51	-
15	CRT	U	102	-	-	10/51/51/51	-
9	BCL	p	104	6	-	16/41/137/137	-
9	BCL	AE	104	6	-	11/41/137/137	-
14	MQ8	y	403	-	-	26/47/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEF	M	406	-	-	11/20/20/50	-
15	CRT	z	101	-	-	3/51/51/51	-
9	BCL	L	305	2	-	14/41/137/137	-
15	CRT	M	404	-	-	11/51/51/51	-
15	CRT	8	101	-	-	6/51/51/51	-
9	BCL	B	101	5	-	13/41/137/137	-
12	PEF	H	303	-	-	13/20/20/50	-
9	BCL	M	401	-	-	10/41/137/137	-
9	BCL	x	301	-	-	10/41/137/137	-
15	CRT	y	404	-	-	9/51/51/51	-
9	BCL	AK	101	5	-	15/41/137/137	-
12	PEF	t	301	-	-	7/20/20/50	-
9	BCL	p	102	5	-	17/41/137/137	-
15	CRT	f	102	-	-	9/51/51/51	-
15	CRT	v	101	-	-	9/51/51/51	-
11	UQ8	x	304	-	-	7/51/75/75	0/1/1/1
9	BCL	AH	103	6	-	24/41/137/137	-
15	CRT	2	101	-	-	7/51/51/51	-
15	CRT	p	103	-	-	9/51/51/51	-
9	BCL	l	102	6	-	14/41/137/137	-
9	BCL	h	101	-	-	9/41/137/137	-
12	PEF	H	301	-	-	7/20/20/50	-
15	CRT	E	101	-	-	8/51/51/51	-
15	CRT	i	101	-	-	11/51/51/51	-
9	BCL	U	101	5	-	15/41/137/137	-
7	HEM	o	502	1	-	5/14/54/54	-
9	BCL	m	102	-	-	16/41/137/137	-
9	BCL	v	102	6	-	13/41/137/137	-
9	BCL	g	101	6	-	19/41/137/137	-
9	BCL	j	101	-	-	21/41/137/137	-
9	BCL	r	101	-	-	18/41/137/137	-
9	BCL	5	102	6	-	17/41/137/137	-
15	CRT	n	101	-	-	19/51/51/51	-
12	PEF	M	408	-	-	12/20/20/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	AA	101	-	-	17/41/137/137	-
7	HEM	C	501	1	-	6/14/54/54	-
15	CRT	X	101	-	-	13/51/51/51	-
12	PEF	H	304	-	-	11/20/20/50	-
12	PEF	m	101	-	-	7/20/20/50	-
9	BCL	i	102	6	-	19/41/137/137	-
17	PGW	S	101	-	-	13/23/23/55	-
12	PEF	y	408	-	-	9/20/20/50	-
7	HEM	C	502	1	-	5/14/54/54	-
9	BCL	A	102	6	-	12/41/137/137	-
9	BCL	3	101	5	-	13/41/137/137	-
9	BCL	x	303	3	-	15/41/137/137	-
9	BCL	4	102	6	-	17/41/137/137	-
9	BCL	m	103	6	-	19/41/137/137	-
15	CRT	A	103	-	-	6/51/51/51	-
15	CRT	e	101	-	-	8/51/51/51	-
9	BCL	R	102	6	-	15/41/137/137	-
9	BCL	AJ	102	6	-	17/41/137/137	-
10	BPH	M	402	-	-	22/37/105/105	0/5/6/6
12	PEF	L	306	-	-	8/11/11/50	-
10	BPH	x	302	-	-	16/37/105/105	0/5/6/6
9	BCL	D	101	5	-	11/41/137/137	-
9	BCL	J	102	6	-	14/41/137/137	-
15	CRT	s	101	-	-	8/51/51/51	-
9	BCL	S	102	5	-	14/41/137/137	-
11	UQ8	L	304	-	-	9/51/75/75	0/1/1/1
9	BCL	8	102	-	-	26/41/137/137	-
9	BCL	I	101	-	-	10/41/137/137	-
9	BCL	u	101	5	-	17/41/137/137	-
9	BCL	w	101	5	-	15/41/137/137	-

The worst 5 of 1215 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	503	HEM	FE-NB	14.24	2.39	1.94
7	C	503	HEM	FE-NB	14.11	2.38	1.94
7	C	504	HEM	FE-NB	13.71	2.37	1.94
7	o	502	HEM	FE-NB	13.49	2.36	1.94

The worst 5 of 2942 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	404	CRT	C2-C1-C4	-19.43	81.03	110.86
15	T	101	CRT	C3-C1-C4	-19.16	81.43	110.86
15	4	101	CRT	C3-C1-C4	-18.20	82.92	110.86
15	s	101	CRT	C2-C1-C4	-18.08	83.10	110.86
15	A	103	CRT	C2-C1-C4	-17.08	84.63	110.86

There are no chirality outliers.

5 of 1812 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	503	HEM	C2B-C3B-CAB-CBB
7	C	503	HEM	C4B-C3B-CAB-CBB
7	o	501	HEM	C2B-C3B-CAB-CBB
7	o	502	HEM	C2B-C3B-CAB-CBB
7	o	502	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

141 monomers are involved in 1156 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	y	406	PEF	4	0
15	4	101	CRT	10	0
9	1	101	BCL	5	0
15	9	102	CRT	14	0
12	x	306	PEF	11	0
15	k	101	CRT	11	0
9	y	401	BCL	11	0
17	AE	101	PGW	1	0
9	AE	102	BCL	6	0
15	AL	101	CRT	11	0
9	AC	102	BCL	8	0
9	Z	102	BCL	9	0
9	O	101	BCL	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	X	102	BCL	12	0
7	o	503	HEM	5	0
9	k	102	BCL	12	0
12	A	101	PEF	3	0
9	L	303	BCL	11	0
9	T	102	BCL	12	0
12	M	407	PEF	5	0
9	K	101	BCL	5	0
15	G	101	CRT	10	0
9	f	101	BCL	10	0
15	R	101	CRT	8	0
7	o	504	HEM	12	0
12	y	407	PEF	2	0
15	AE	103	CRT	13	0
15	c	101	CRT	6	0
9	d	101	BCL	9	0
9	AI	101	BCL	11	0
9	AL	102	BCL	10	0
7	C	504	HEM	11	0
9	x	305	BCL	17	0
9	Q	101	BCL	5	0
9	G	102	BCL	7	0
9	l	101	BCL	13	0
9	AB	101	BCL	10	0
9	e	102	BCL	11	0
9	F	101	BCL	10	0
12	p	101	PEF	5	0
9	P	101	BCL	6	0
9	7	101	BCL	8	0
15	J	101	CRT	12	0
9	L	301	BCL	11	0
7	o	501	HEM	9	0
9	s	102	BCL	4	0
9	z	102	BCL	6	0
15	6	101	CRT	5	0
15	AH	102	CRT	8	0
9	5	101	BCL	9	0
15	T	101	CRT	13	0
9	9	103	BCL	10	0
10	L	302	BPH	14	0
9	AD	101	BCL	12	0
9	0	101	BCL	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	101	BCL	12	0
15	N	101	CRT	15	0
10	y	402	BPH	14	0
15	P	102	CRT	9	0
15	AC	101	CRT	7	0
15	AD	102	CRT	10	0
14	M	403	MQ8	9	0
15	AJ	101	CRT	10	0
9	AH	101	BCL	13	0
9	D	102	BCL	7	0
9	Y	101	BCL	13	0
12	t	303	PEF	8	0
9	N	102	BCL	5	0
16	y	405	PO4	1	0
9	V	101	BCL	9	0
7	C	503	HEM	7	0
9	c	102	BCL	7	0
15	Z	101	CRT	9	0
15	U	102	CRT	5	0
9	p	104	BCL	6	0
9	AE	104	BCL	7	0
14	y	403	MQ8	10	0
12	M	406	PEF	2	0
15	z	101	CRT	3	0
9	L	305	BCL	10	0
15	M	404	CRT	11	0
15	8	101	CRT	14	0
9	B	101	BCL	9	0
12	H	303	PEF	3	0
9	M	401	BCL	12	0
9	x	301	BCL	12	0
15	y	404	CRT	10	0
9	AK	101	BCL	7	0
12	t	301	PEF	5	0
9	p	102	BCL	12	0
15	f	102	CRT	12	0
15	v	101	CRT	7	0
11	x	304	UQ8	20	0
9	AH	103	BCL	9	0
15	2	101	CRT	14	0
15	p	103	CRT	9	0
9	1	102	BCL	9	0

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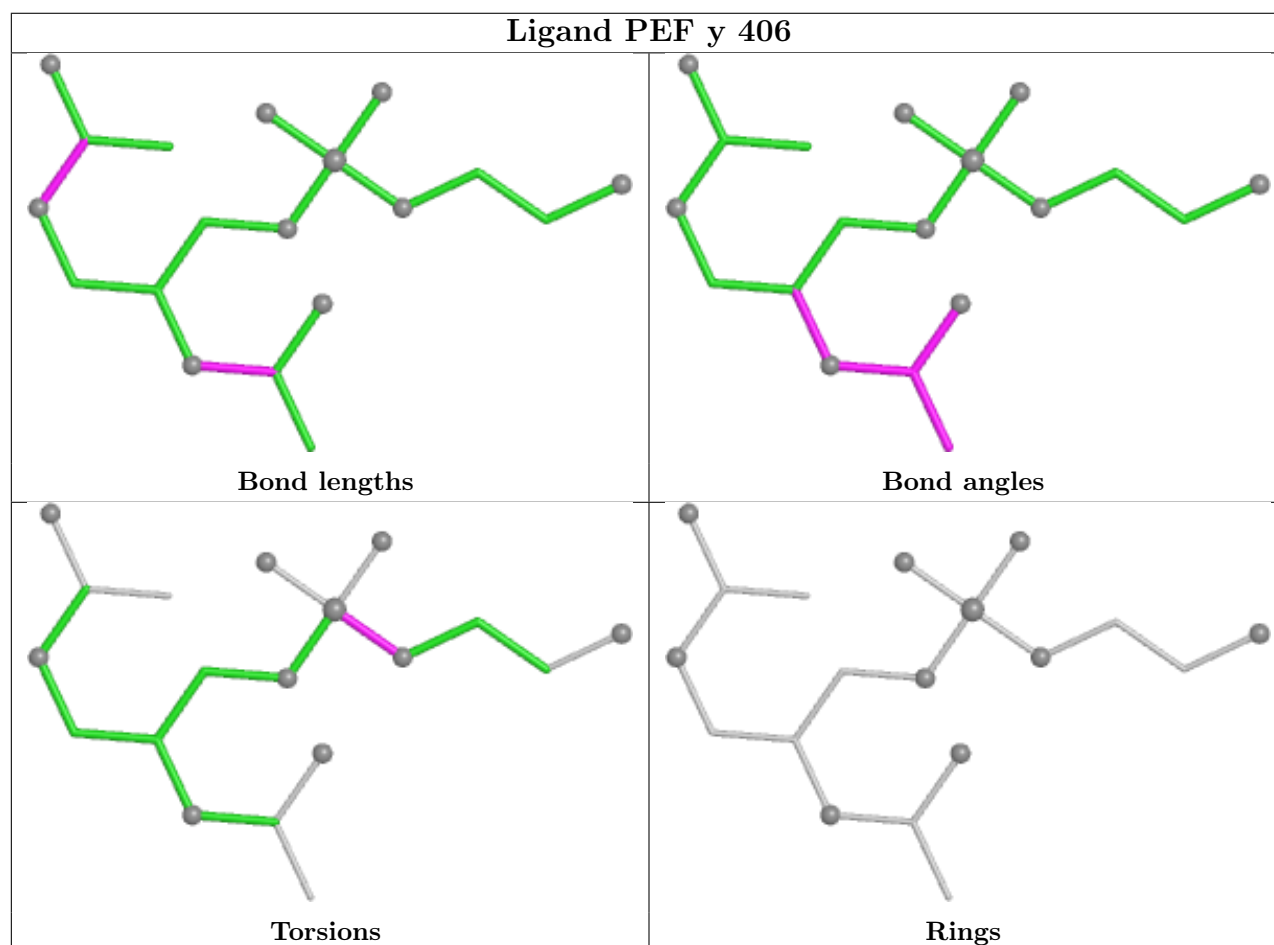
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	h	101	BCL	10	0
12	H	301	PEF	4	0
15	E	101	CRT	9	0
15	i	101	CRT	6	0
9	U	101	BCL	10	0
7	o	502	HEM	10	0
9	m	102	BCL	4	0
9	v	102	BCL	9	0
9	g	101	BCL	12	0
9	j	101	BCL	11	0
9	r	101	BCL	12	0
9	5	102	BCL	5	0
15	n	101	CRT	15	0
12	M	408	PEF	3	0
9	AA	101	BCL	8	0
7	C	501	HEM	10	0
15	X	101	CRT	12	0
12	H	304	PEF	6	0
12	m	101	PEF	4	0
9	i	102	BCL	8	0
17	S	101	PGW	3	0
12	y	408	PEF	3	0
7	C	502	HEM	5	0
9	A	102	BCL	9	0
9	3	101	BCL	11	0
9	x	303	BCL	9	0
9	4	102	BCL	13	0
9	m	103	BCL	9	0
15	A	103	CRT	8	0
15	e	101	CRT	11	0
9	R	102	BCL	6	0
9	AJ	102	BCL	5	0
10	M	402	BPH	13	0
12	L	306	PEF	1	0
10	x	302	BPH	12	0
9	D	101	BCL	11	0
9	J	102	BCL	12	0
15	s	101	CRT	13	0
9	S	102	BCL	8	0
11	L	304	UQ8	18	0
9	8	102	BCL	14	0
9	I	101	BCL	9	0

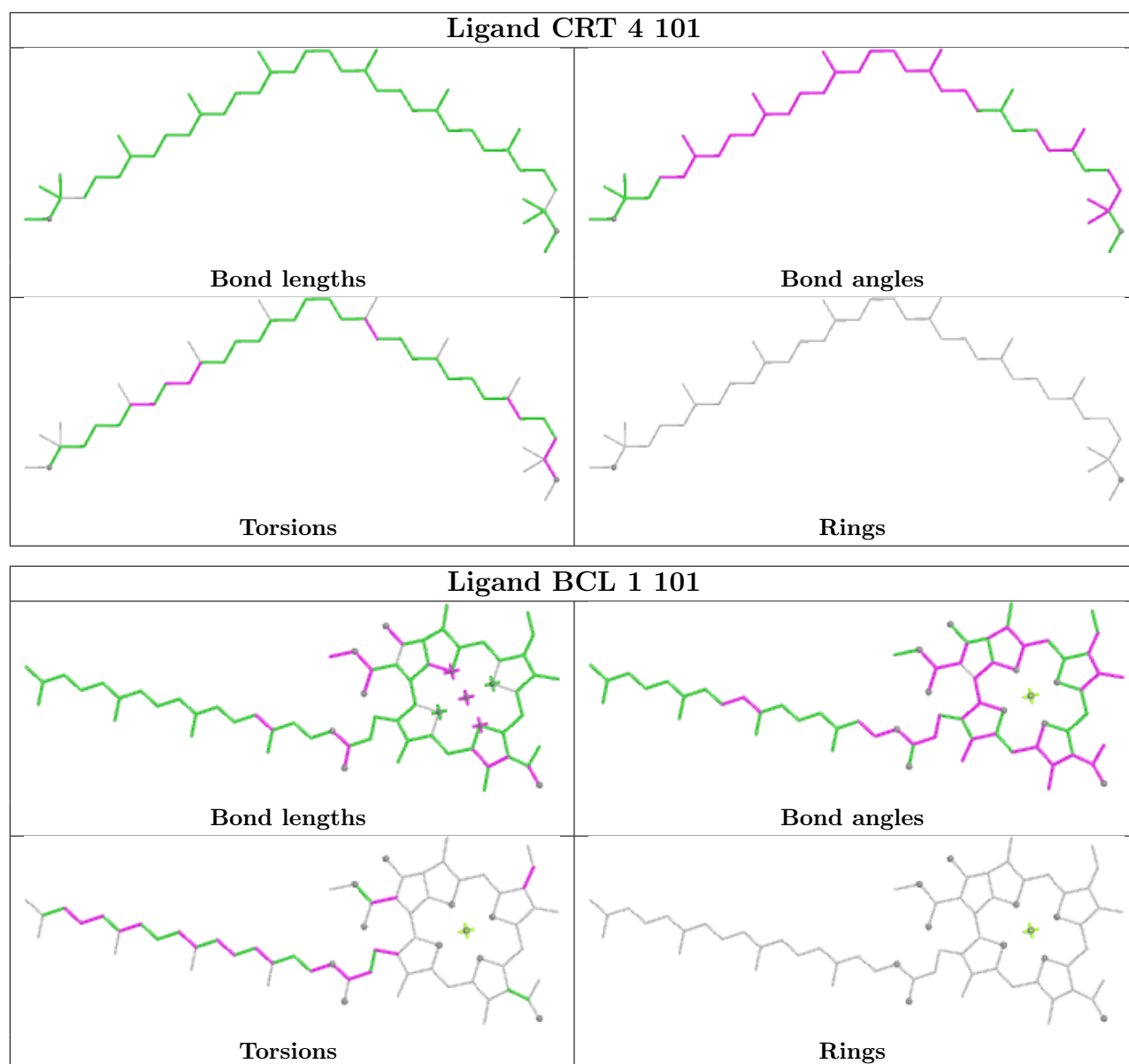
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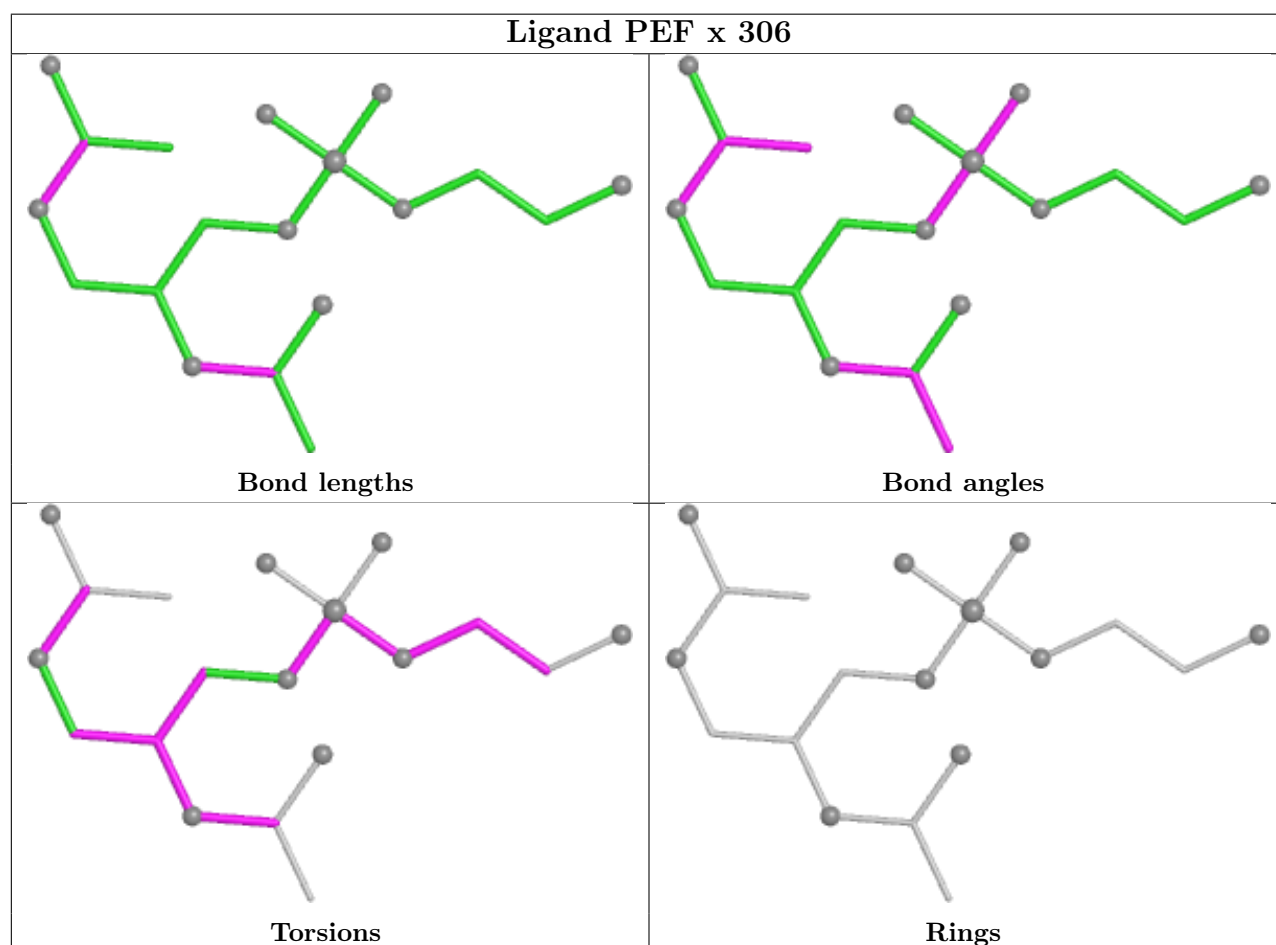
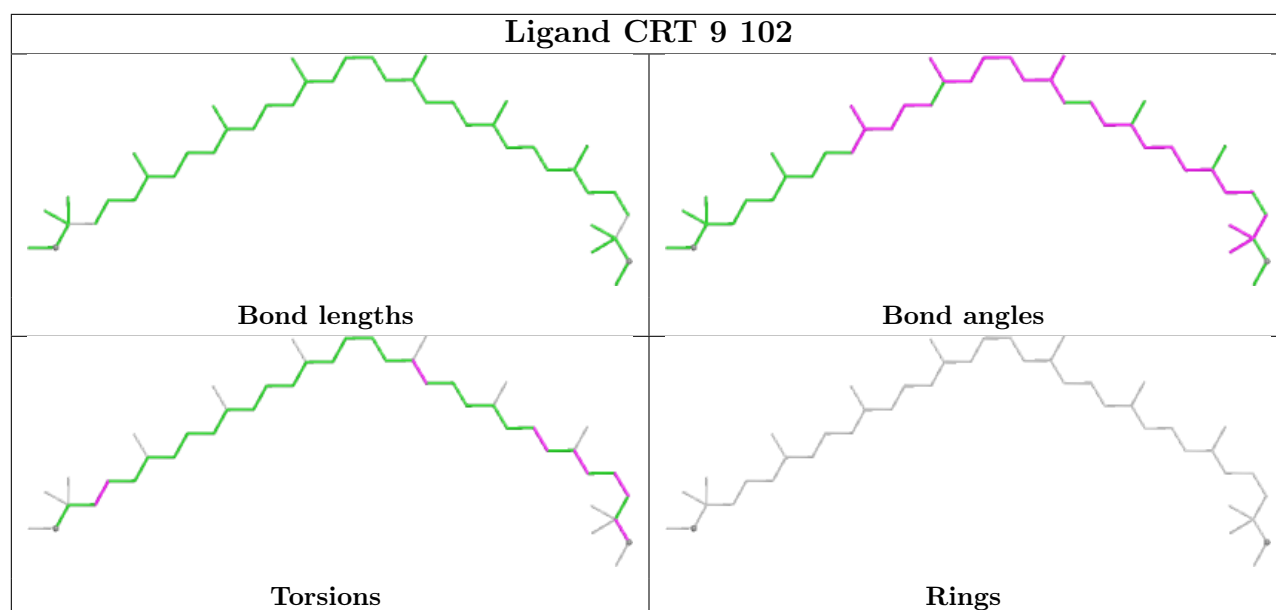
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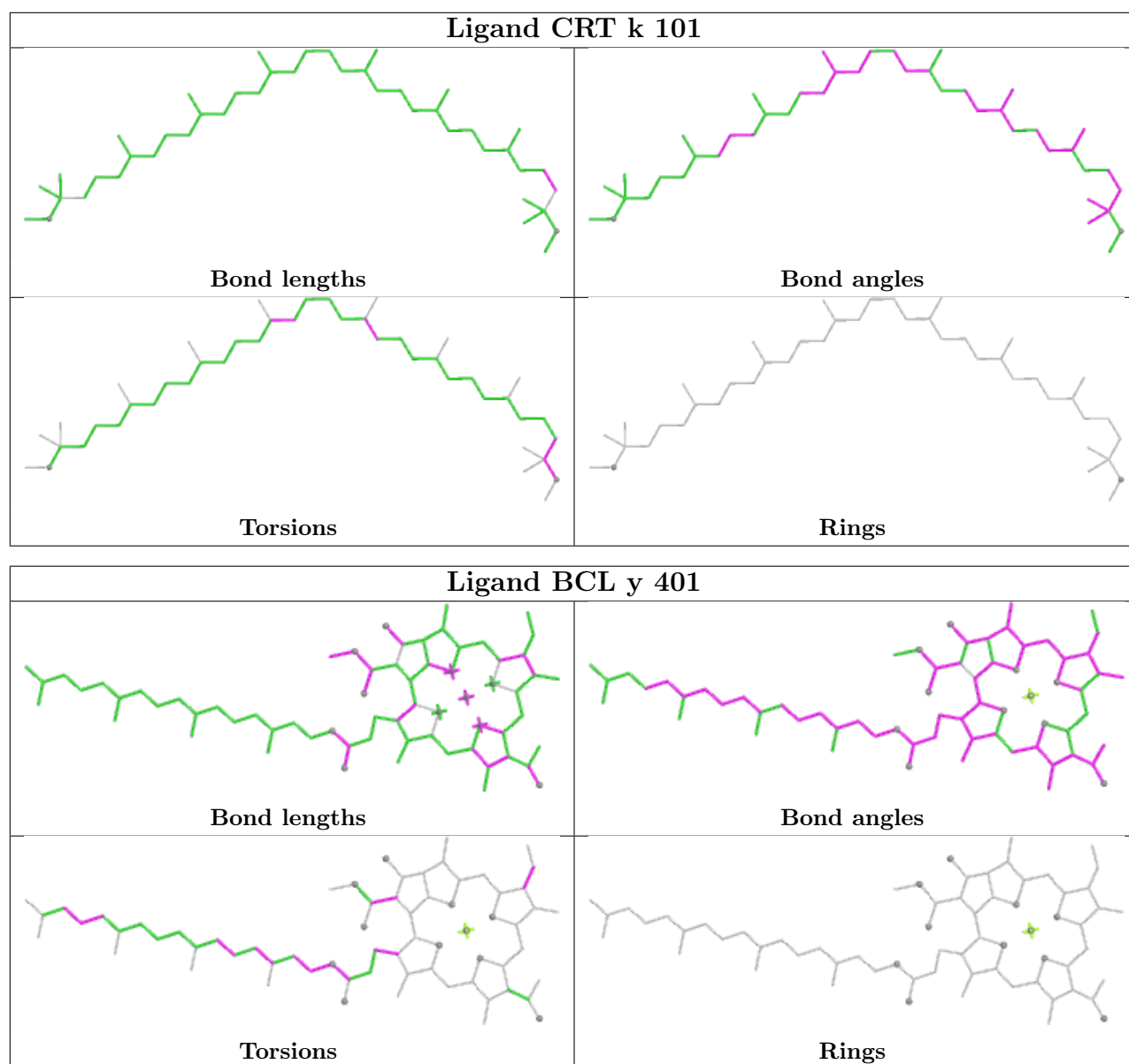
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	u	101	BCL	9	0
9	w	101	BCL	12	0

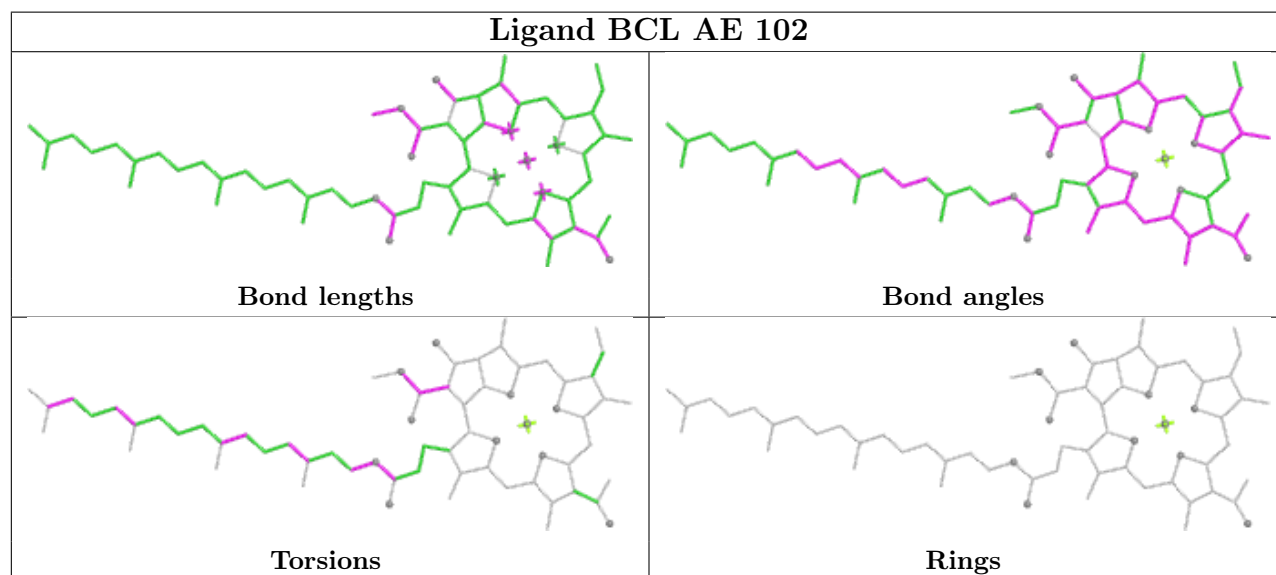
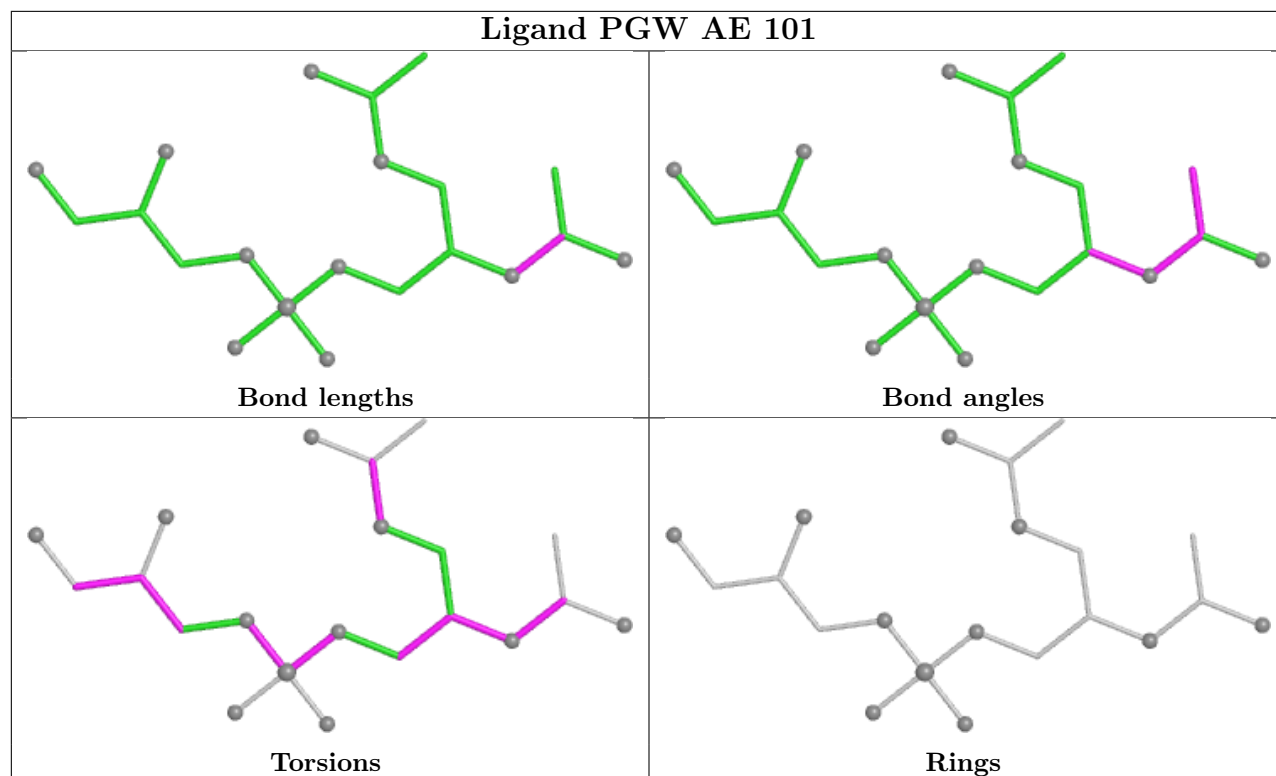
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

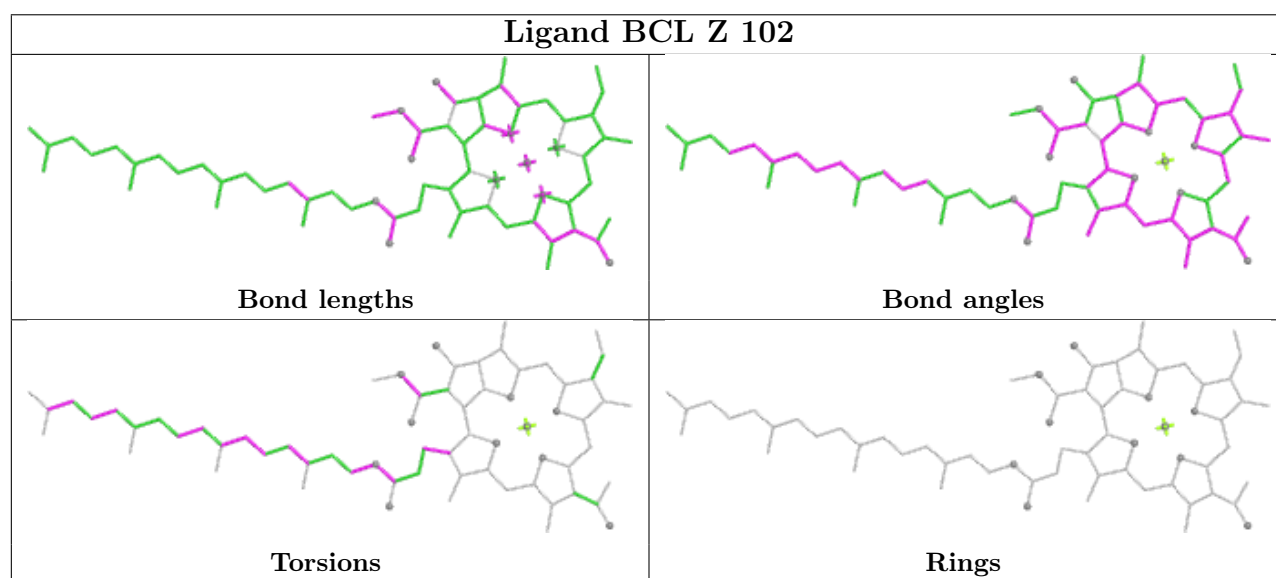
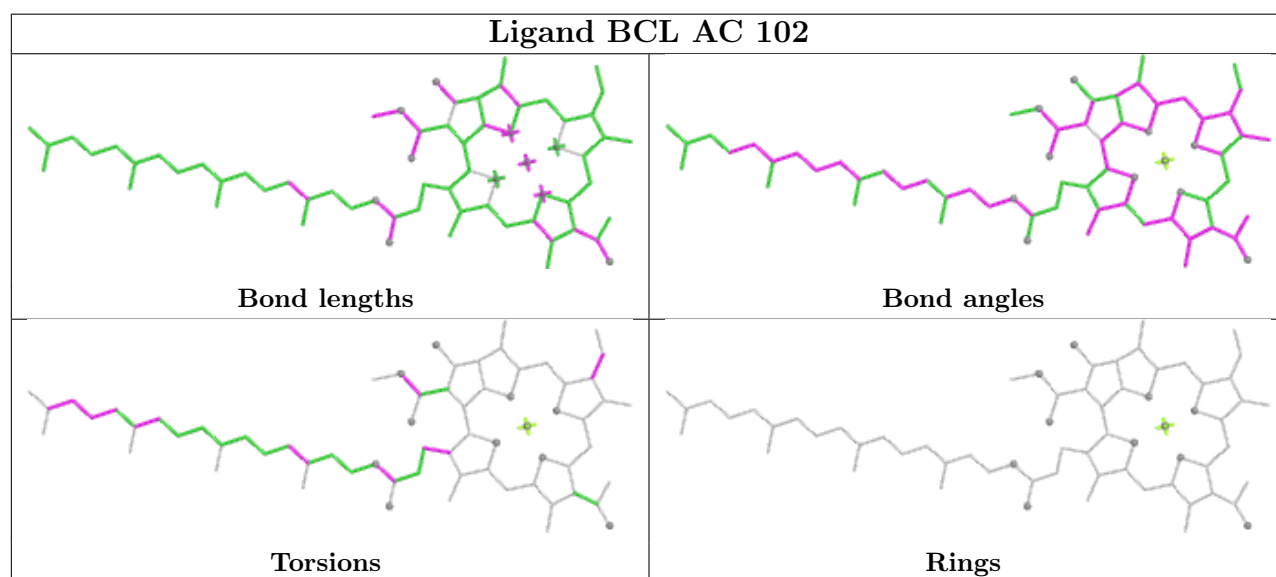
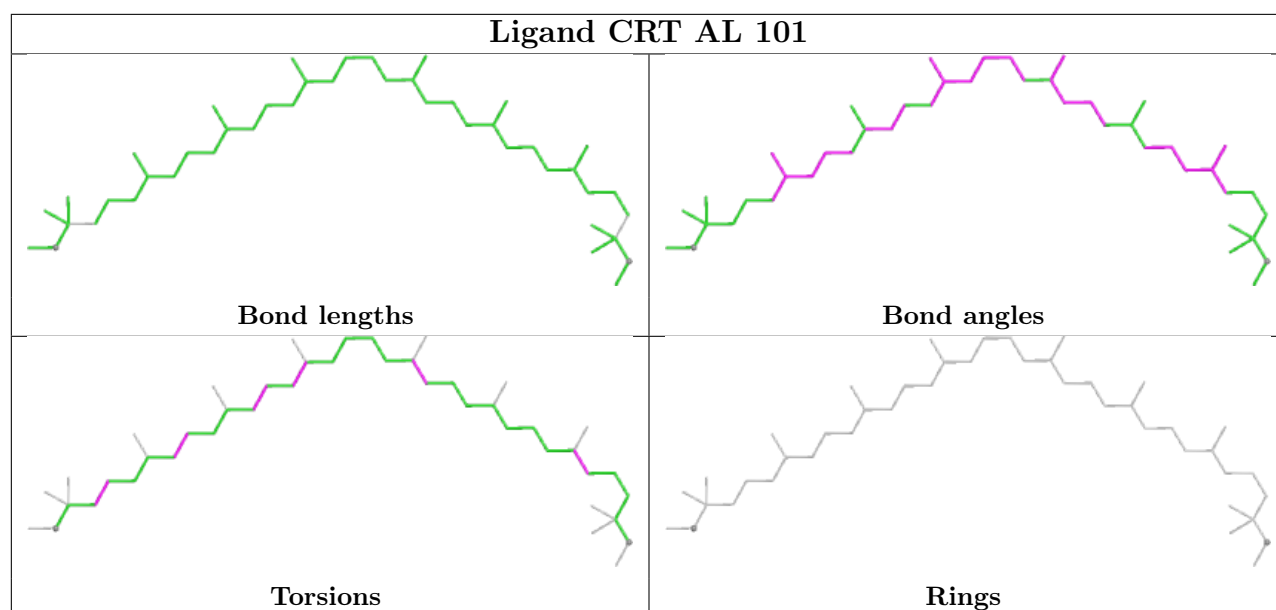


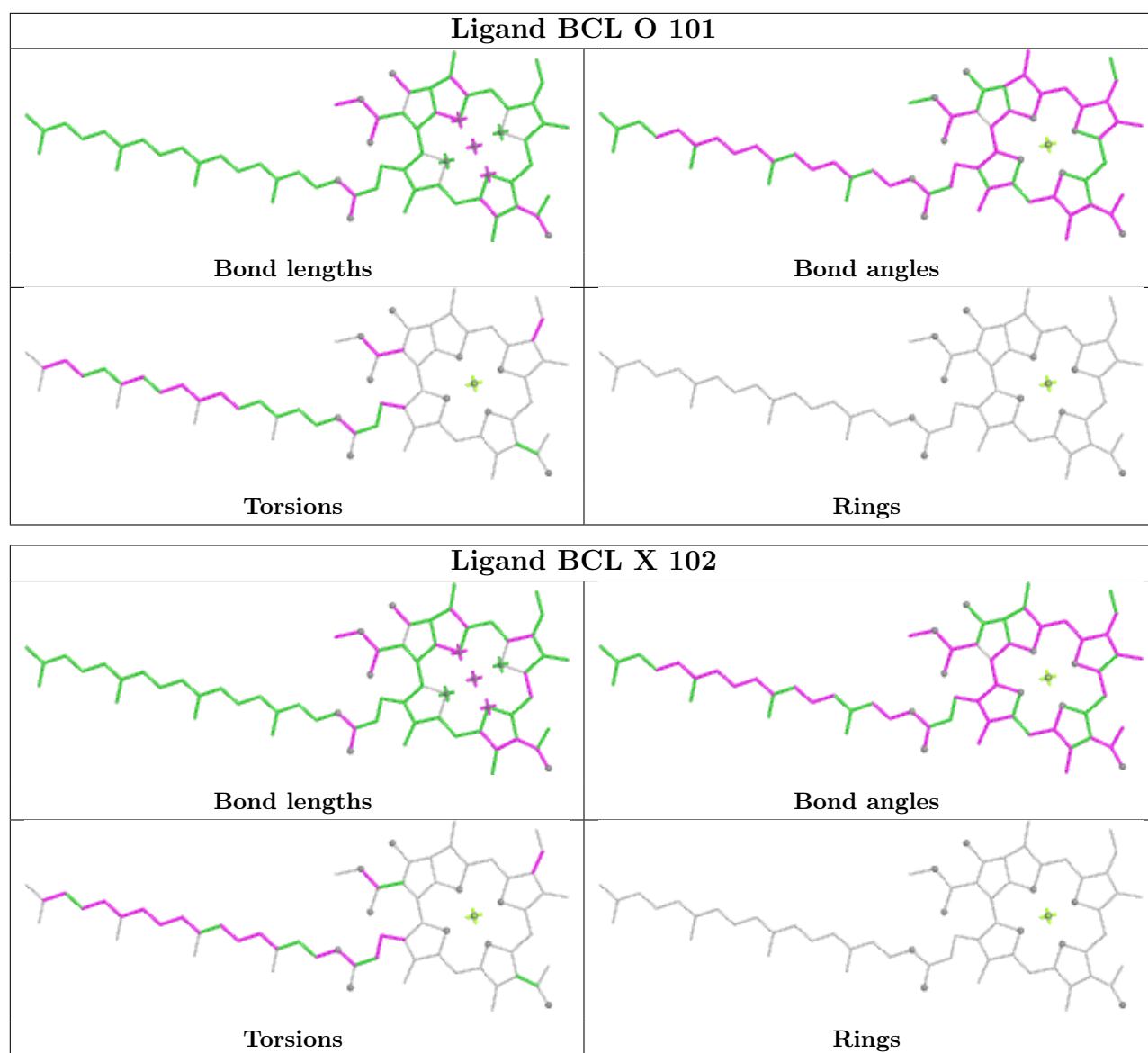




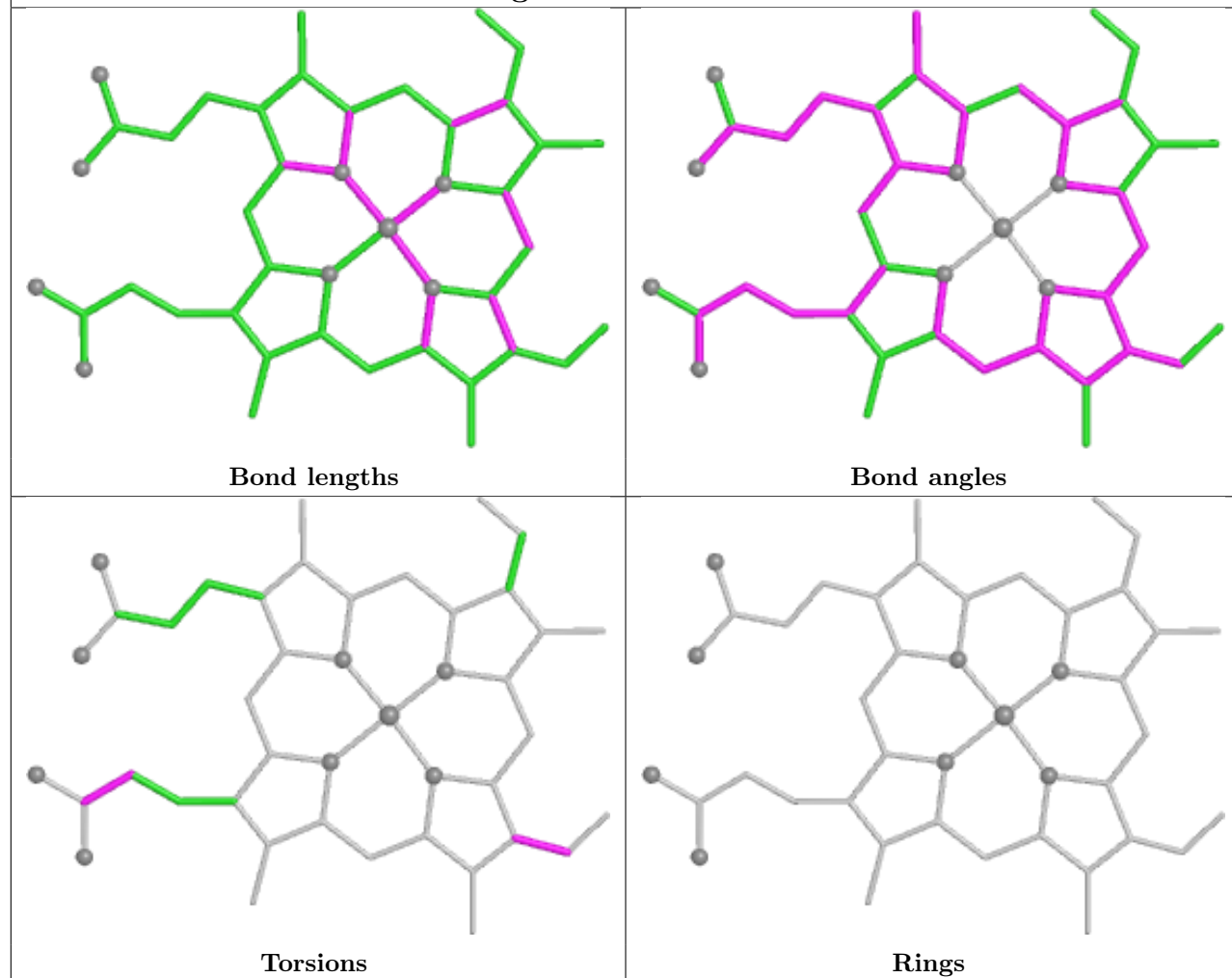




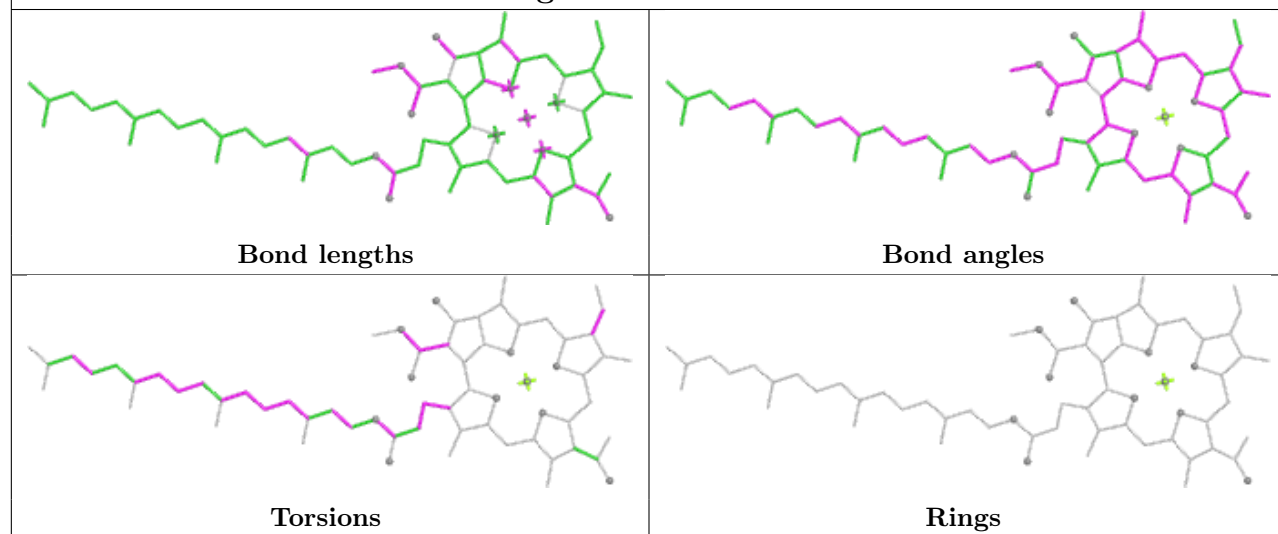




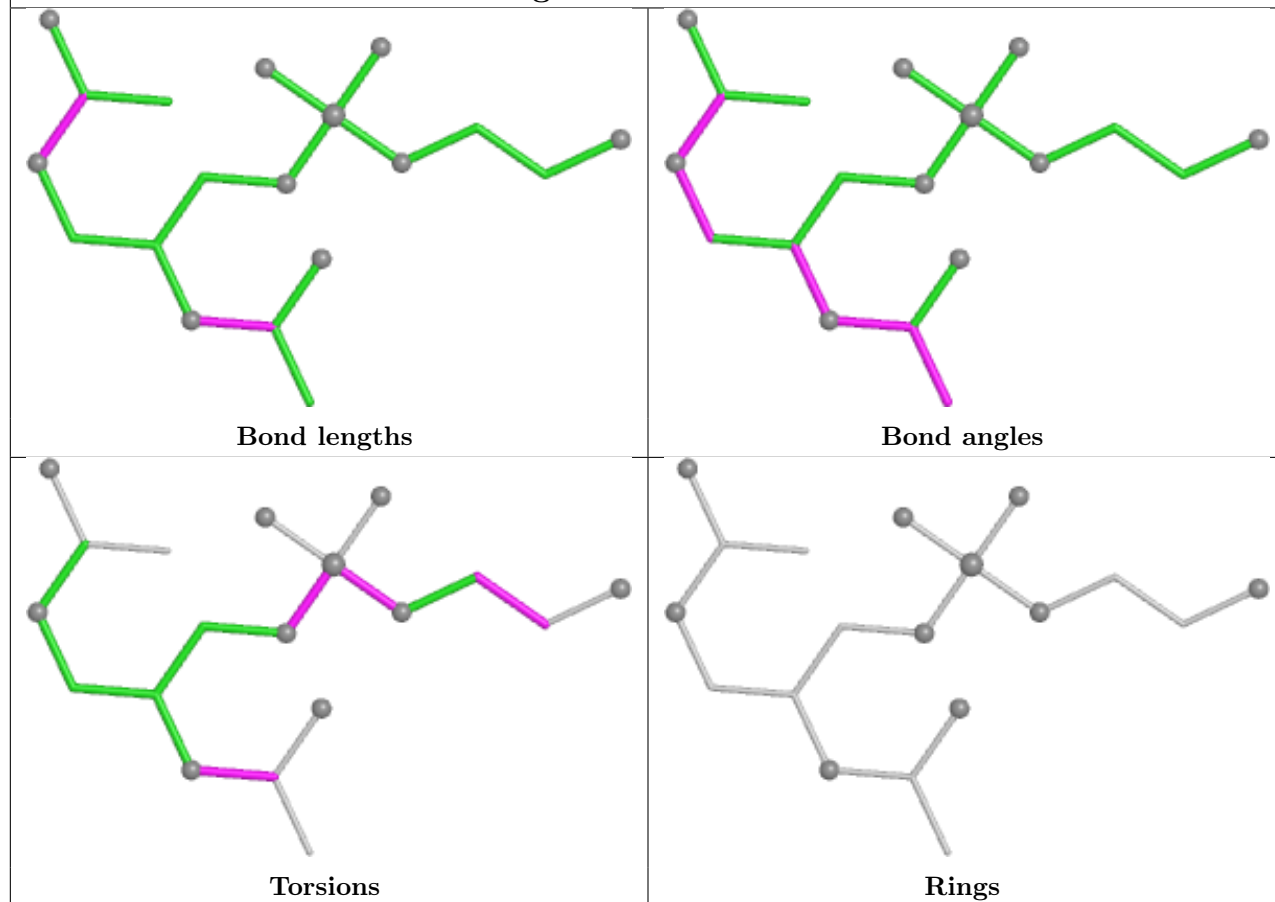
Ligand HEM o 503



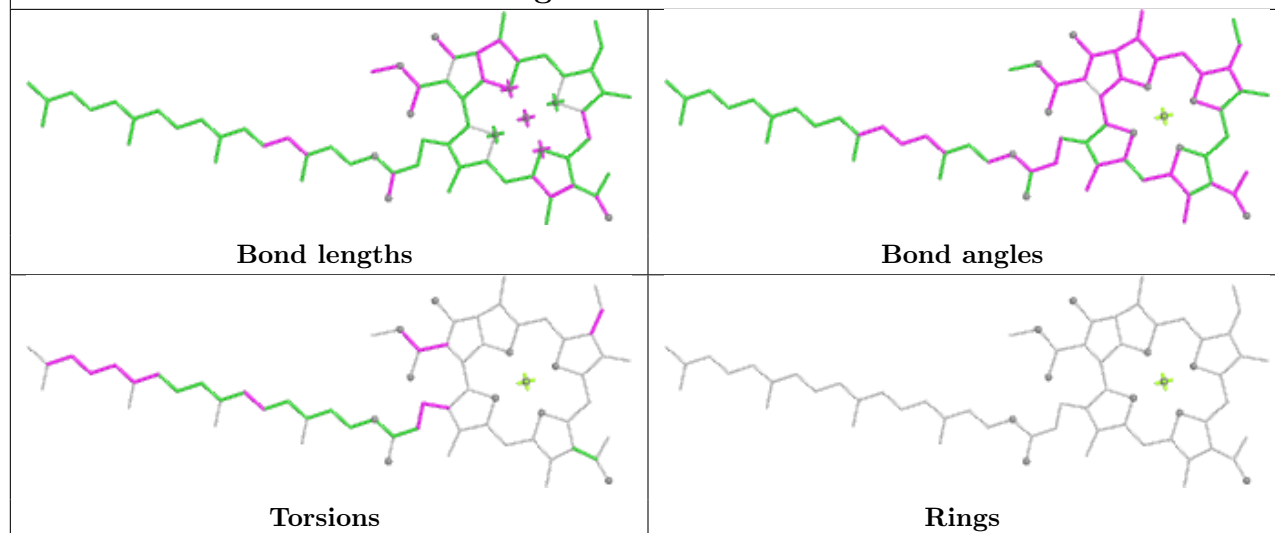
Ligand BCL k 102

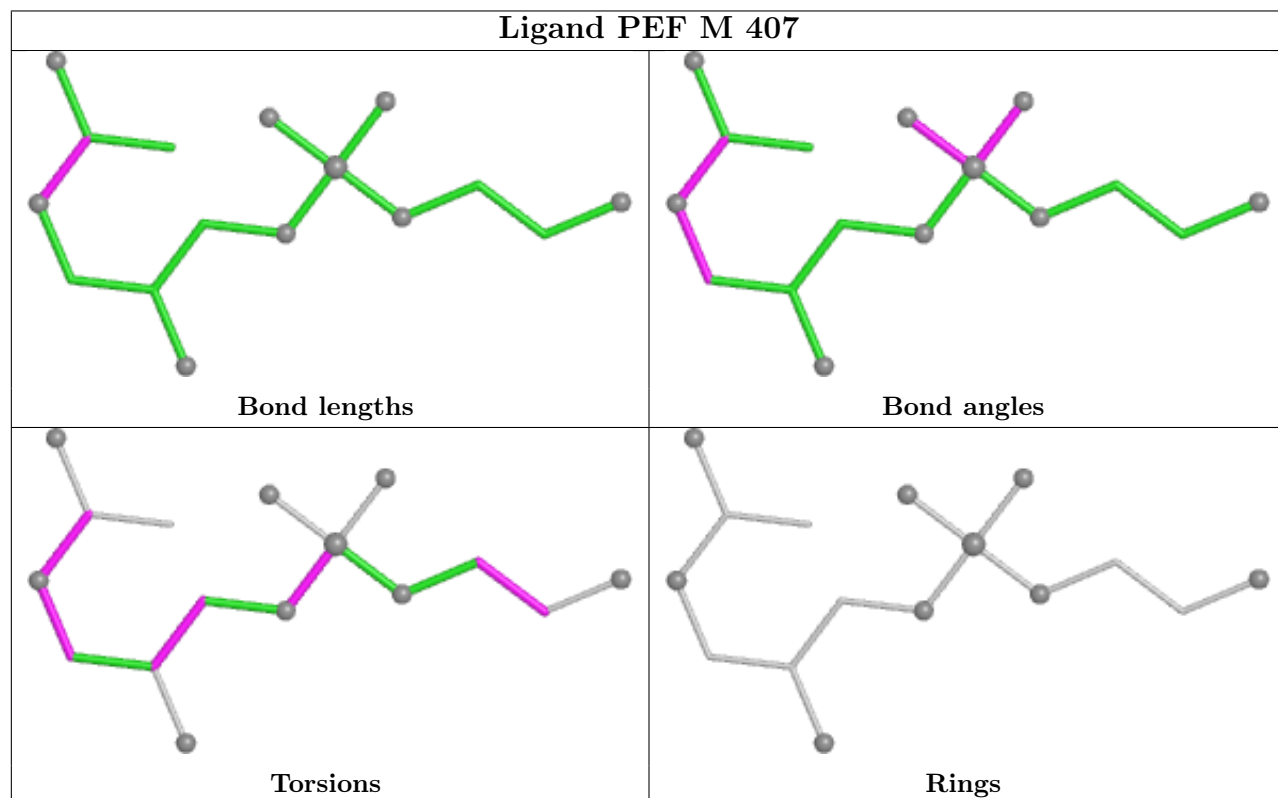
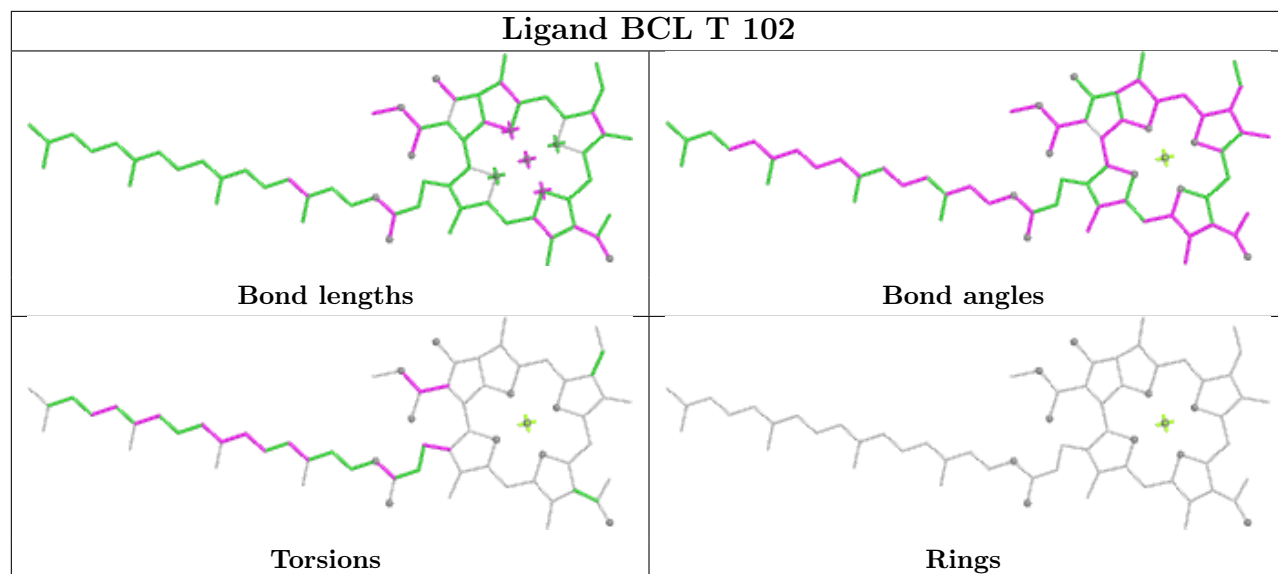


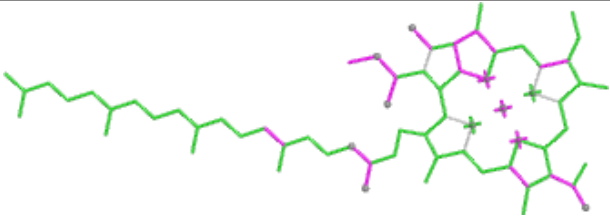
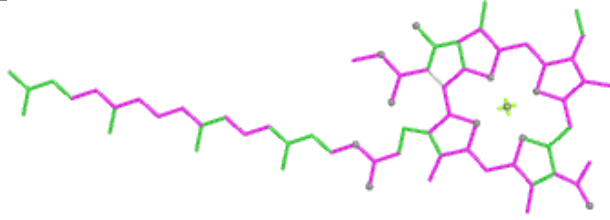
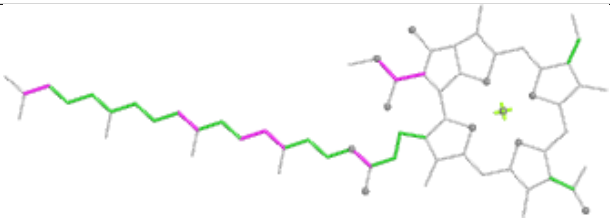
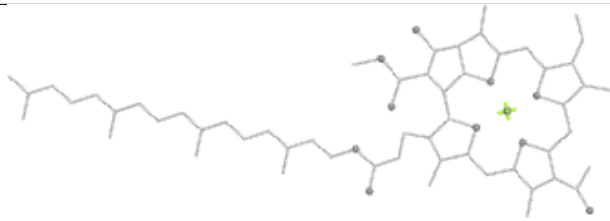
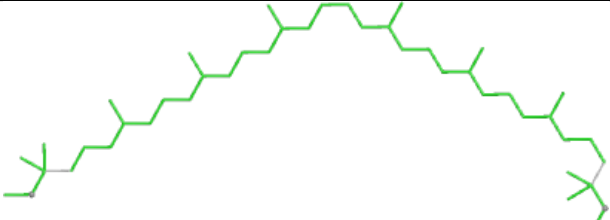
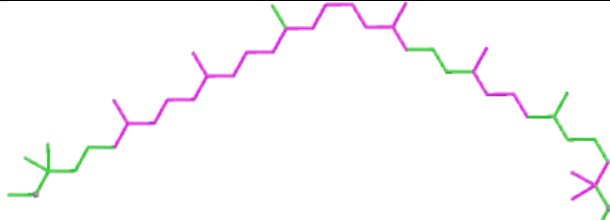
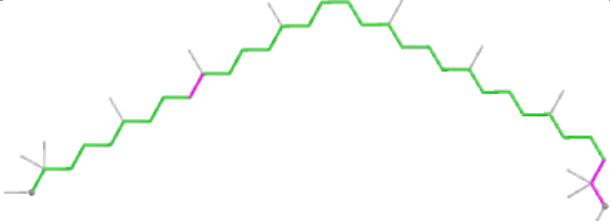
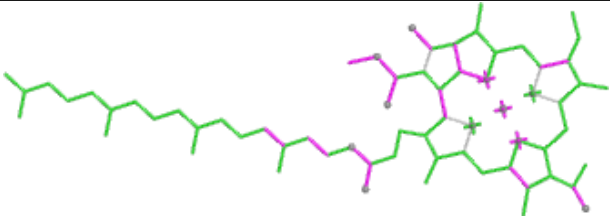
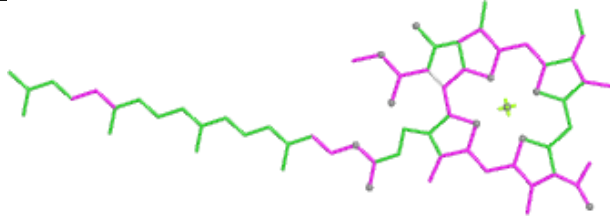
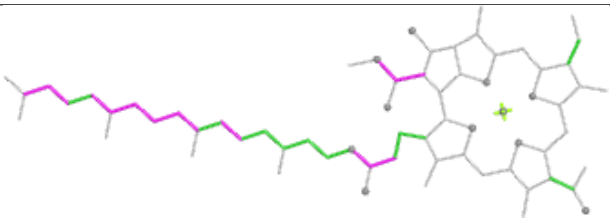
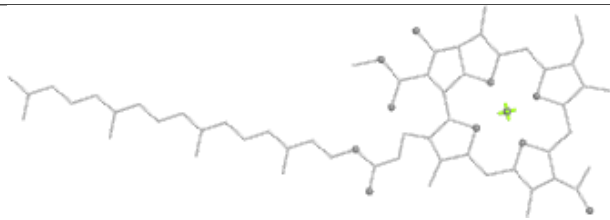
Ligand PEF A 101

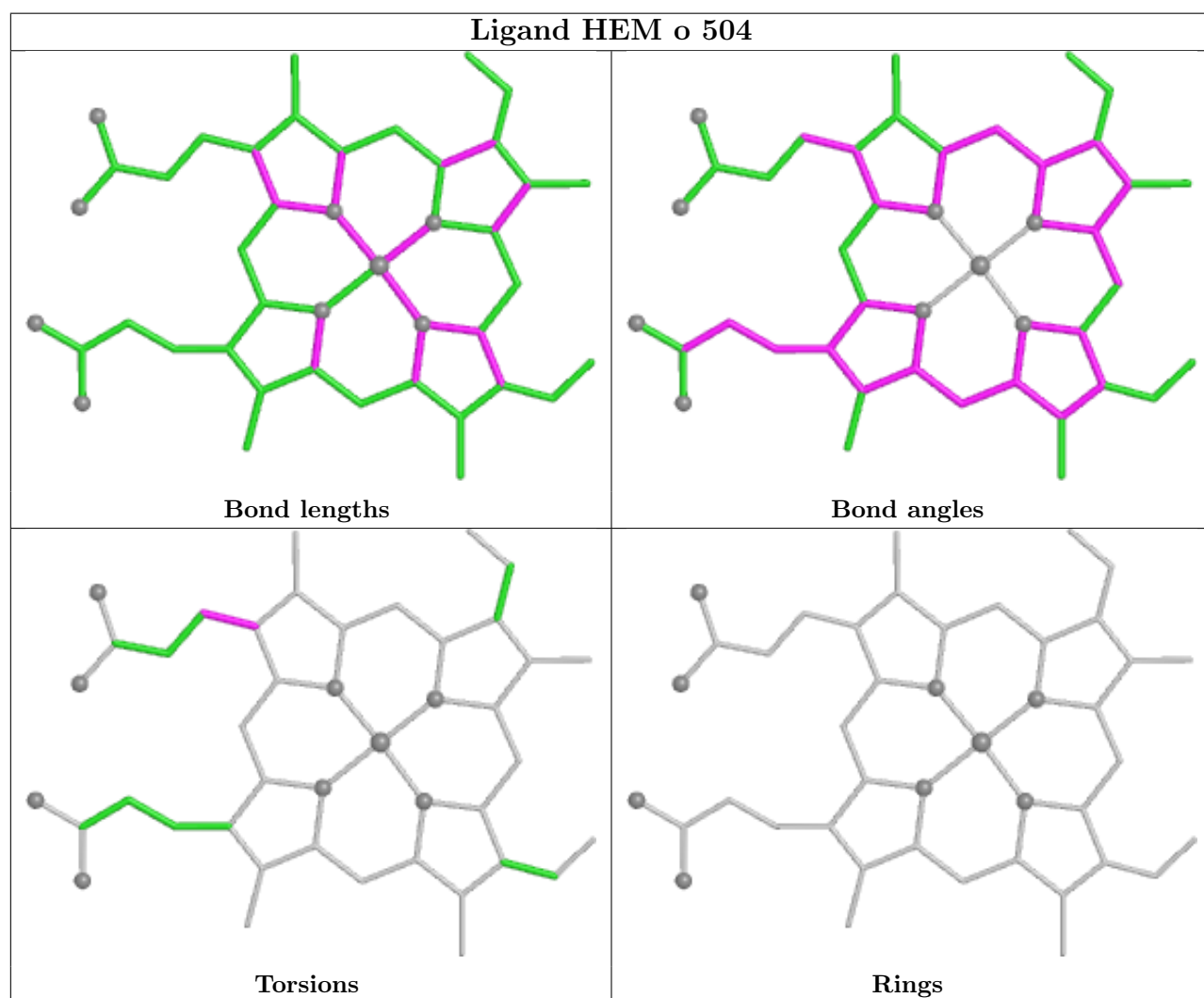
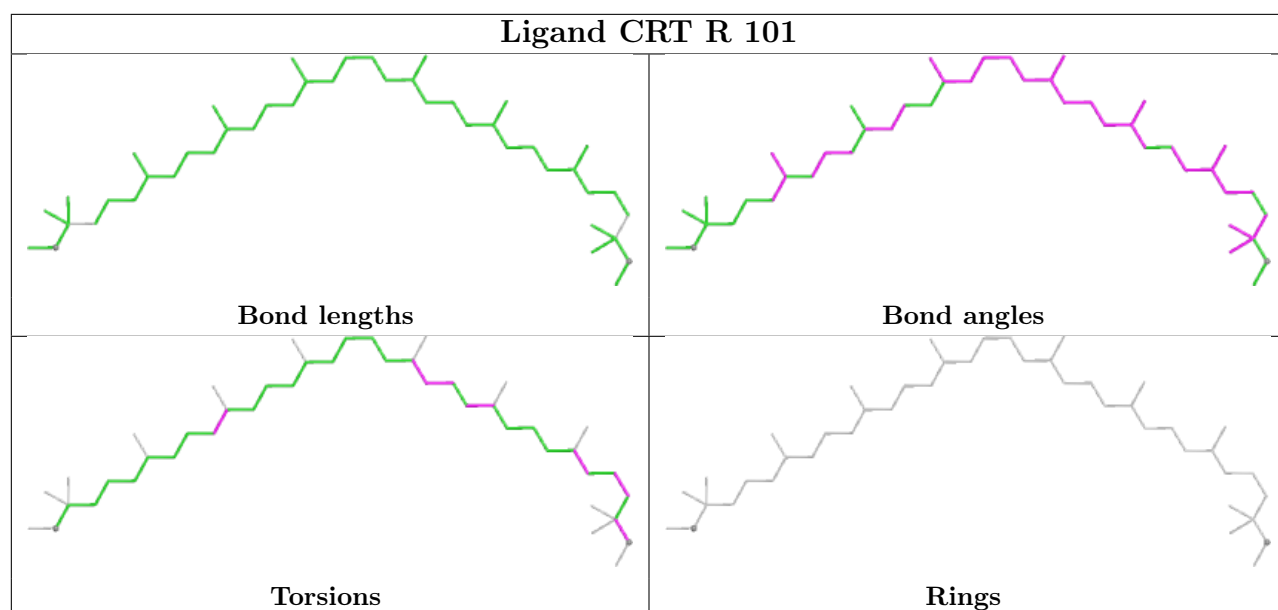


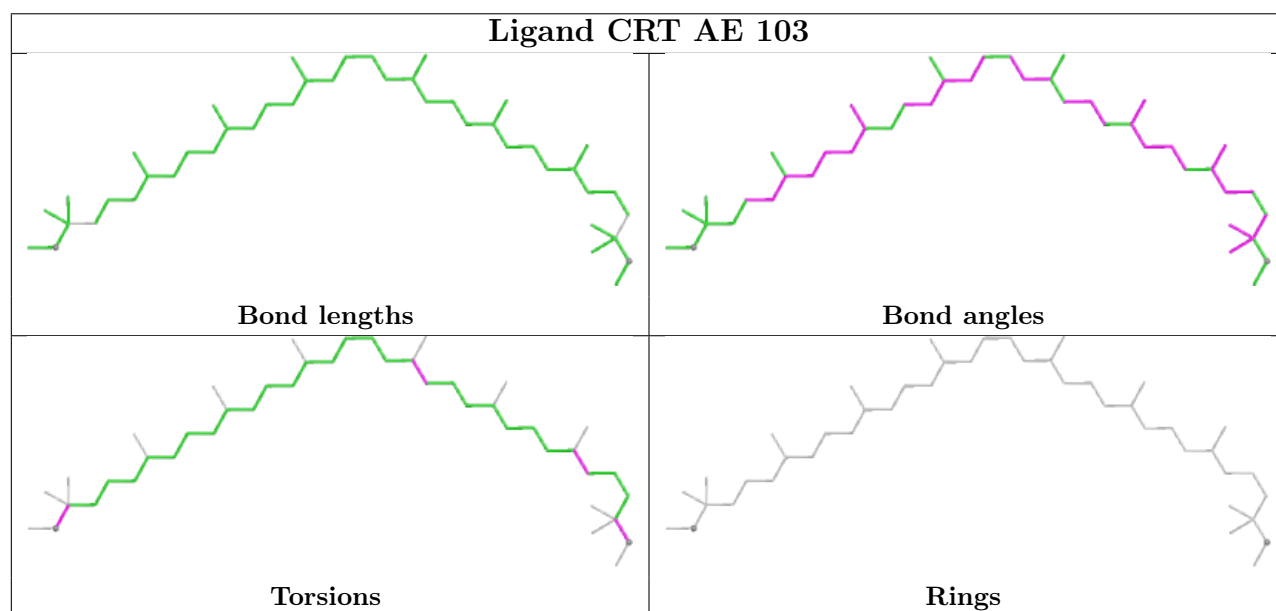
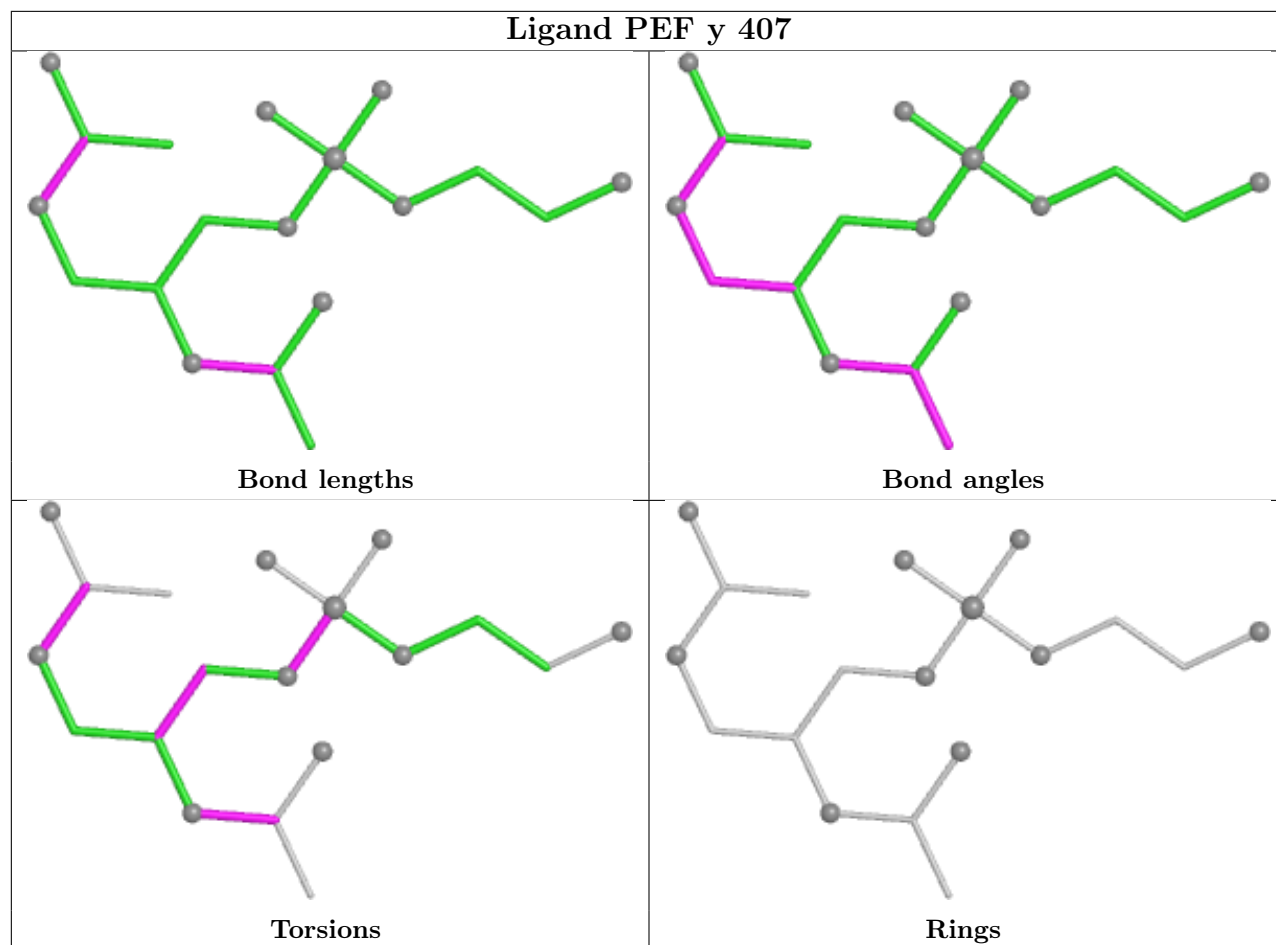
Ligand BCL L 303

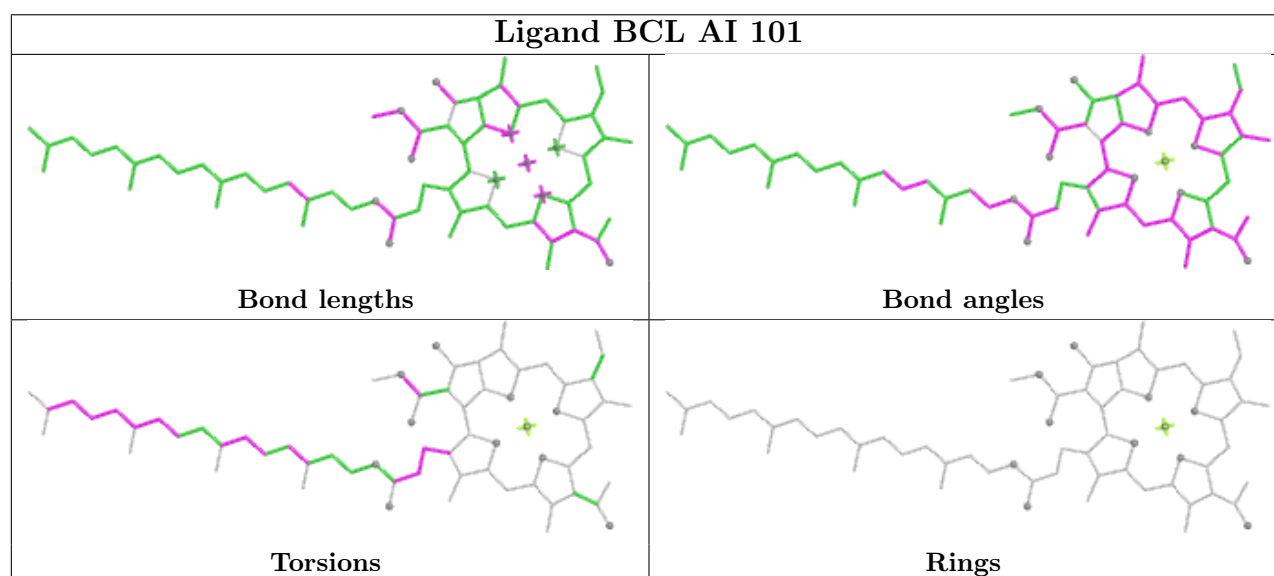
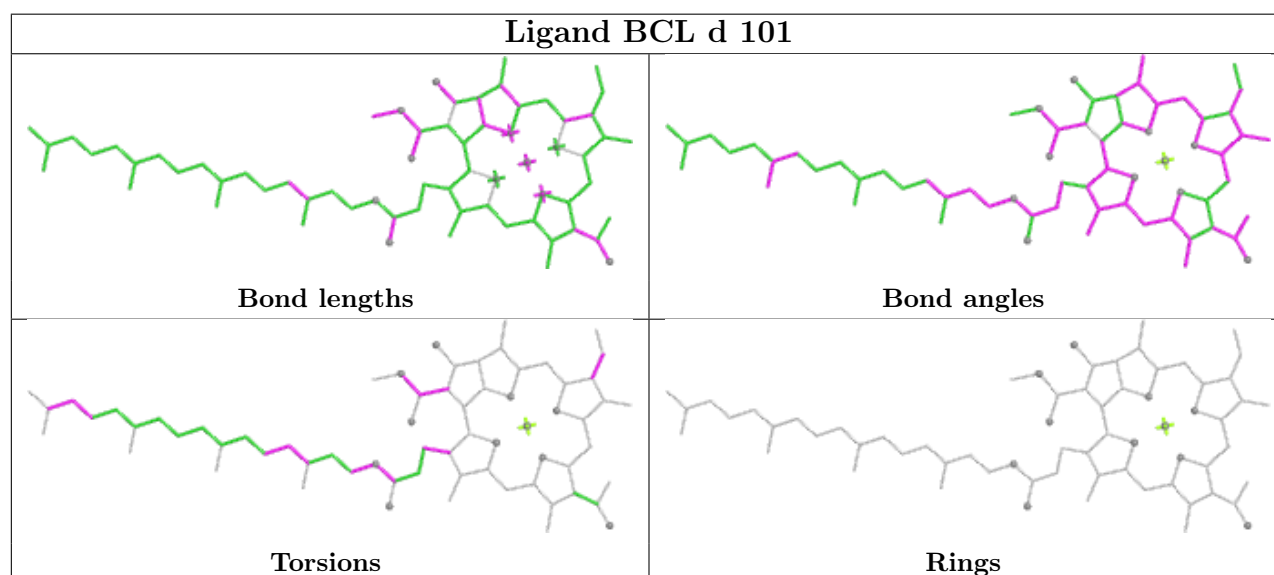
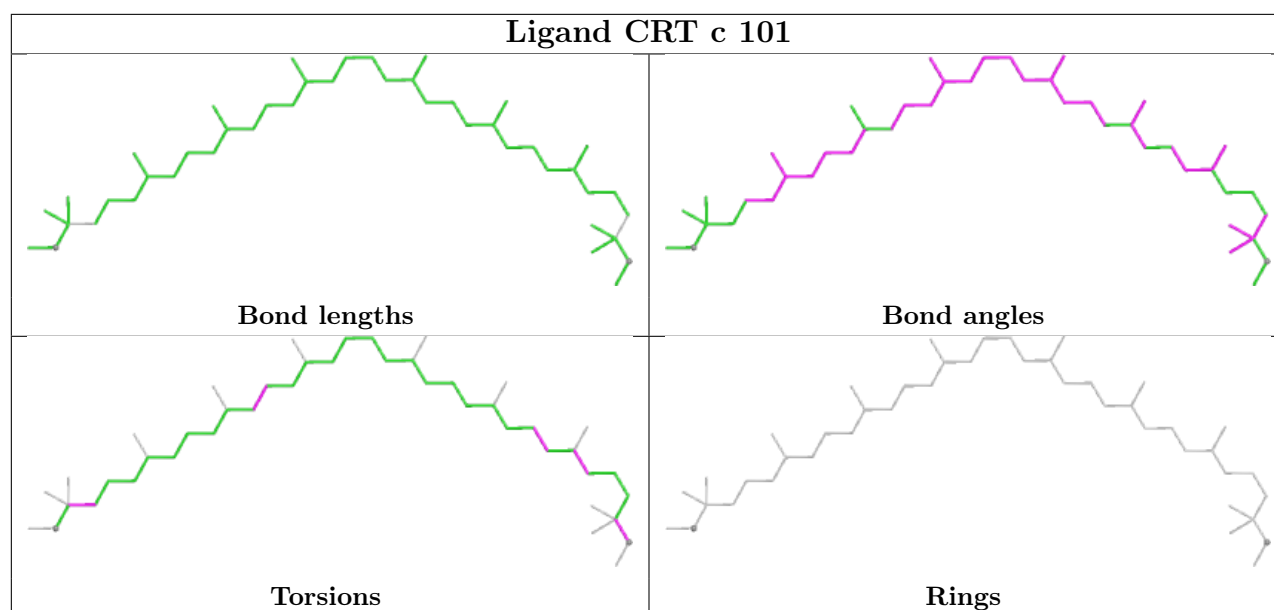


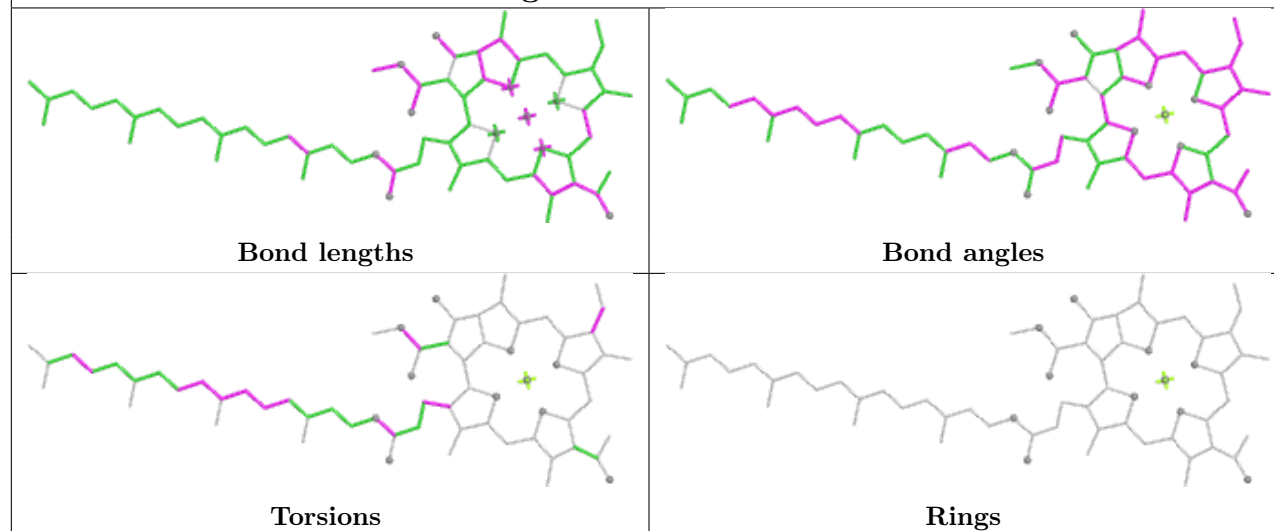
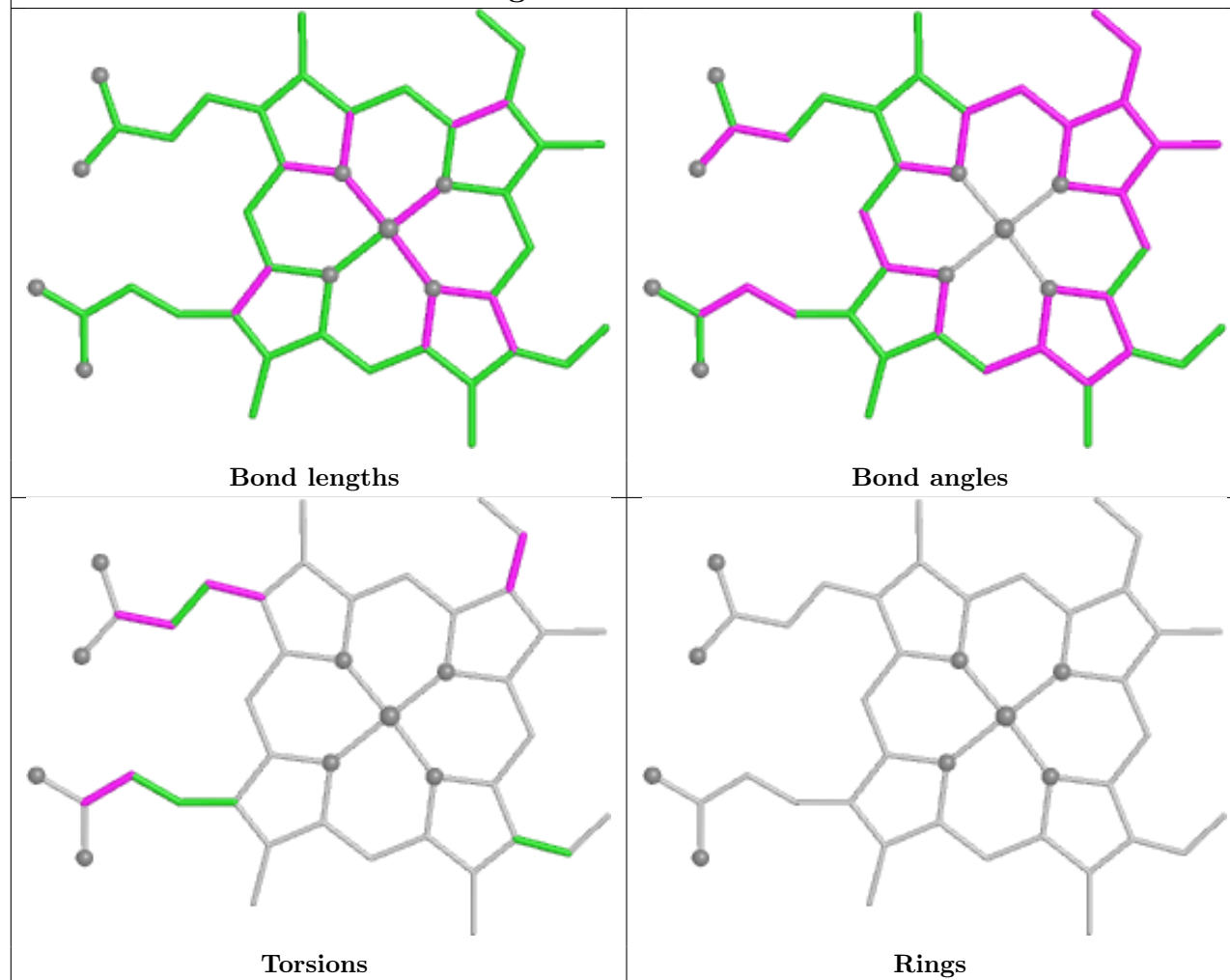


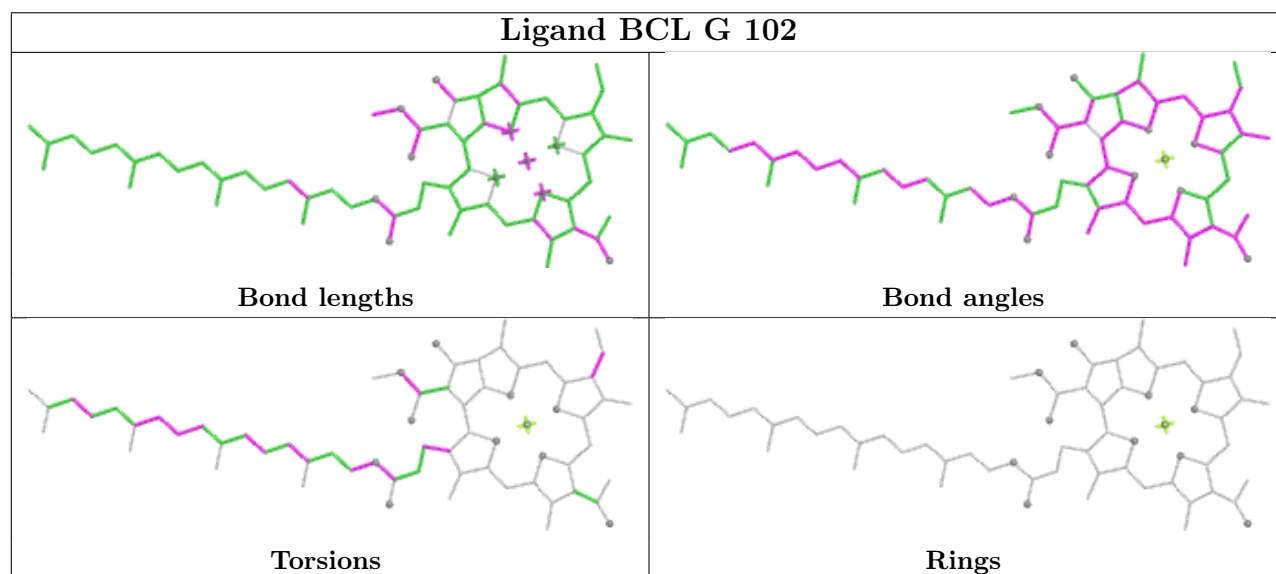
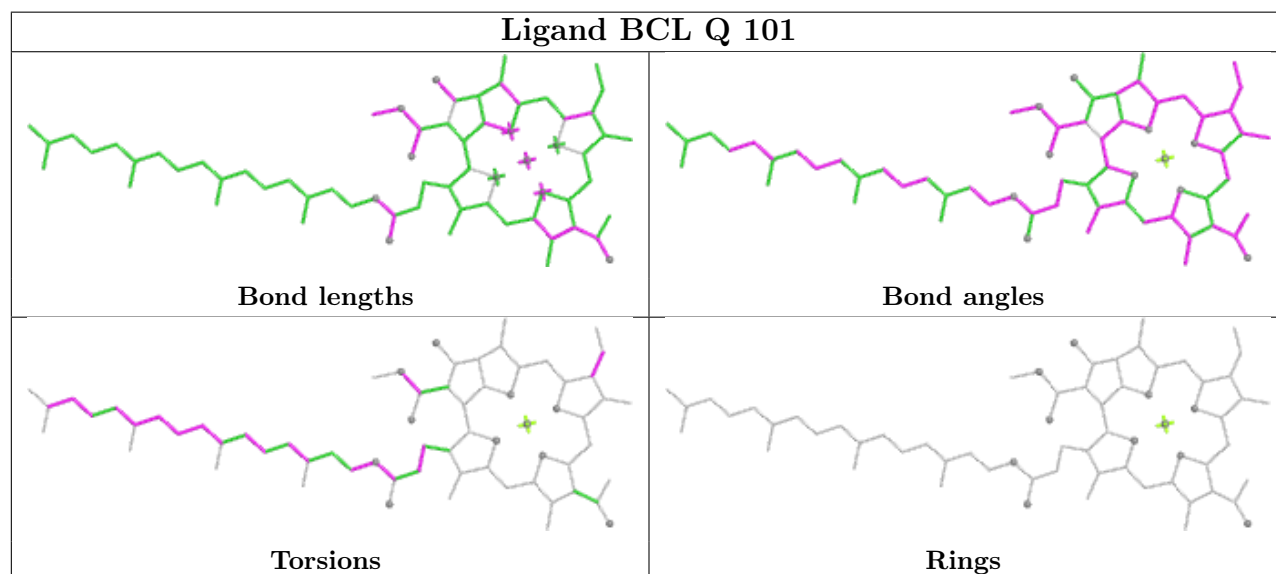
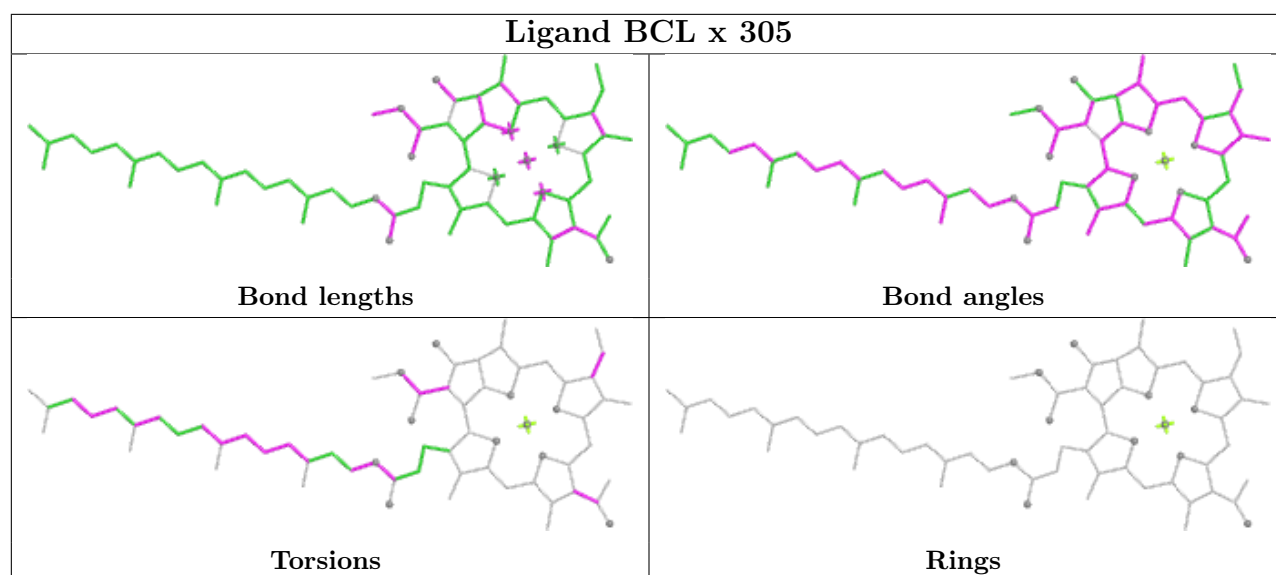
Ligand BCL K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CRT G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL f 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

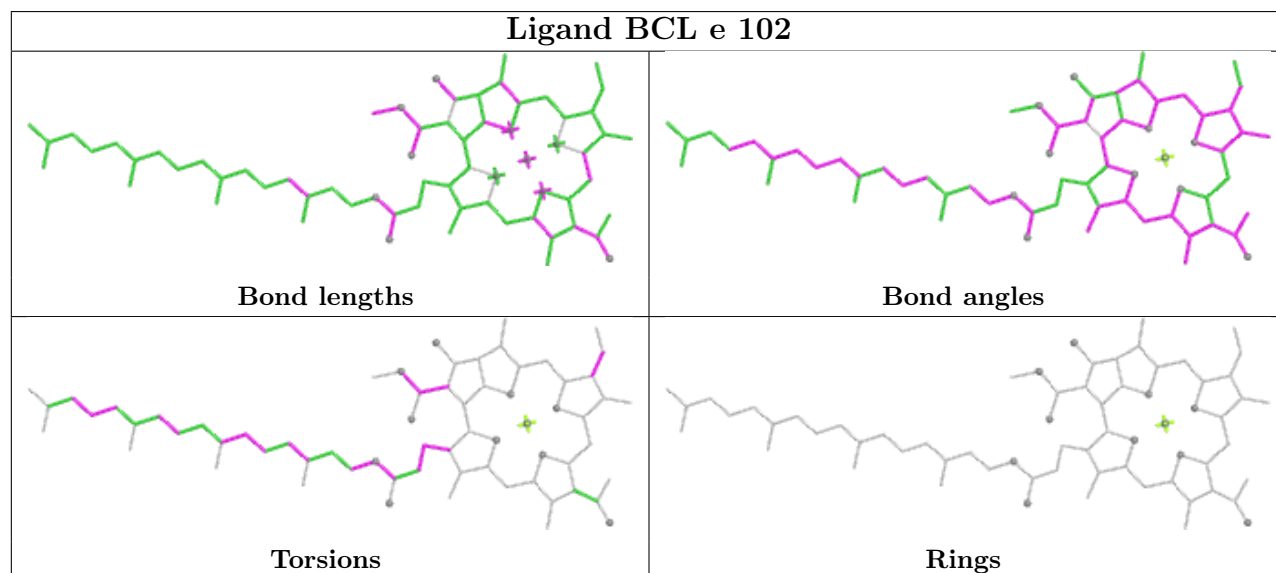
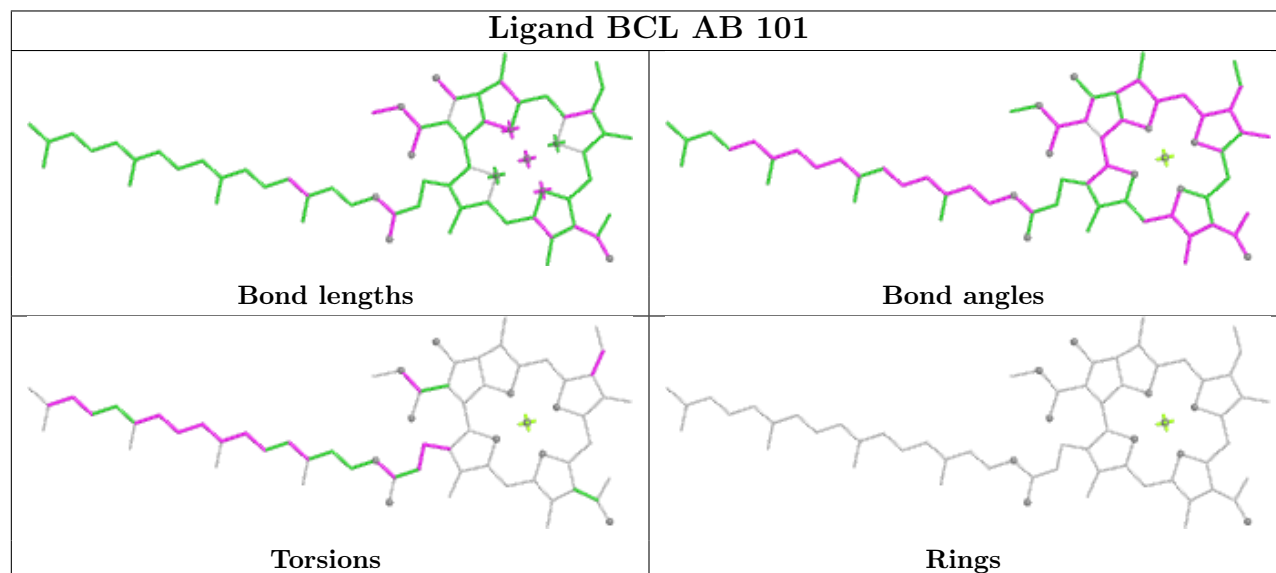
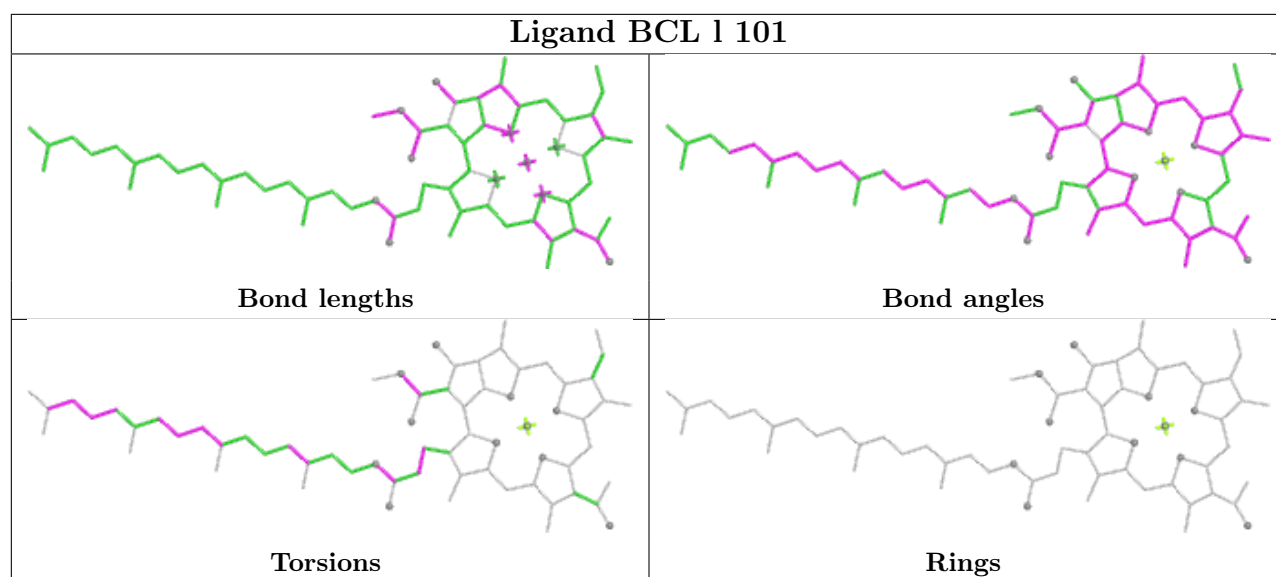


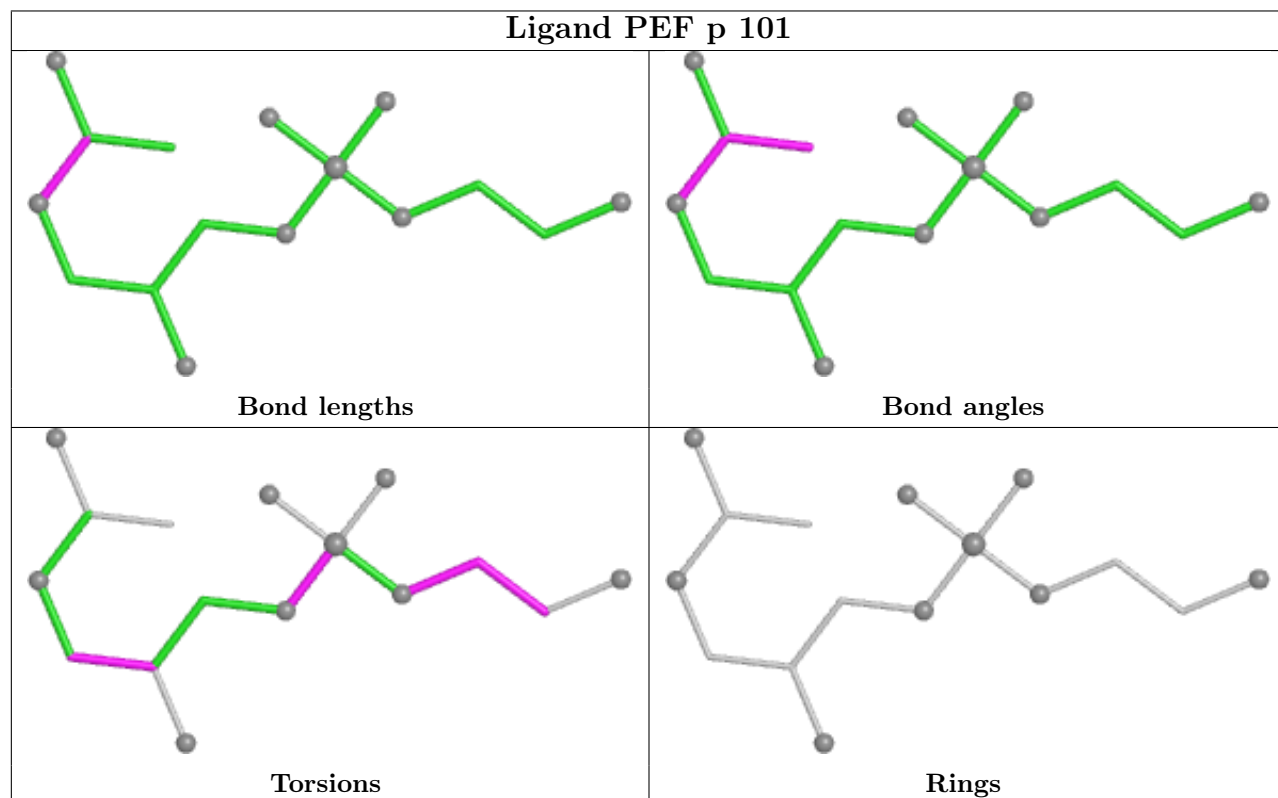
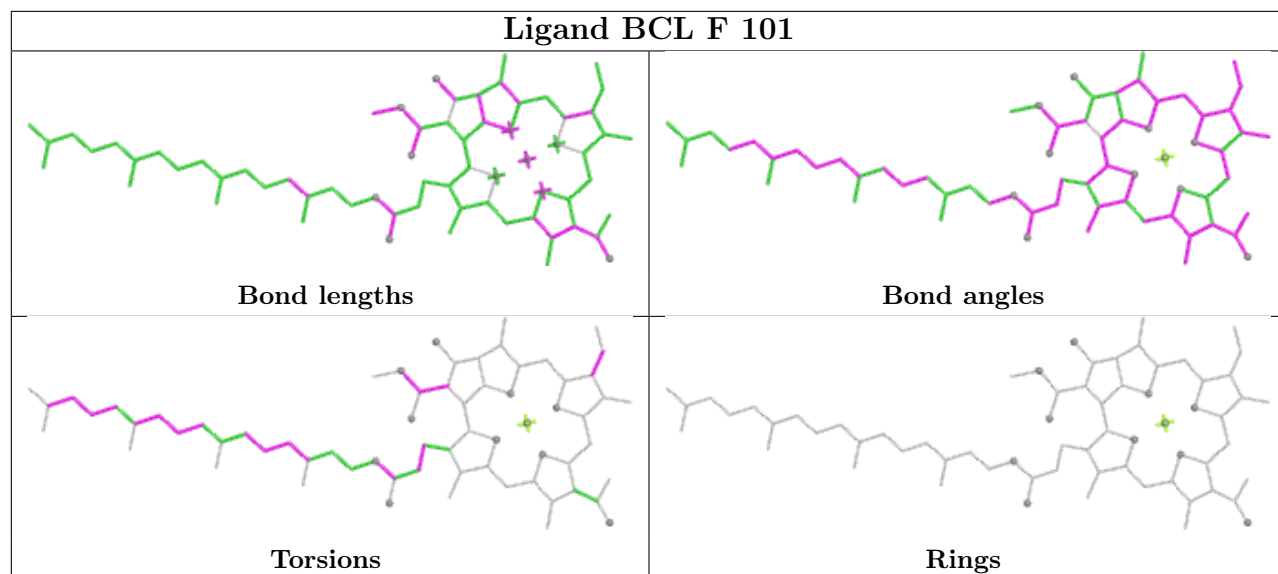


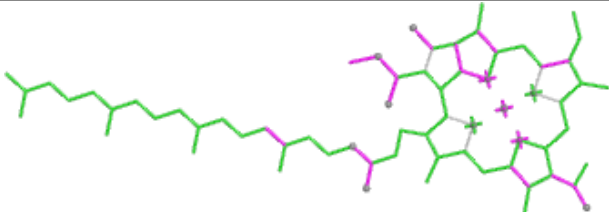
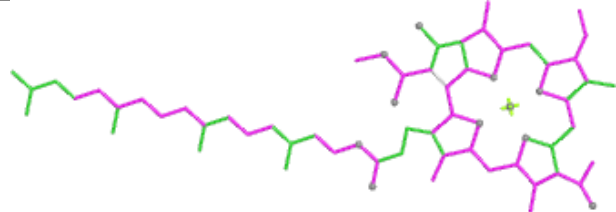
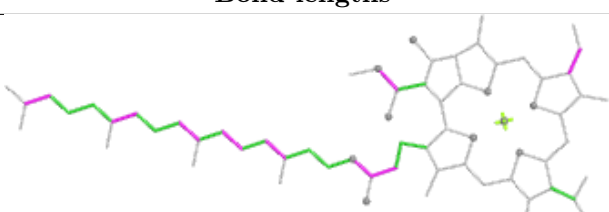
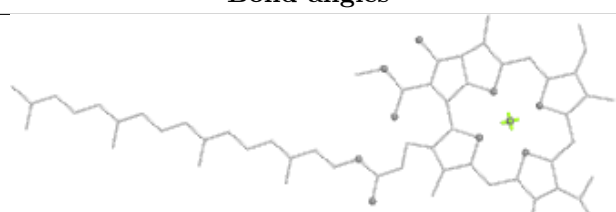
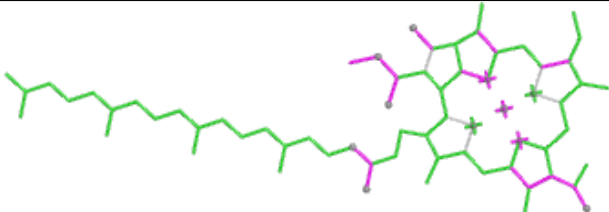
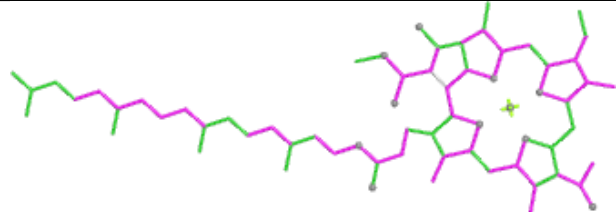
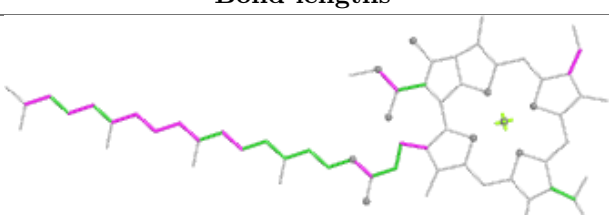
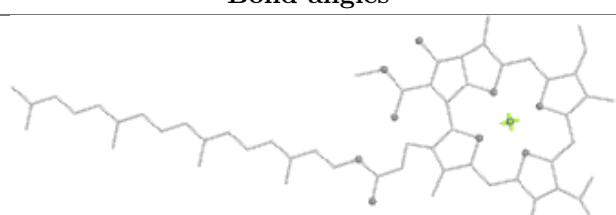
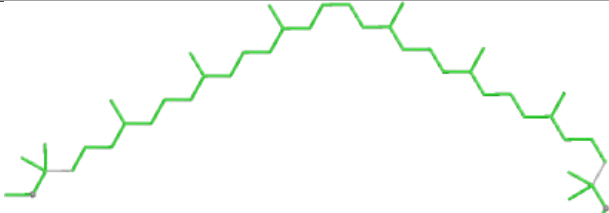
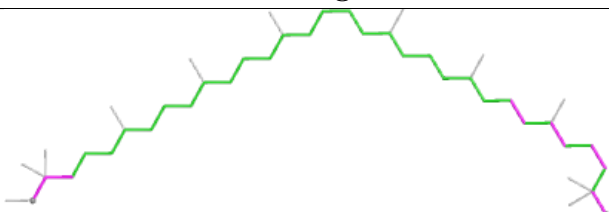
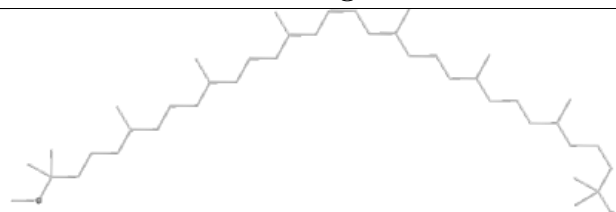


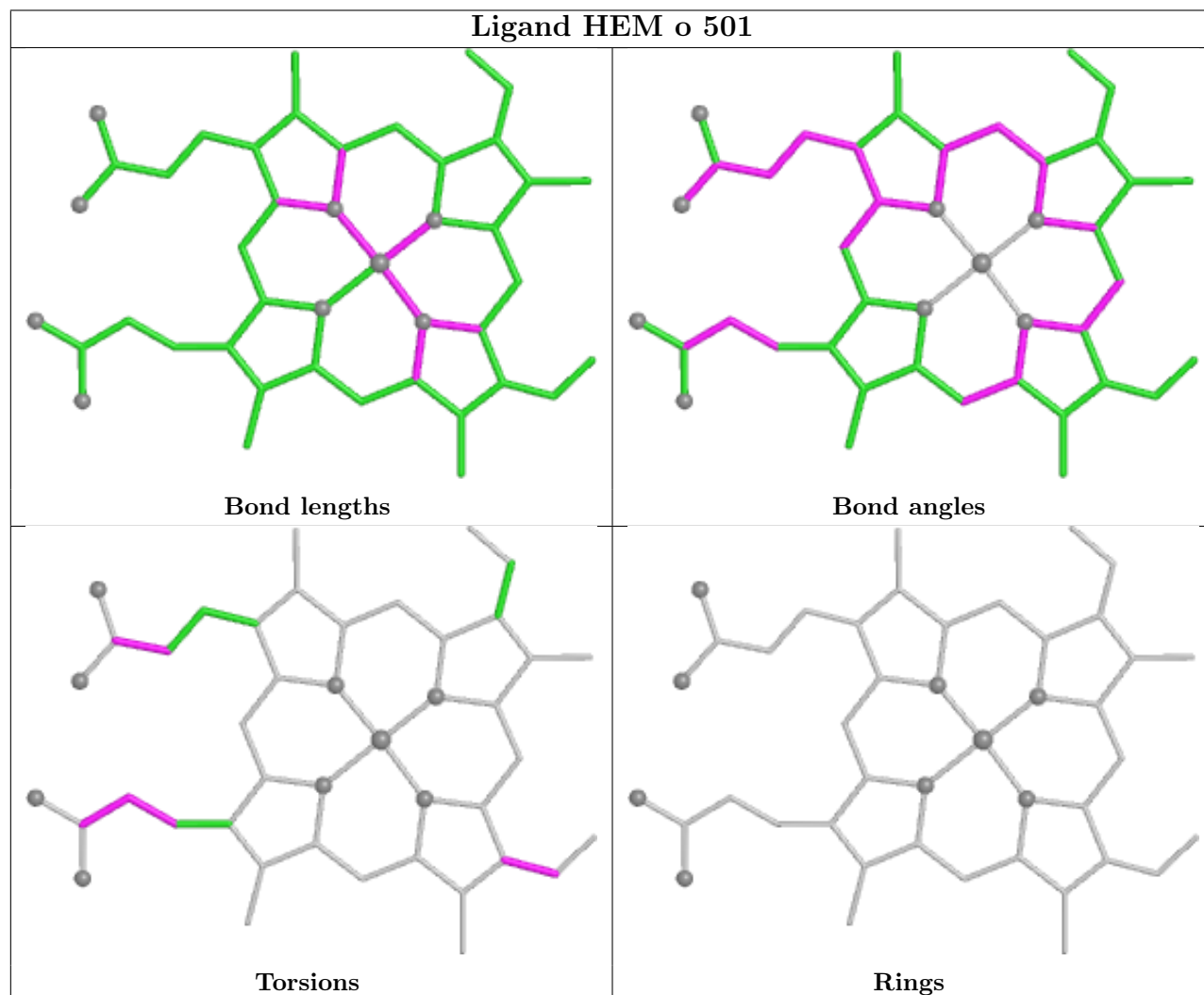
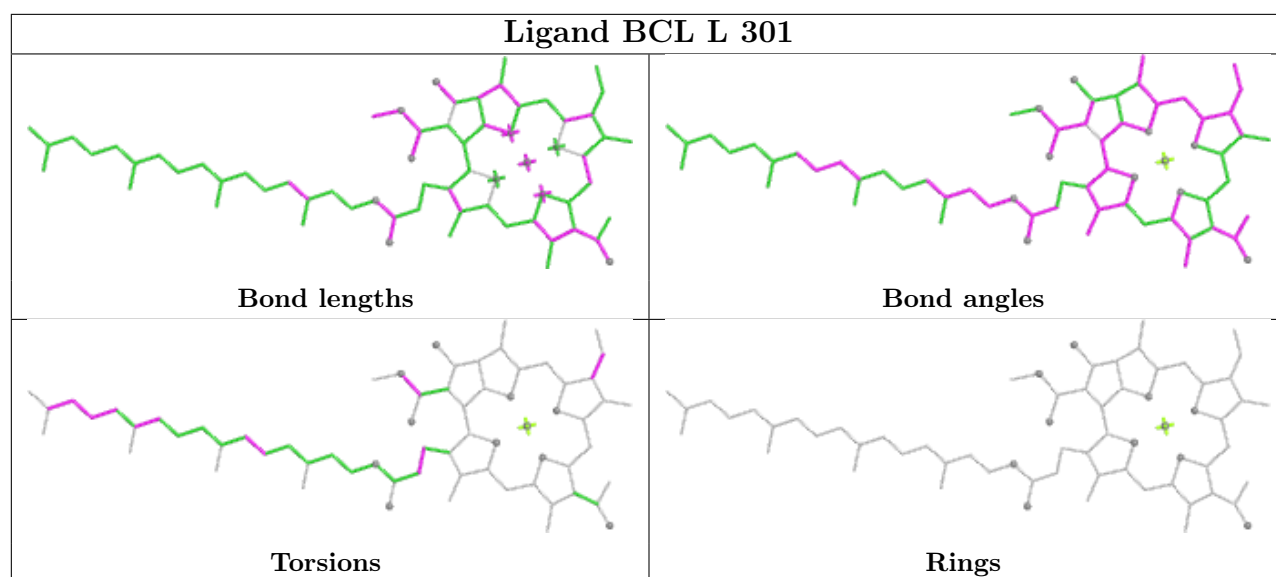
Ligand BCL AL 102**Ligand HEM C 504**

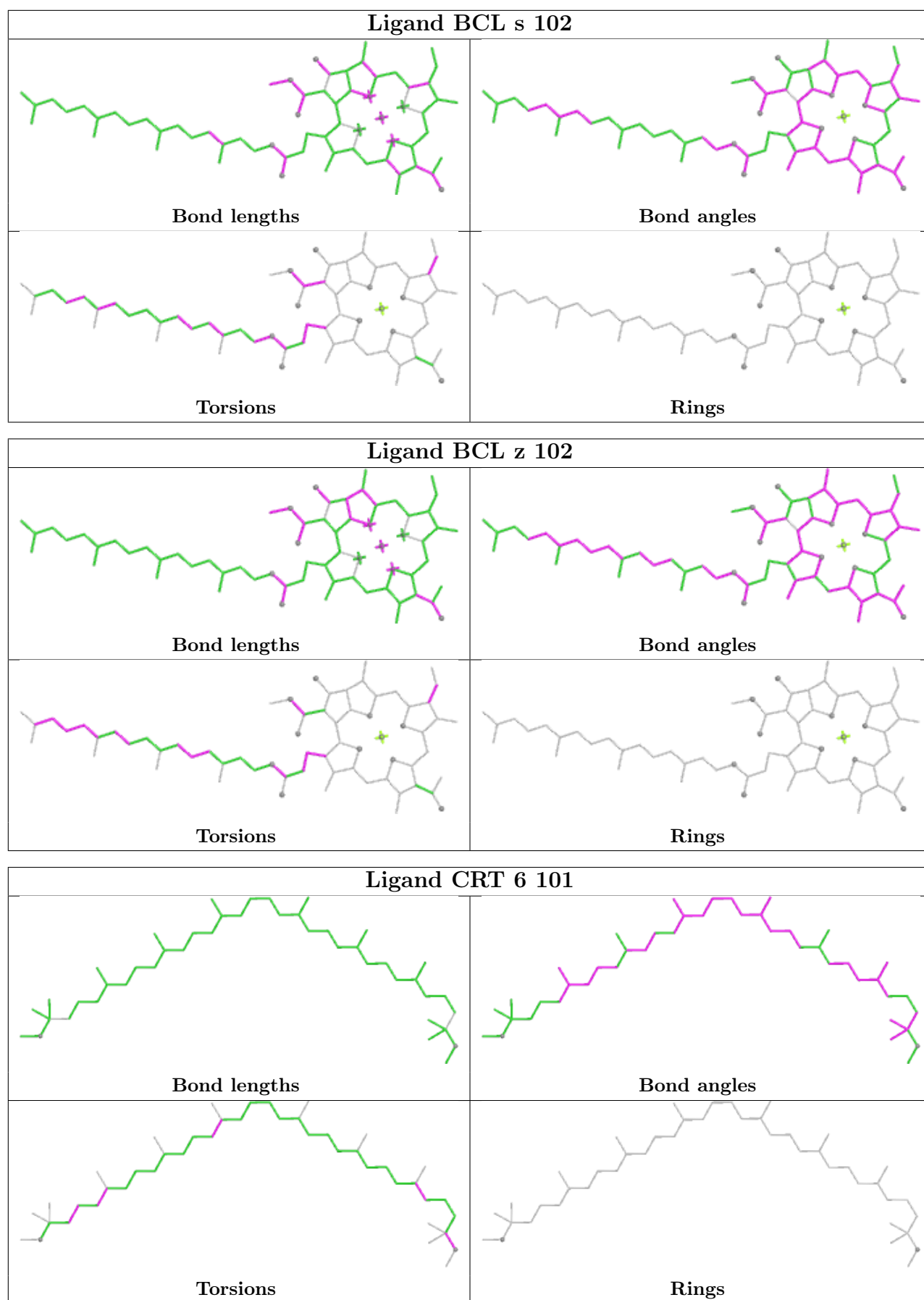


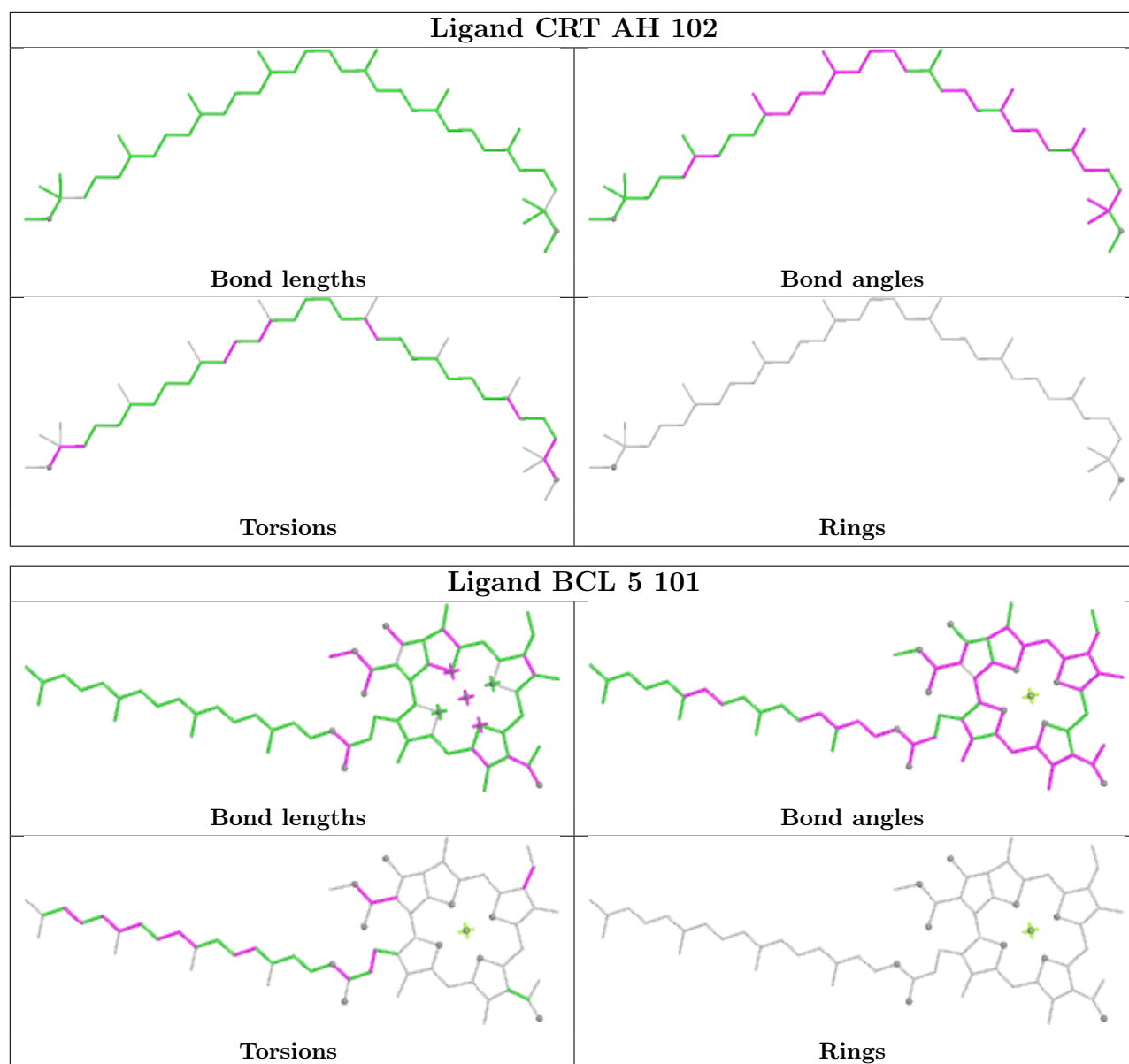


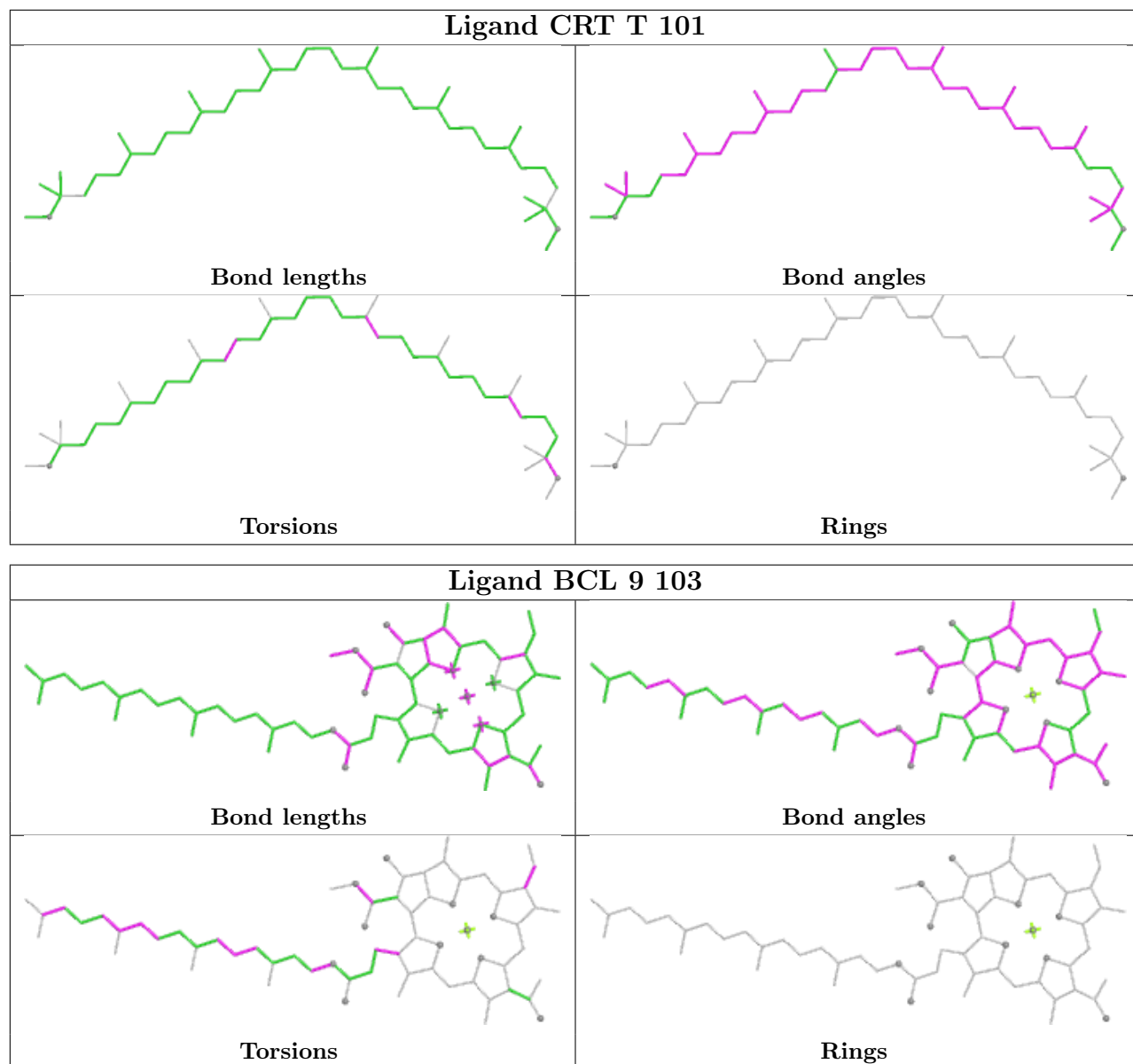


Ligand BCL P 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL 7 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CRT J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

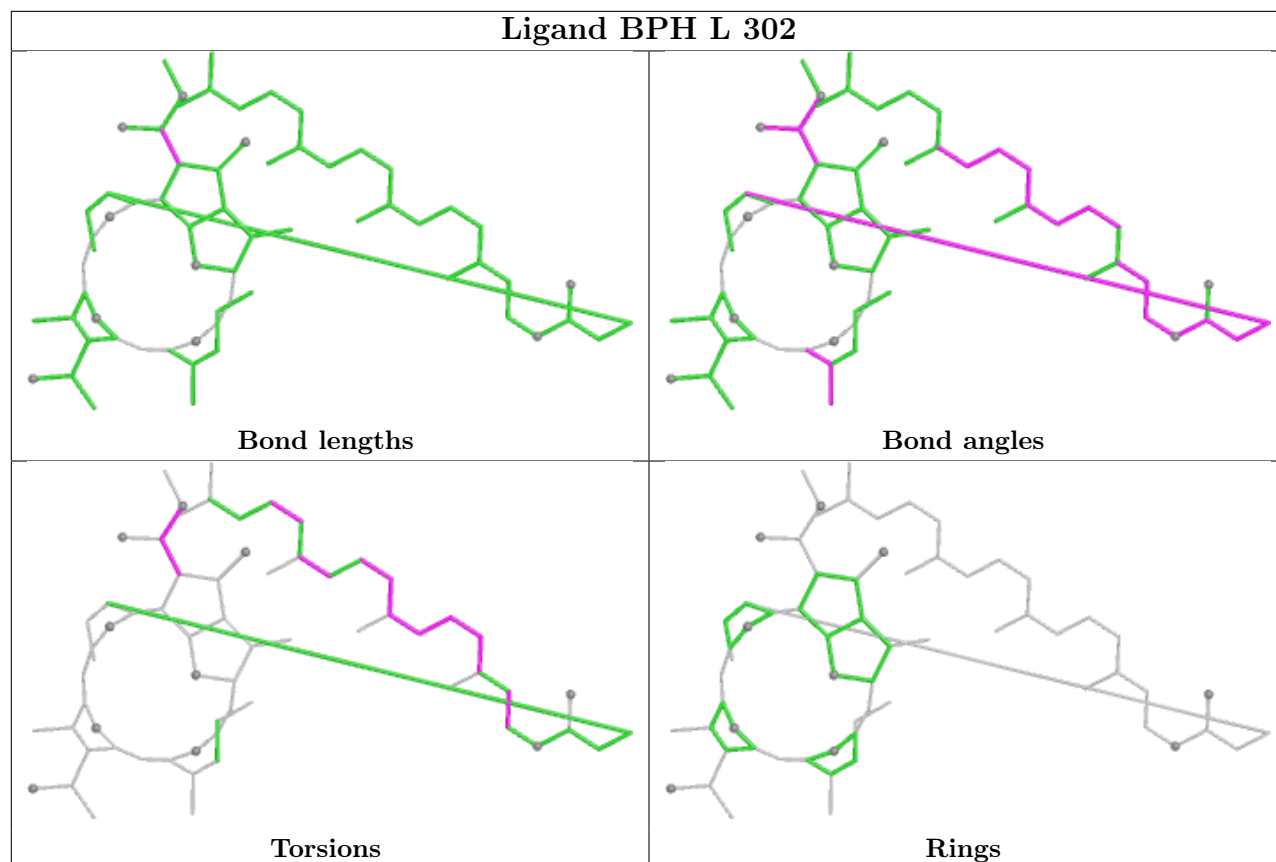




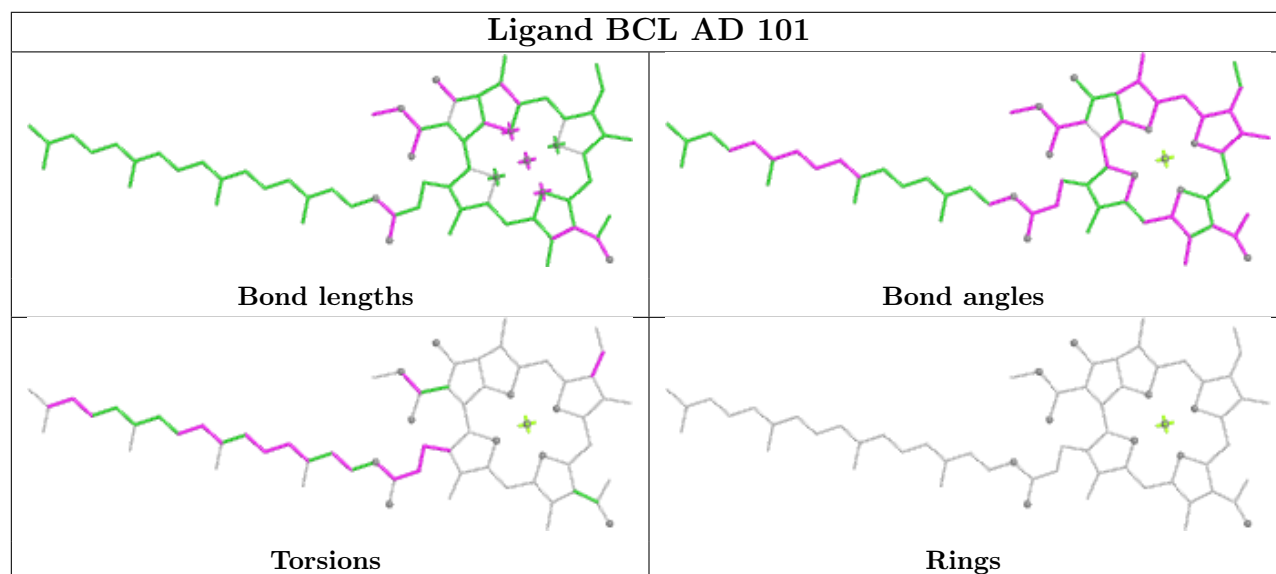


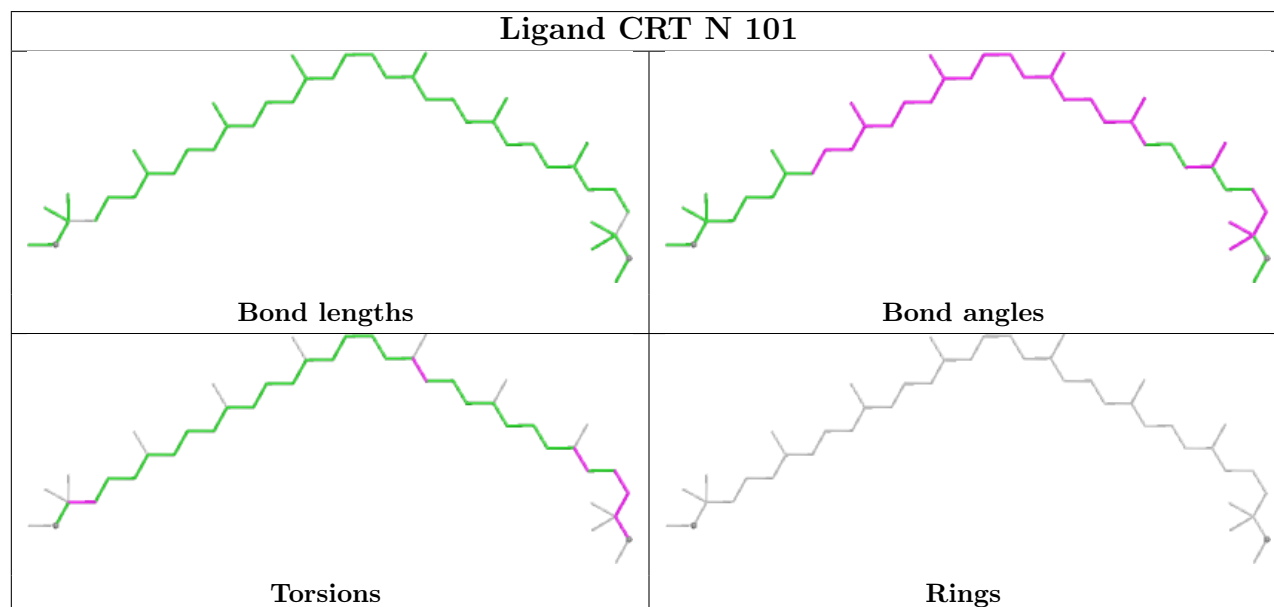
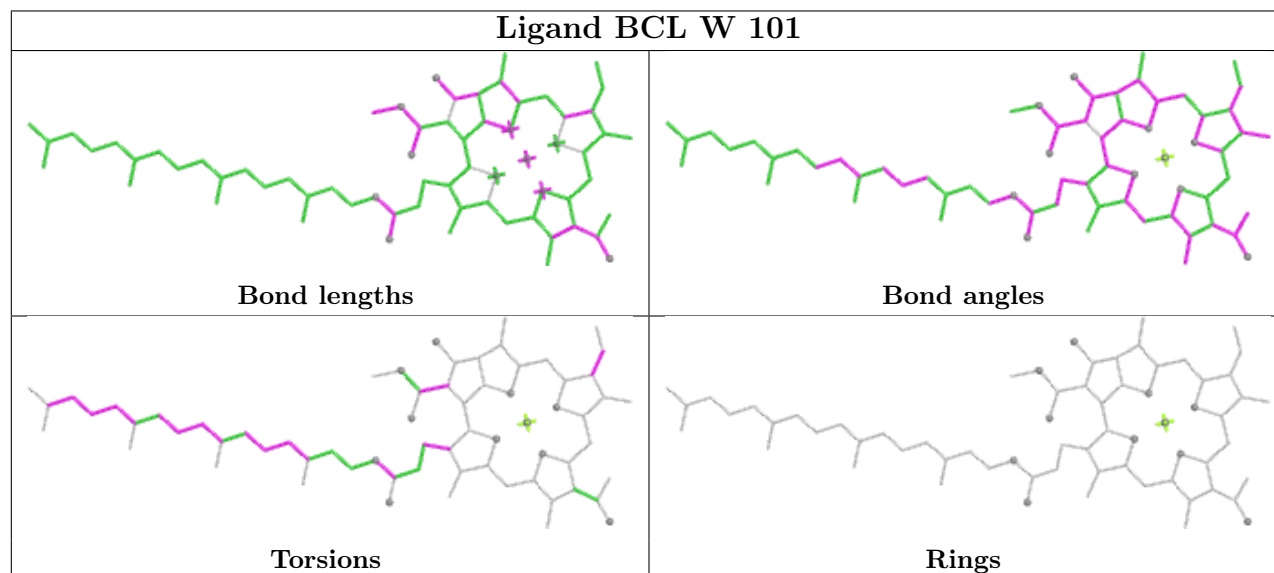
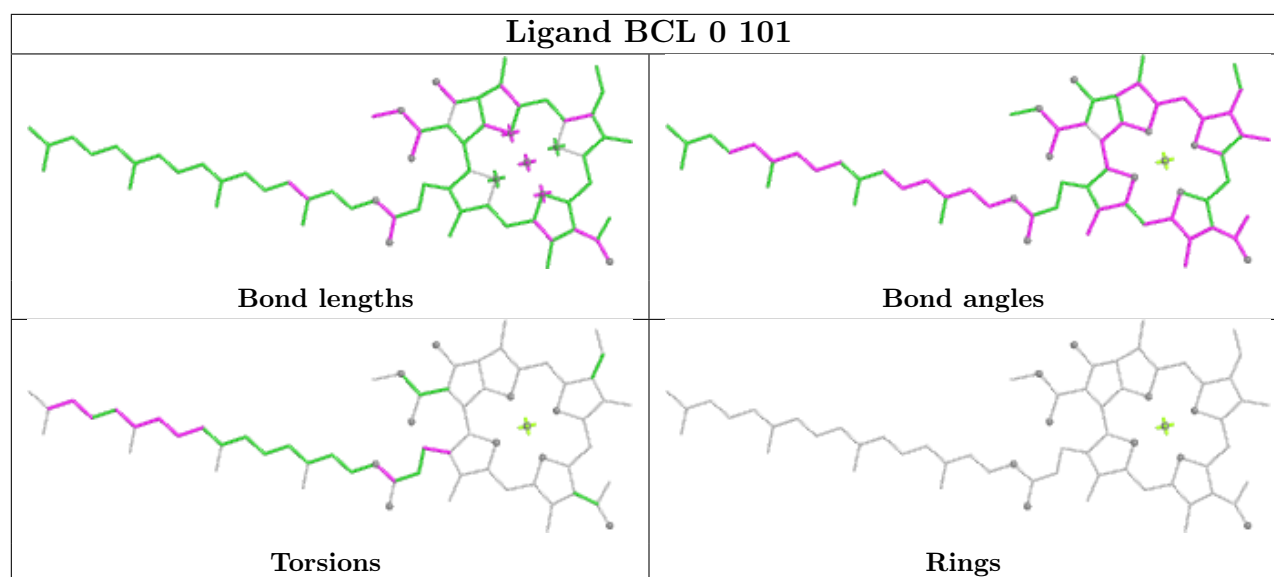


Ligand BPH L 302

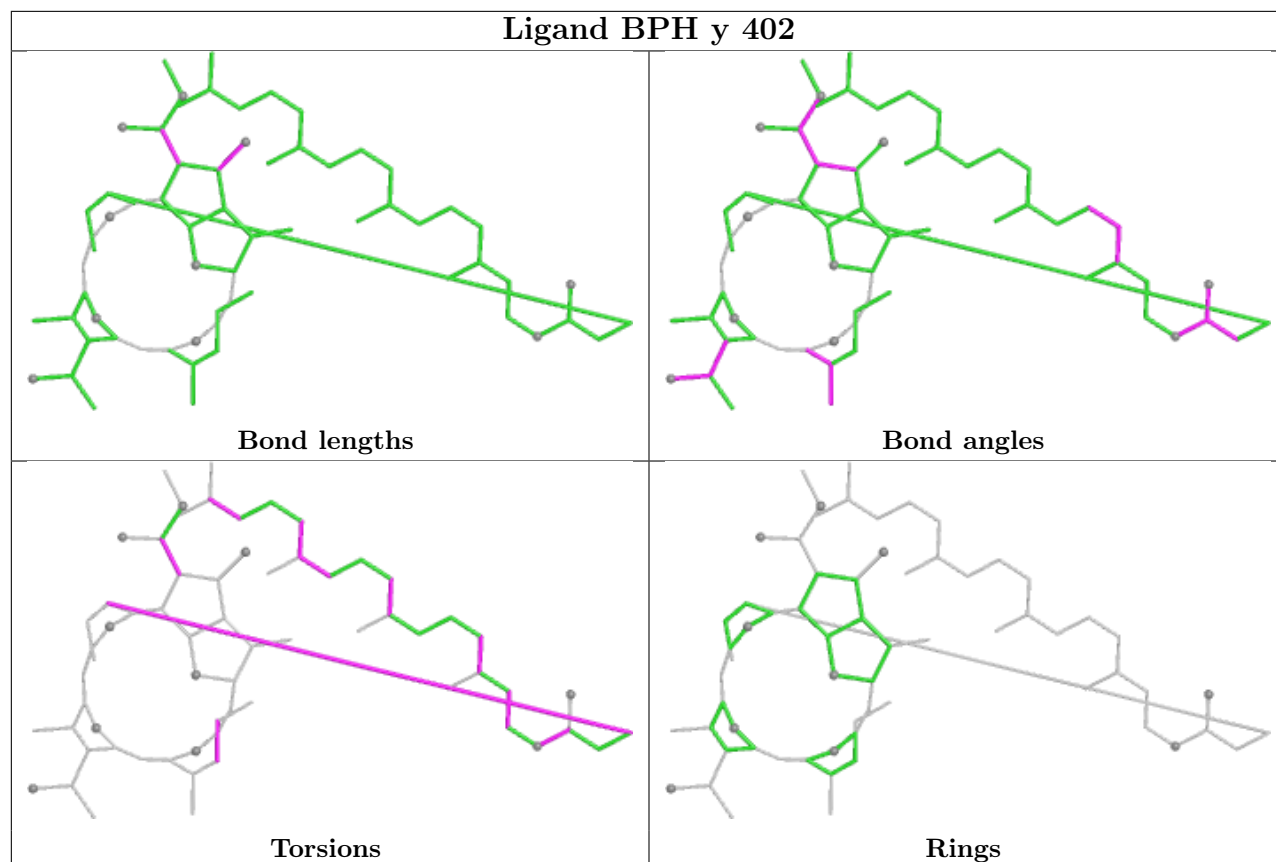


Ligand BCL AD 101

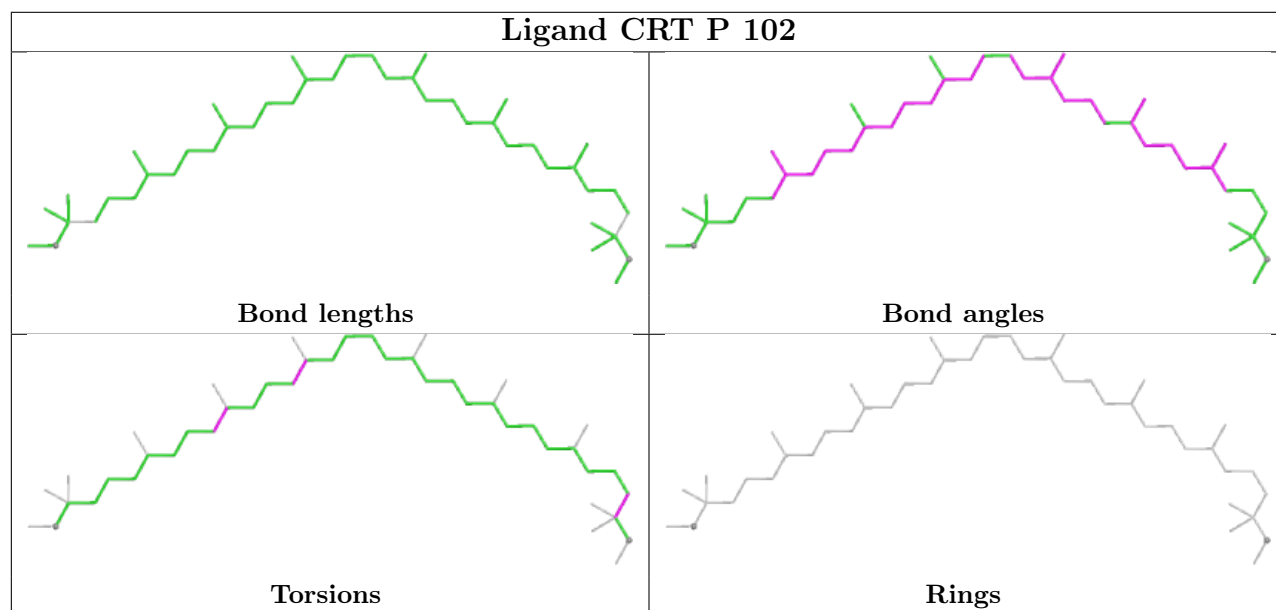


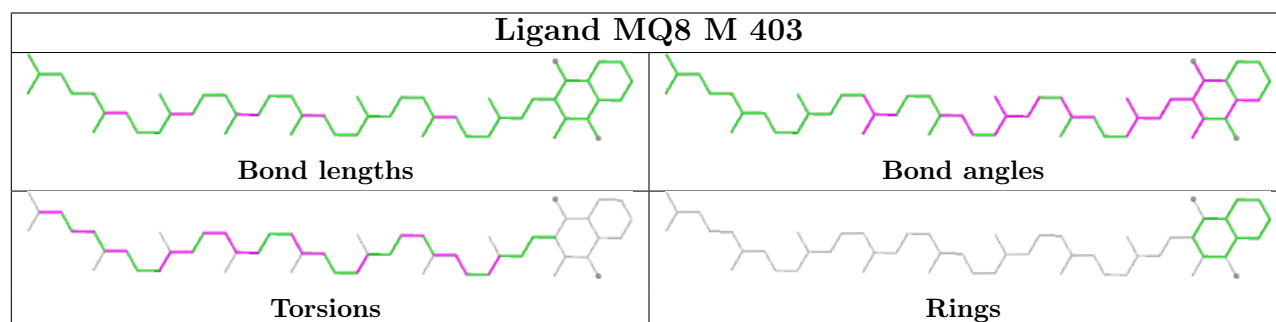
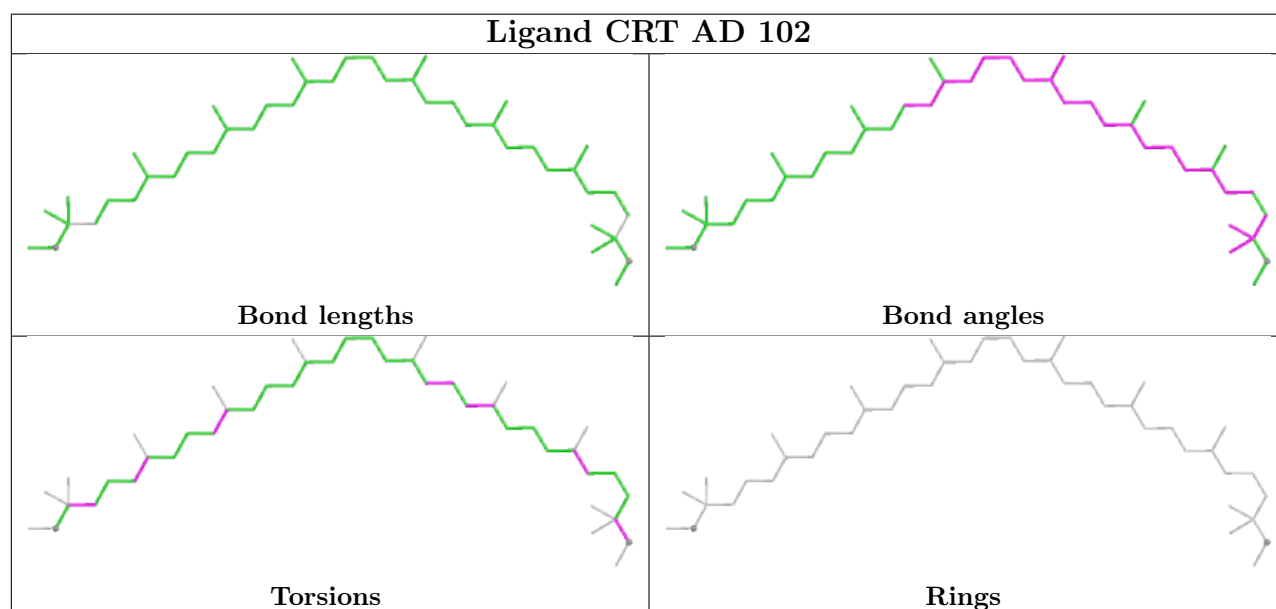
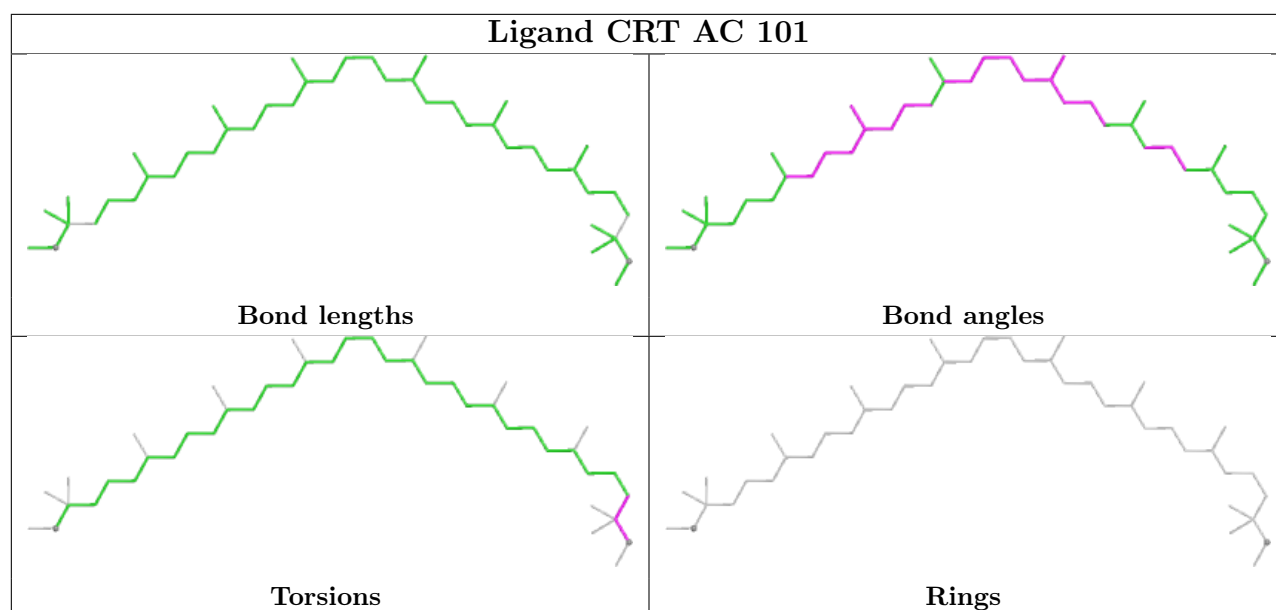


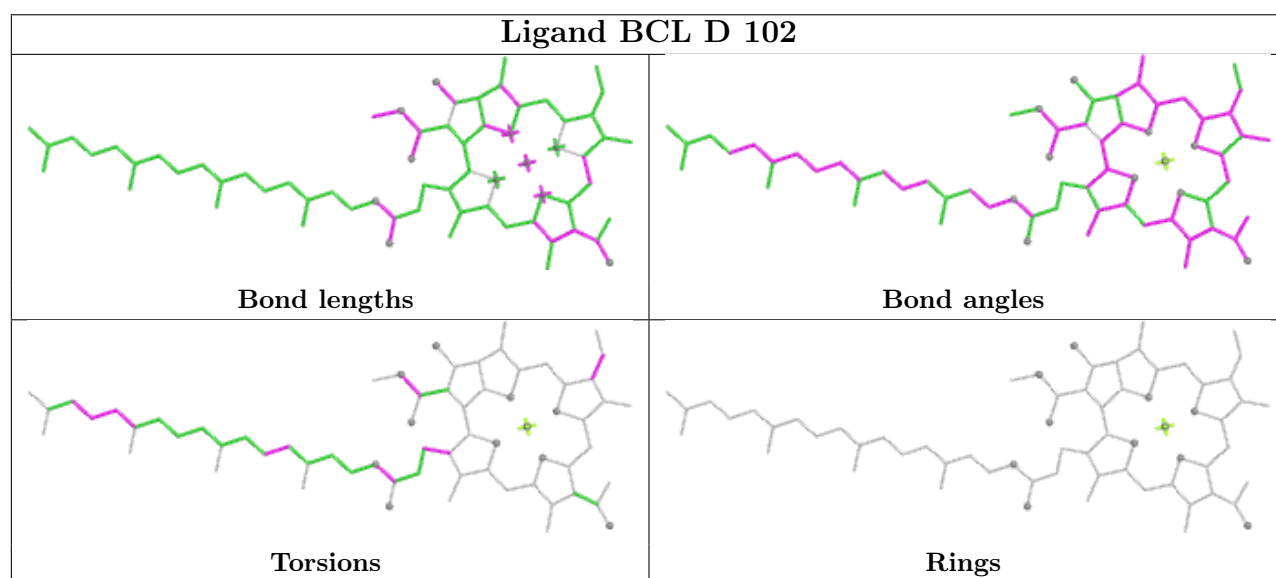
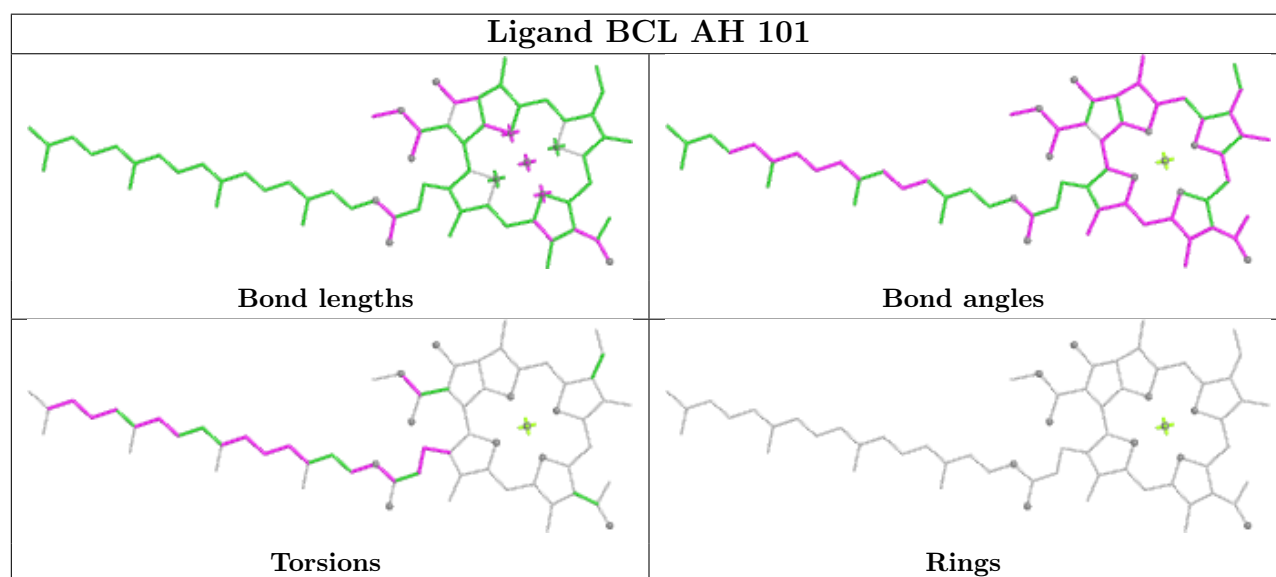
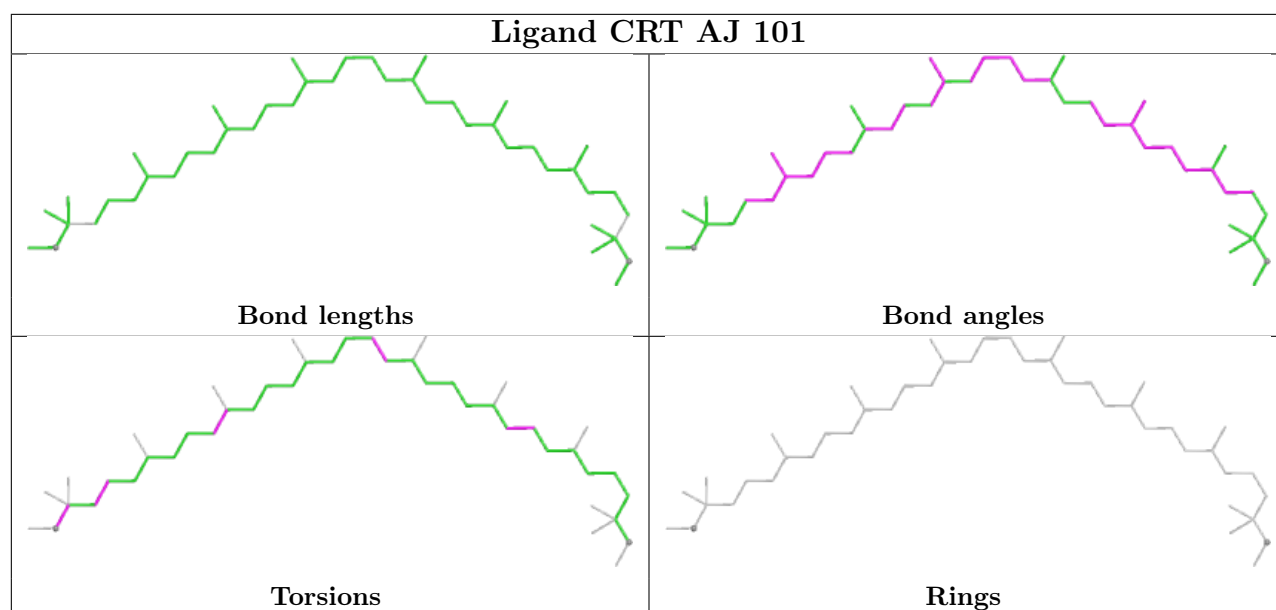
Ligand BPH y 402

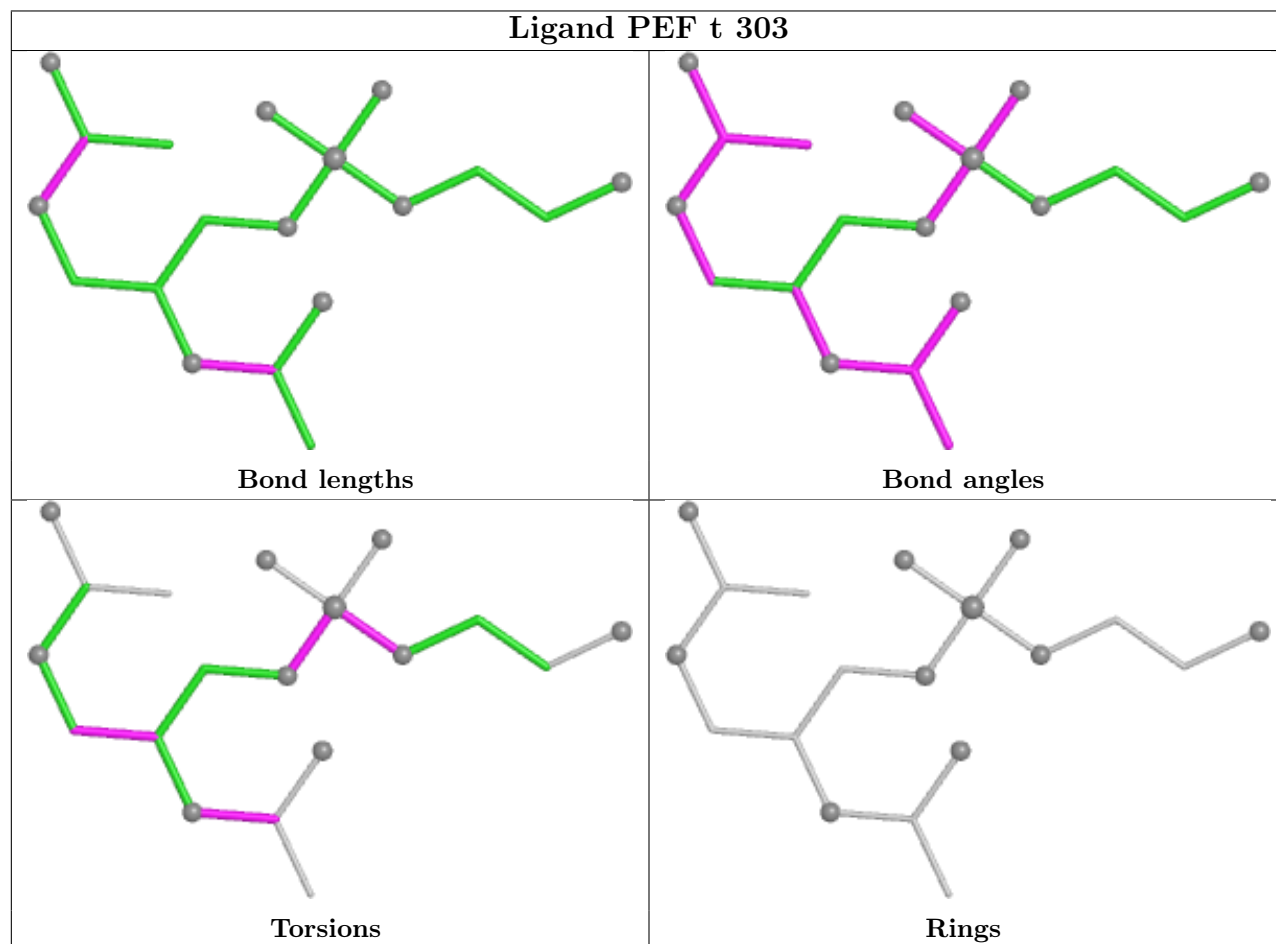
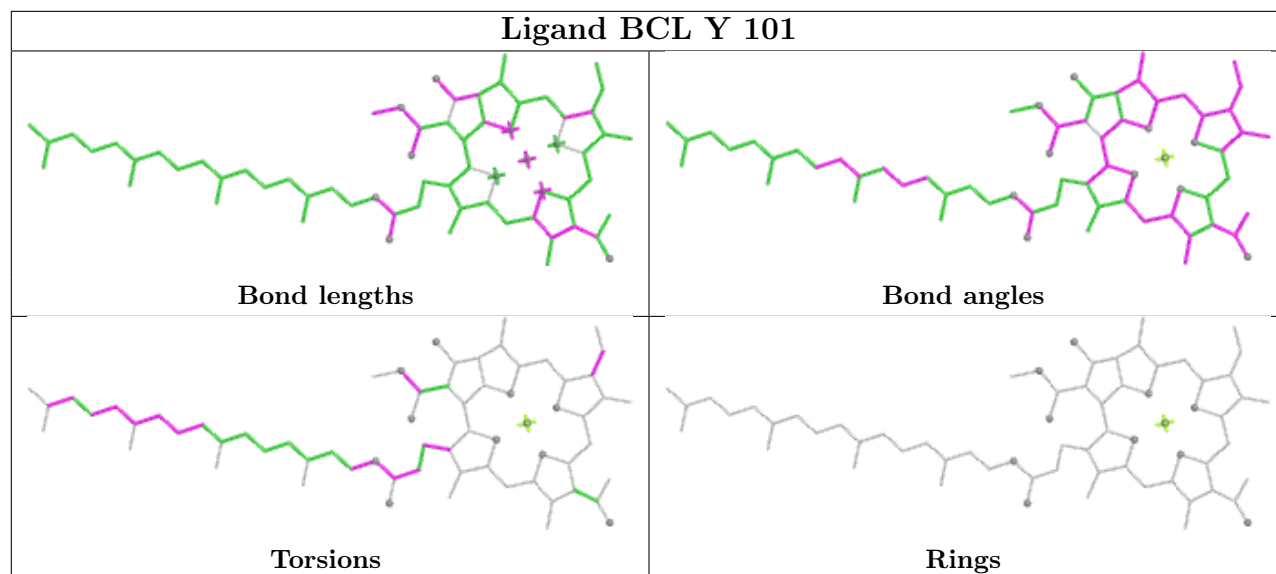


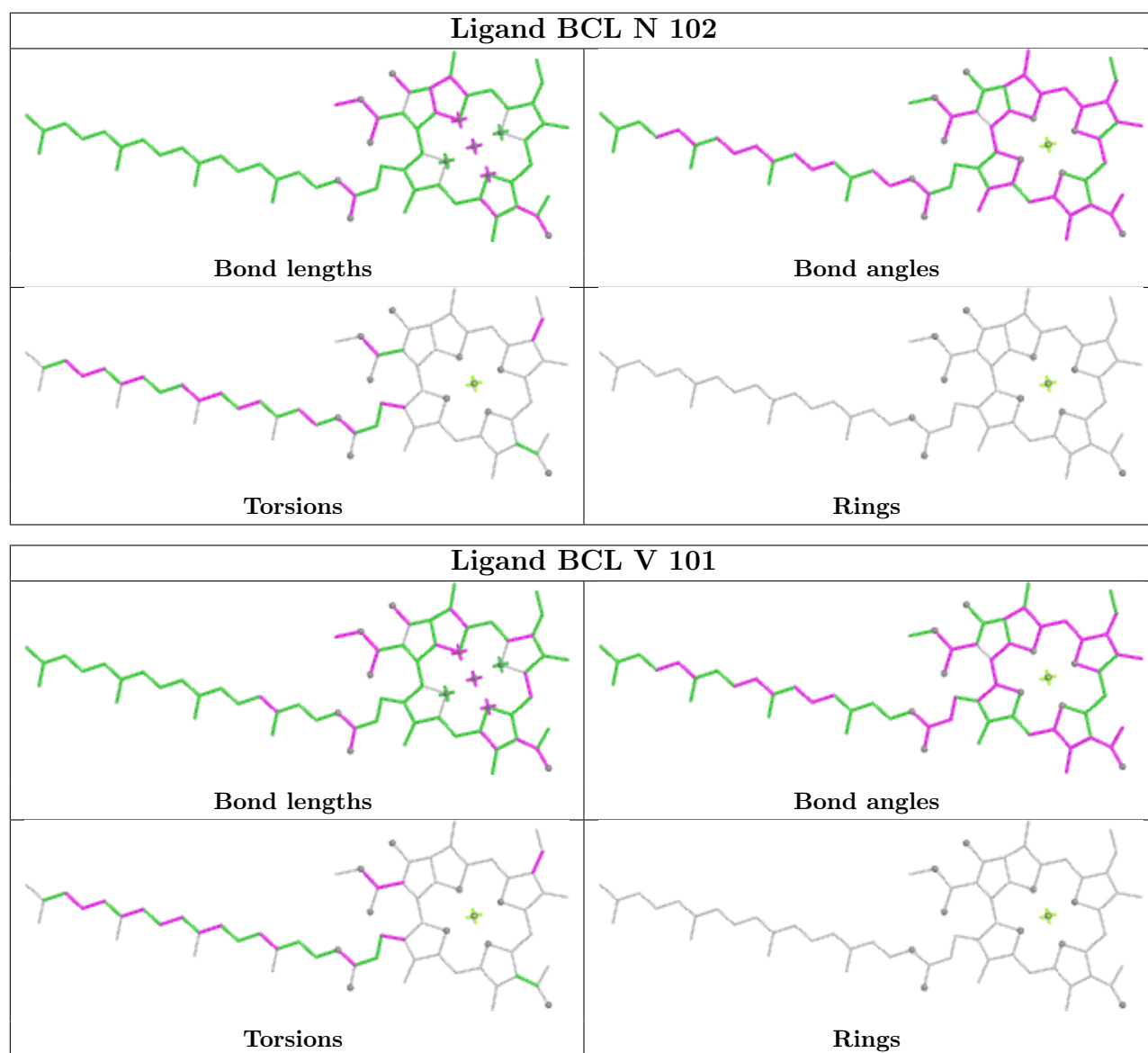
Ligand CRT P 102

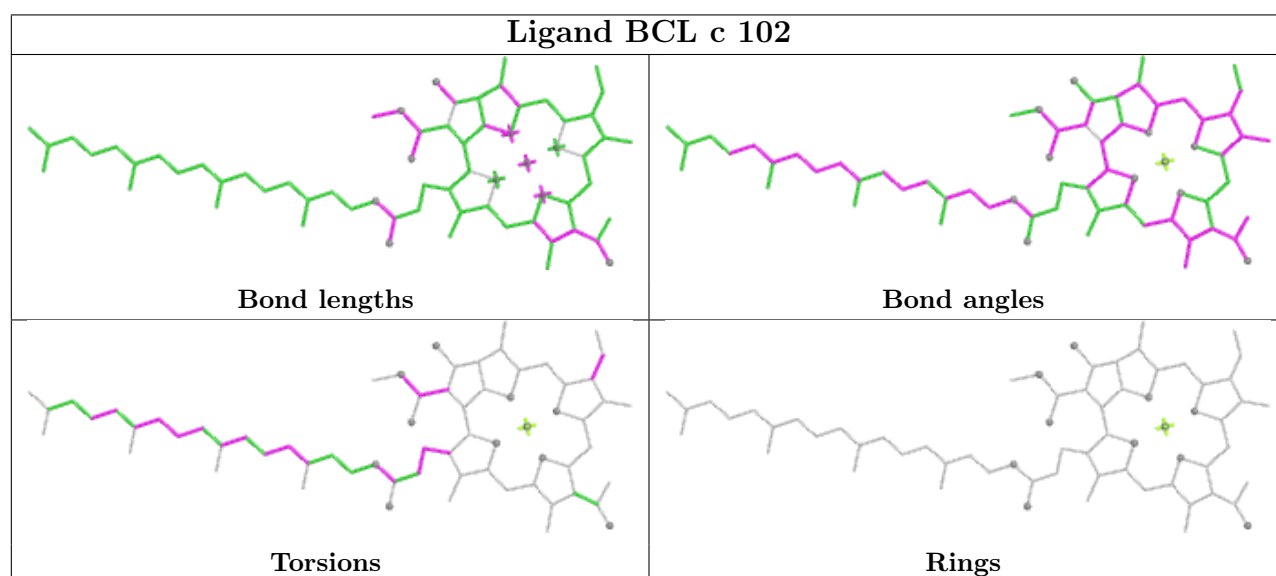
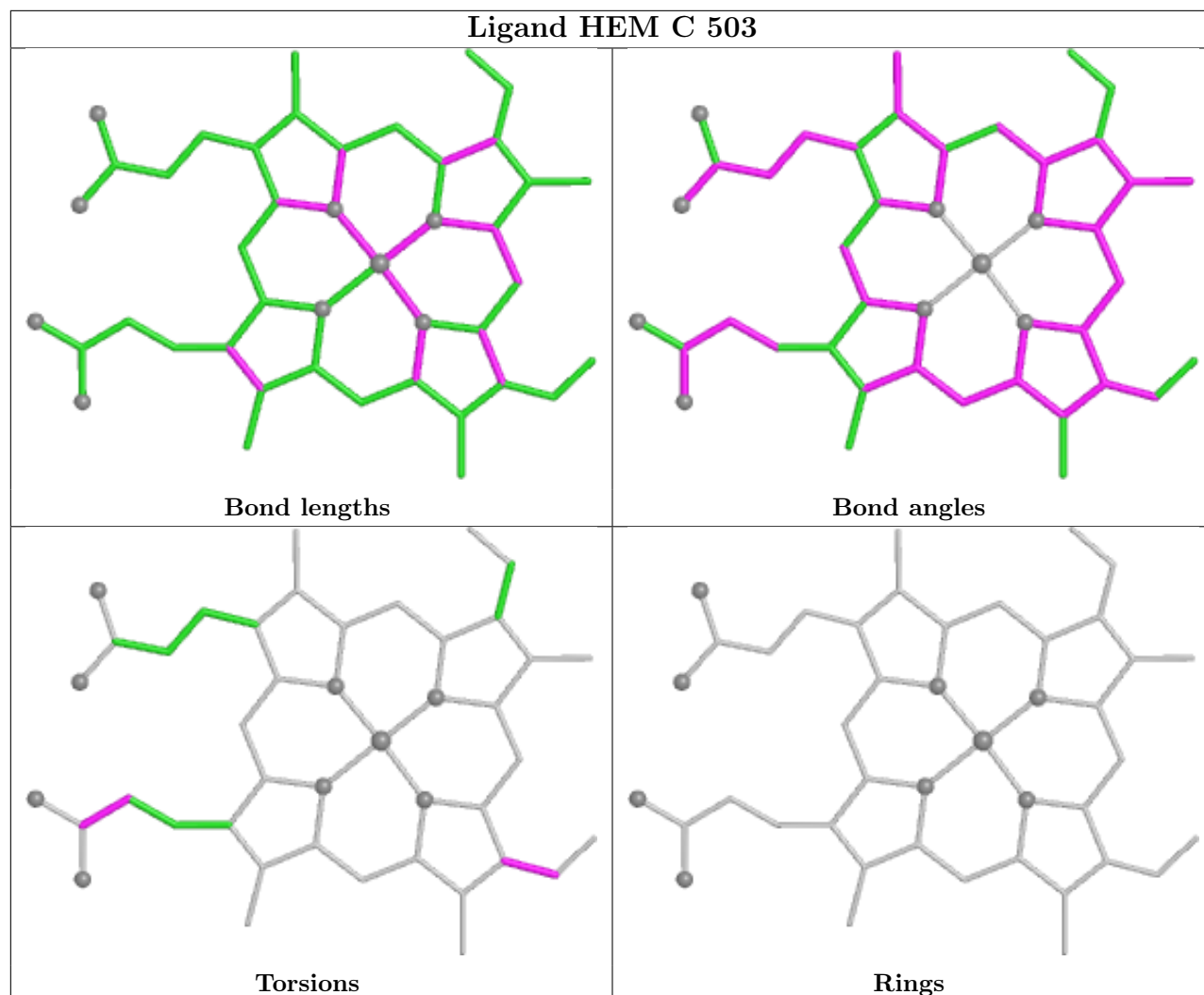


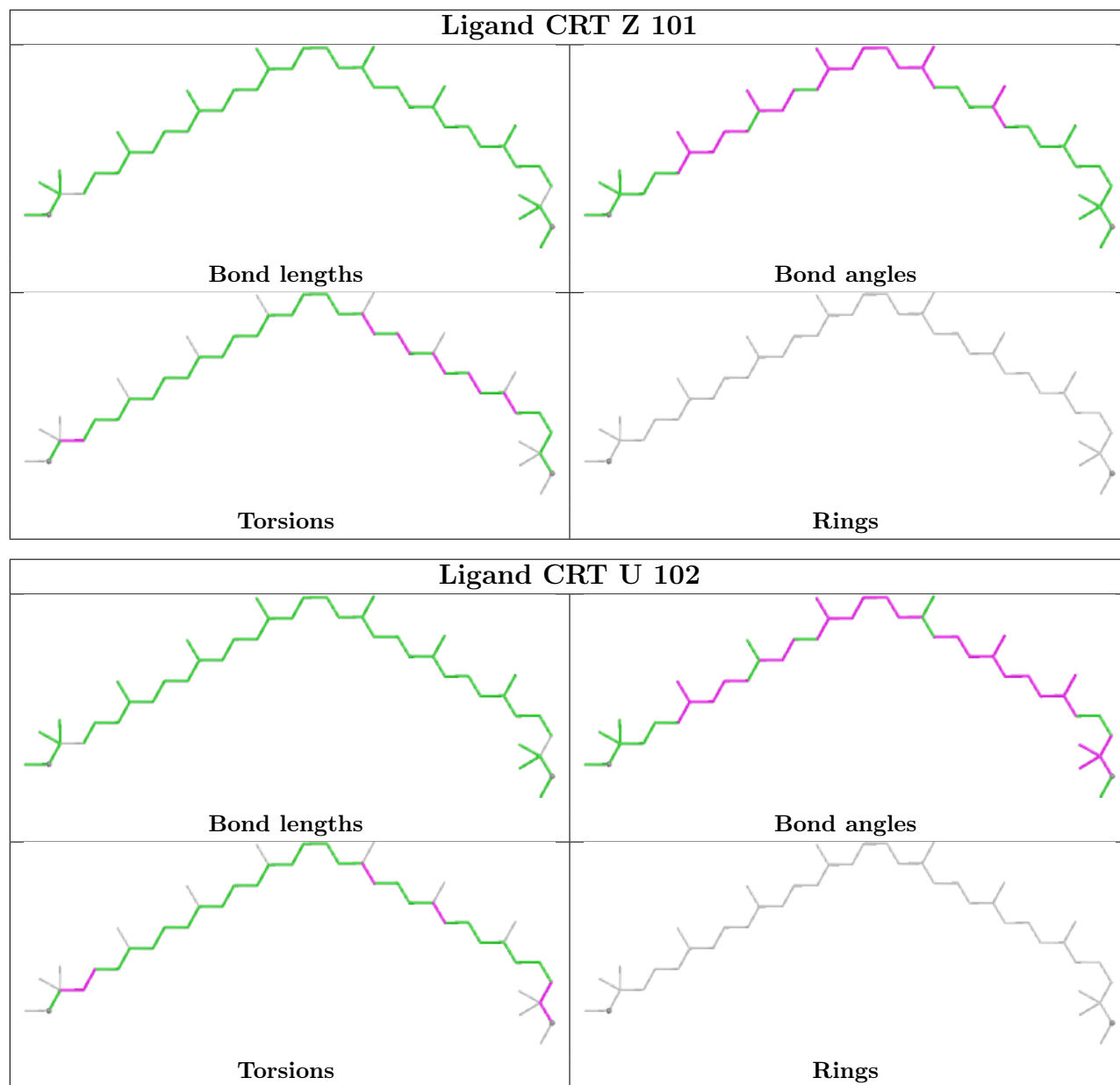


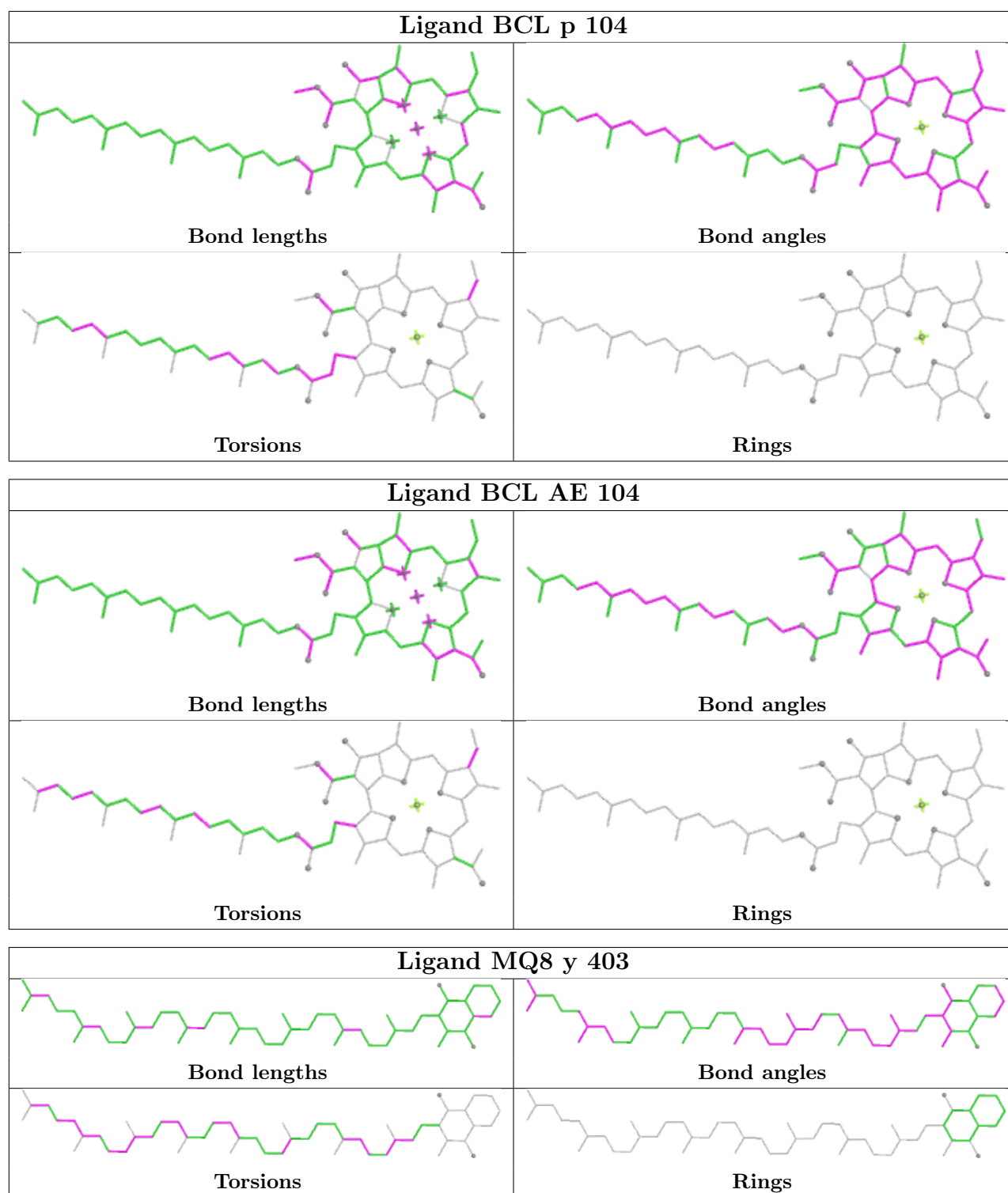


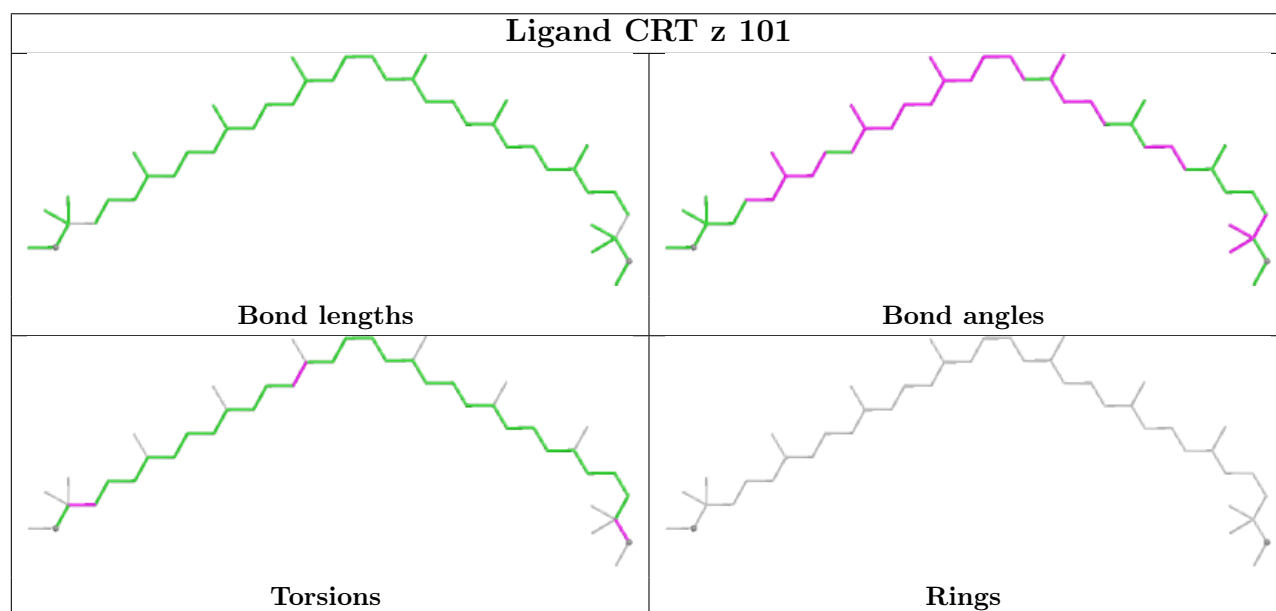
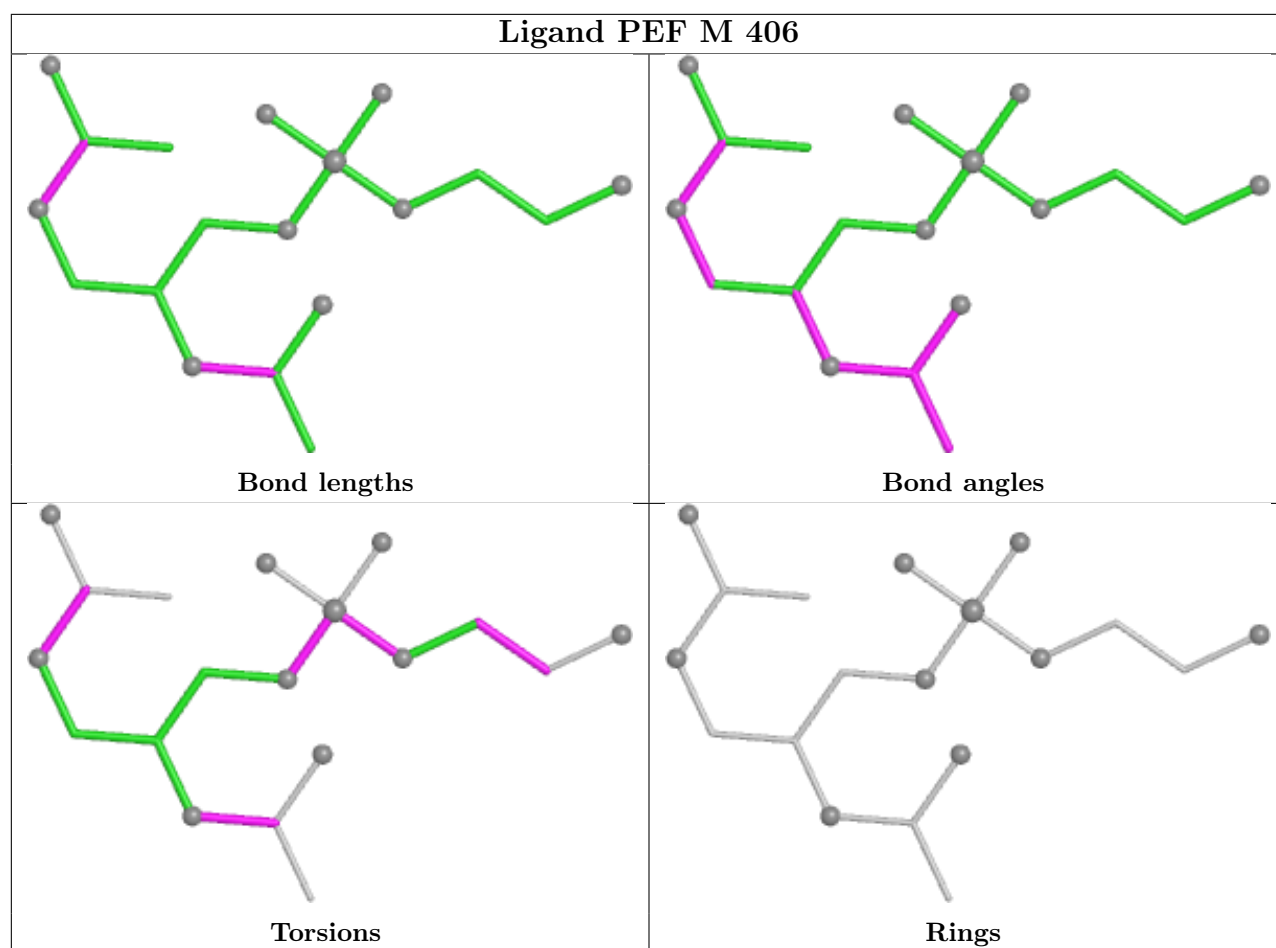


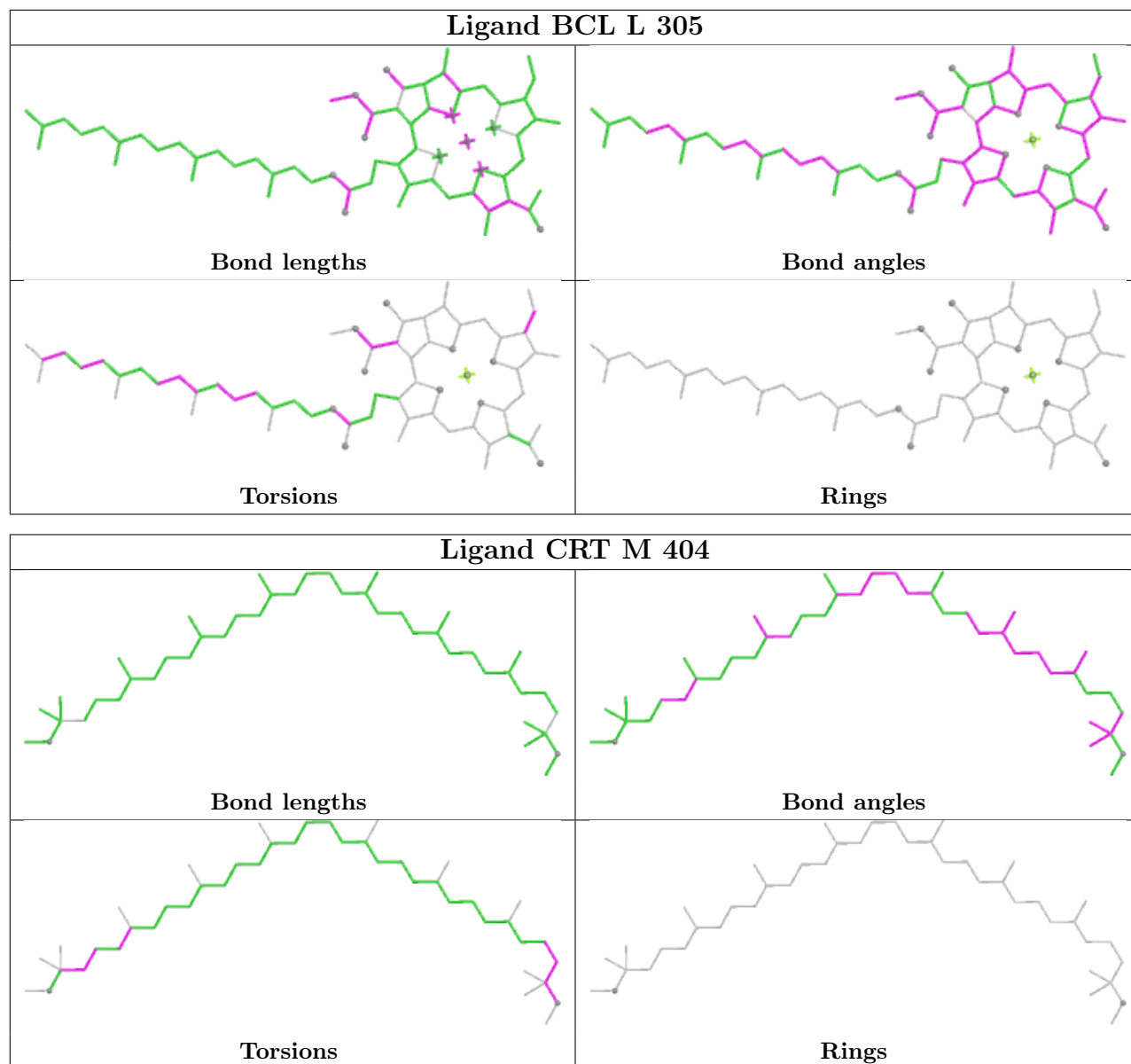


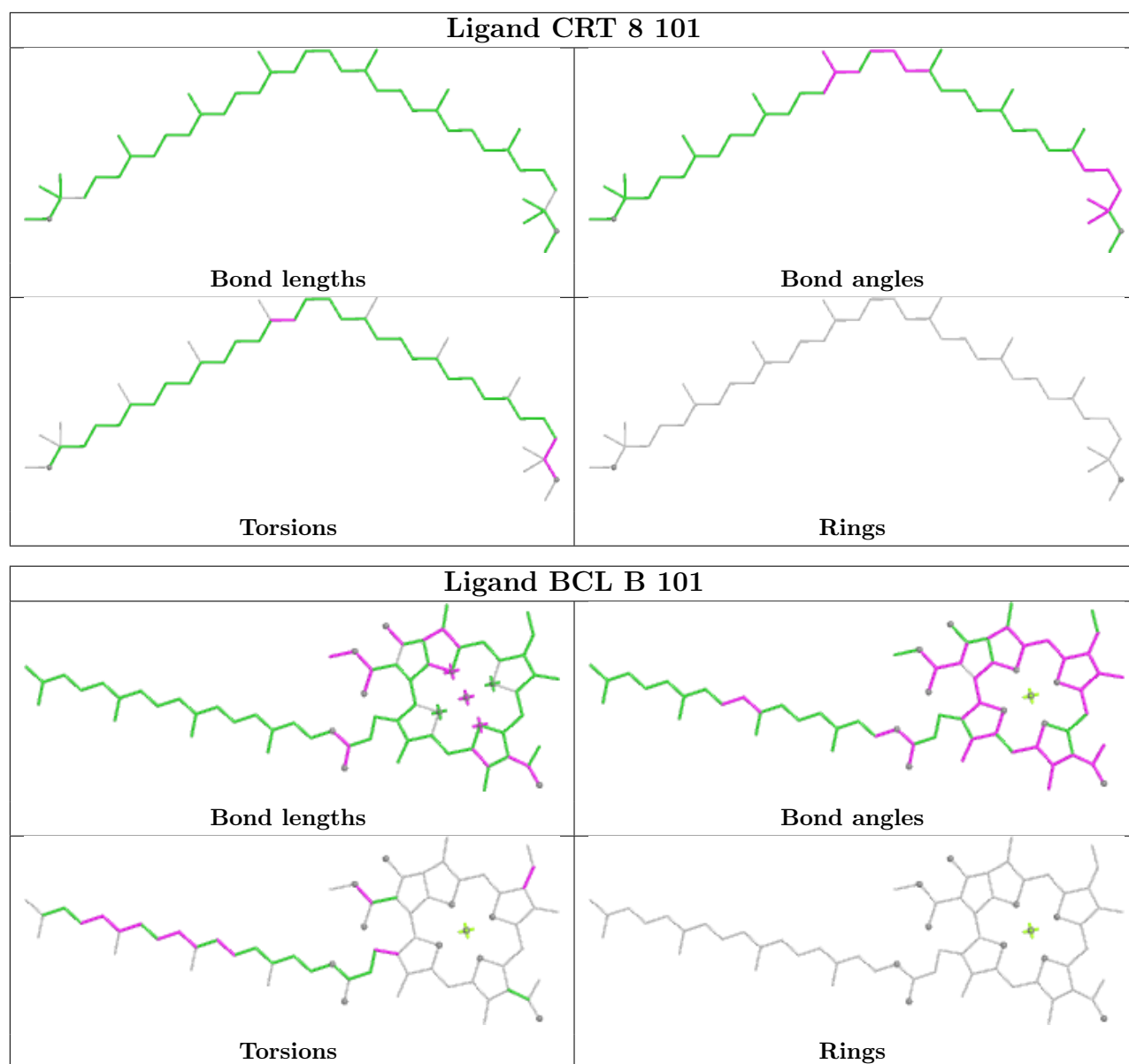




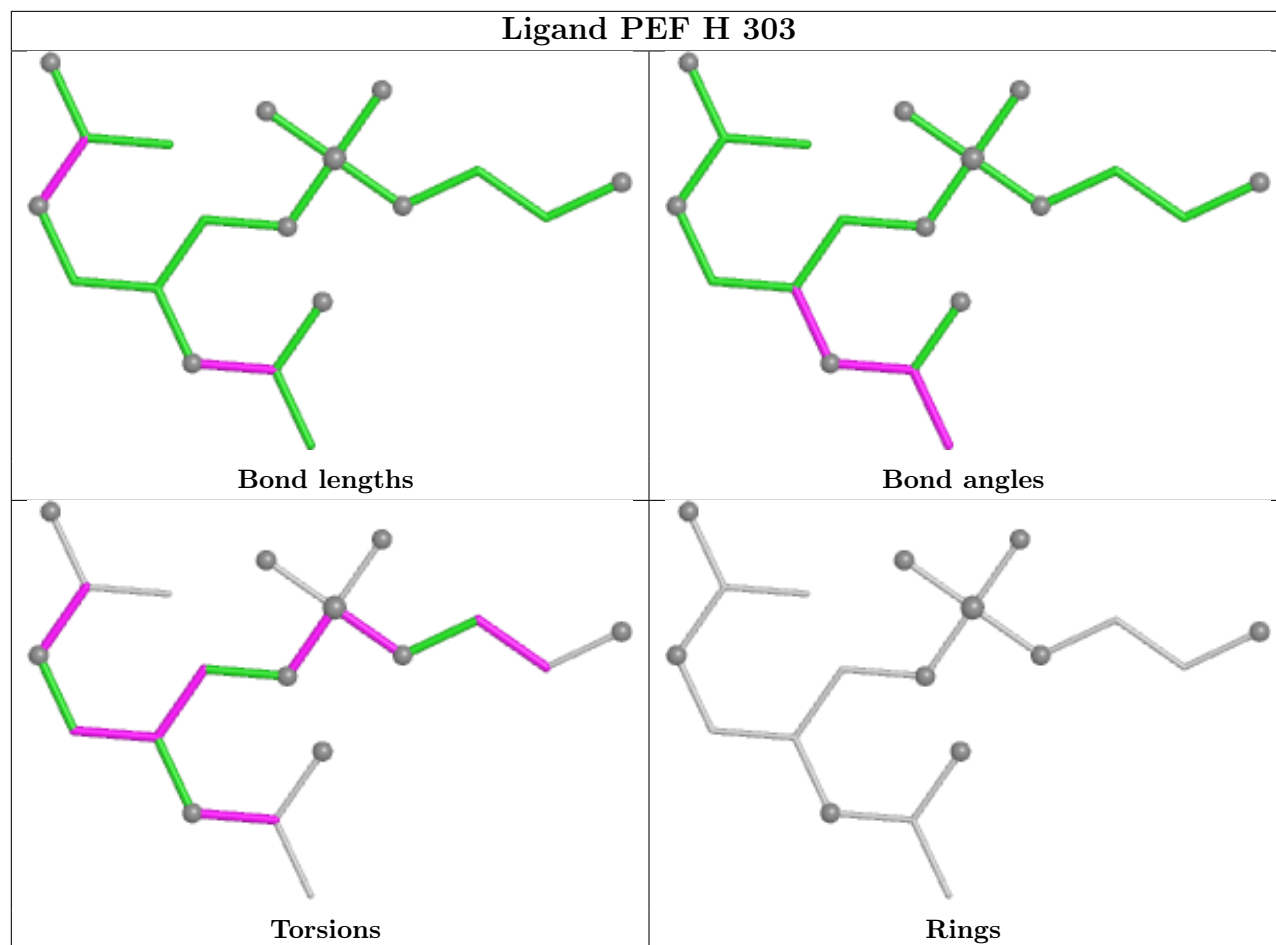




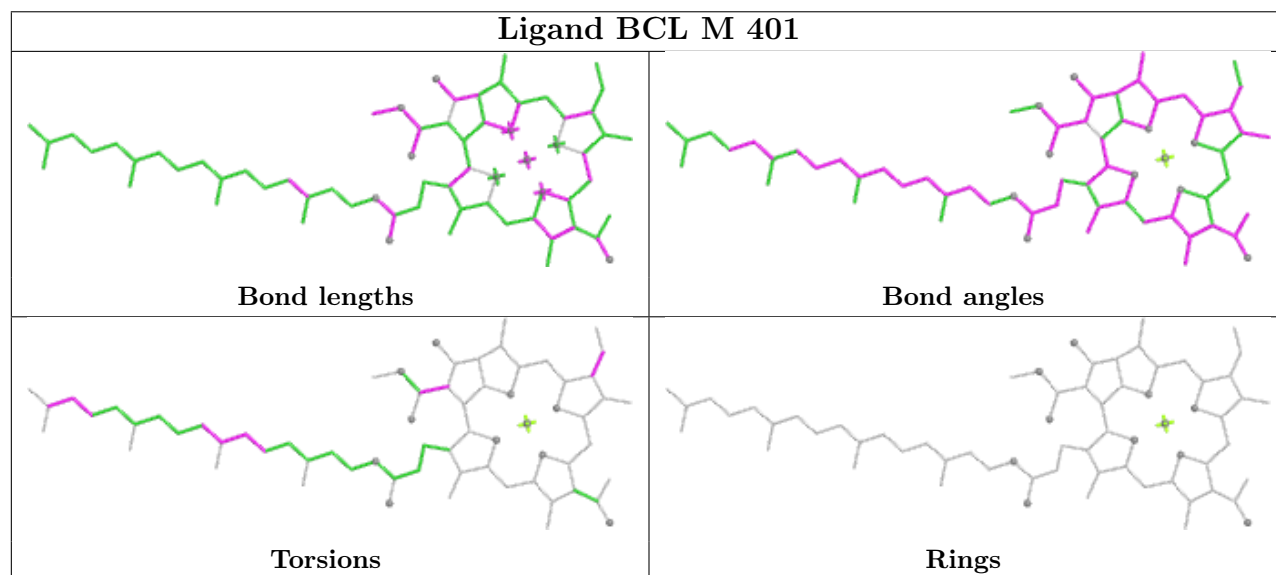


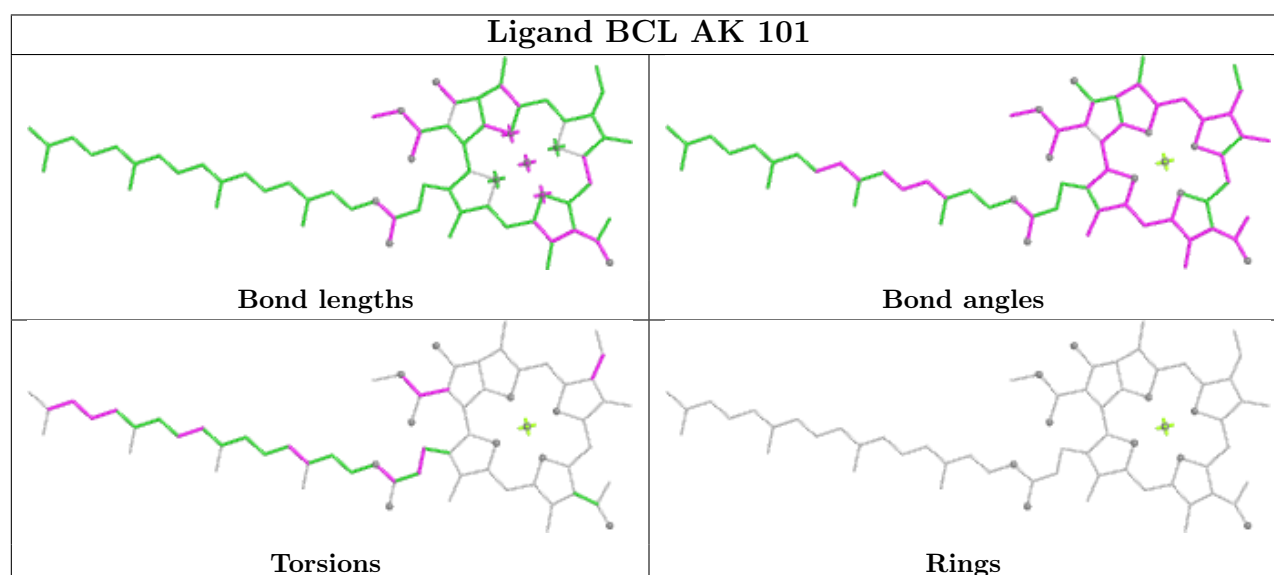
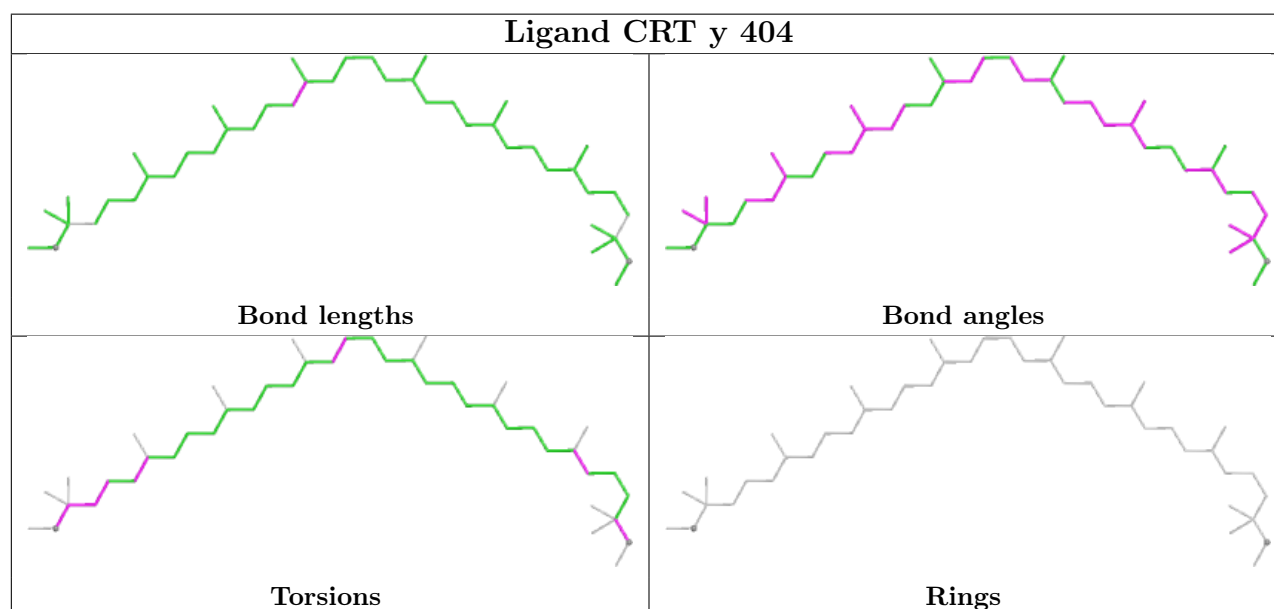
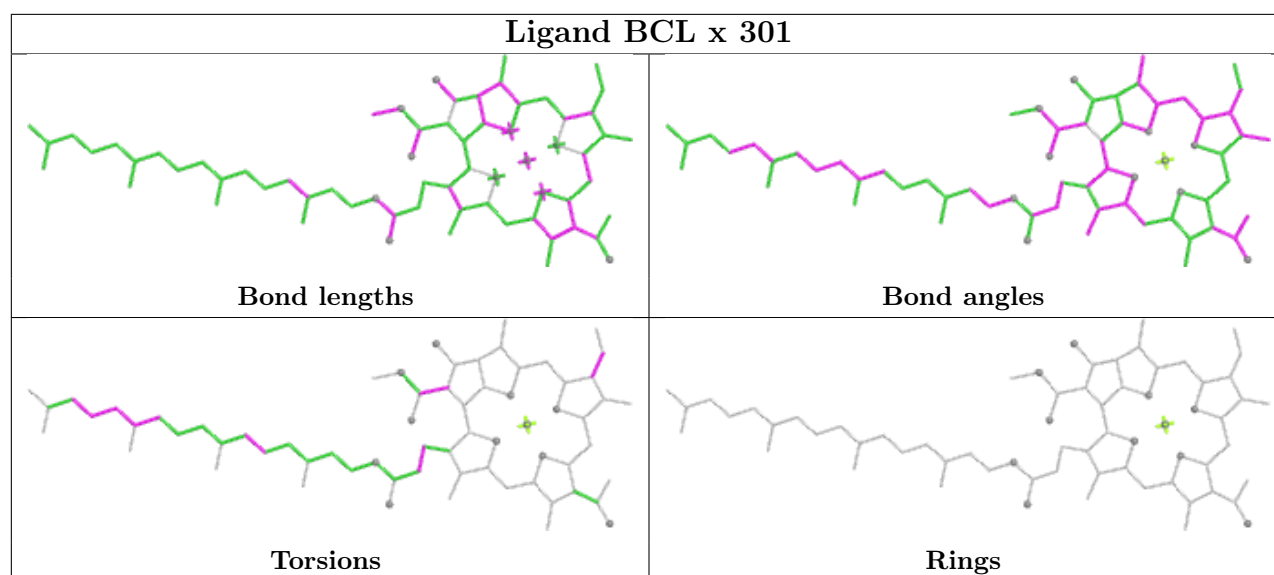


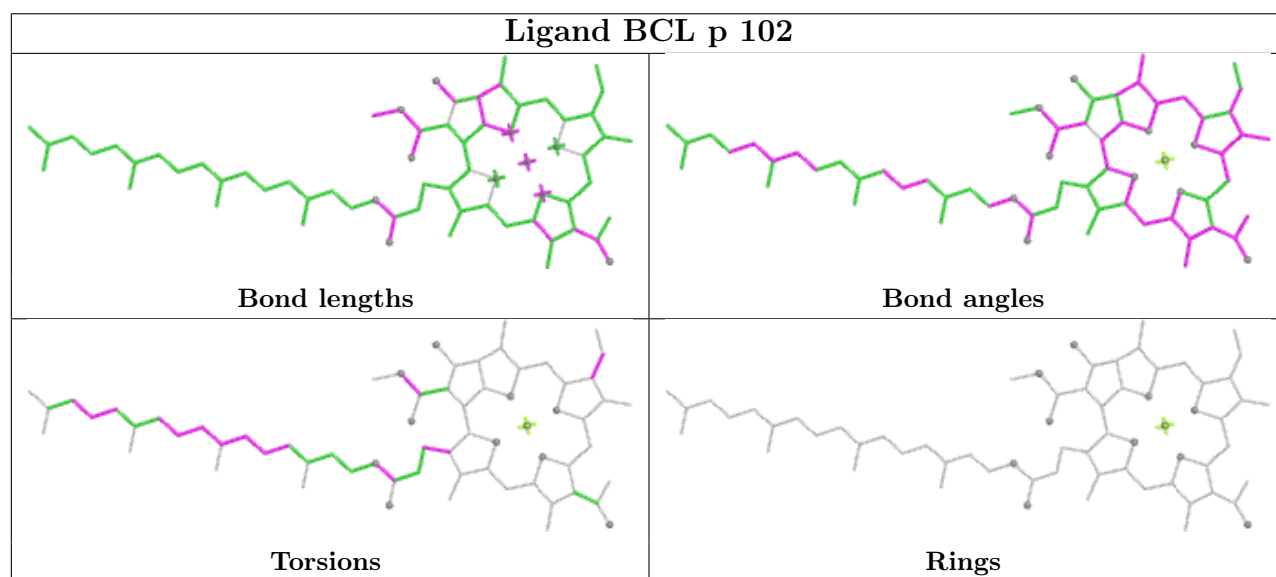
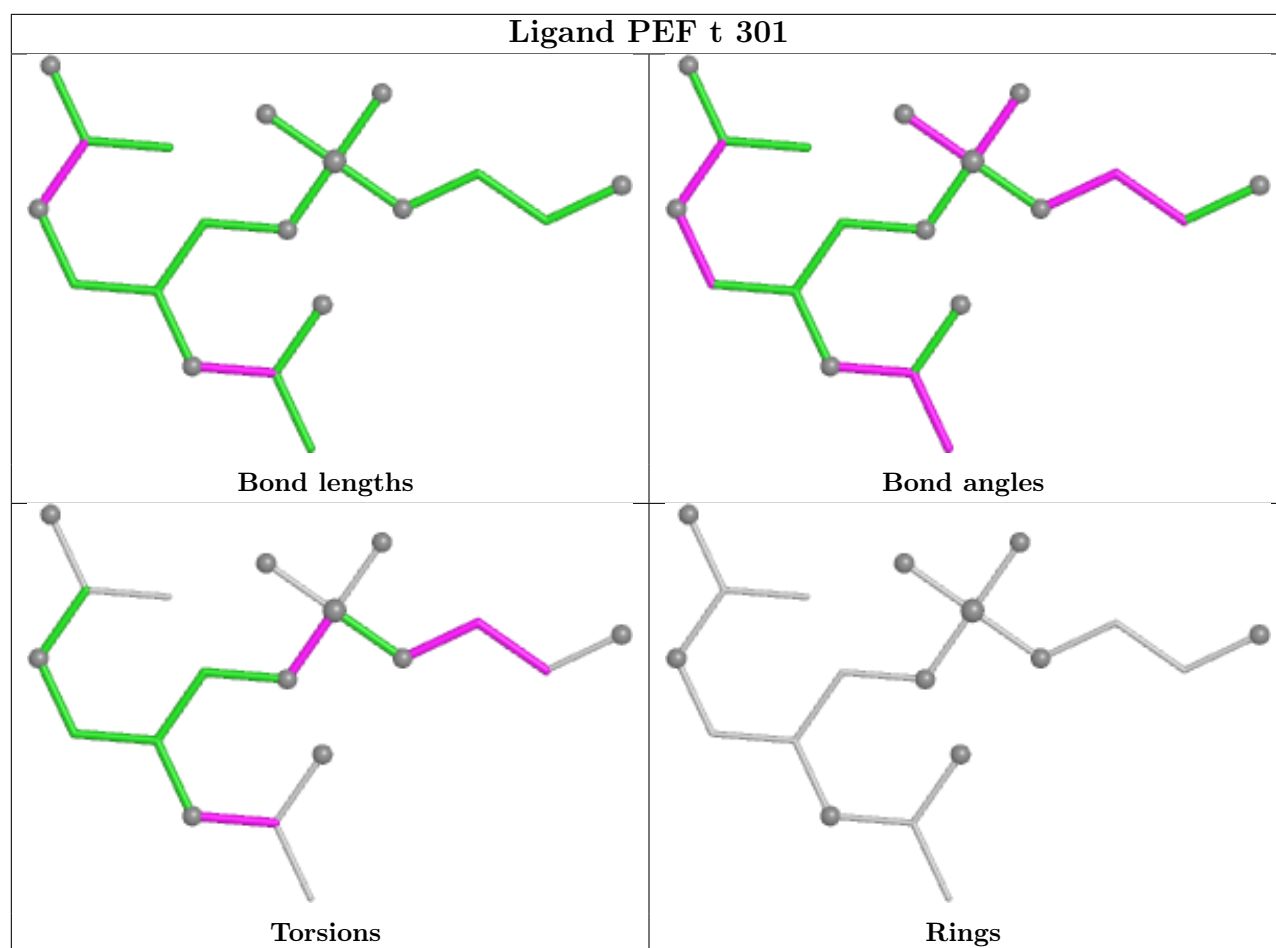
Ligand PEF H 303

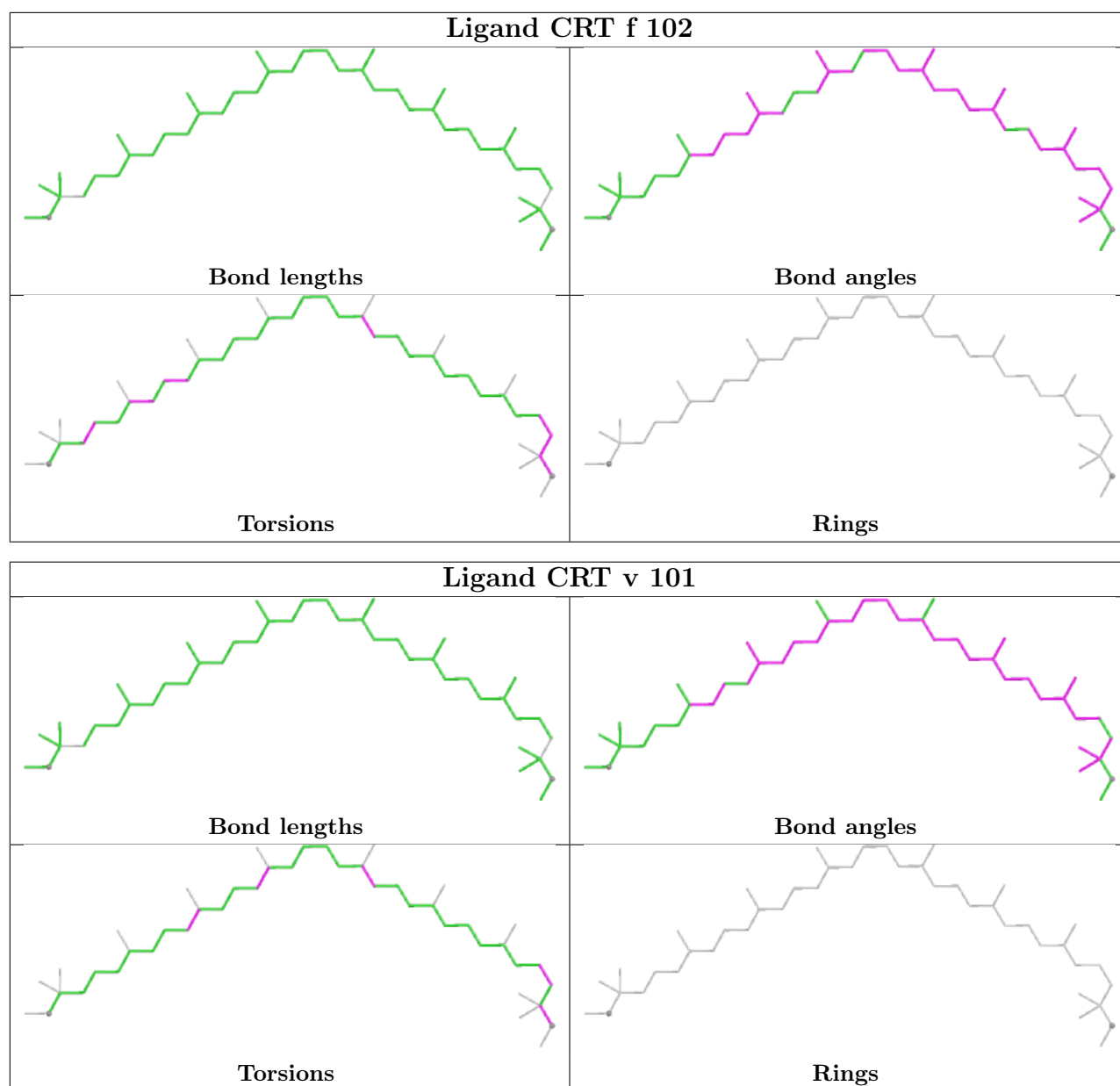


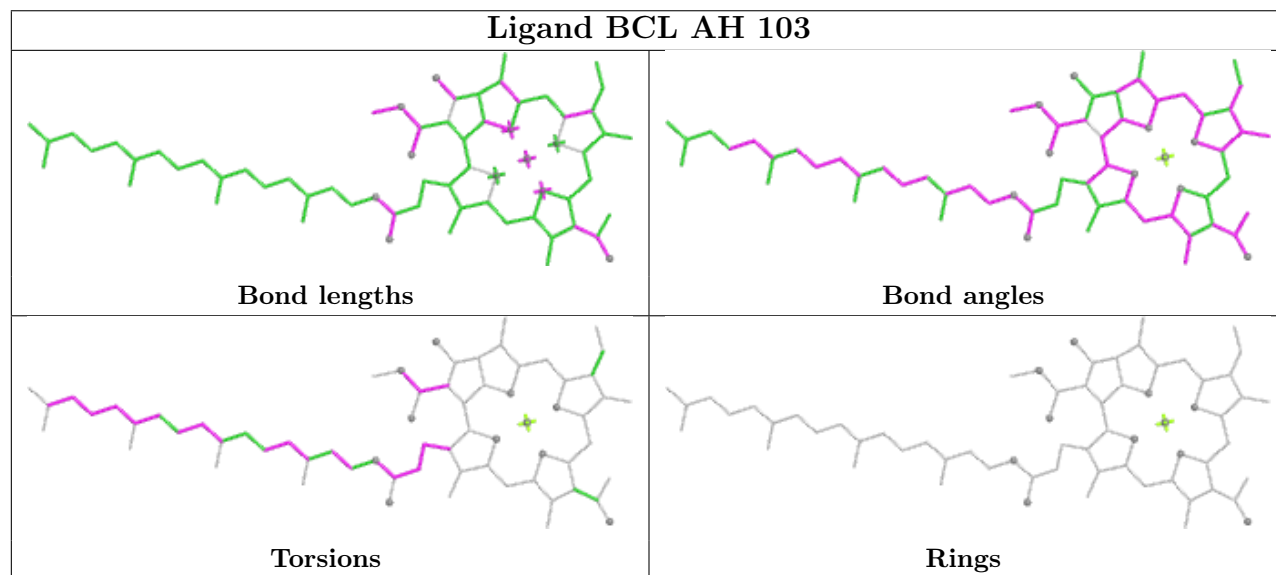
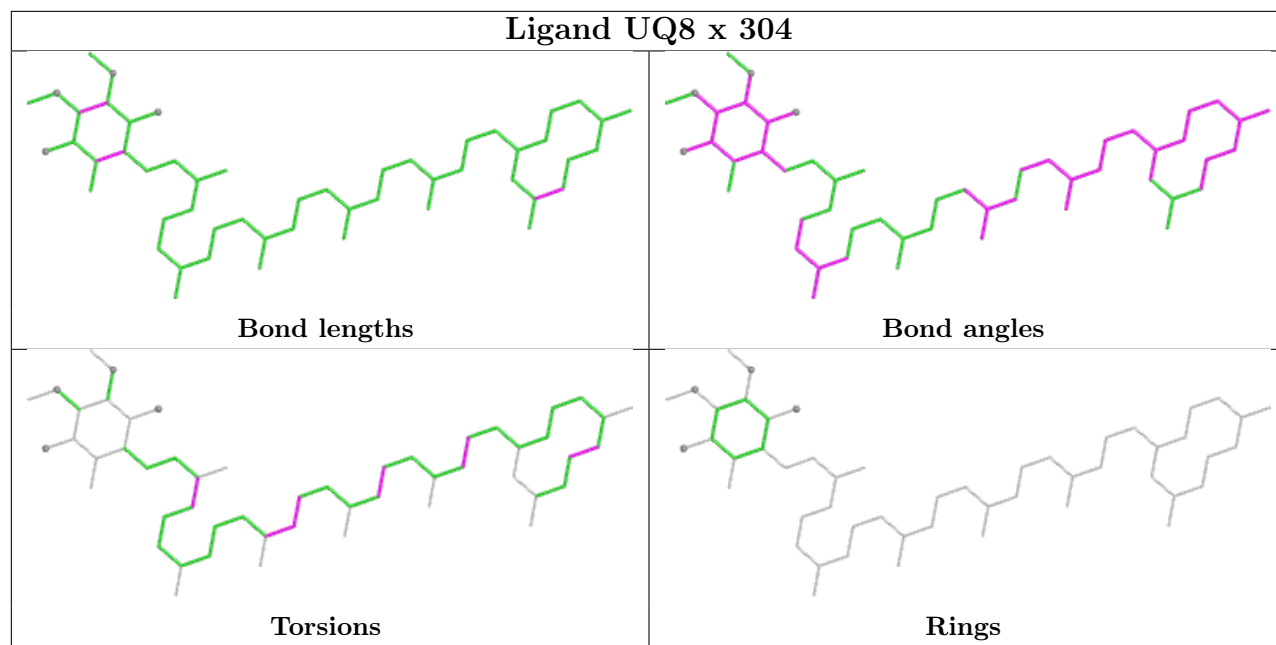
Ligand BCL M 401

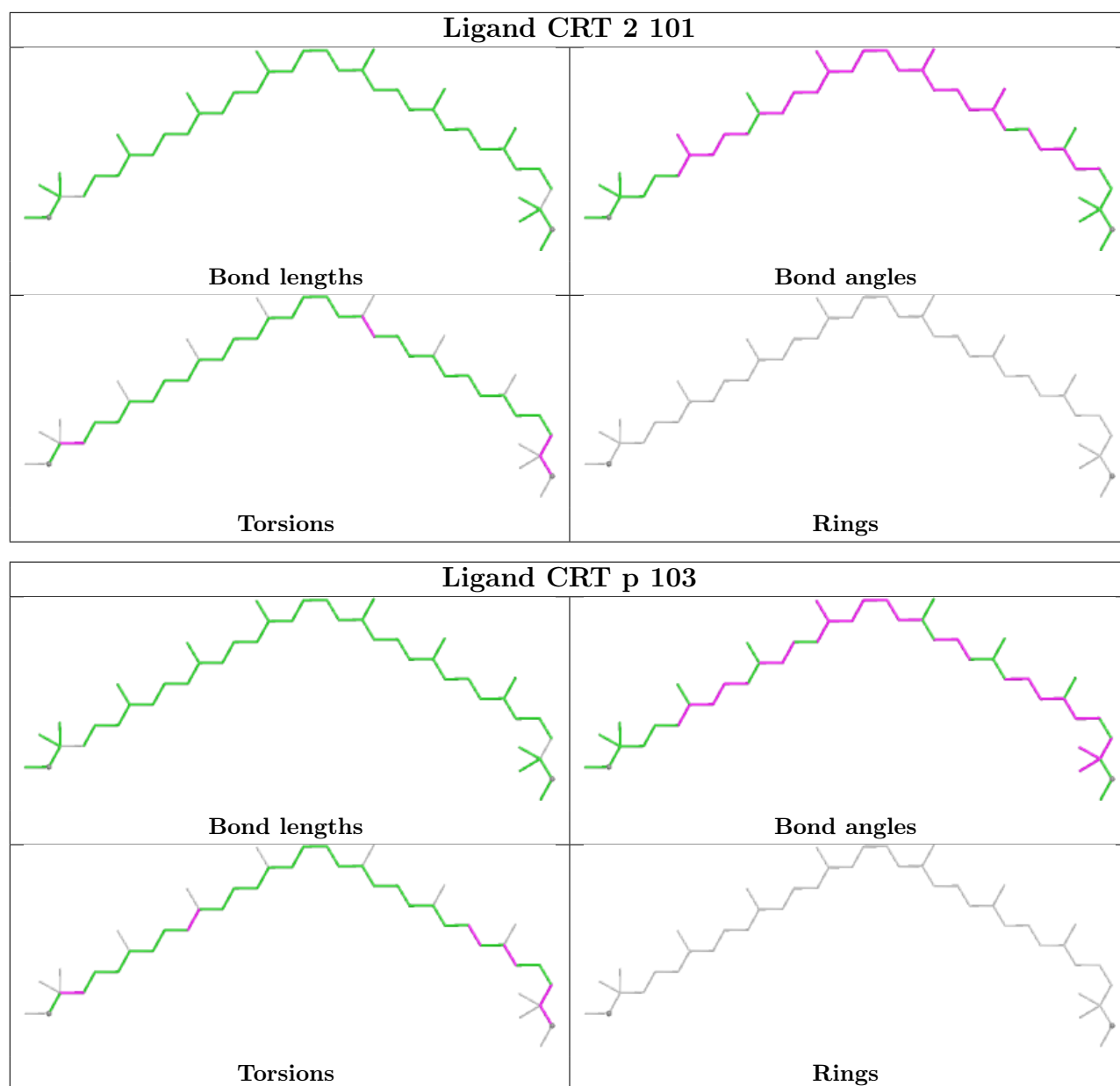


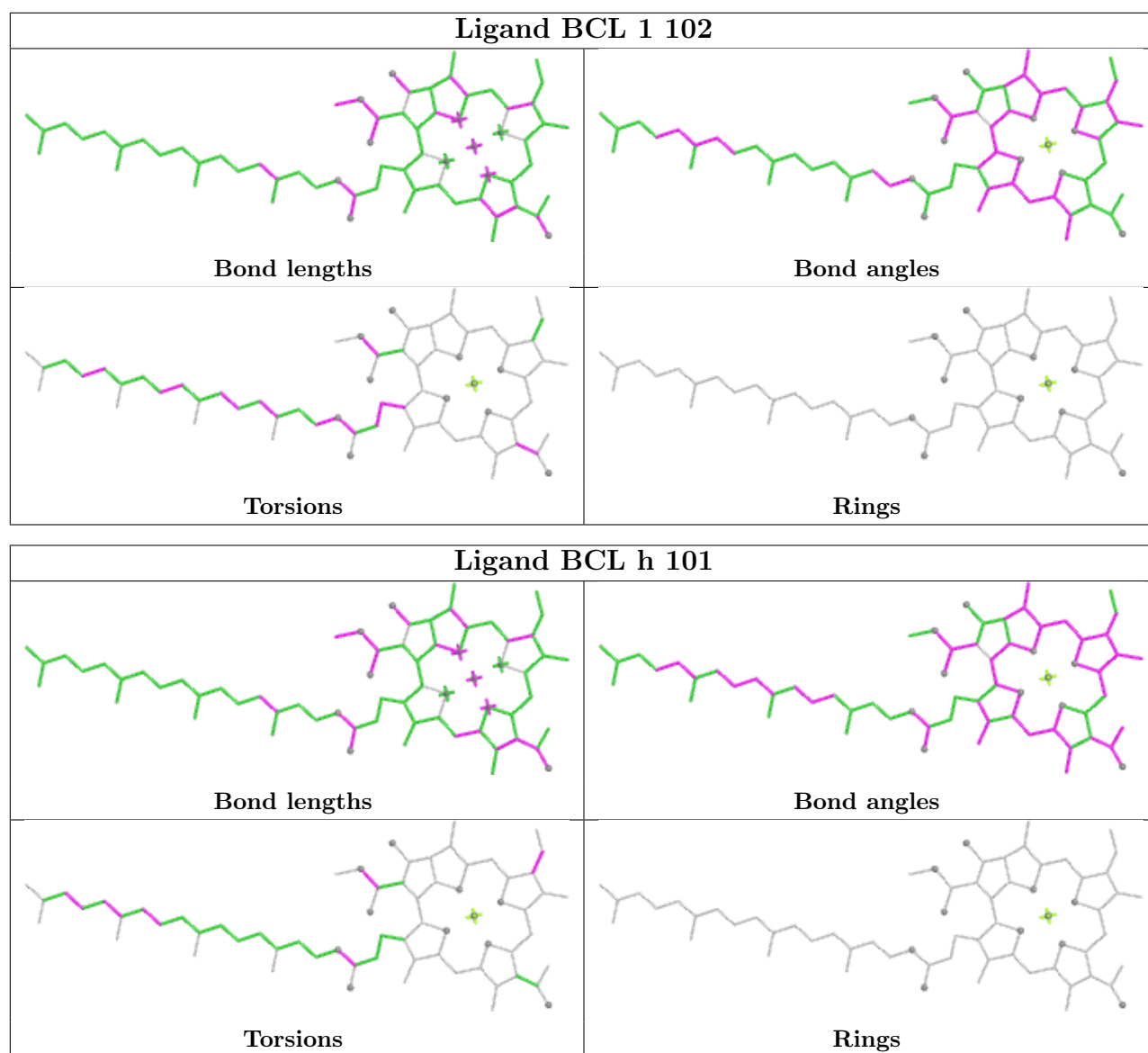


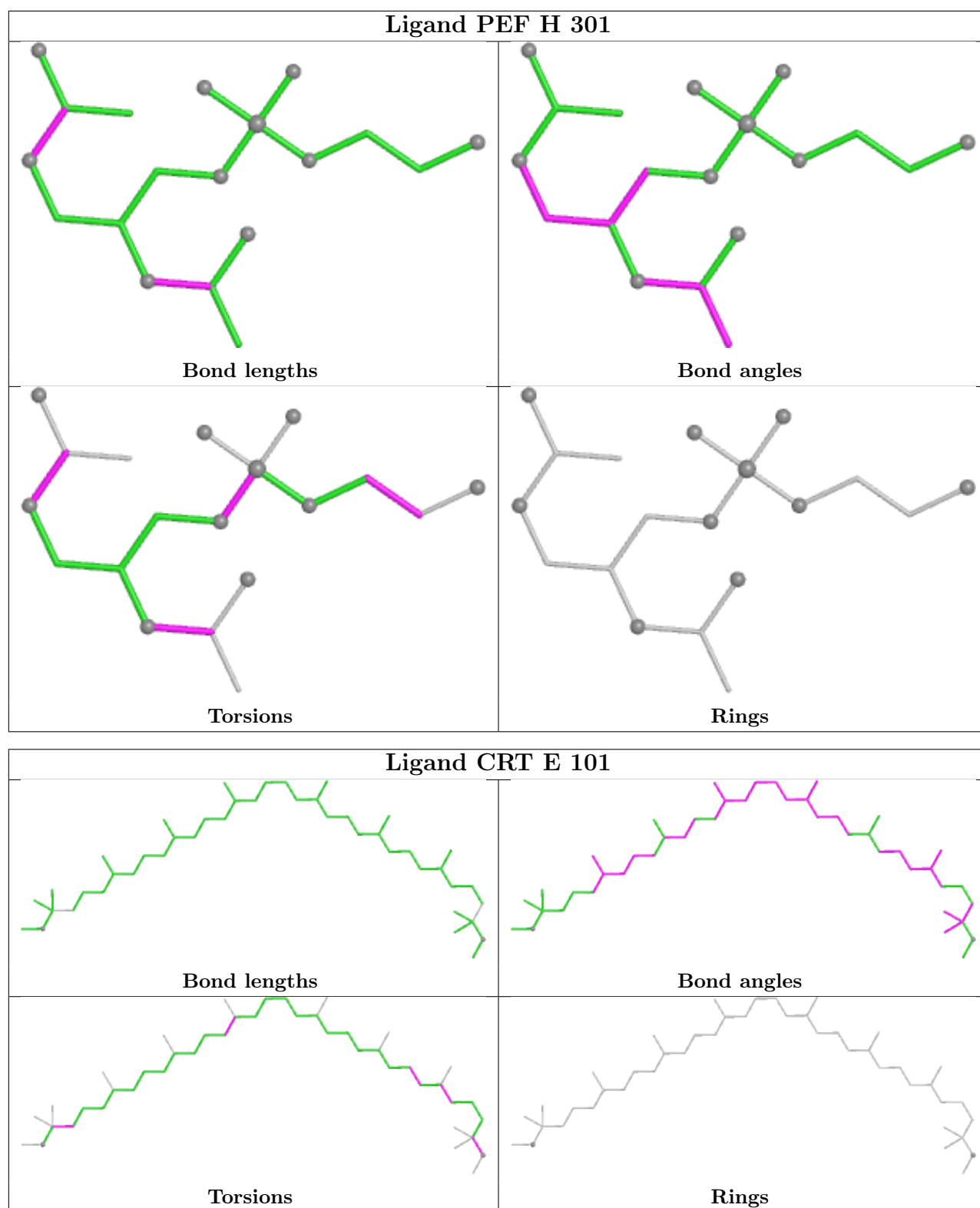


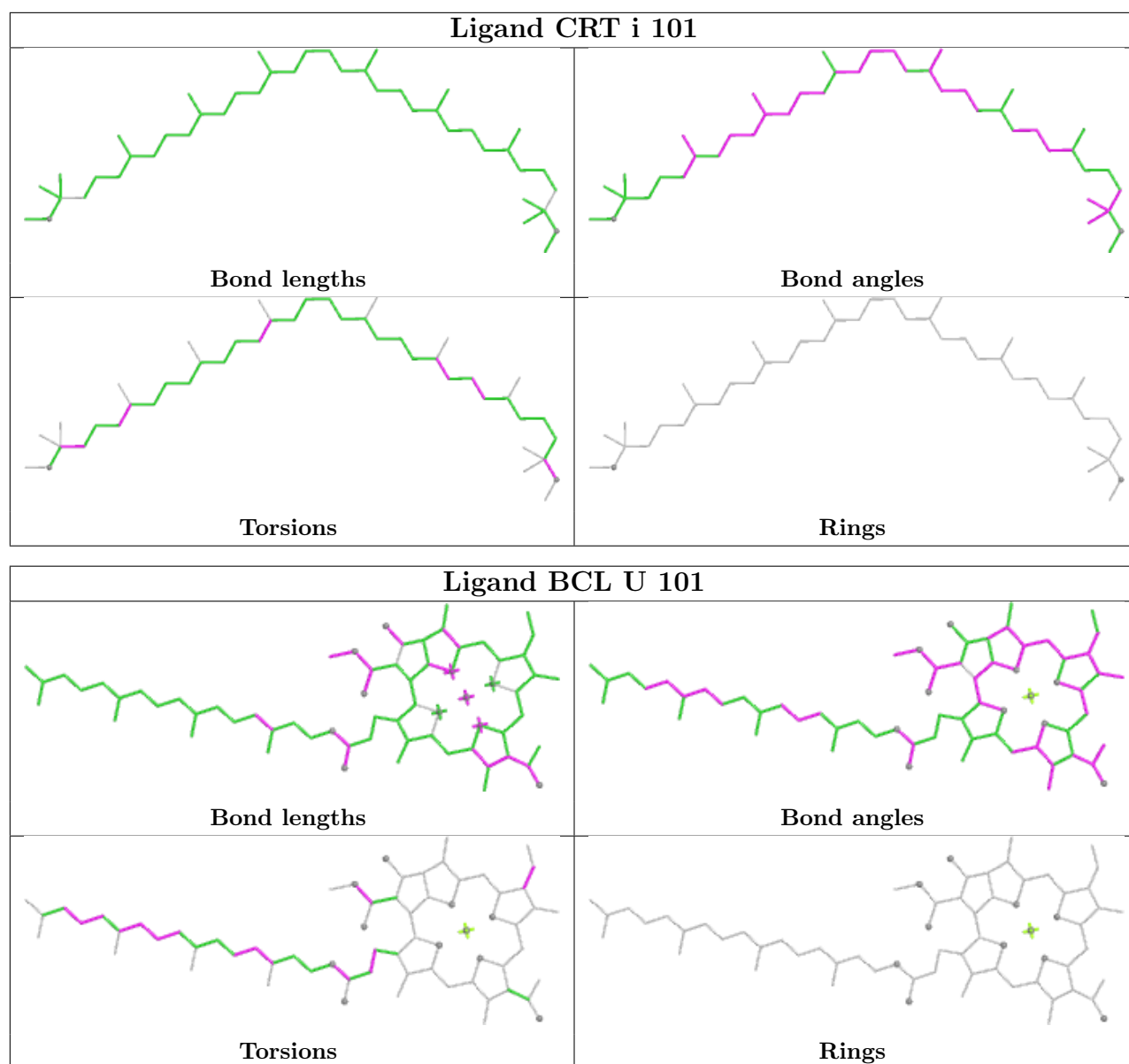




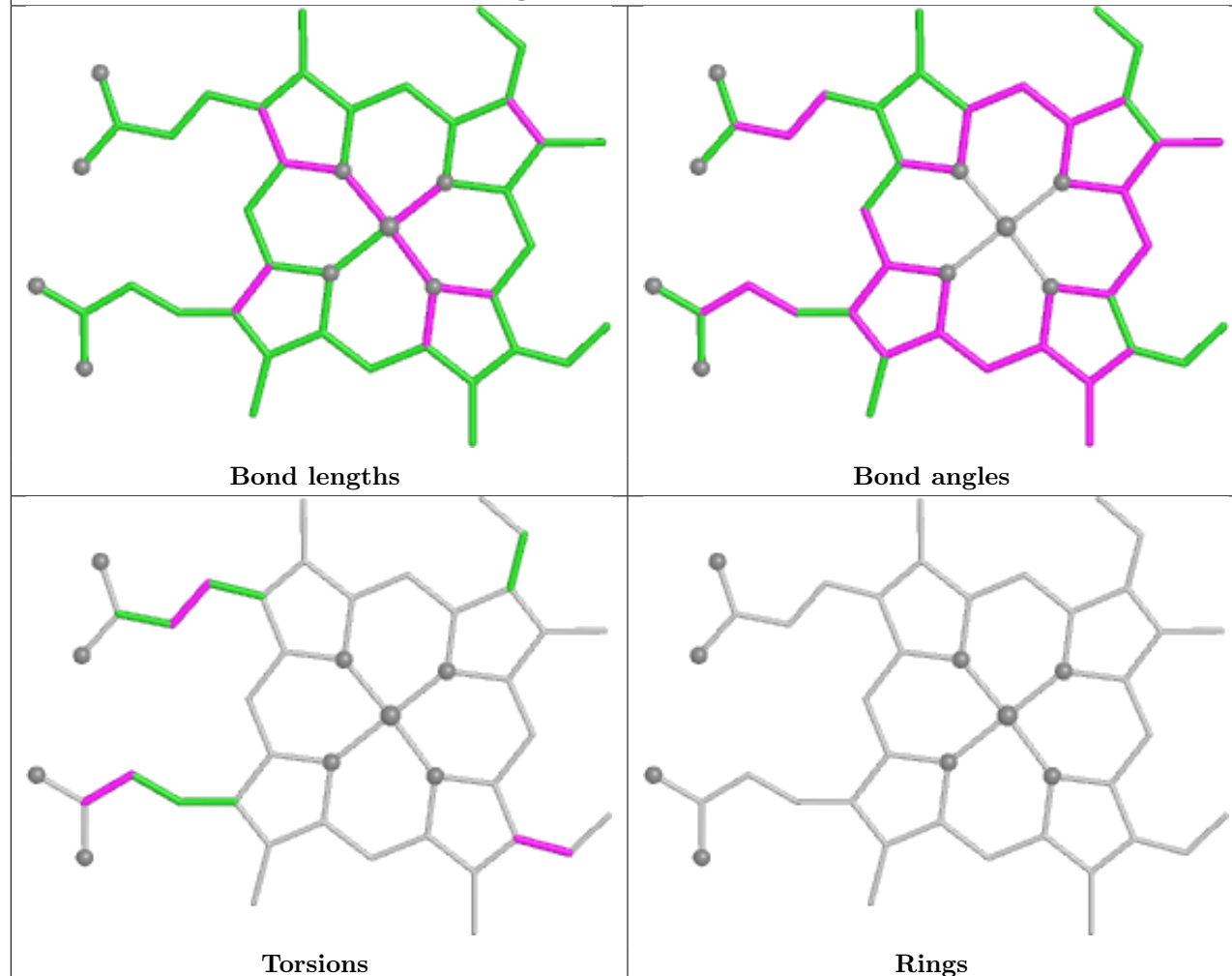




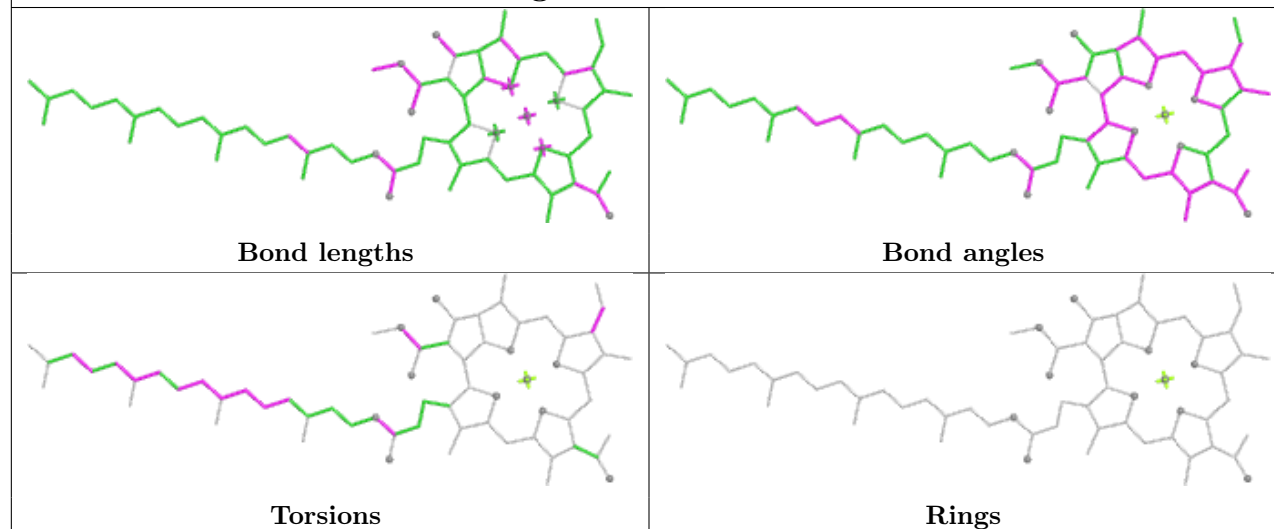


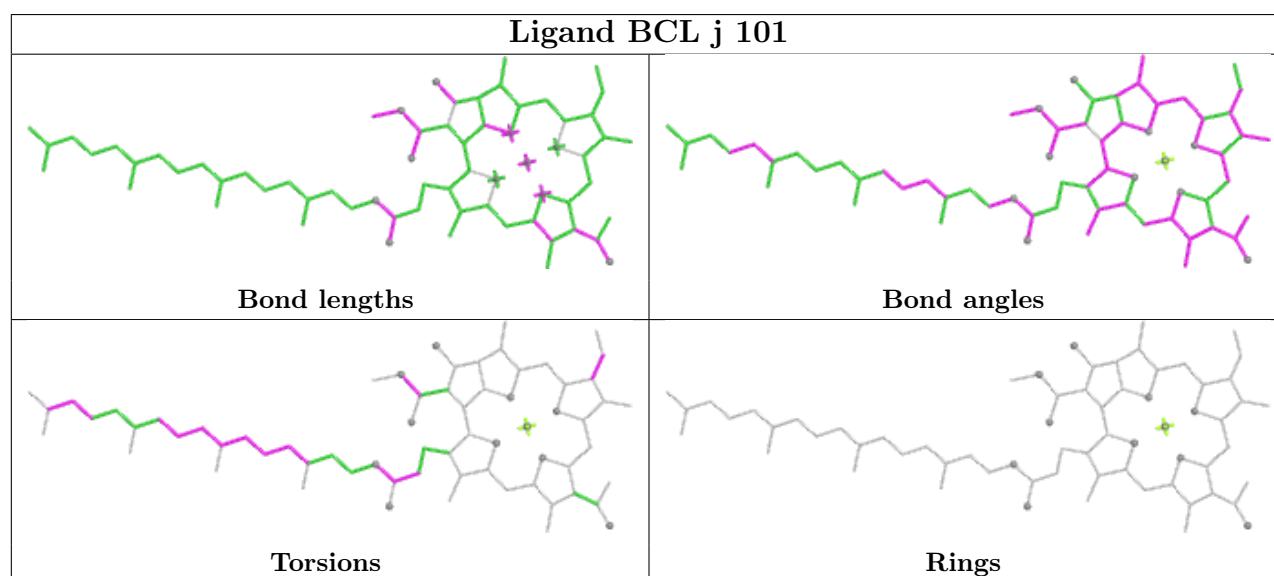
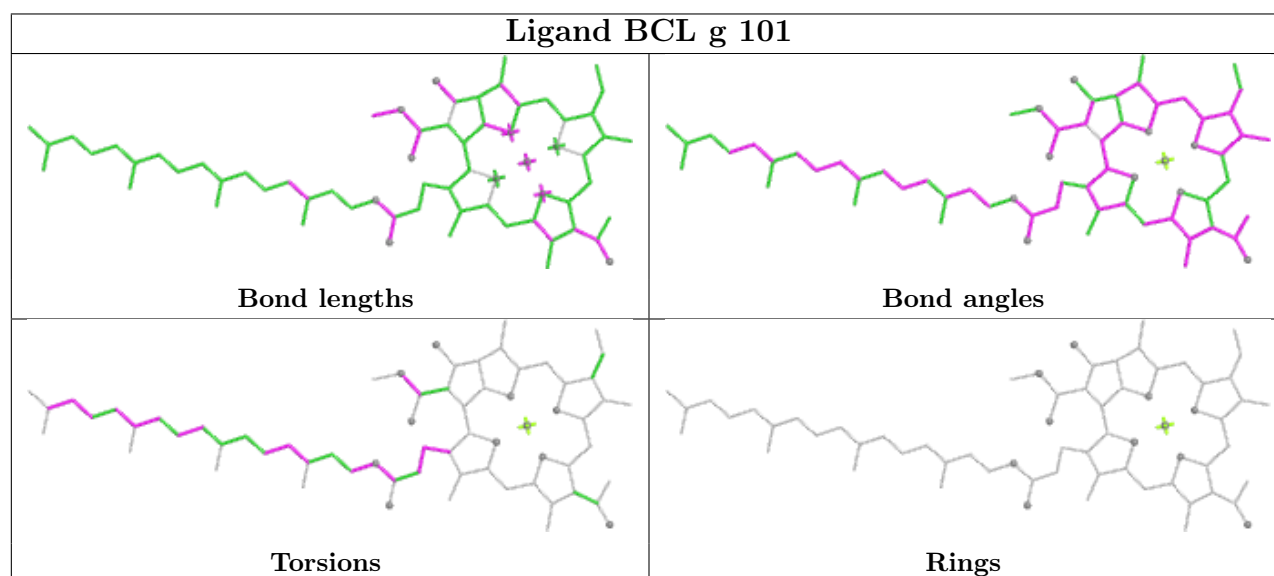
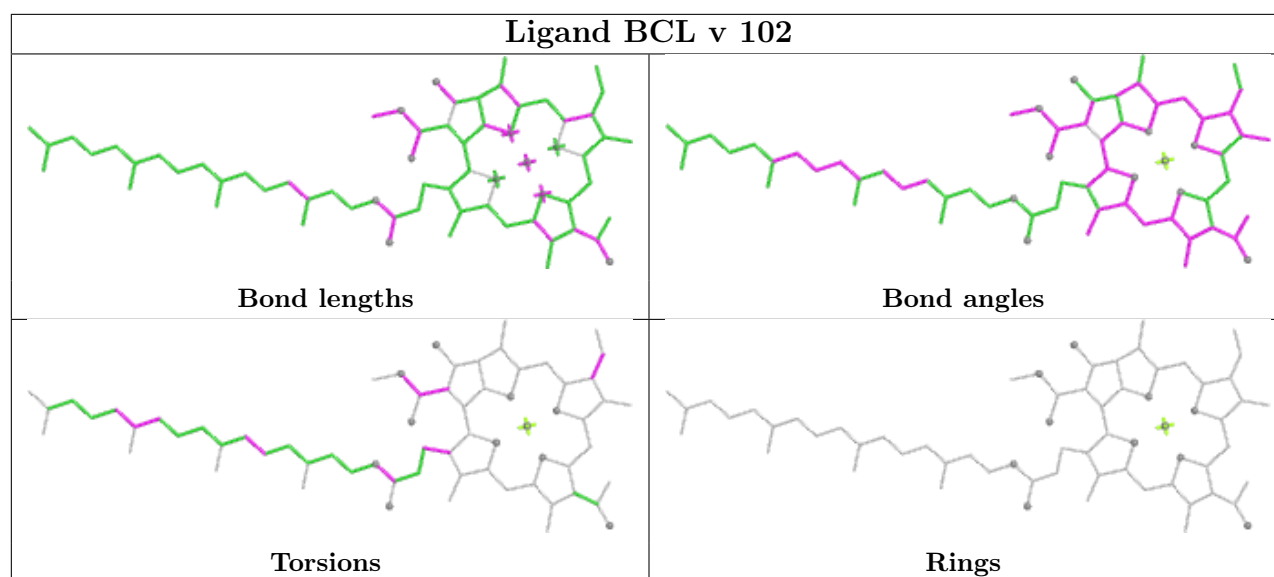


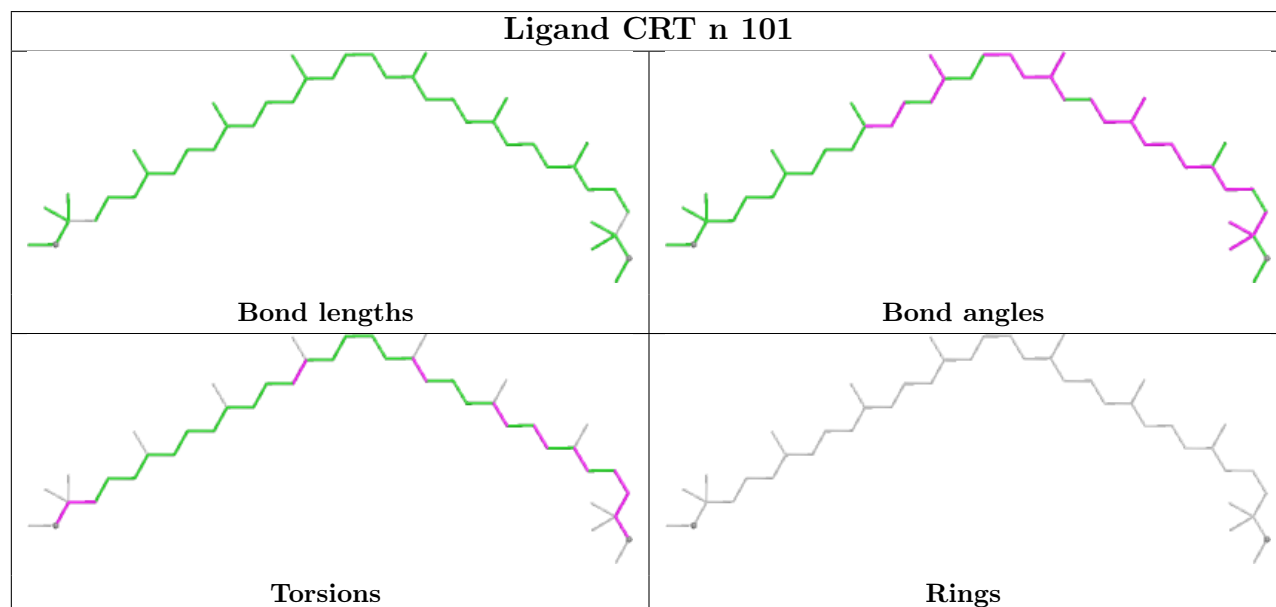
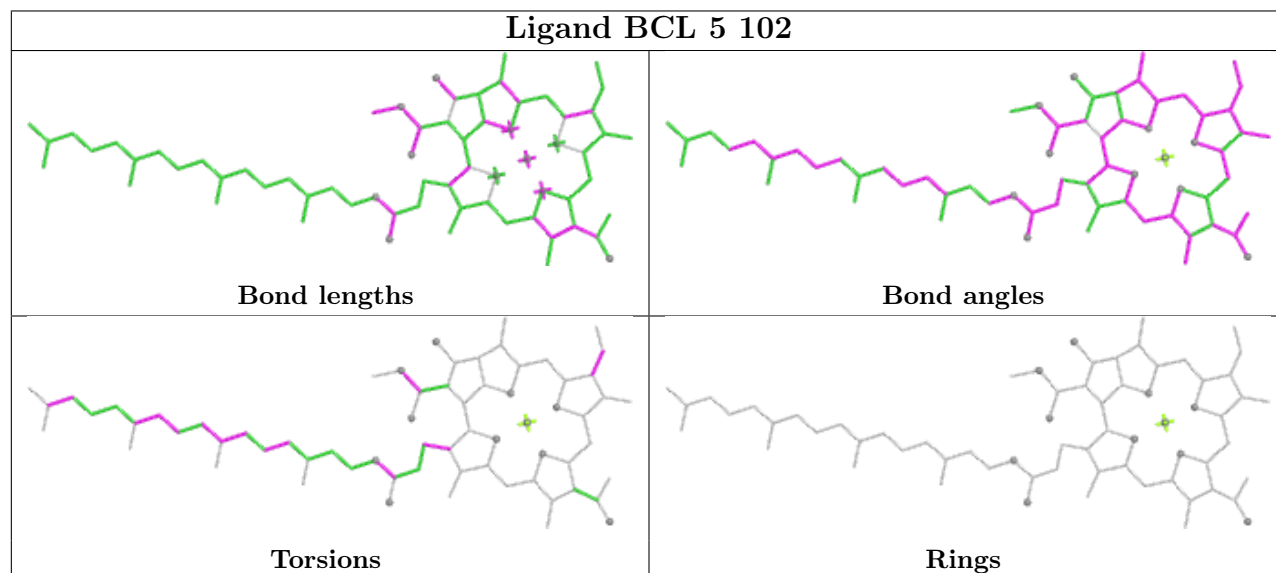
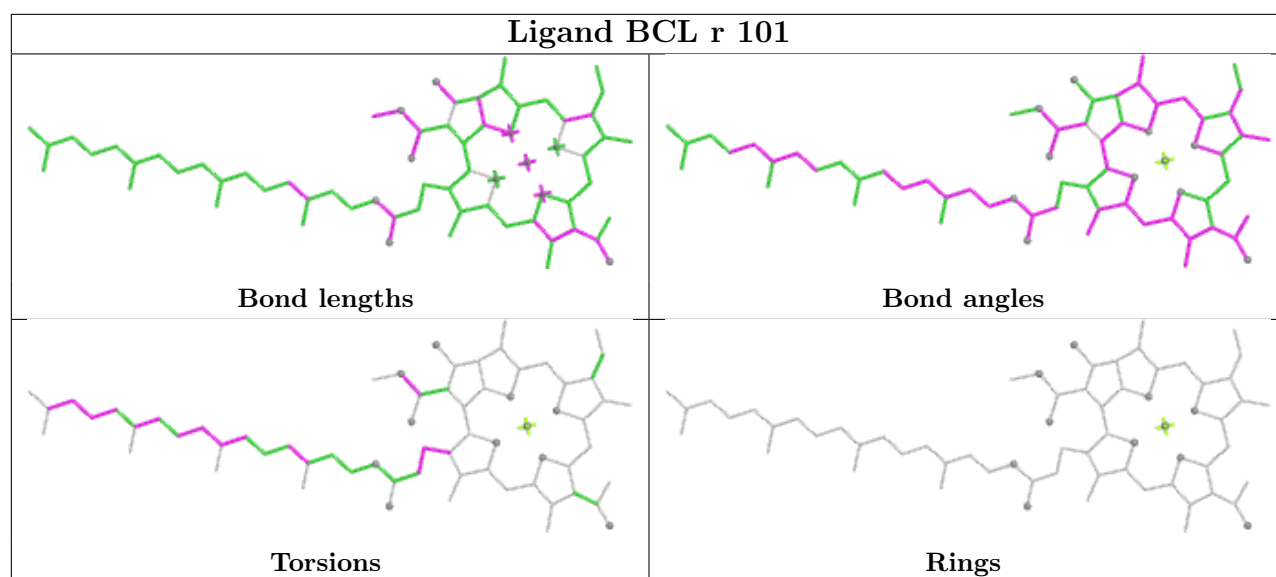
Ligand HEM o 502

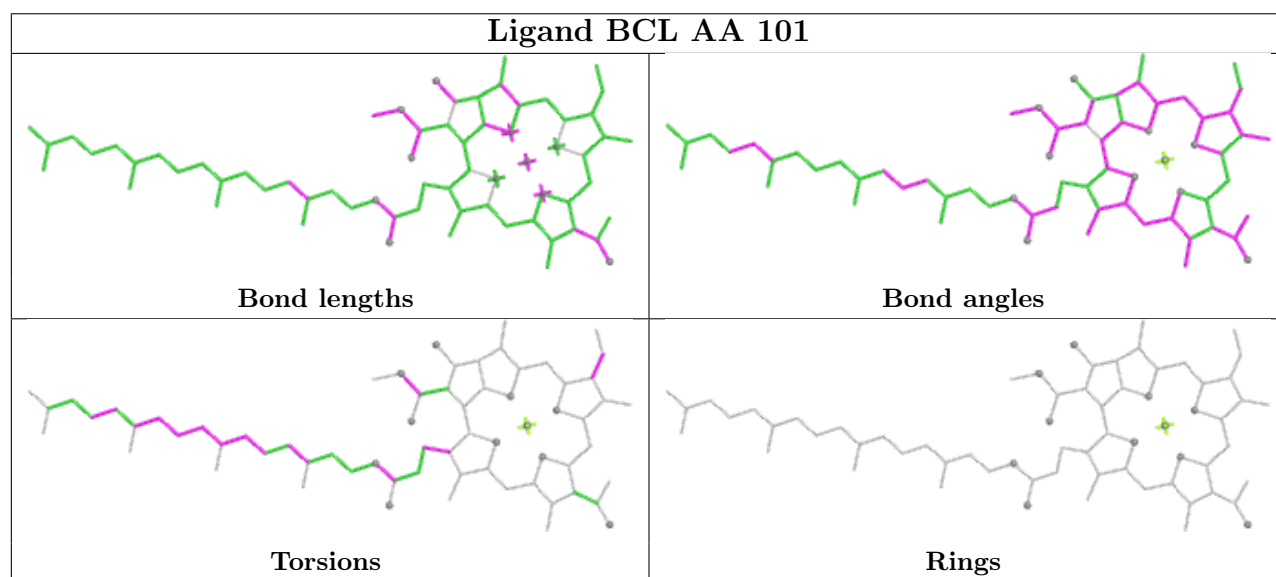
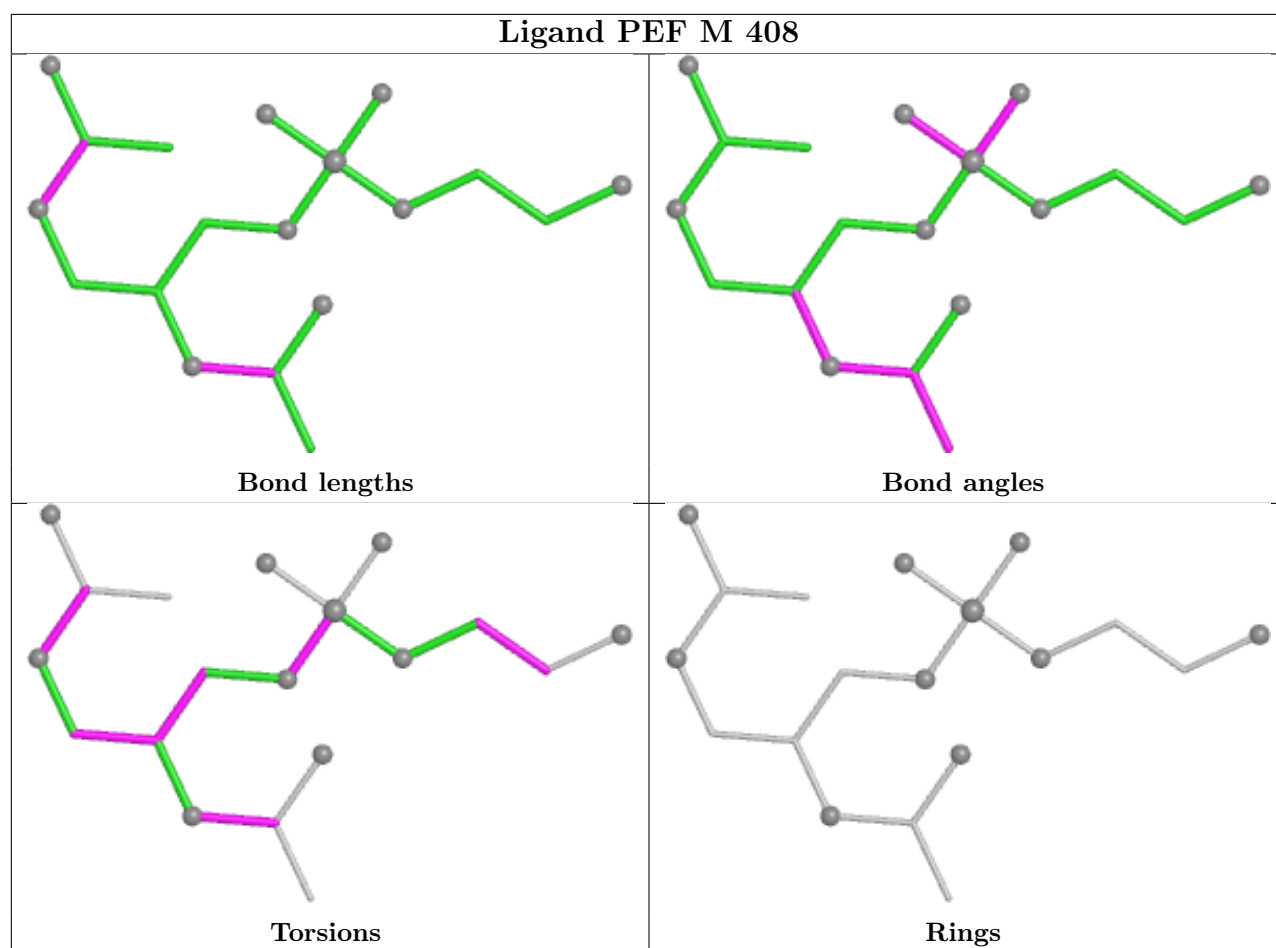


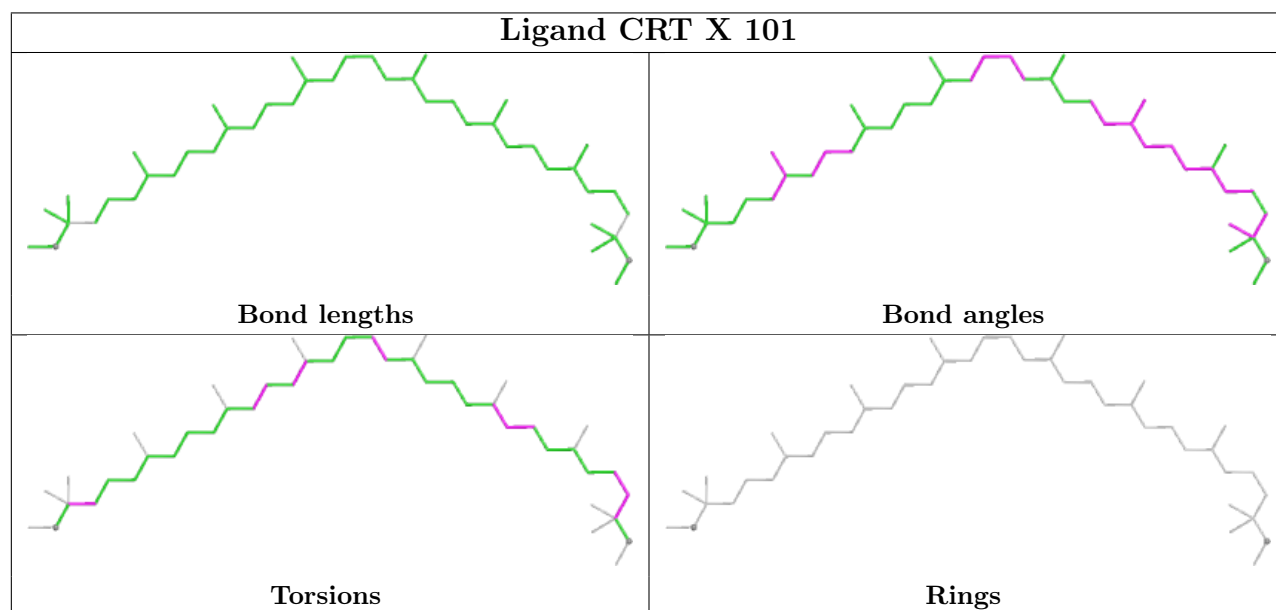
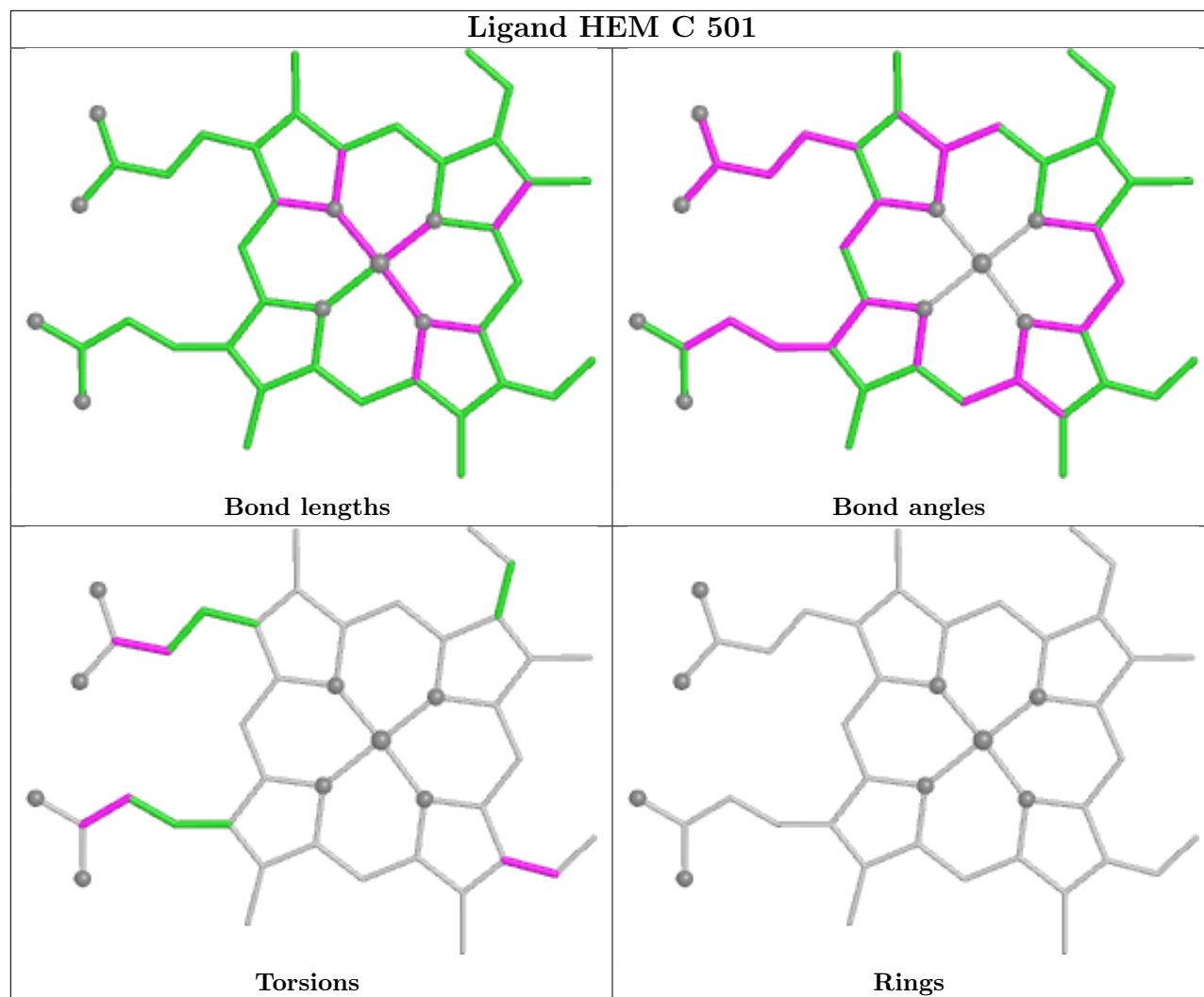
Ligand BCL m 102



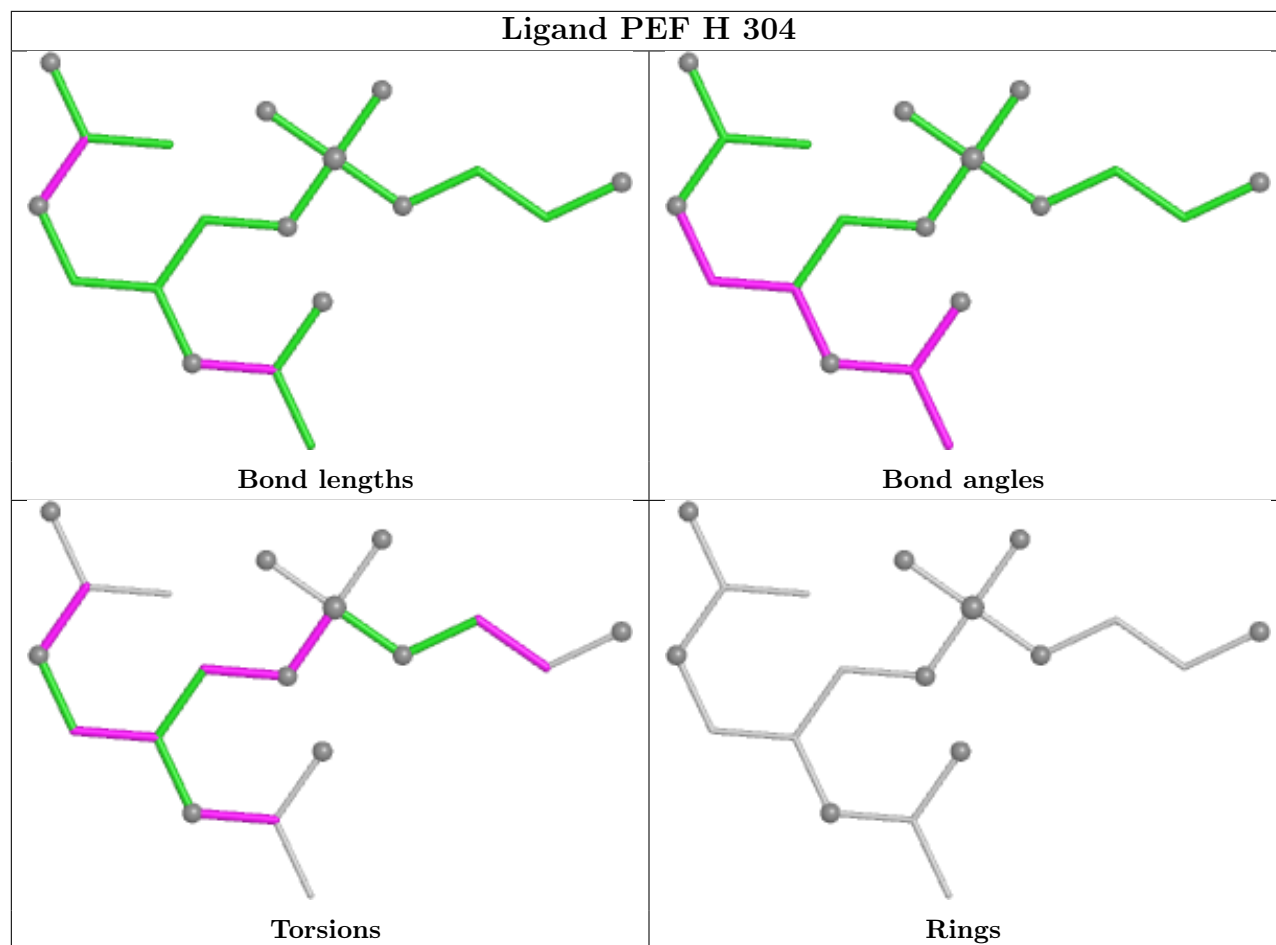


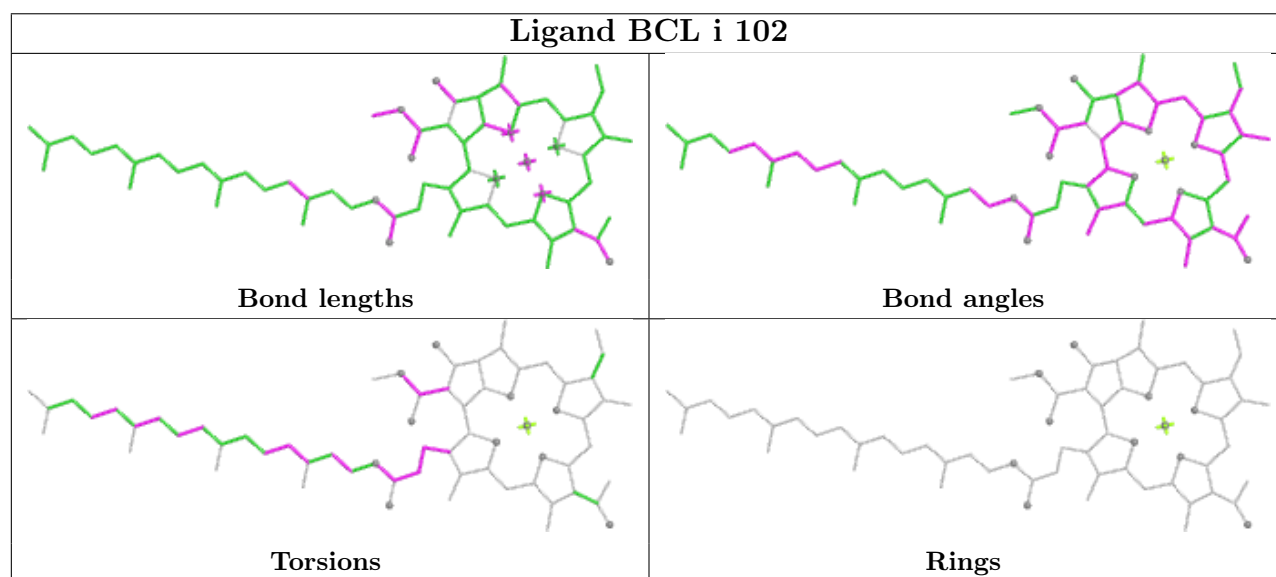
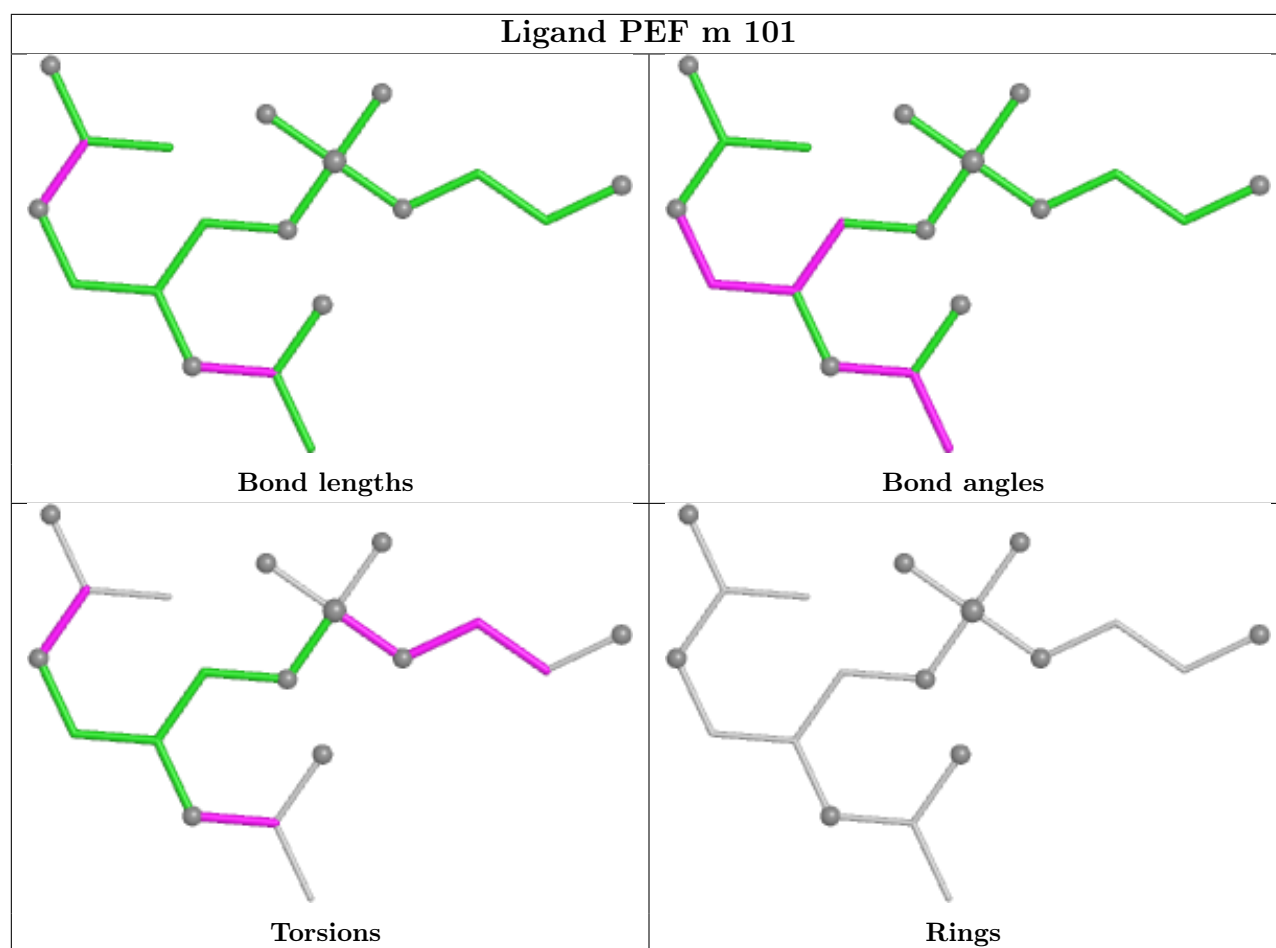


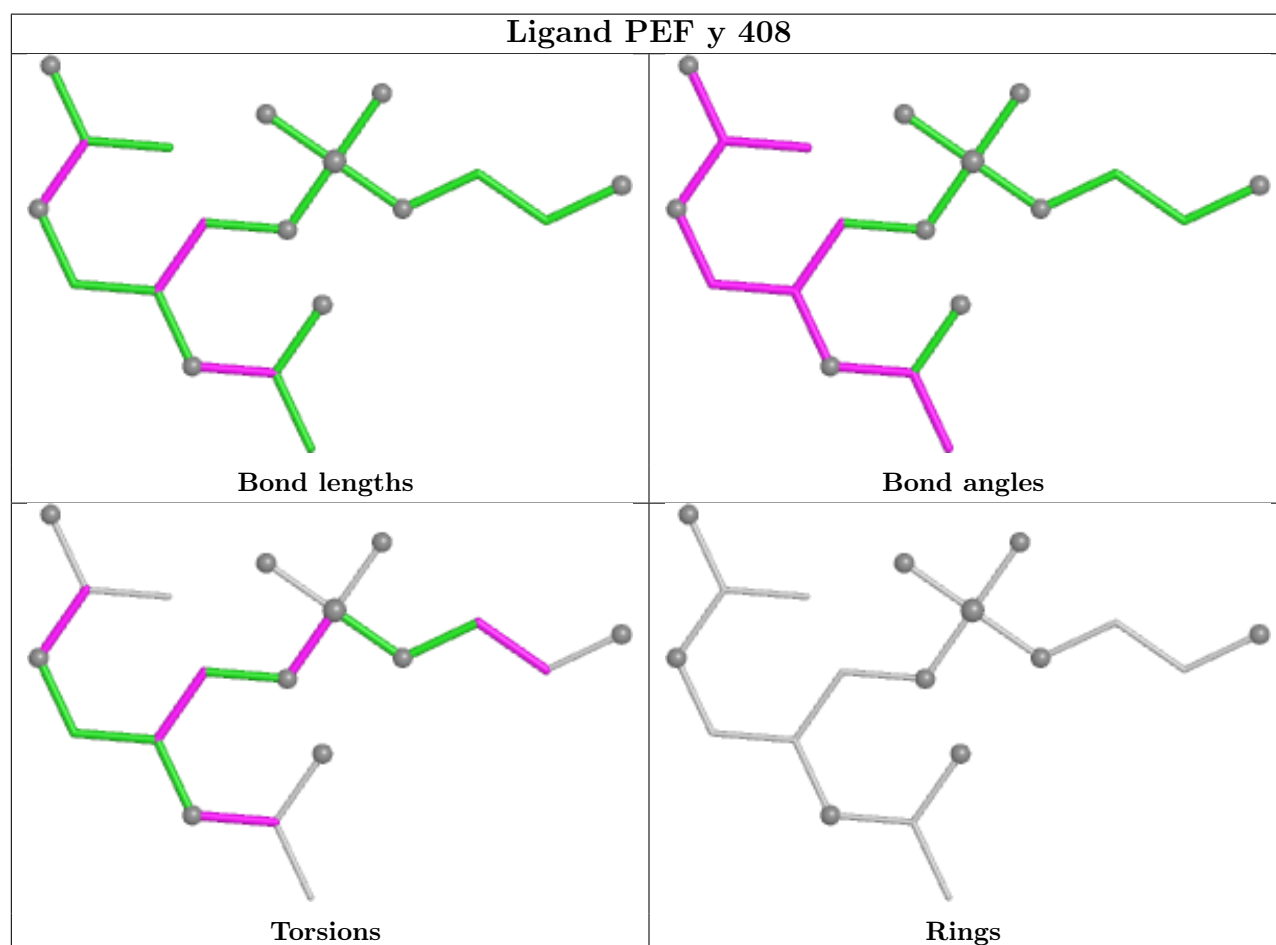
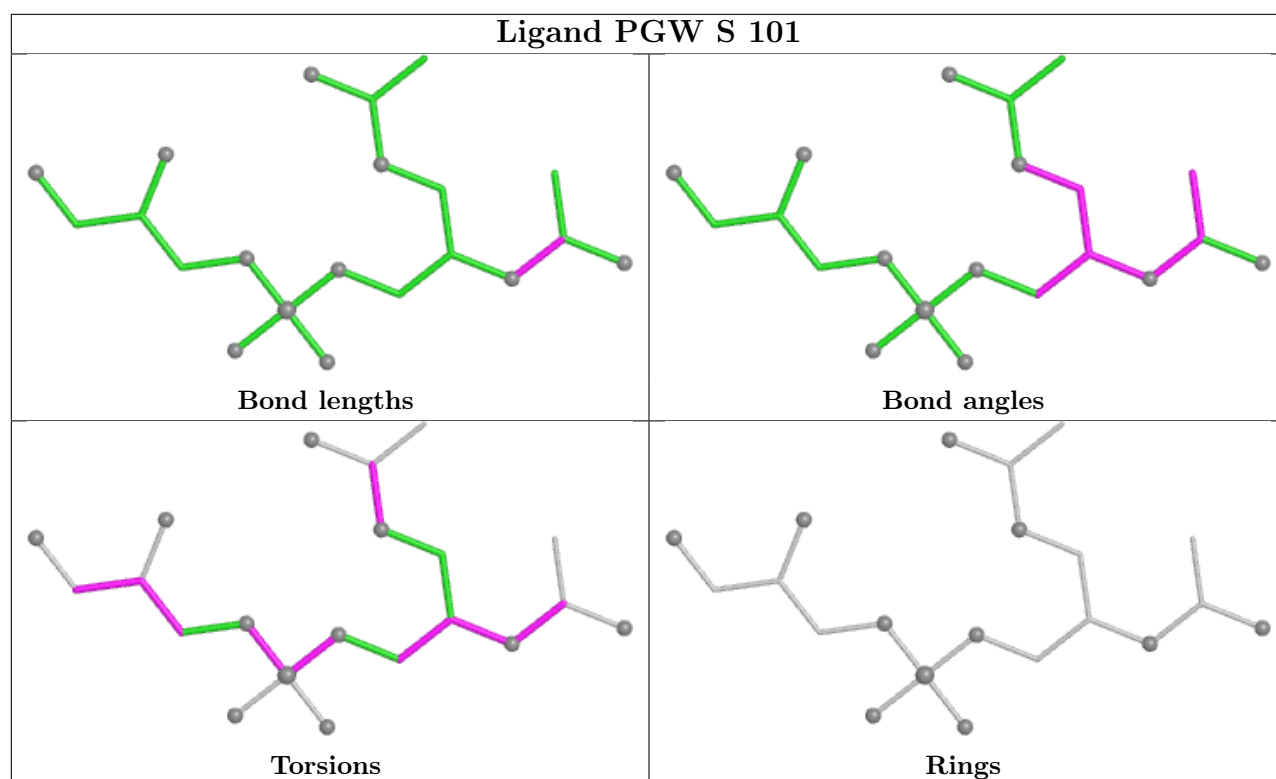


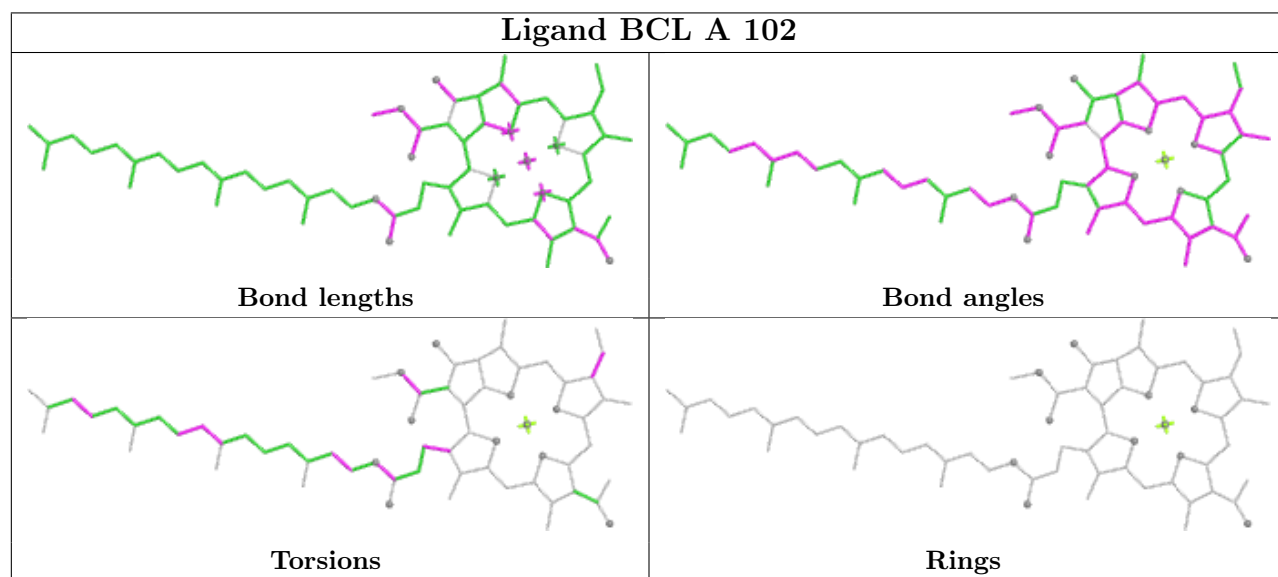
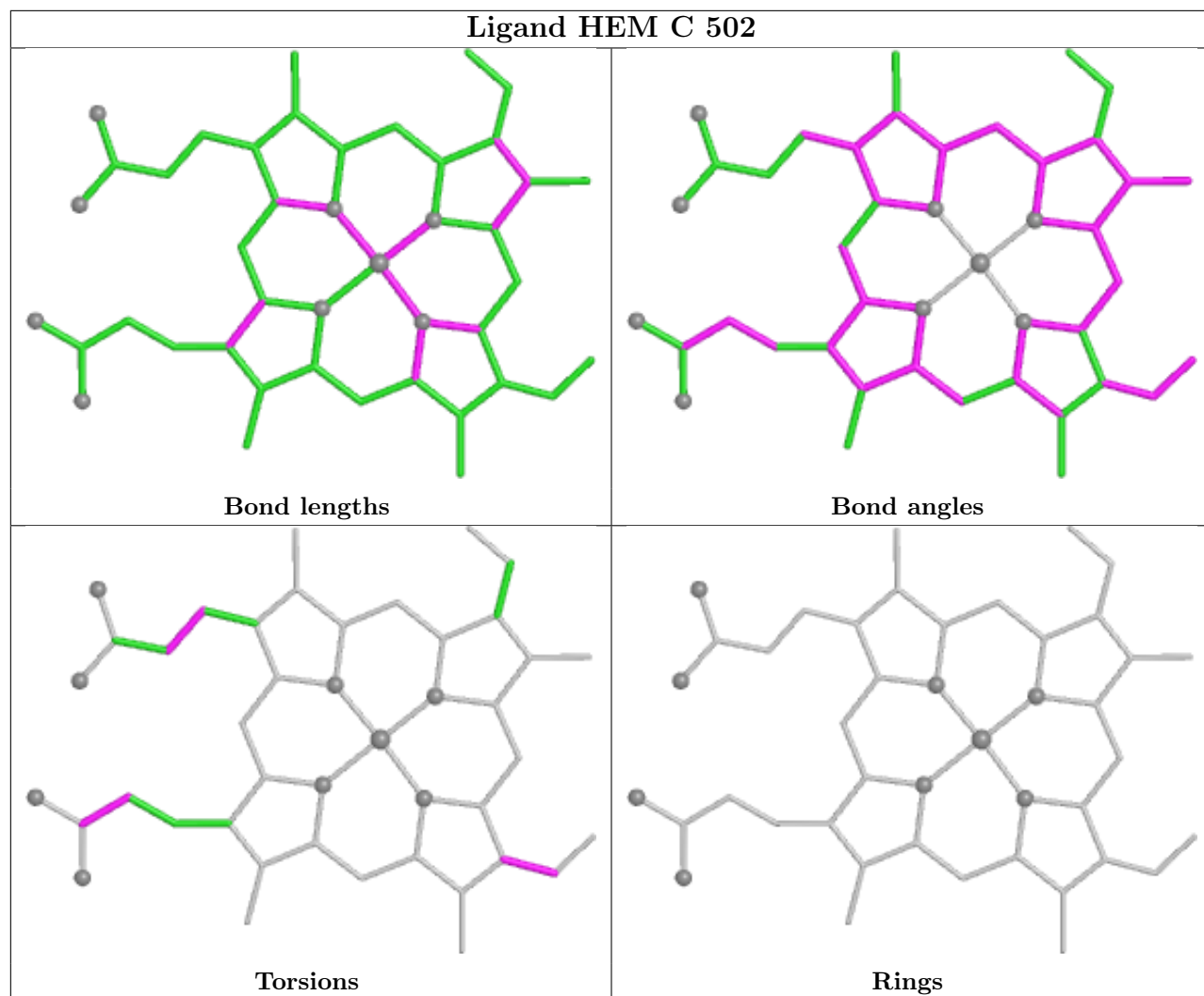


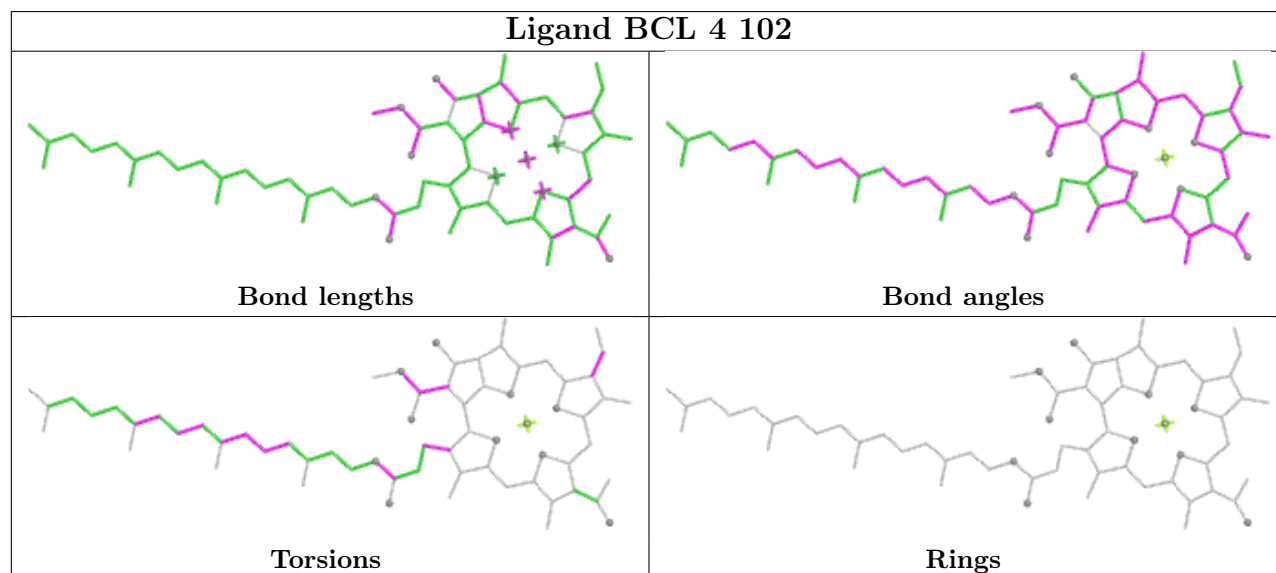
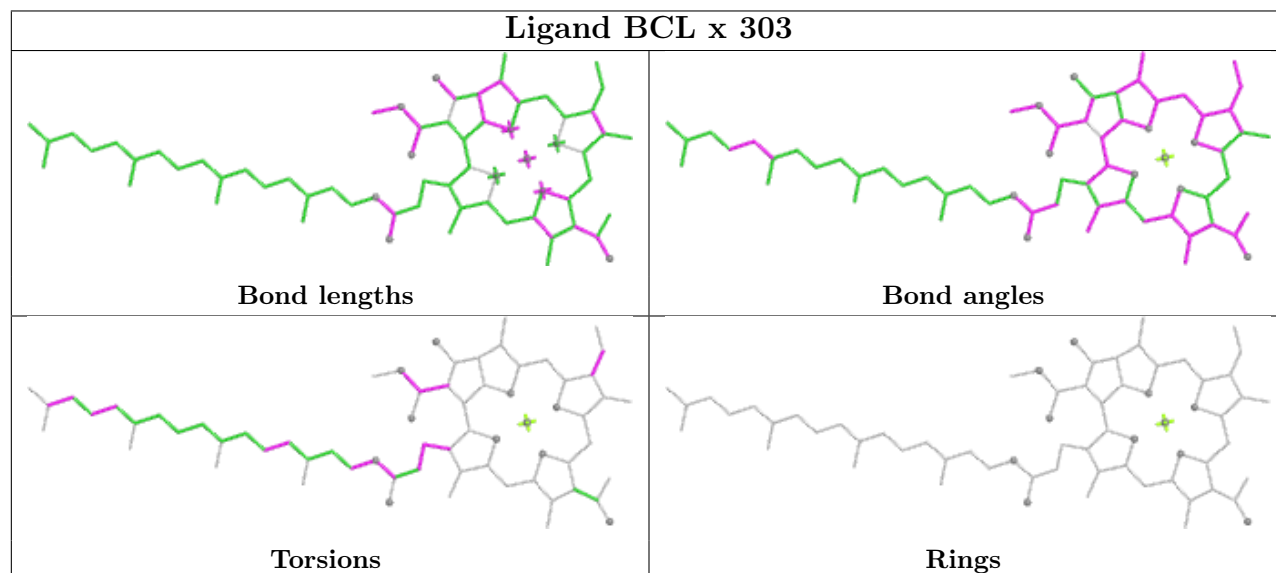
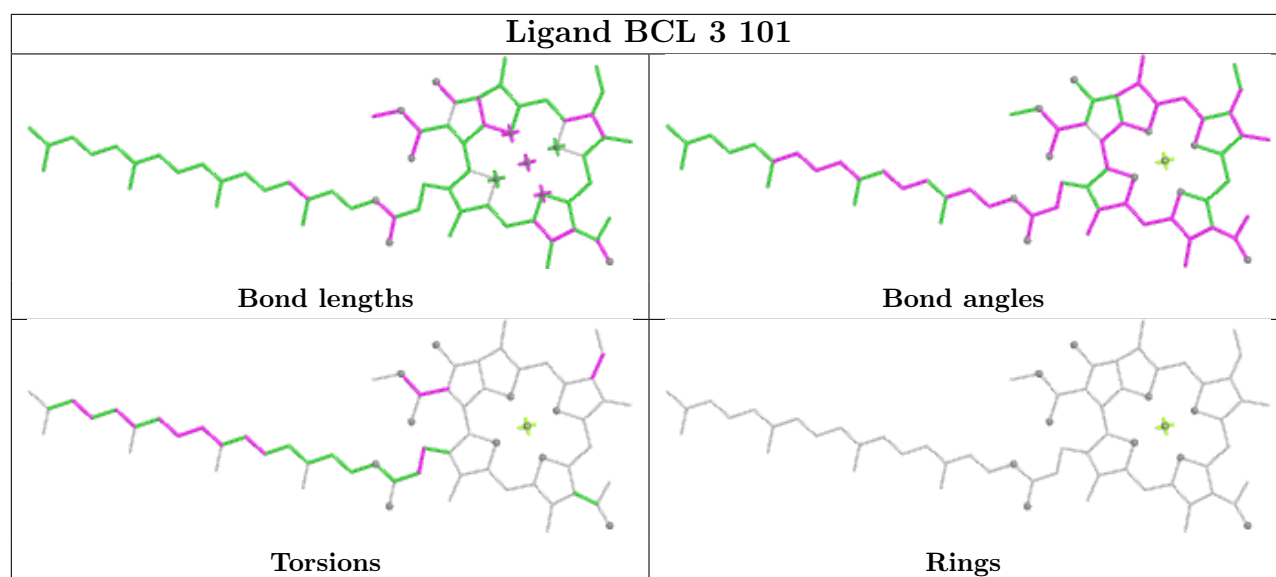
Ligand PEF H 304

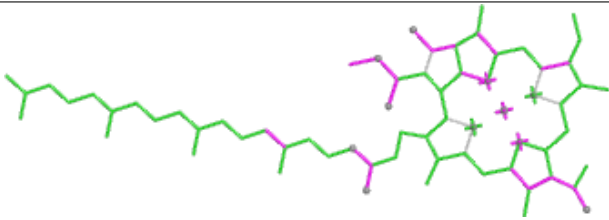
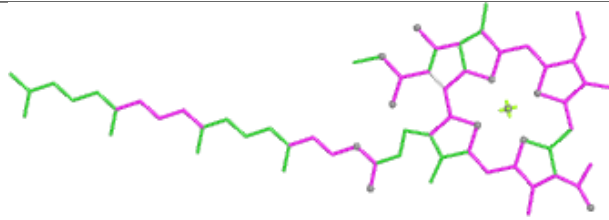
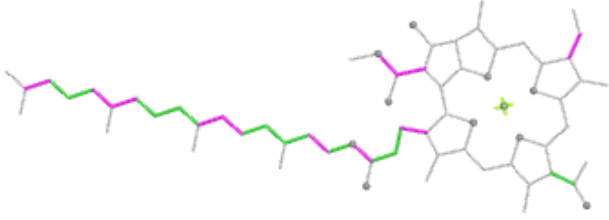
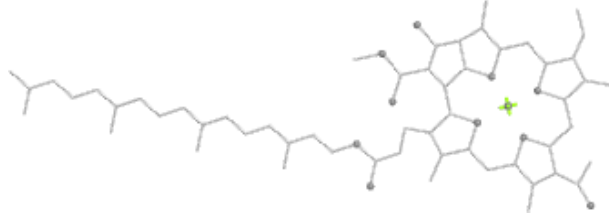


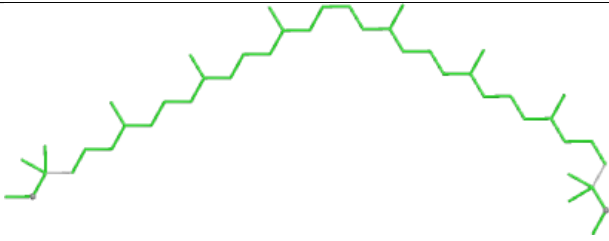
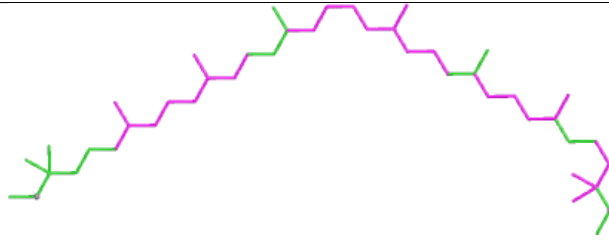
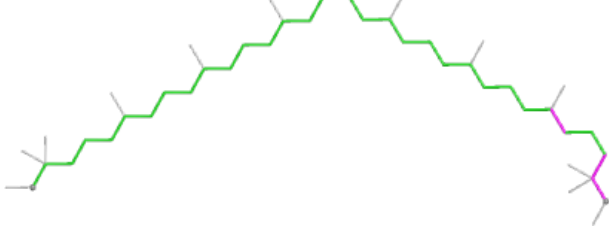


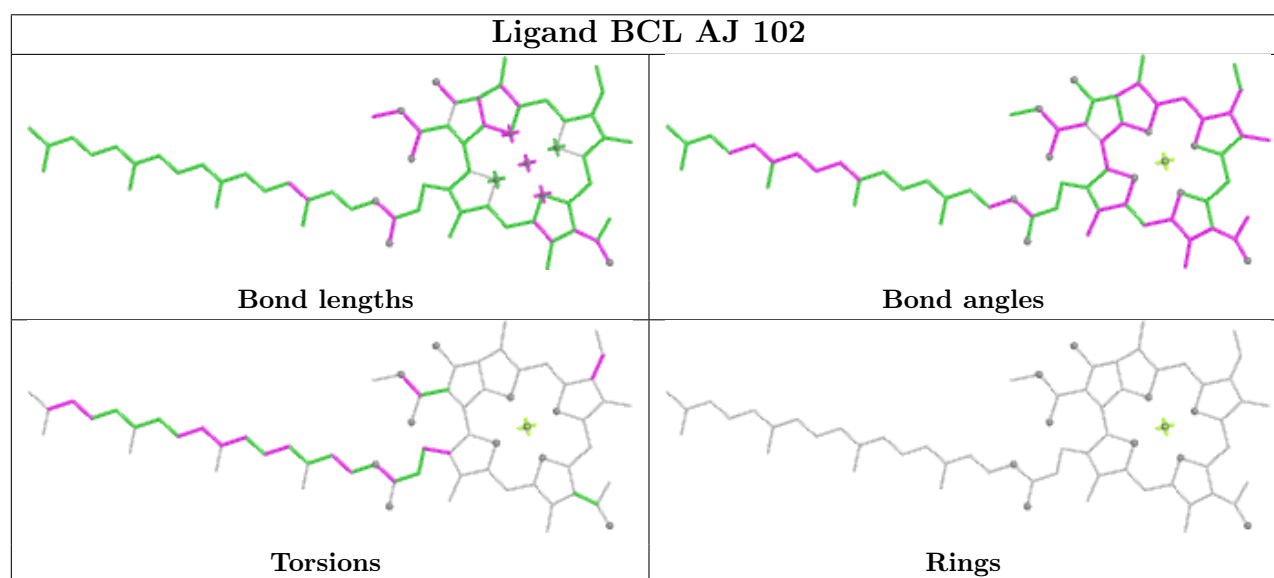
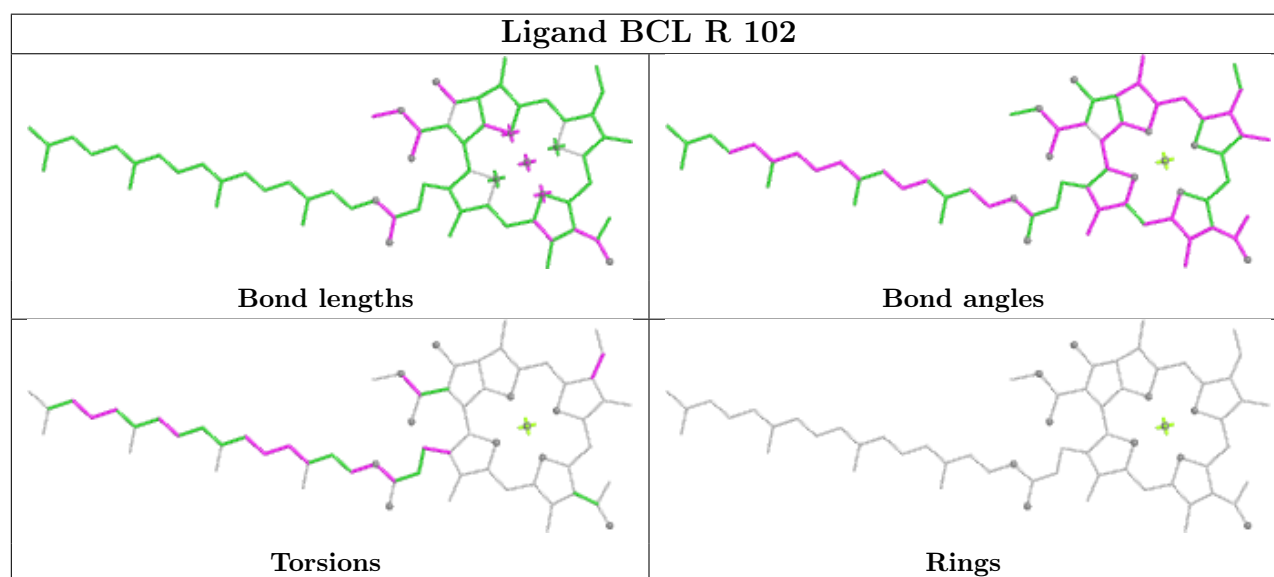
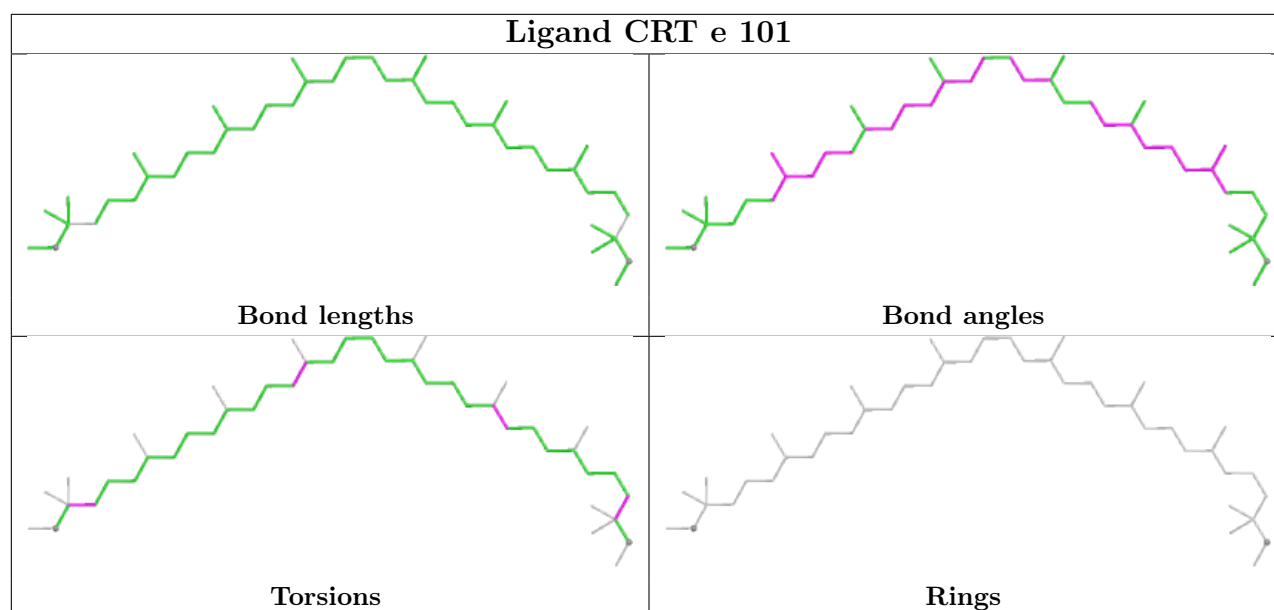


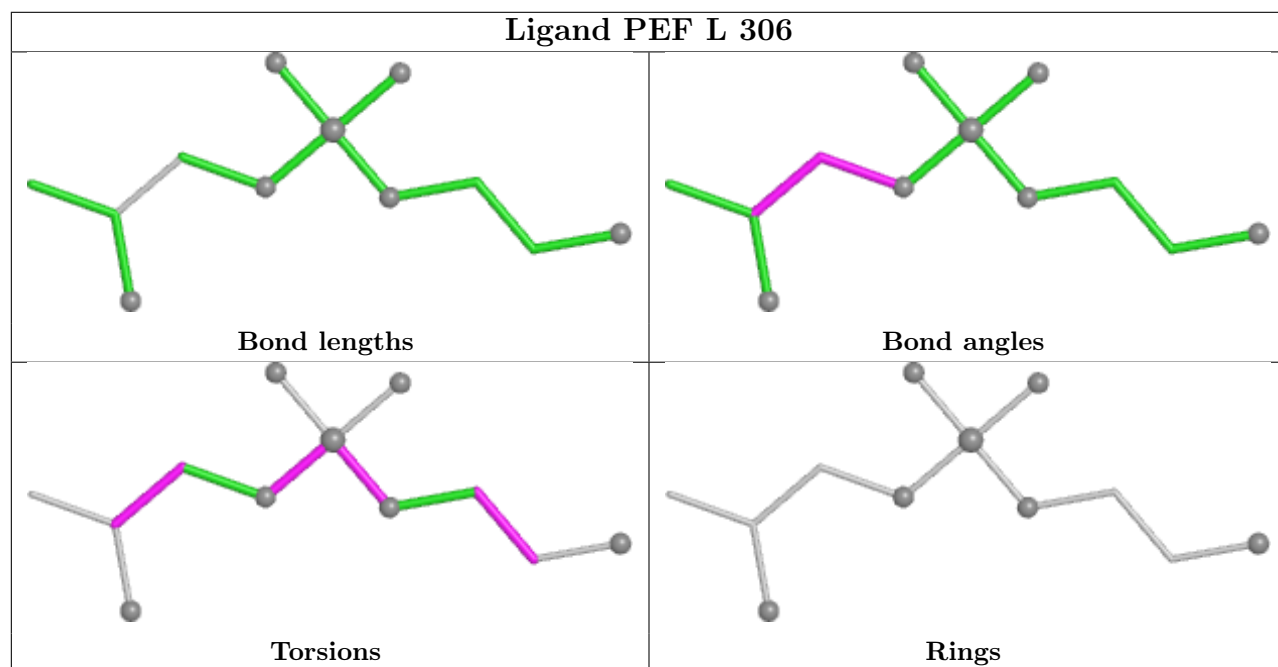
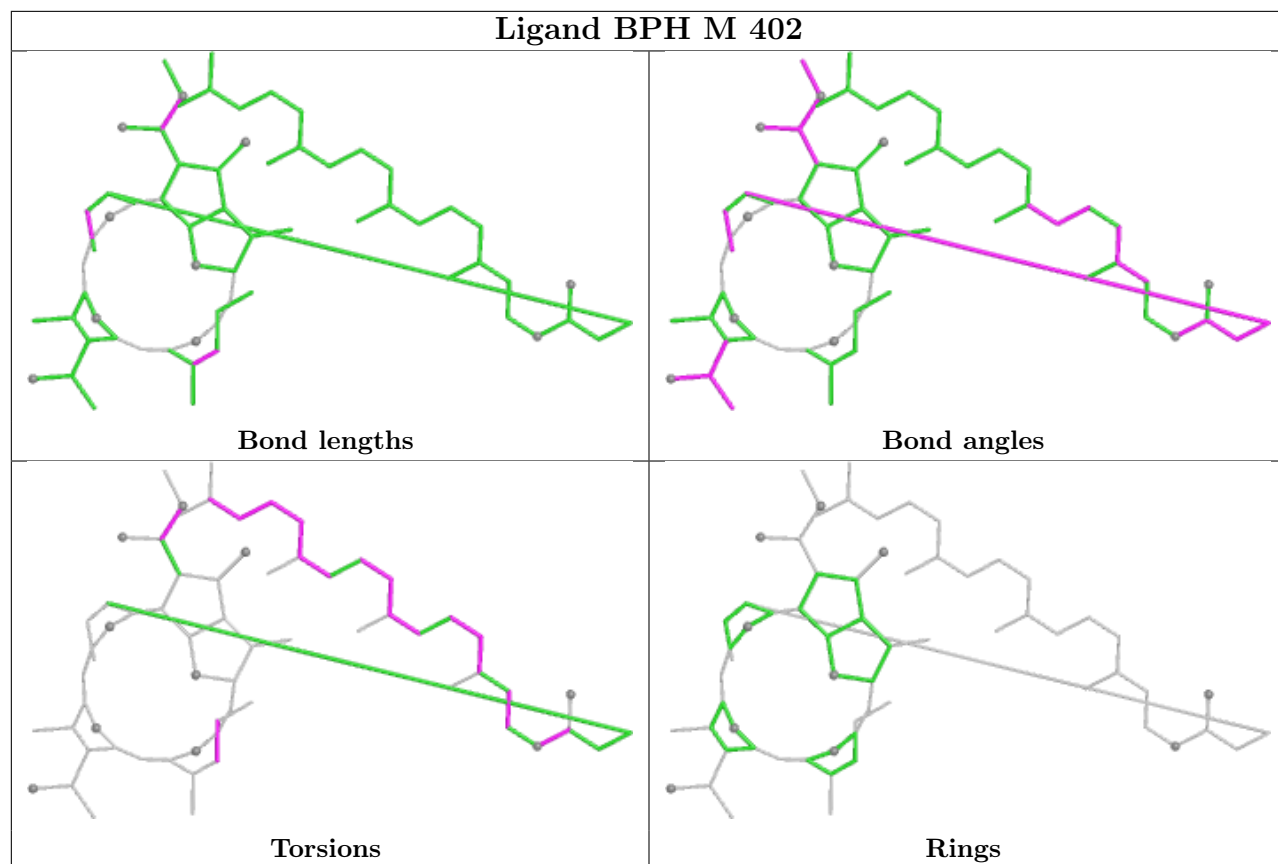




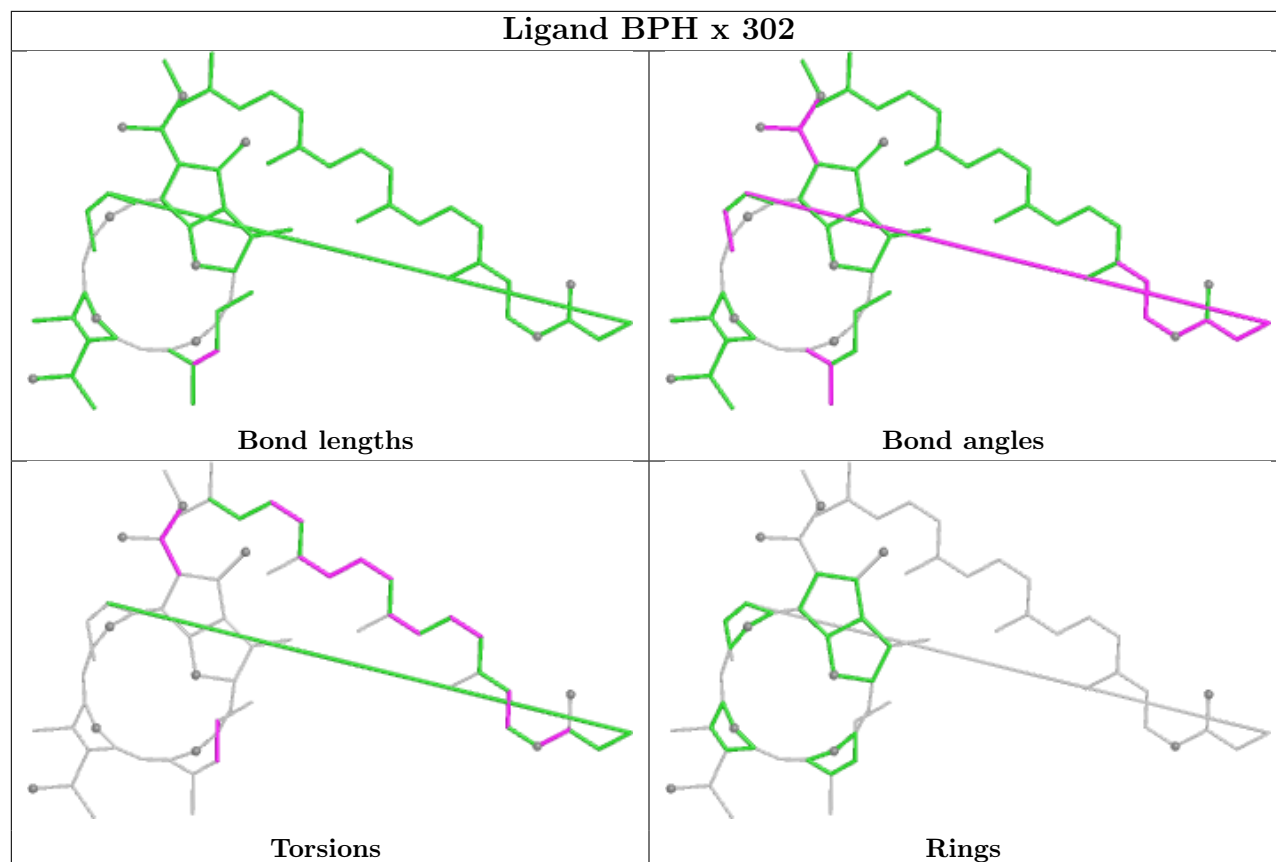
Ligand BCL m 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CRT A 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

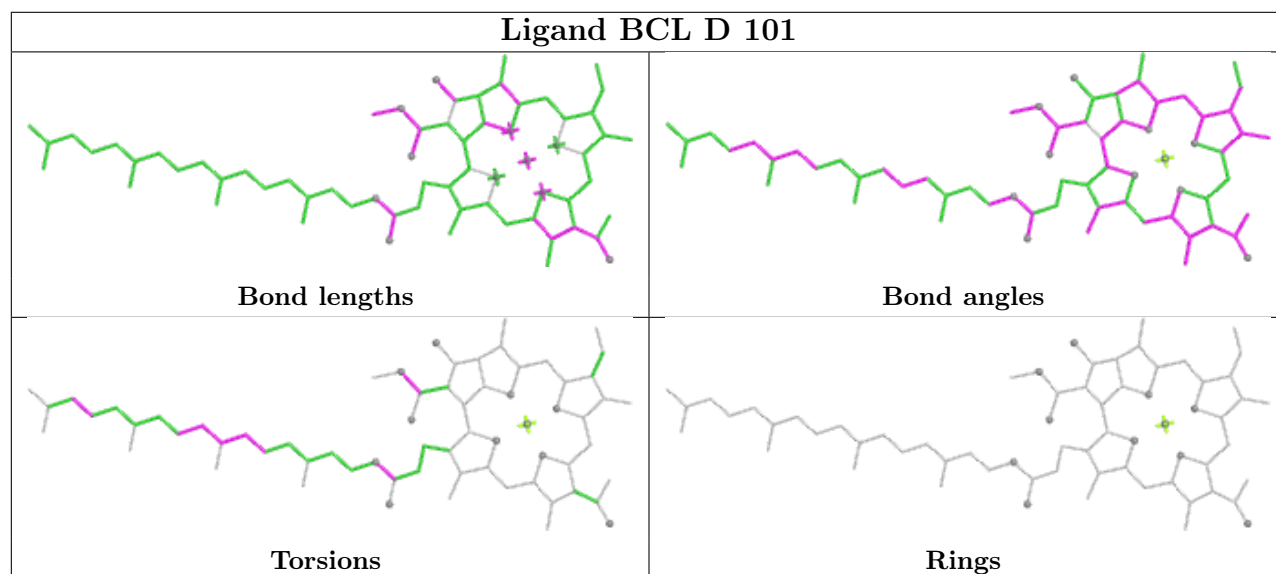


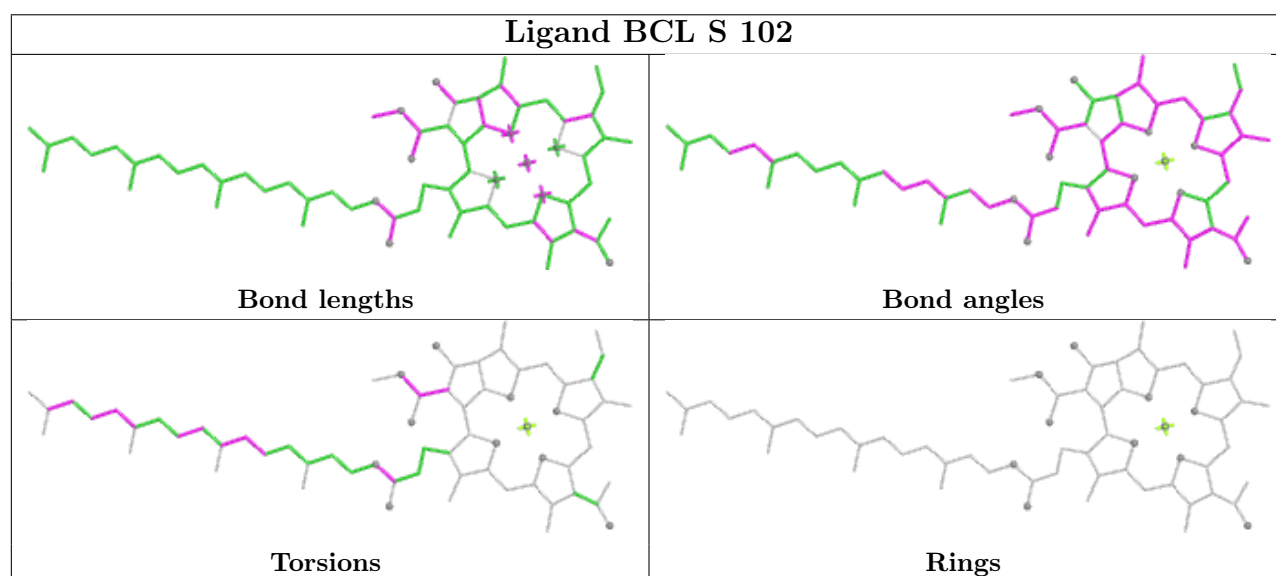
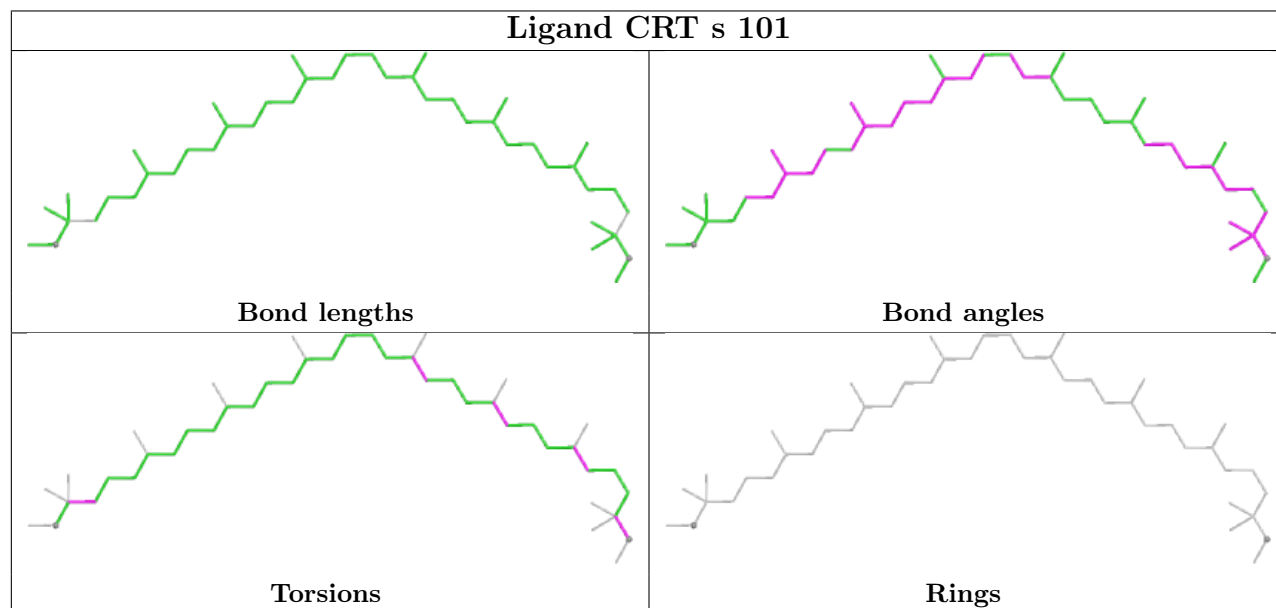
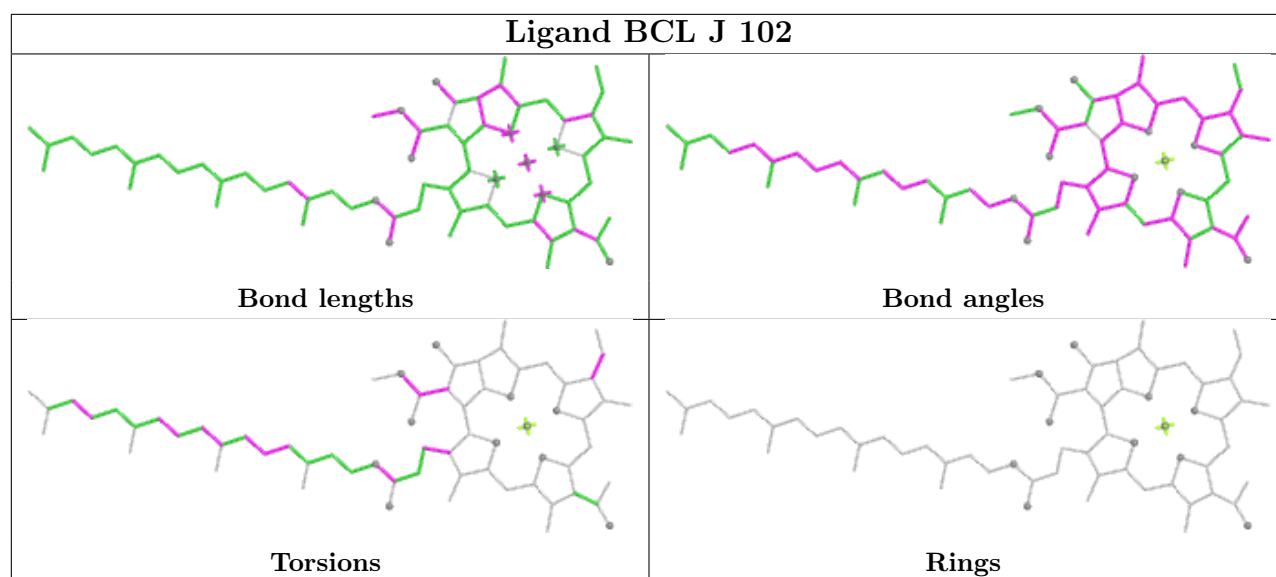


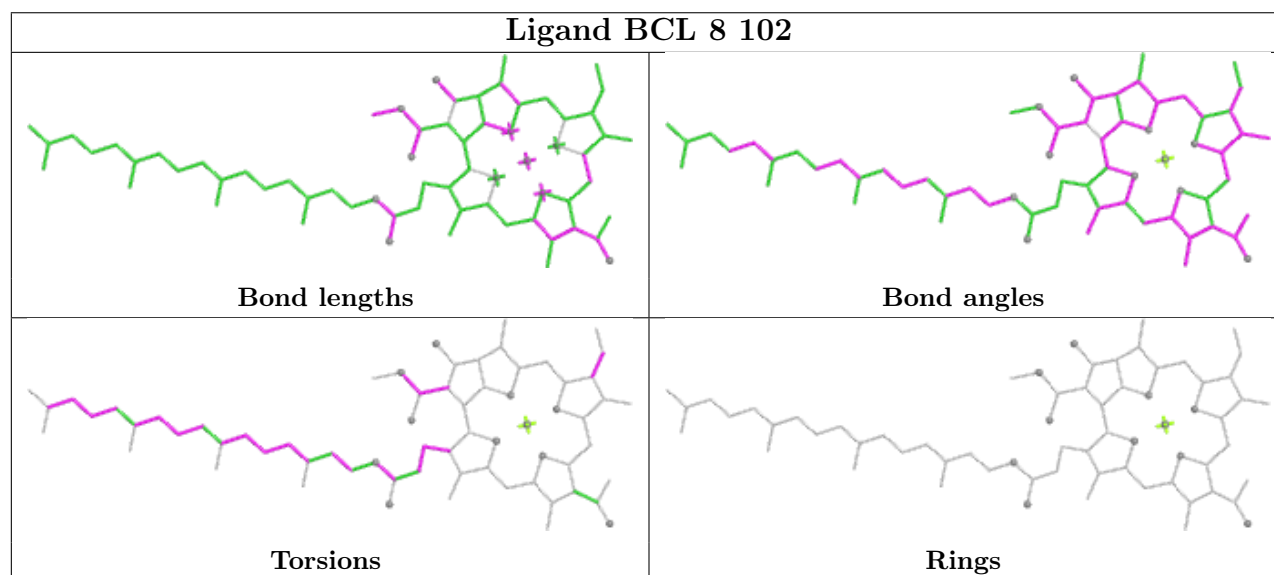
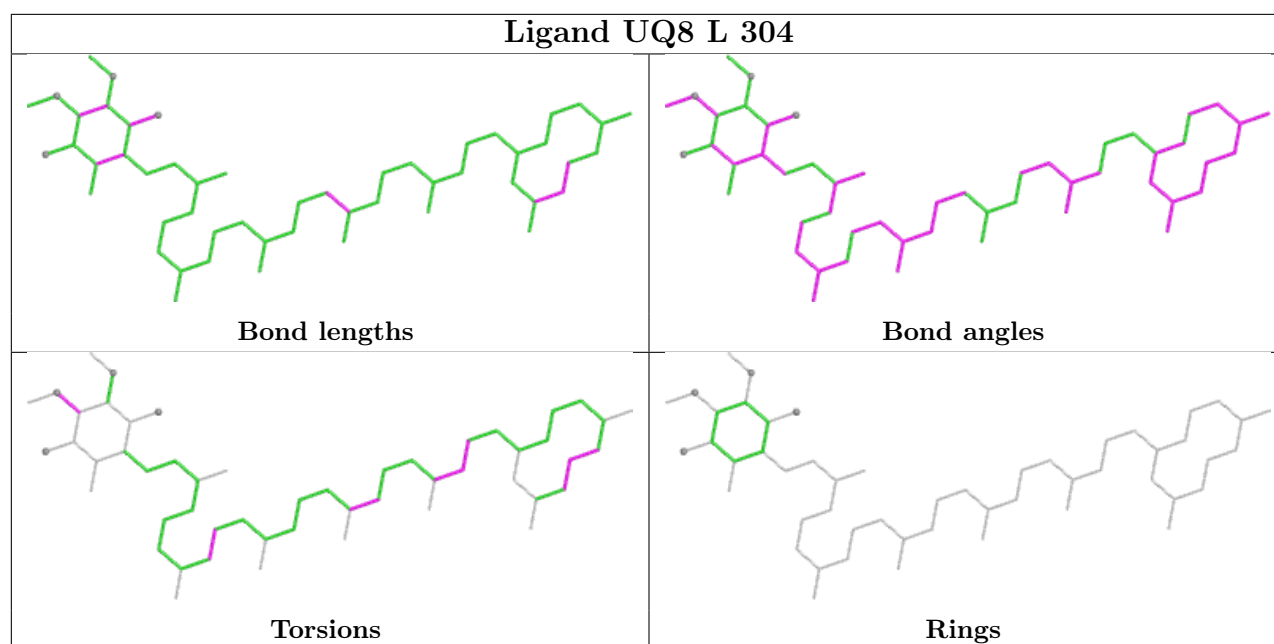
Ligand BPH x 302

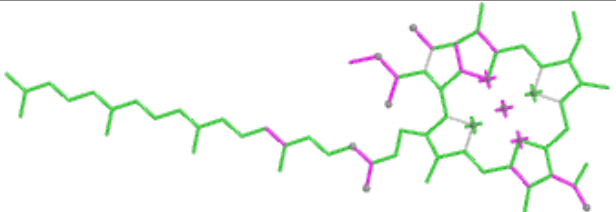
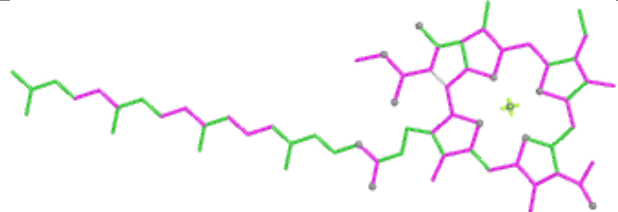
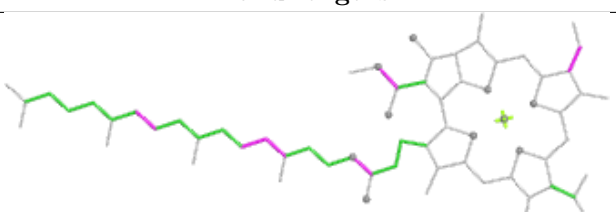
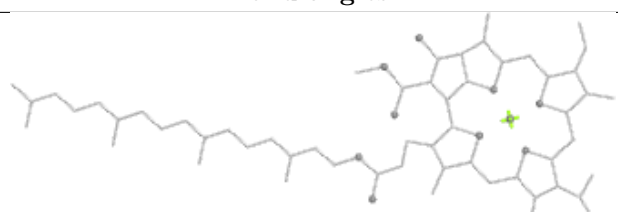


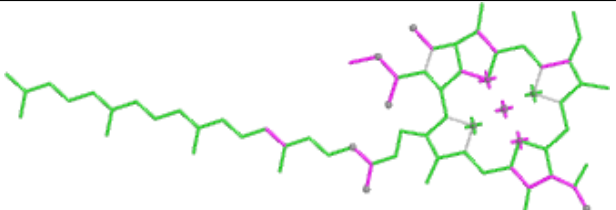
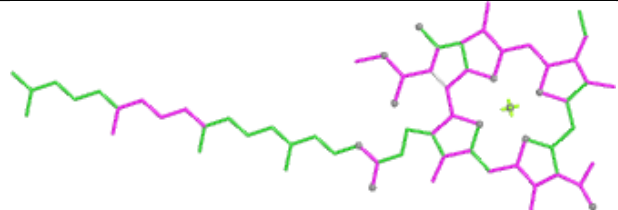
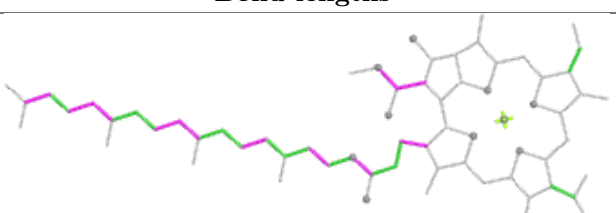
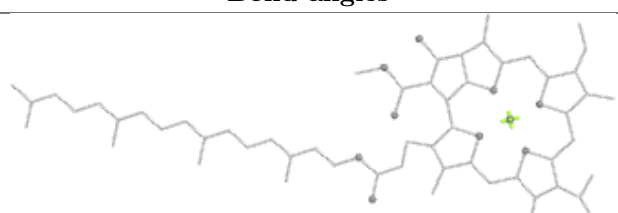
Ligand BCL D 101

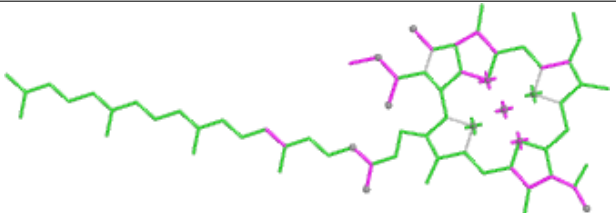
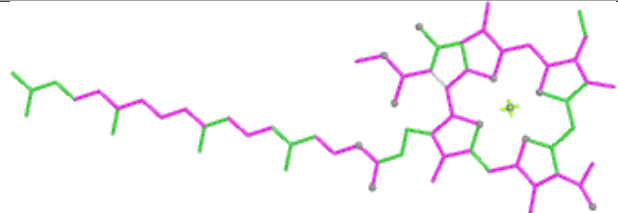
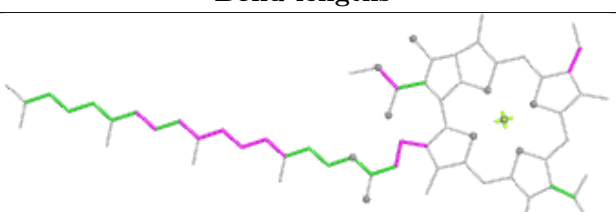
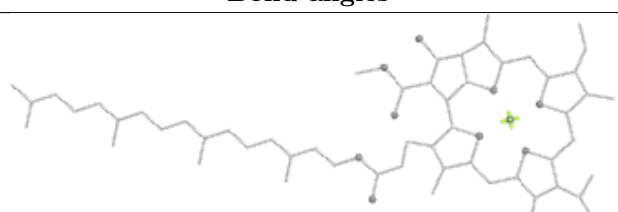






Ligand BCL I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL u 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL w 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.05	5 (1%) 70 52	79, 112, 143, 161	0
1	o	317/333 (95%)	0.08	10 (3%) 50 34	96, 133, 172, 190	0
2	L	280/281 (99%)	0.20	11 (3%) 43 29	60, 95, 154, 189	0
2	x	280/281 (99%)	0.21	11 (3%) 43 29	63, 97, 147, 181	0
3	M	318/319 (99%)	0.04	9 (2%) 55 36	65, 100, 140, 160	0
3	y	318/319 (99%)	0.10	6 (1%) 66 48	61, 111, 158, 187	0
4	H	258/259 (99%)	-0.09	6 (2%) 61 42	77, 105, 171, 274	0
4	t	258/259 (99%)	-0.08	8 (3%) 51 35	77, 106, 143, 251	0
5	1	60/61 (98%)	-0.00	1 (1%) 69 50	130, 158, 212, 237	0
5	3	60/61 (98%)	0.18	3 (5%) 34 23	129, 157, 225, 232	0
5	5	60/61 (98%)	-0.07	0 100 100	137, 174, 239, 244	0
5	7	60/61 (98%)	0.14	0 100 100	159, 188, 259, 272	0
5	9	60/61 (98%)	0.17	3 (5%) 34 23	163, 204, 239, 243	0
5	A	60/61 (98%)	0.11	4 (6%) 24 16	170, 210, 257, 260	0
5	AA	60/61 (98%)	0.01	2 (3%) 49 33	165, 216, 280, 292	0
5	AC	60/61 (98%)	0.03	1 (1%) 69 50	176, 225, 276, 279	0
5	AE	60/61 (98%)	0.05	3 (5%) 34 23	100, 230, 263, 270	1 (1%)
5	AG	60/61 (98%)	0.01	3 (5%) 34 23	177, 216, 274, 278	0
5	AI	60/61 (98%)	0.15	2 (3%) 49 33	159, 194, 255, 261	0
5	AK	60/61 (98%)	0.20	3 (5%) 34 23	151, 180, 247, 264	0
5	D	60/61 (98%)	-0.07	0 100 100	170, 217, 266, 269	0
5	F	60/61 (98%)	-0.04	0 100 100	174, 215, 261, 264	0
5	I	60/61 (98%)	-0.01	0 100 100	179, 222, 268, 269	0
5	K	60/61 (98%)	-0.15	1 (1%) 69 50	164, 214, 288, 303	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	O	60/61 (98%)	0.02	1 (1%) 69 50	143, 195, 279, 284	0
5	Q	60/61 (98%)	0.15	2 (3%) 49 33	139, 185, 264, 270	0
5	S	60/61 (98%)	0.03	1 (1%) 69 50	81, 193, 256, 260	1 (1%)
5	U	60/61 (98%)	0.12	1 (1%) 69 50	138, 179, 250, 256	0
5	W	60/61 (98%)	-0.15	0 100 100	126, 164, 228, 235	0
5	Y	60/61 (98%)	0.14	1 (1%) 69 50	123, 153, 233, 264	0
5	d	60/61 (98%)	-0.04	2 (3%) 49 33	147, 181, 240, 252	0
5	f	60/61 (98%)	0.07	3 (5%) 34 23	157, 180, 247, 253	0
5	h	60/61 (98%)	-0.07	1 (1%) 69 50	154, 189, 257, 267	0
5	j	60/61 (98%)	-0.17	0 100 100	157, 191, 243, 257	0
5	l	60/61 (98%)	0.11	3 (5%) 34 23	147, 187, 241, 251	0
5	m	60/61 (98%)	0.07	1 (1%) 69 50	146, 186, 255, 259	0
5	p	60/61 (98%)	0.26	3 (5%) 34 23	135, 189, 258, 262	0
5	r	60/61 (98%)	-0.05	2 (3%) 49 33	139, 186, 274, 280	0
5	u	60/61 (98%)	-0.05	4 (6%) 24 16	156, 202, 257, 263	0
5	w	60/61 (98%)	-0.20	1 (1%) 69 50	168, 218, 271, 277	0
6	0	40/47 (85%)	-0.24	0 100 100	178, 236, 246, 250	0
6	2	40/47 (85%)	-0.23	0 100 100	164, 177, 210, 219	0
6	4	40/47 (85%)	-0.29	0 100 100	166, 181, 200, 210	0
6	6	40/47 (85%)	-0.37	0 100 100	178, 203, 222, 224	0
6	8	40/47 (85%)	-0.05	1 (2%) 58 39	194, 230, 240, 241	0
6	AB	40/47 (85%)	0.03	0 100 100	198, 237, 255, 258	0
6	AD	40/47 (85%)	-0.21	0 100 100	210, 245, 256, 257	0
6	AF	40/47 (85%)	-0.04	1 (2%) 58 39	230, 249, 257, 257	0
6	AH	40/47 (85%)	-0.19	1 (2%) 58 39	224, 241, 251, 254	0
6	AJ	40/47 (85%)	-0.30	0 100 100	199, 230, 241, 243	0
6	AL	40/47 (85%)	0.11	0 100 100	190, 211, 236, 238	0
6	B	40/47 (85%)	-0.24	0 100 100	188, 239, 250, 254	0
6	E	40/47 (85%)	-0.19	2 (5%) 34 23	193, 239, 251, 252	0
6	G	40/47 (85%)	-0.04	2 (5%) 34 23	187, 239, 252, 255	0
6	J	40/47 (85%)	-0.06	0 100 100	191, 243, 258, 262	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	N	40/47 (85%)	-0.07	1 (2%) 58 39	175, 225, 247, 254	0
6	P	40/47 (85%)	-0.29	1 (2%) 58 39	170, 220, 241, 245	0
6	R	40/47 (85%)	-0.20	1 (2%) 58 39	170, 223, 236, 236	0
6	T	40/47 (85%)	-0.22	1 (2%) 58 39	184, 218, 236, 237	0
6	V	40/47 (85%)	-0.34	0 100 100	171, 205, 226, 234	0
6	X	40/47 (85%)	-0.15	2 (5%) 34 23	160, 186, 205, 209	0
6	Z	40/47 (85%)	-0.55	0 100 100	159, 173, 197, 202	0
6	c	40/47 (85%)	-0.21	1 (2%) 58 39	160, 217, 245, 247	0
6	e	40/47 (85%)	-0.21	2 (5%) 34 23	189, 204, 236, 240	0
6	g	40/47 (85%)	-0.16	2 (5%) 34 23	195, 213, 235, 239	0
6	i	40/47 (85%)	-0.31	0 100 100	199, 223, 240, 241	0
6	k	40/47 (85%)	-0.30	0 100 100	195, 233, 251, 255	0
6	n	40/47 (85%)	0.01	1 (2%) 58 39	153, 214, 249, 253	0
6	q	40/47 (85%)	-0.41	1 (2%) 58 39	156, 199, 239, 246	0
6	s	40/47 (85%)	0.03	1 (2%) 58 39	151, 198, 236, 238	0
6	v	40/47 (85%)	0.10	2 (5%) 34 23	182, 205, 244, 247	0
6	z	40/47 (85%)	0.03	1 (2%) 58 39	184, 224, 266, 271	0
All	All	5546/5840 (94%)	-0.00	142 (2%) 57 38	60, 169, 252, 303	2 (0%)

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	3	44	LEU	7.4
6	AF	11	ASP	6.8
5	AK	13	LEU	5.8
6	v	45	TRP	5.8
5	p	47	LEU	5.7

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
12	PEF	y	406	19/47	0.55	0.12	124,132,141,146	0
8	SR	I	102	1/1	0.59	0.17	284,284,284,284	0
16	PO4	y	405	5/5	0.59	0.14	138,141,147,148	0
17	PGW	AE	101	21/51	0.60	0.14	149,167,181,187	0
8	SR	K	102	1/1	0.63	0.19	270,270,270,270	0
12	PEF	A	101	19/47	0.65	0.14	141,149,161,165	0
8	SR	9	101	1/1	0.66	0.19	236,236,236,236	0
12	PEF	m	101	19/47	0.67	0.18	124,130,143,146	0
17	PGW	S	101	21/51	0.68	0.13	118,132,142,148	0
12	PEF	x	306	19/47	0.69	0.10	96,102,108,108	0
15	CRT	J	101	44/44	0.72	0.14	196,214,220,222	0
15	CRT	AL	101	44/44	0.76	0.14	140,190,233,236	0
12	PEF	L	306	12/47	0.76	0.10	113,119,126,127	0
8	SR	7	102	1/1	0.76	0.20	221,221,221,221	0
8	SR	AI	103	1/1	0.76	0.17	228,228,228,228	0
15	CRT	N	101	44/44	0.77	0.14	179,199,209,214	0
16	PO4	t	302	5/5	0.77	0.11	138,140,144,147	0
15	CRT	AH	102	44/44	0.77	0.15	163,220,243,244	0
12	PEF	y	408	19/47	0.77	0.10	93,103,113,116	0
8	SR	5	103	1/1	0.78	0.09	197,197,197,197	0
12	PEF	H	303	19/47	0.78	0.10	164,173,184,191	0
12	PEF	t	303	19/47	0.78	0.11	83,87,94,95	0
12	PEF	y	407	19/47	0.79	0.09	91,96,102,105	0
8	SR	p	105	1/1	0.79	0.12	265,265,265,265	0
15	CRT	p	103	44/44	0.79	0.14	158,177,182,187	0
9	BCL	AE	104	66/66	0.80	0.09	208,235,262,264	0
16	PO4	H	302	5/5	0.80	0.07	170,172,178,179	0
8	SR	D	103	1/1	0.81	0.11	269,269,269,269	0
15	CRT	c	101	44/44	0.82	0.14	179,196,203,207	0
15	CRT	8	101	44/44	0.82	0.15	174,203,220,223	0
8	SR	Q	102	1/1	0.82	0.16	256,256,256,256	0
12	PEF	t	301	19/47	0.82	0.10	94,98,103,104	0
12	PEF	H	304	19/47	0.82	0.09	92,98,106,108	0
15	CRT	i	101	44/44	0.82	0.12	163,197,220,226	0
8	SR	U	103	1/1	0.83	0.12	233,233,233,233	0
12	PEF	p	101	16/47	0.83	0.15	132,144,152,156	0
9	BCL	1	101	66/66	0.83	0.12	115,148,161,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	PEF	M	406	19/47	0.83	0.08	107,115,119,124	0
9	BCL	AC	102	66/66	0.83	0.12	205,236,259,261	0
14	MQ8	M	403	53/53	0.84	0.10	75,98,159,170	0
15	CRT	E	101	44/44	0.84	0.12	182,217,225,226	0
15	CRT	G	101	44/44	0.84	0.12	187,217,225,228	0
12	PEF	M	407	16/47	0.84	0.10	79,83,87,89	0
9	BCL	j	101	66/66	0.84	0.11	177,199,217,223	0
15	CRT	R	101	44/44	0.84	0.14	157,189,197,198	0
9	BCL	m	103	66/66	0.84	0.10	178,209,237,245	0
9	BCL	AH	103	66/66	0.84	0.14	195,211,245,252	0
15	CRT	z	101	44/44	0.84	0.16	179,205,209,210	0
11	UQ8	L	304	53/53	0.85	0.13	75,80,82,83	0
15	CRT	AC	101	44/44	0.85	0.13	195,211,216,218	0
8	SR	j	102	1/1	0.85	0.09	233,233,233,233	0
15	CRT	AJ	101	44/44	0.85	0.11	147,203,240,241	0
9	BCL	G	102	66/66	0.85	0.11	203,233,249,251	0
15	CRT	e	101	44/44	0.85	0.15	149,194,237,241	0
15	CRT	f	102	44/44	0.85	0.12	152,190,223,230	0
9	BCL	N	102	66/66	0.85	0.12	187,219,242,244	0
15	CRT	k	101	44/44	0.85	0.11	172,200,217,220	0
12	PEF	M	408	19/47	0.85	0.07	87,92,97,100	0
9	BCL	T	102	66/66	0.85	0.12	164,188,236,238	0
15	CRT	X	101	44/44	0.85	0.10	118,164,193,198	0
15	CRT	2	101	44/44	0.85	0.09	128,165,195,200	0
9	BCL	f	101	66/66	0.85	0.12	157,181,196,203	0
8	SR	f	103	1/1	0.85	0.06	208,208,208,208	0
9	BCL	S	102	66/66	0.86	0.12	129,190,203,213	0
15	CRT	n	101	44/44	0.86	0.15	173,188,197,201	0
8	SR	AE	105	1/1	0.86	0.07	257,257,257,257	0
15	CRT	s	101	44/44	0.86	0.11	155,177,181,183	0
15	CRT	v	101	44/44	0.86	0.11	165,192,198,200	0
9	BCL	AD	101	66/66	0.86	0.10	193,224,242,252	0
8	SR	O	102	1/1	0.86	0.11	254,254,254,254	0
12	PEF	H	301	19/47	0.86	0.11	140,163,175,180	0
11	UQ8	x	304	53/53	0.86	0.12	73,85,92,93	0
15	CRT	4	101	44/44	0.86	0.12	136,169,192,198	0
9	BCL	AK	101	66/66	0.87	0.12	168,180,199,220	0
9	BCL	d	101	66/66	0.87	0.11	138,175,187,197	0
9	BCL	K	101	66/66	0.87	0.11	181,215,235,242	0
9	BCL	v	102	66/66	0.87	0.13	182,211,260,262	0
9	BCL	k	102	66/66	0.87	0.11	181,211,246,260	0
8	SR	5	104	1/1	0.87	0.21	206,206,206,206	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	BCL	R	102	66/66	0.87	0.10	174,203,233,235	0
9	BCL	AE	102	66/66	0.87	0.10	169,228,244,254	0
9	BCL	1	102	66/66	0.87	0.12	140,153,192,205	0
9	BCL	AH	101	66/66	0.87	0.10	199,218,233,243	0
9	BCL	9	103	66/66	0.87	0.13	169,202,226,235	0
9	BCL	AJ	102	66/66	0.87	0.11	177,189,226,232	0
14	MQ8	y	403	53/53	0.87	0.13	71,88,135,144	0
15	CRT	A	103	44/44	0.87	0.13	186,214,224,225	0
9	BCL	h	101	66/66	0.88	0.10	168,188,207,212	0
9	BCL	z	102	66/66	0.88	0.11	193,228,269,271	0
9	BCL	AB	101	66/66	0.88	0.11	197,232,260,262	0
15	CRT	U	102	44/44	0.88	0.11	132,179,205,208	0
10	BPH	L	302	65/65	0.88	0.14	68,81,108,115	0
15	CRT	M	404	44/44	0.88	0.12	75,96,139,150	0
10	BPH	x	302	65/65	0.88	0.14	71,78,102,105	0
9	BCL	u	101	66/66	0.88	0.12	120,199,218,223	0
9	BCL	p	102	66/66	0.88	0.12	124,199,217,224	0
15	CRT	y	404	44/44	0.89	0.12	96,117,155,166	0
8	SR	AA	102	1/1	0.89	0.06	273,273,273,273	0
9	BCL	J	102	66/66	0.89	0.11	202,233,255,257	0
8	SR	W	102	1/1	0.89	0.10	205,205,205,205	0
15	CRT	T	101	44/44	0.89	0.13	145,187,206,207	0
8	SR	AI	102	1/1	0.89	0.06	245,245,245,245	0
9	BCL	5	102	66/66	0.89	0.11	150,176,224,240	0
9	BCL	c	102	66/66	0.89	0.09	177,211,249,251	0
9	BCL	L	303	66/66	0.89	0.15	62,70,78,83	0
9	BCL	m	102	66/66	0.89	0.10	160,202,221,229	0
9	BCL	D	102	66/66	0.90	0.11	202,232,246,247	0
9	BCL	F	101	66/66	0.90	0.11	184,220,238,242	0
9	BCL	AL	102	66/66	0.90	0.14	167,178,209,221	0
8	SR	w	103	1/1	0.90	0.18	260,260,260,260	0
15	CRT	AD	102	44/44	0.90	0.13	192,225,232,234	0
9	BCL	w	101	66/66	0.90	0.10	174,206,228,234	0
9	BCL	g	101	66/66	0.90	0.11	169,190,234,245	0
9	BCL	W	101	66/66	0.90	0.10	146,162,172,181	0
9	BCL	AA	101	66/66	0.90	0.09	177,212,237,244	0
9	BCL	Z	102	66/66	0.90	0.10	141,150,181,191	0
9	BCL	I	101	66/66	0.90	0.10	141,226,243,247	0
8	SR	S	103	1/1	0.90	0.12	235,235,235,235	0
8	SR	l	102	1/1	0.90	0.06	245,245,245,245	0
16	PO4	M	405	5/5	0.90	0.11	120,126,128,129	0
15	CRT	6	101	44/44	0.90	0.12	153,180,198,203	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SR	AC	103	1/1	0.90	0.11	265,265,265,265	0
9	BCL	O	101	66/66	0.90	0.10	179,211,234,235	0
9	BCL	P	101	66/66	0.90	0.10	171,205,223,228	0
9	BCL	AI	101	66/66	0.90	0.13	177,195,210,216	0
9	BCL	l	101	66/66	0.91	0.08	161,201,221,228	0
9	BCL	D	101	66/66	0.91	0.11	149,221,243,245	0
8	SR	L	307	1/1	0.91	0.09	205,205,205,205	0
8	SR	w	102	1/1	0.91	0.05	263,263,263,263	0
10	BPH	y	402	65/65	0.91	0.12	80,90,143,155	0
8	SR	A	104	1/1	0.91	0.18	256,256,256,256	0
9	BCL	s	102	66/66	0.91	0.12	171,202,247,248	0
8	SR	m	104	1/1	0.91	0.11	253,253,253,253	0
9	BCL	3	101	66/66	0.91	0.10	134,153,169,173	0
9	BCL	i	102	66/66	0.91	0.10	173,197,242,261	0
9	BCL	L	305	66/66	0.91	0.11	76,88,106,115	0
15	CRT	AE	103	44/44	0.91	0.10	182,236,248,249	0
9	BCL	7	101	66/66	0.91	0.12	162,184,202,209	0
9	BCL	Q	101	66/66	0.92	0.11	165,201,216,224	0
15	CRT	Z	101	44/44	0.92	0.10	114,157,190,195	0
9	BCL	Y	101	66/66	0.92	0.10	139,149,163,175	0
9	BCL	8	102	66/66	0.92	0.07	177,207,239,244	0
8	SR	Y	102	1/1	0.92	0.17	191,191,191,191	0
10	BPH	M	402	65/65	0.92	0.10	72,77,113,123	0
15	CRT	9	102	44/44	0.92	0.14	188,217,226,230	0
9	BCL	x	301	66/66	0.92	0.14	75,81,87,90	0
9	BCL	y	401	66/66	0.92	0.14	78,88,101,108	0
8	SR	AK	102	1/1	0.92	0.08	203,203,203,203	0
8	SR	d	102	1/1	0.92	0.09	198,198,198,198	0
15	CRT	P	102	44/44	0.92	0.10	169,193,199,202	0
9	BCL	V	101	66/66	0.92	0.13	159,175,219,232	0
9	BCL	r	101	66/66	0.92	0.09	154,192,211,214	0
9	BCL	5	101	66/66	0.92	0.11	141,165,182,188	0
9	BCL	0	101	66/66	0.93	0.09	190,224,244,245	0
7	HEM	o	501	43/43	0.93	0.15	142,155,165,169	0
9	BCL	U	101	66/66	0.93	0.11	151,179,188,195	0
9	BCL	4	102	66/66	0.93	0.09	138,159,198,209	0
7	HEM	C	501	43/43	0.93	0.13	110,120,129,134	0
8	SR	x	307	1/1	0.93	0.04	168,168,168,168	0
9	BCL	M	401	66/66	0.93	0.10	74,82,88,94	0
9	BCL	e	102	66/66	0.93	0.11	166,180,213,225	0
9	BCL	A	102	66/66	0.93	0.10	202,230,242,244	0
8	SR	L	308	1/1	0.93	0.04	145,145,145,145	0

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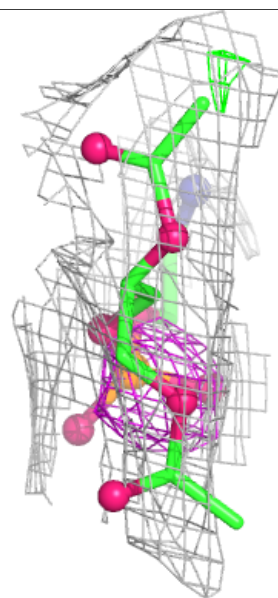
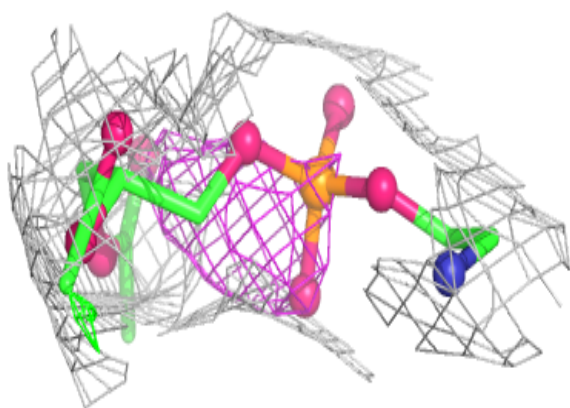
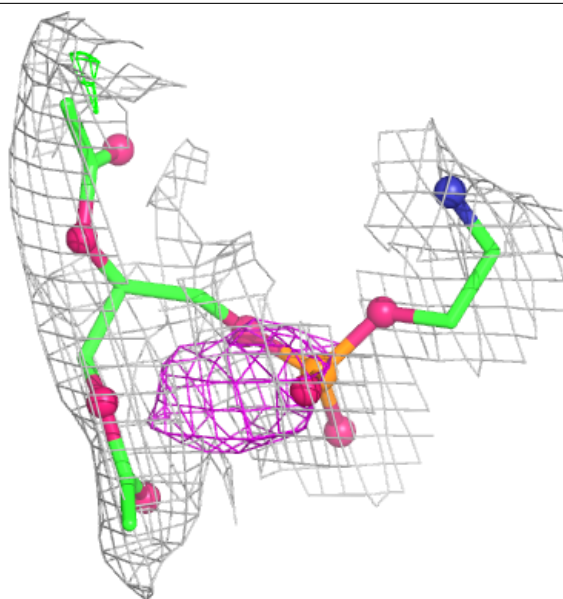
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SR	C	505	1/1	0.94	0.06	113,113,113,113	0
9	BCL	x	303	66/66	0.94	0.10	73,82,94,98	0
9	BCL	x	305	66/66	0.94	0.10	72,82,91,99	0
9	BCL	X	102	66/66	0.94	0.10	142,155,182,199	0
8	SR	l	103	1/1	0.94	0.12	176,176,176,176	0
8	SR	F	102	1/1	0.94	0.13	262,262,262,262	0
9	BCL	L	301	66/66	0.94	0.12	67,74,92,98	0
9	BCL	p	104	66/66	0.94	0.10	170,202,241,242	0
8	SR	x	308	1/1	0.94	0.05	196,196,196,196	0
7	HEM	o	503	43/43	0.94	0.17	94,106,122,126	0
7	HEM	o	504	43/43	0.95	0.14	112,116,123,124	0
9	BCL	B	101	66/66	0.95	0.09	187,218,239,241	0
8	SR	r	102	1/1	0.95	0.07	252,252,252,252	0
7	HEM	C	503	43/43	0.96	0.17	85,100,116,119	0
7	HEM	C	504	43/43	0.96	0.16	97,99,104,107	0
8	SR	o	505	1/1	0.96	0.05	111,111,111,111	0
7	HEM	o	502	43/43	0.97	0.13	125,134,142,145	0
7	HEM	C	502	43/43	0.97	0.12	97,104,111,113	0
8	SR	h	102	1/1	0.98	0.11	220,220,220,220	0
13	FE	L	309	1/1	0.98	0.06	65,65,65,65	0
13	FE	x	309	1/1	0.99	0.05	65,65,65,65	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.

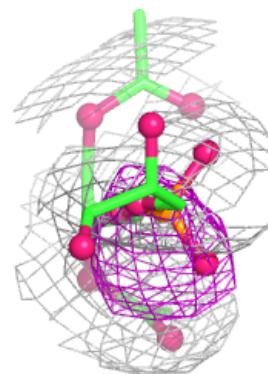
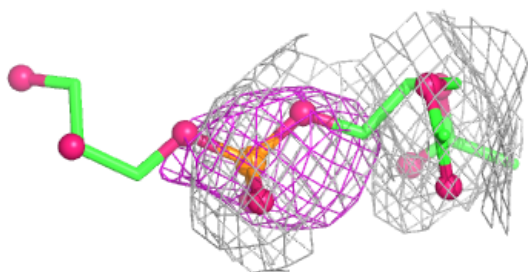
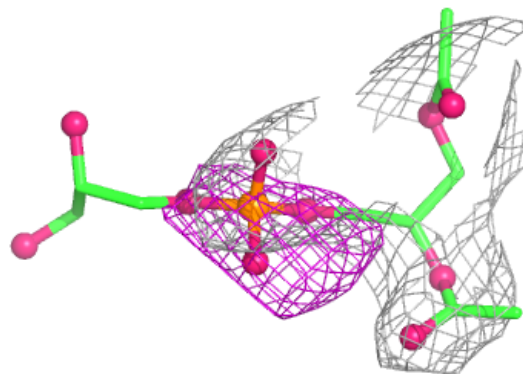
Electron density around PEF y 406:

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



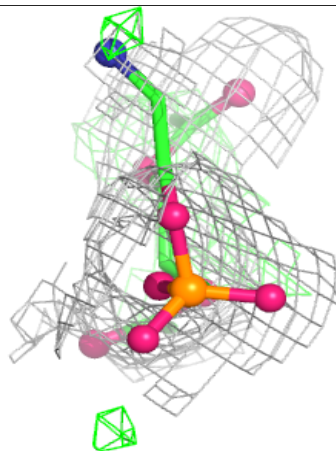
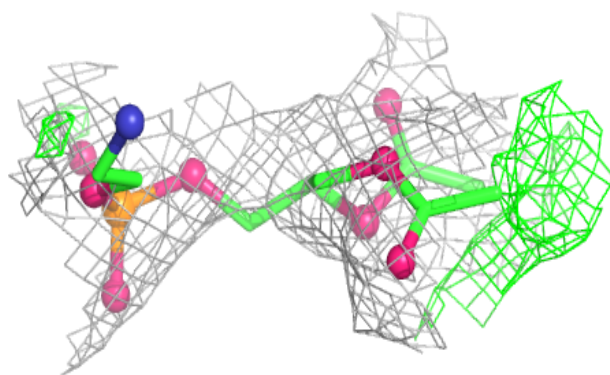
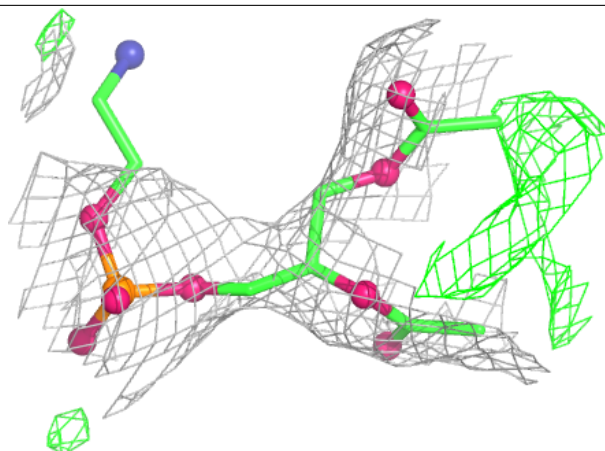
Electron density around PGW AE 101:

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



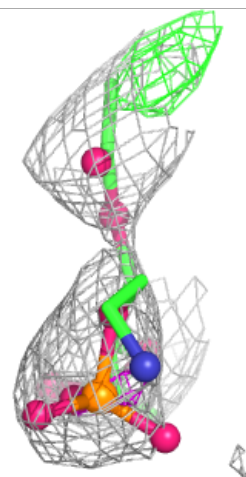
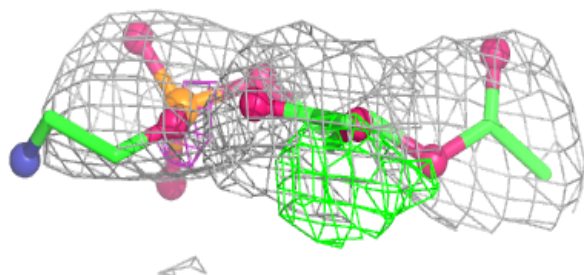
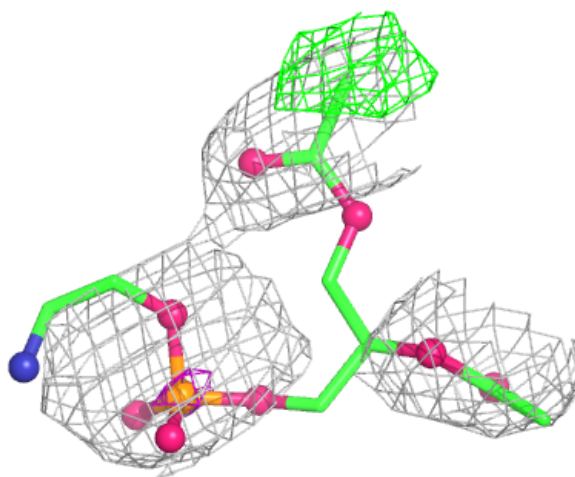
Electron density around PEF A 101:

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



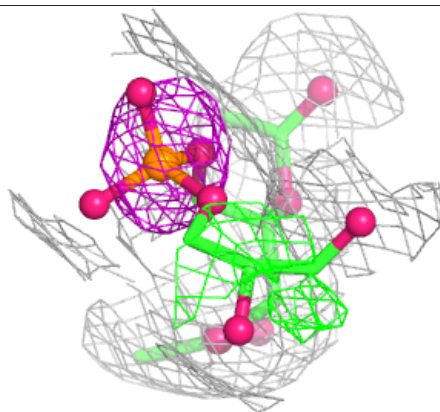
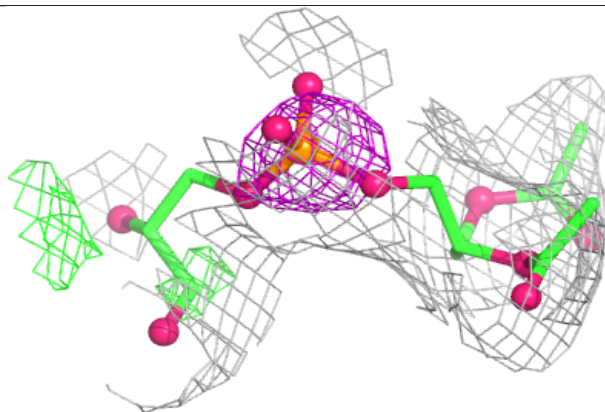
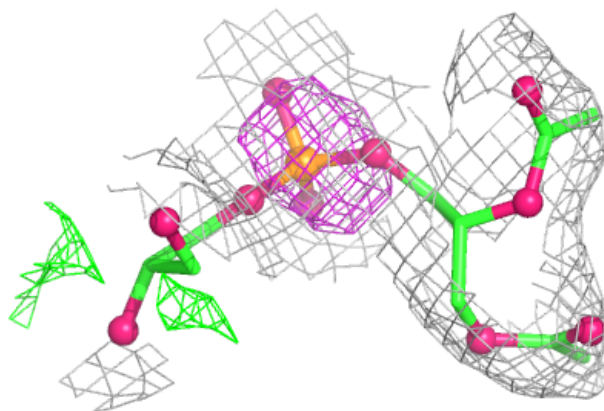
Electron density around PEF m 101:

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



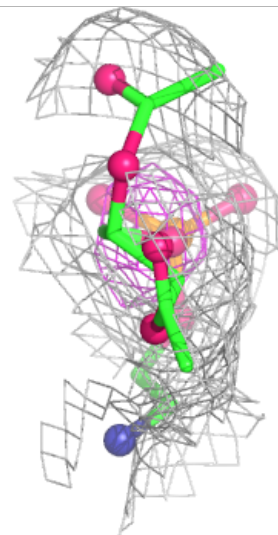
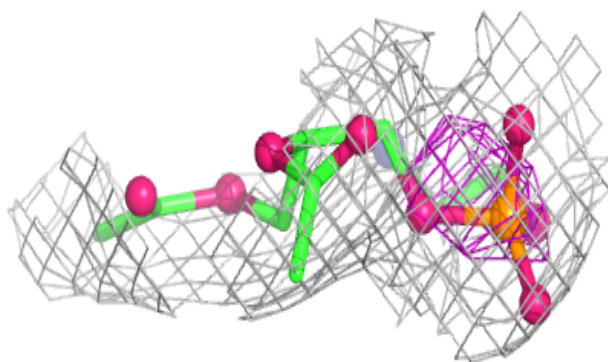
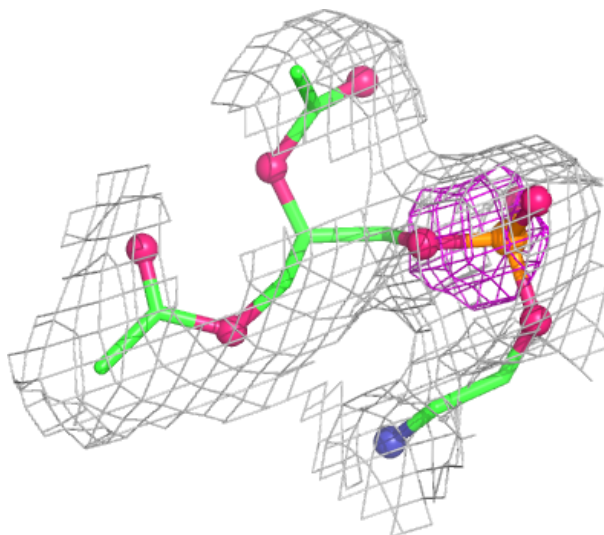
Electron density around PGW S 101:

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



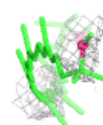
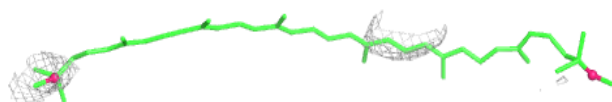
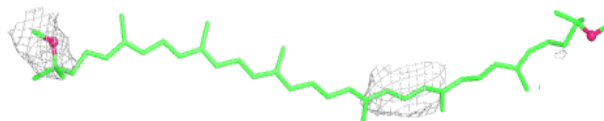
Electron density around PEF x 306:

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

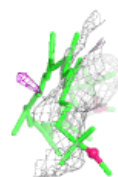
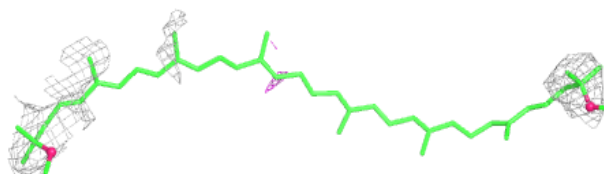


Electron density around CRT J 101:

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

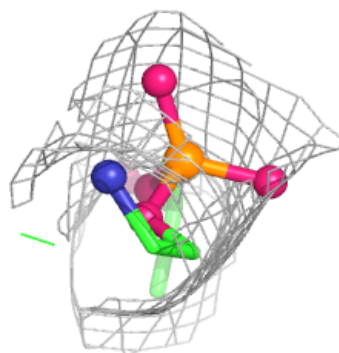
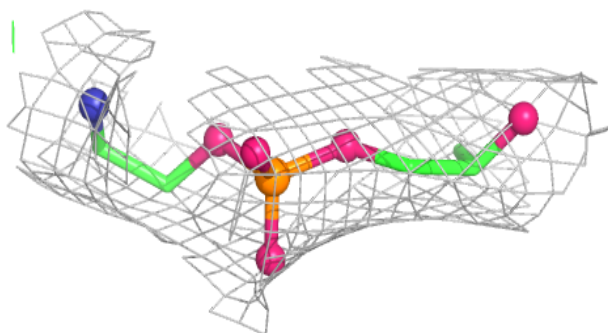
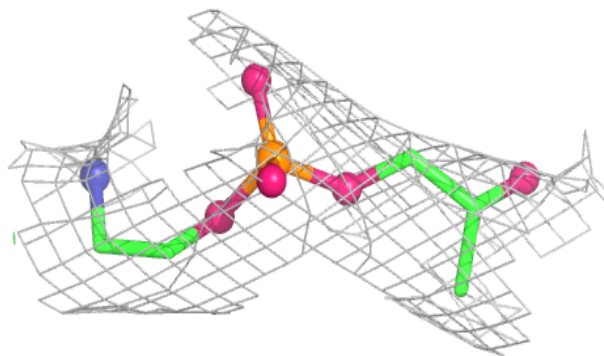
**Electron density around CRT AL 101:**

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

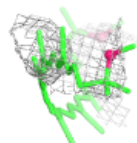
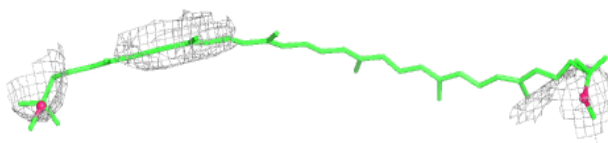
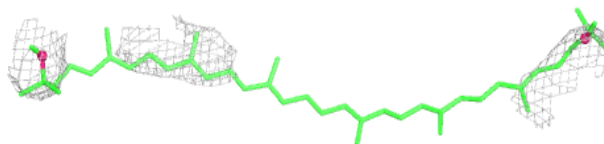


Electron density around PEF L 306:

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

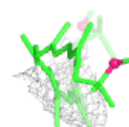
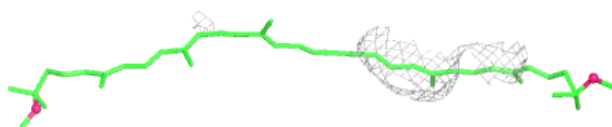
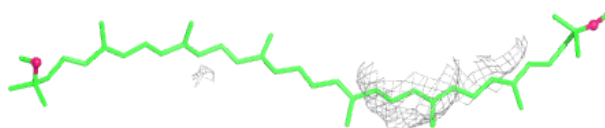
**Electron density around CRT N 101:**

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

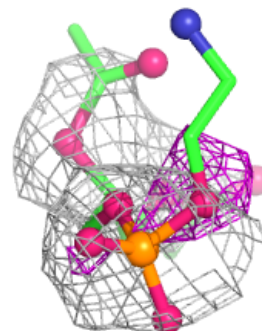
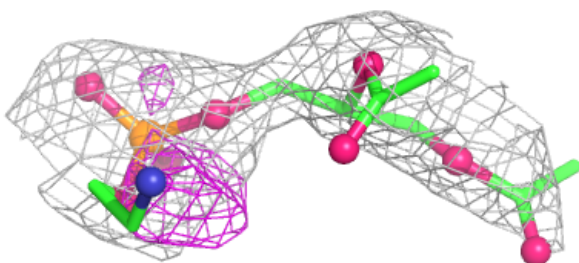
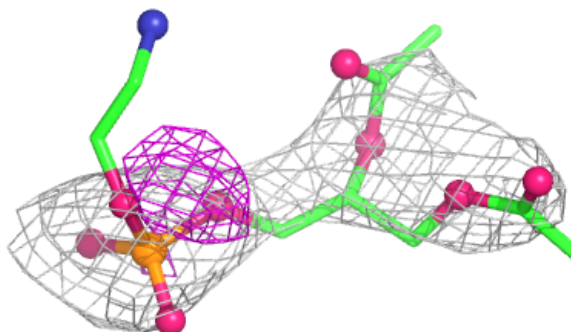


Electron density around CRT AH 102:

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

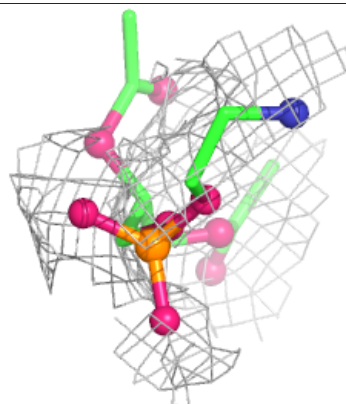
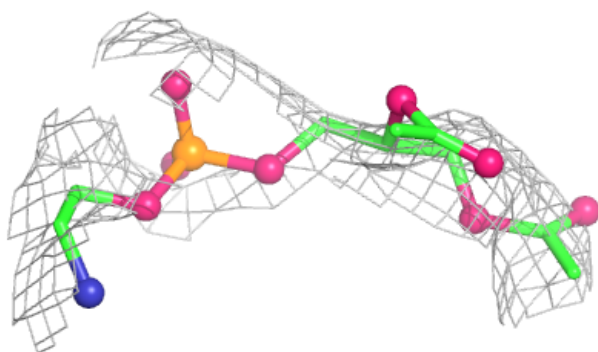
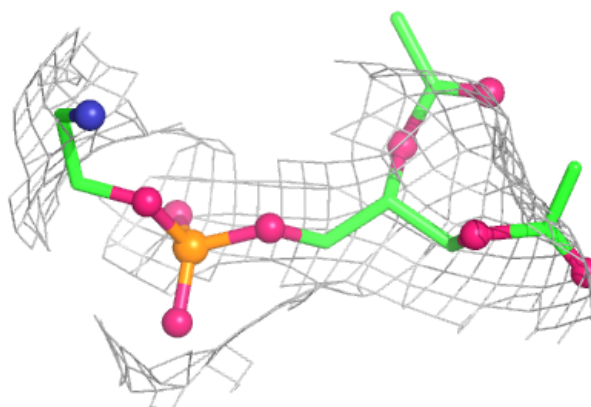
**Electron density around PEF y 408:**

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



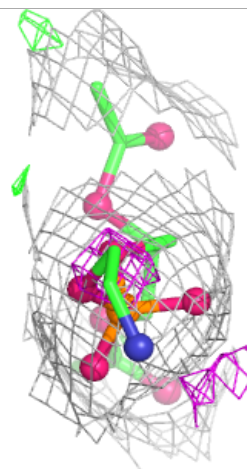
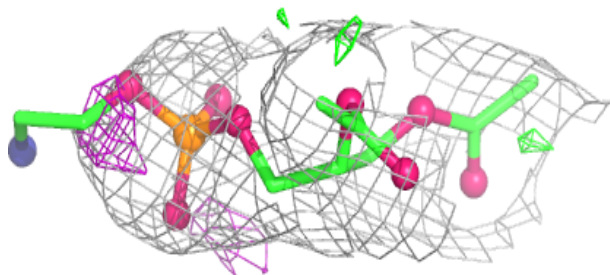
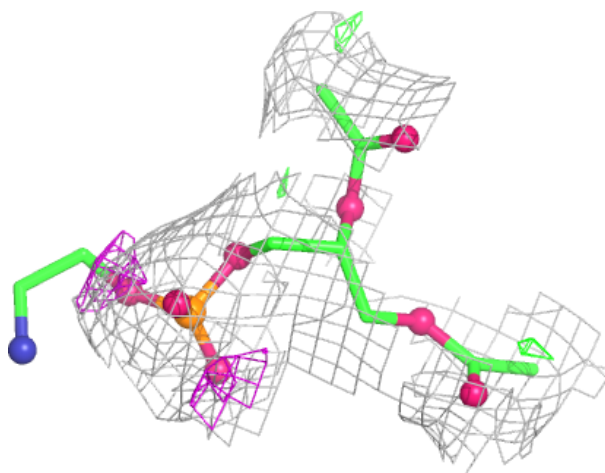
Electron density around PEF H 303:

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



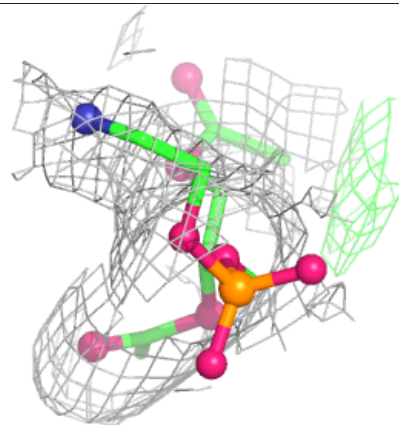
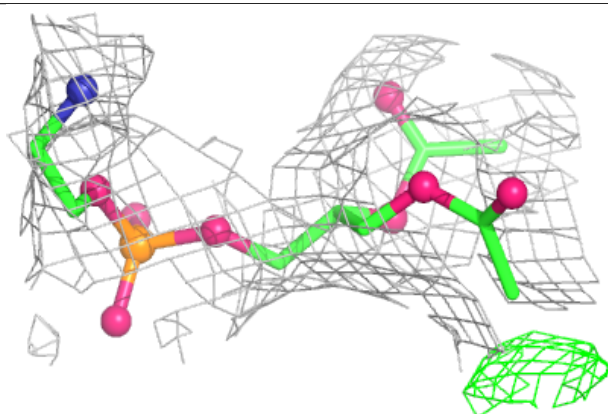
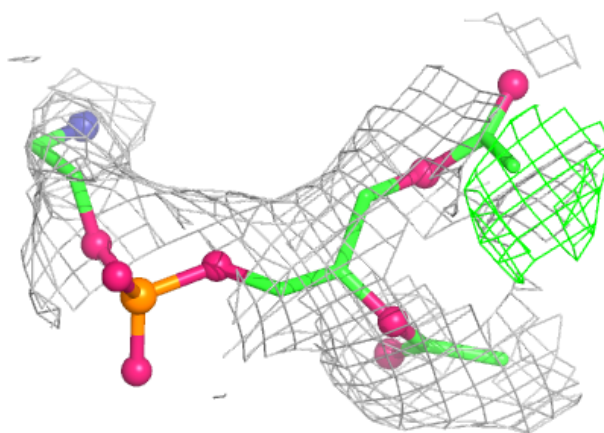
Electron density around PEF t 303:

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

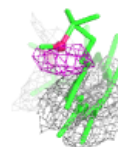
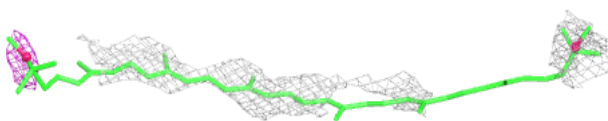
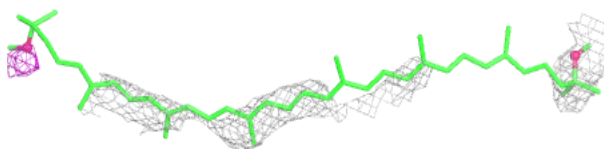


Electron density around PEF y 407:

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

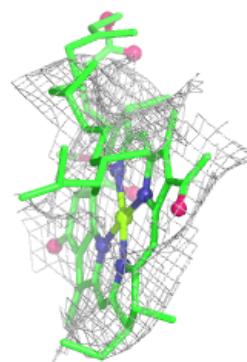
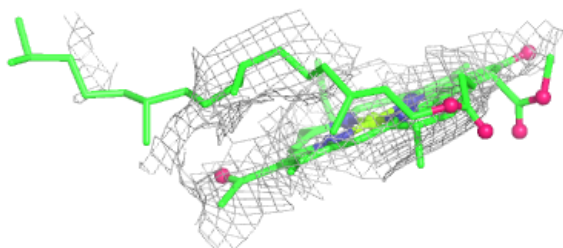
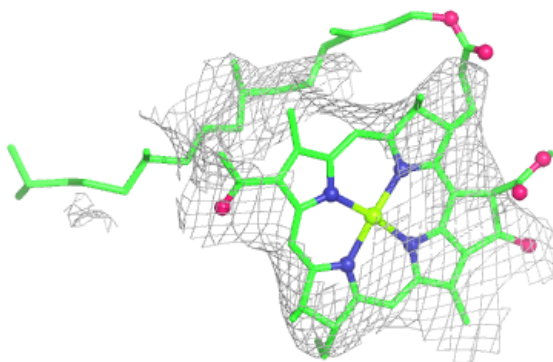
**Electron density around CRT p 103:**

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

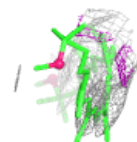
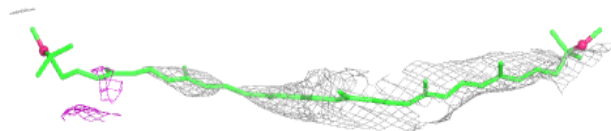
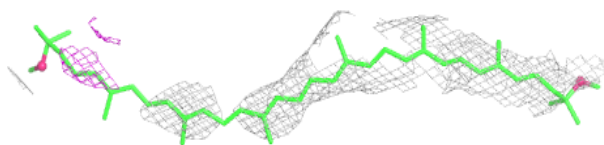


Electron density around BCL AE 104:

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

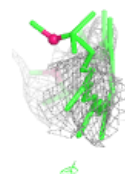
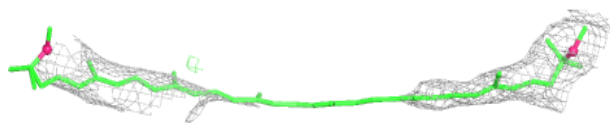
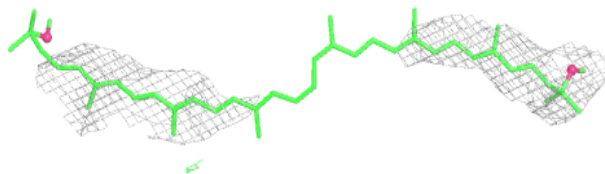
**Electron density around CRT c 101:**

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



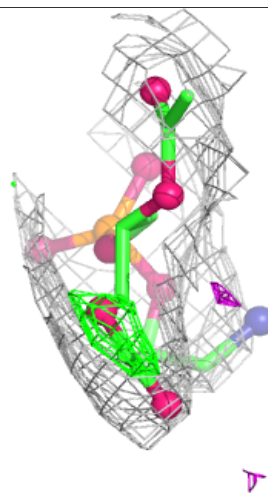
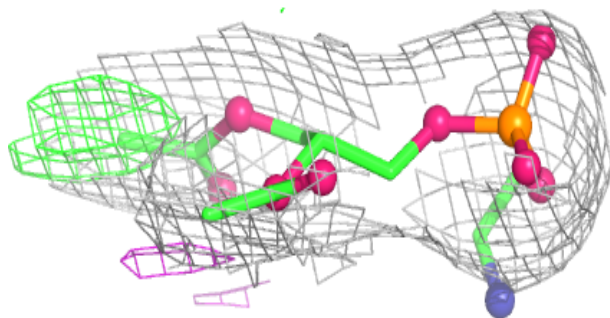
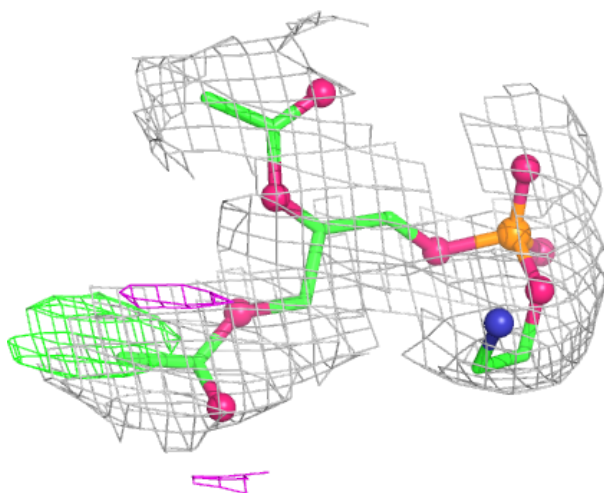
Electron density around CRT 8 101:

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



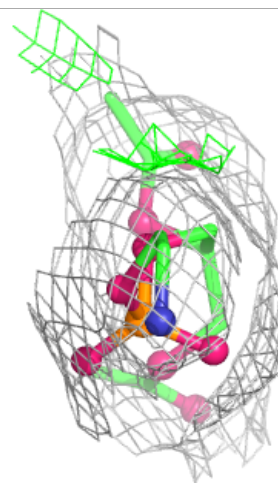
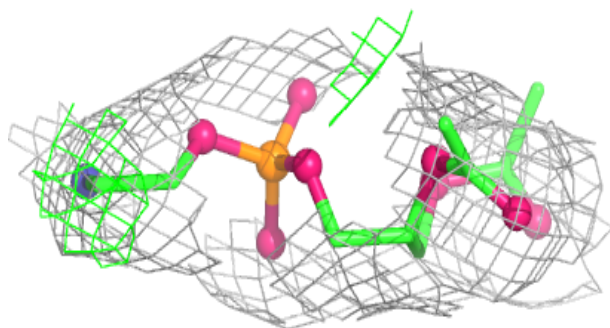
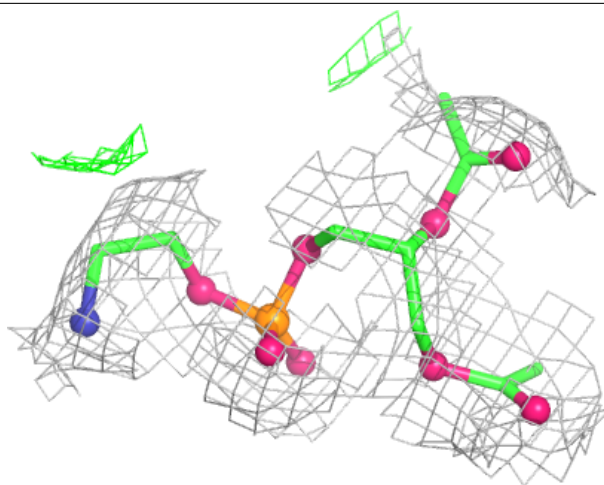
Electron density around PEF t 301:

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



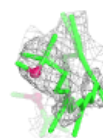
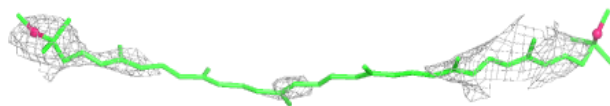
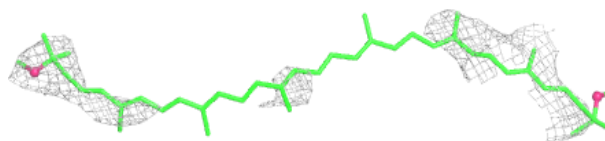
Electron density around PEF H 304:

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



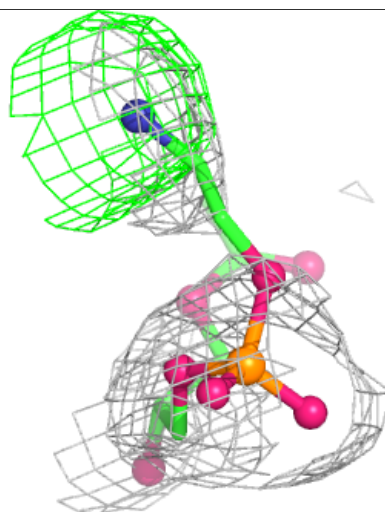
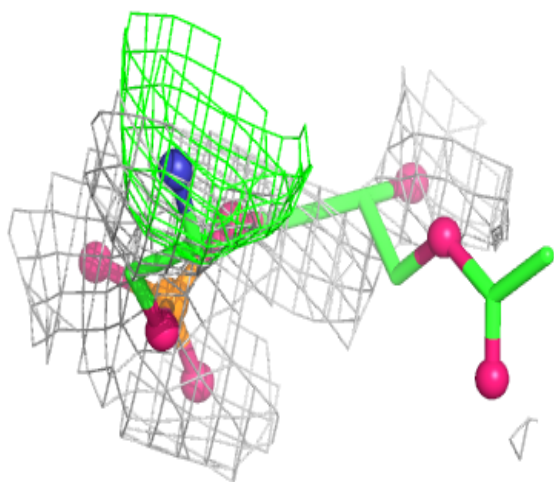
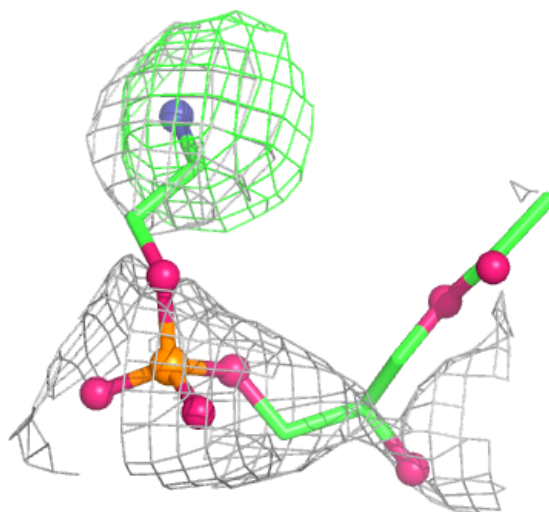
Electron density around CRT i 101:

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



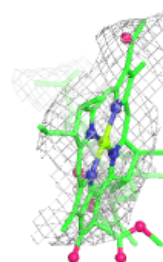
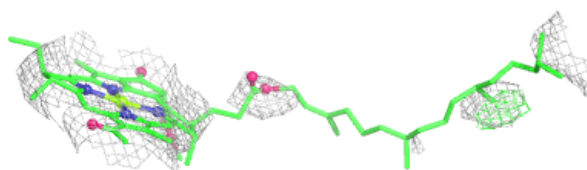
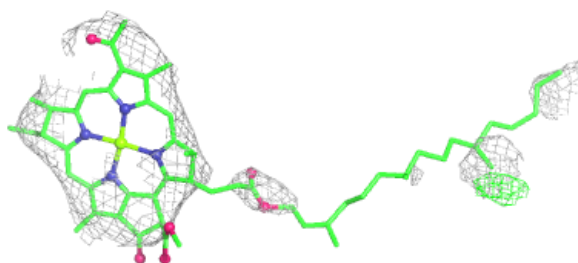
Electron density around PEF p 101:

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



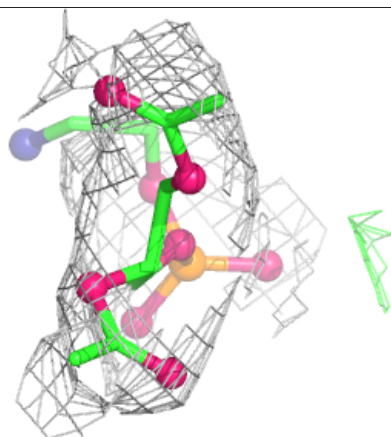
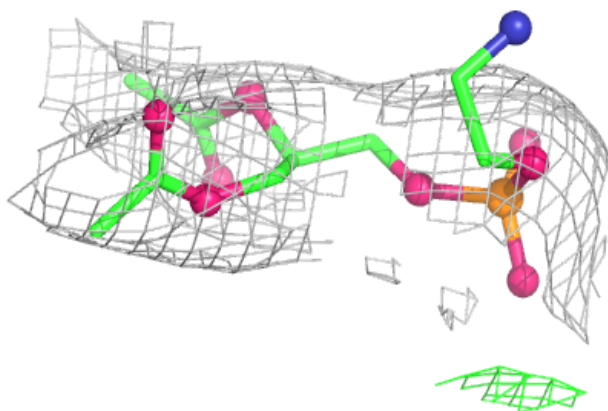
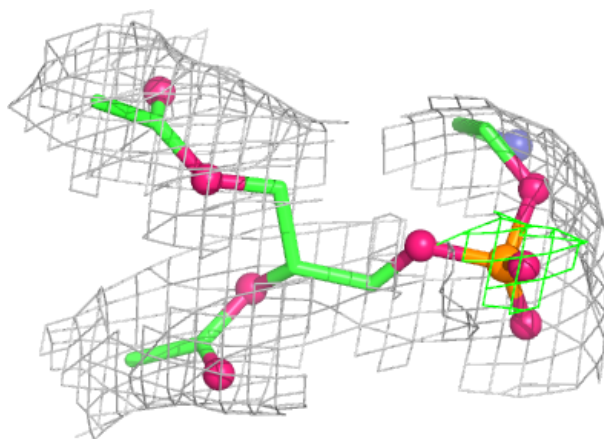
Electron density around BCL 1 101:

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



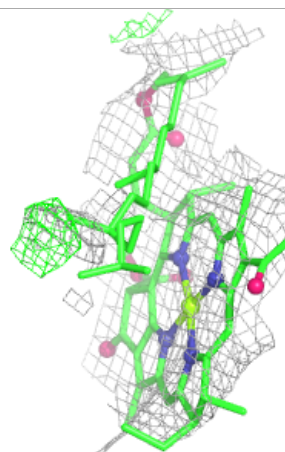
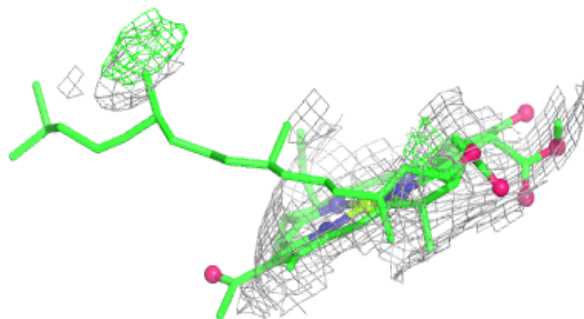
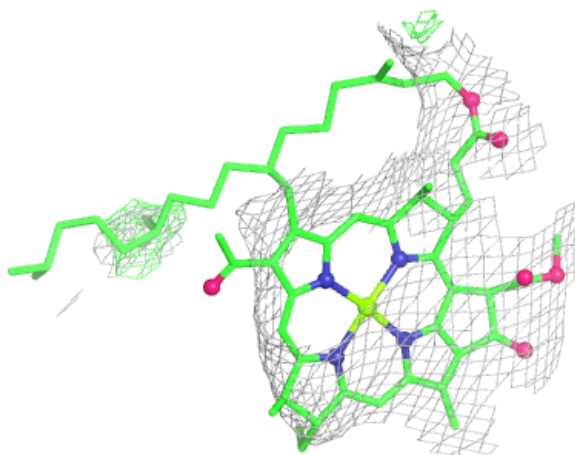
Electron density around PEF M 406:

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



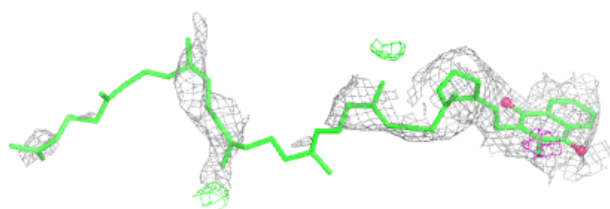
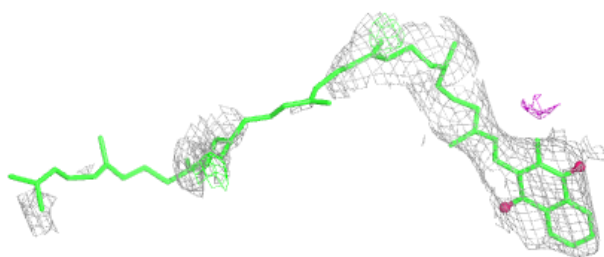
Electron density around BCL AC 102:

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

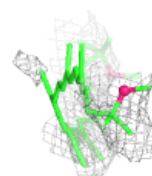
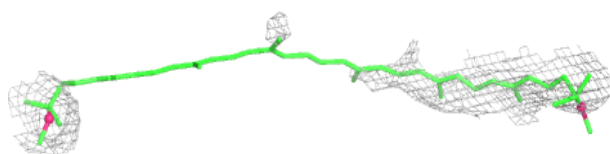
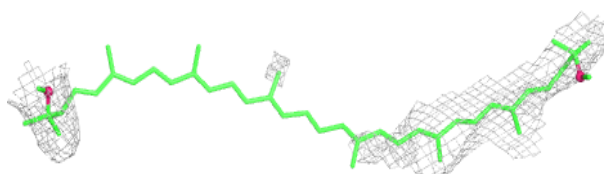


Electron density around MQ8 M 403:

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

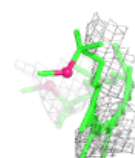
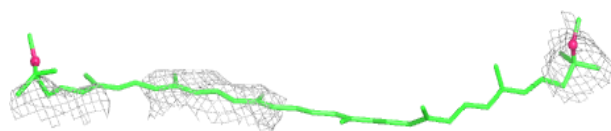
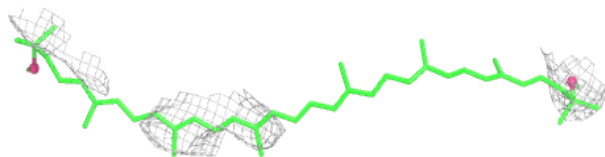
**Electron density around CRT E 101:**

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

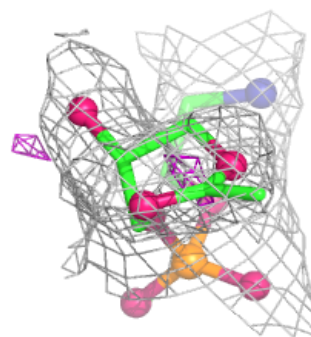
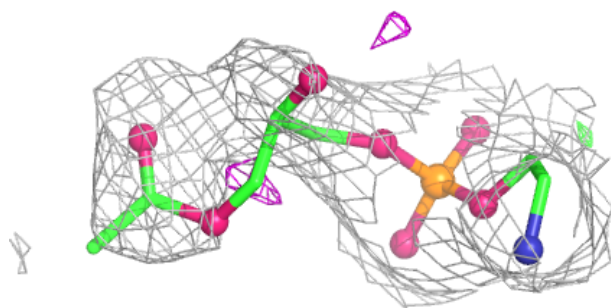
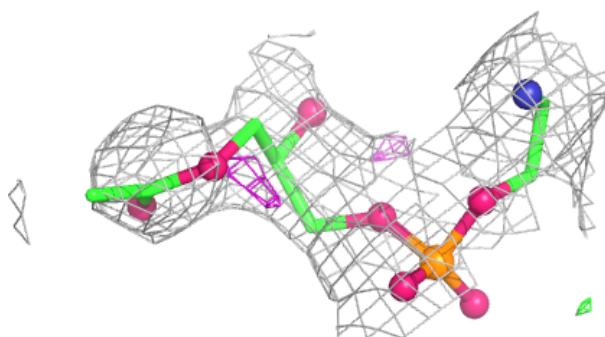


Electron density around CRT G 101:

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

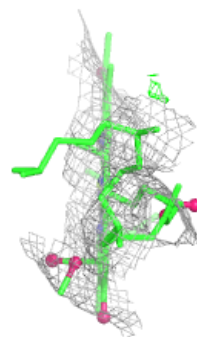
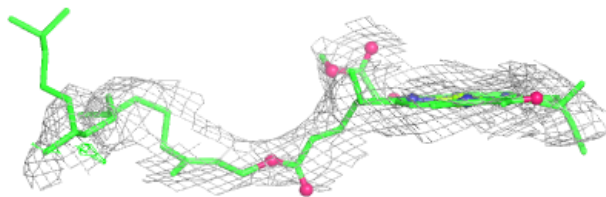
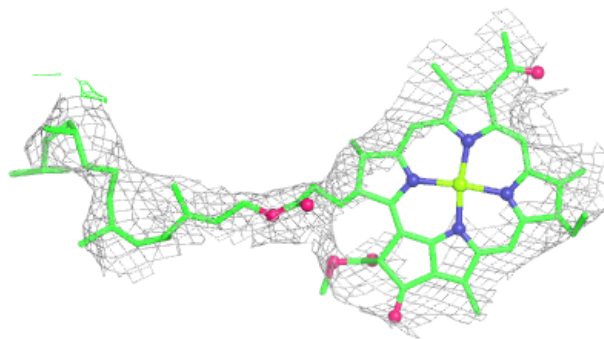
**Electron density around PEF M 407:**

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

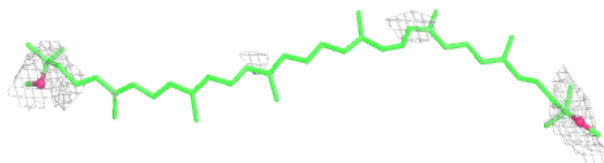


Electron density around BCL j 101:

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

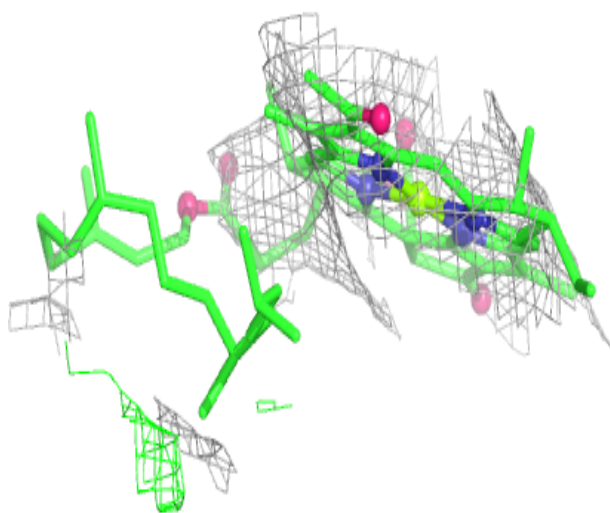
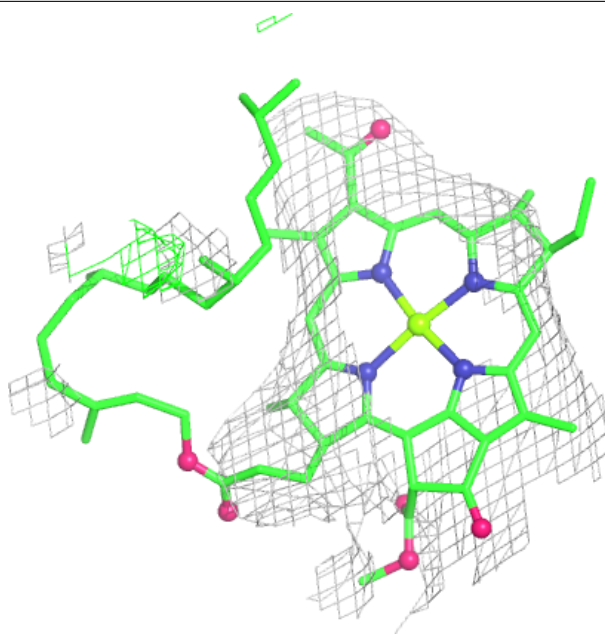
**Electron density around CRT R 101:**

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



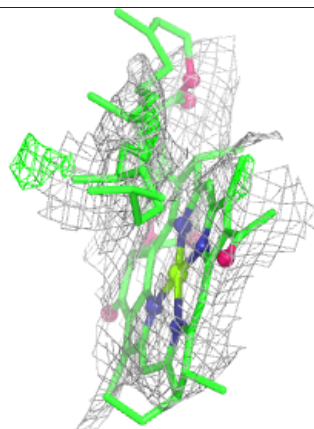
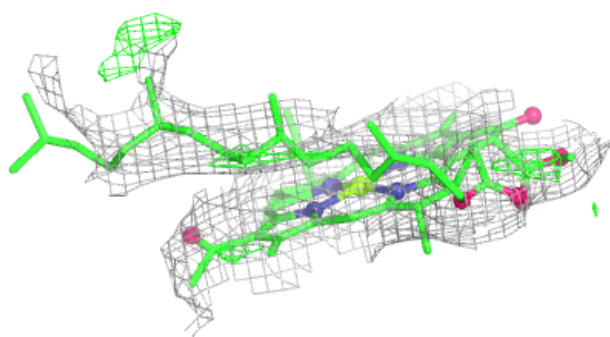
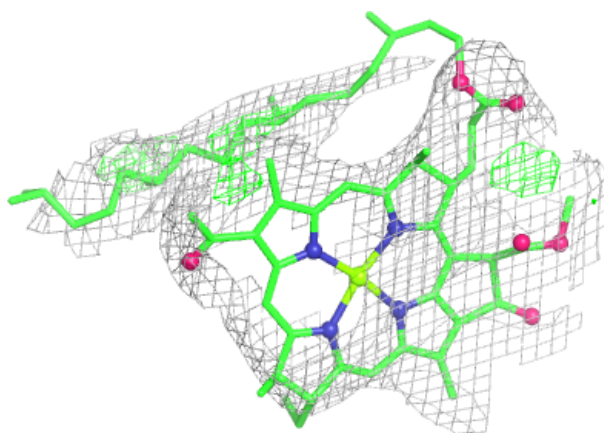
Electron density around BCL m 103:

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

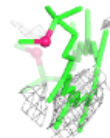
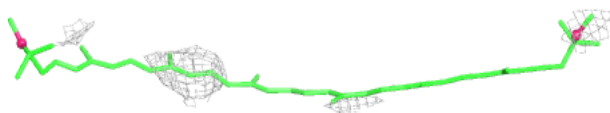
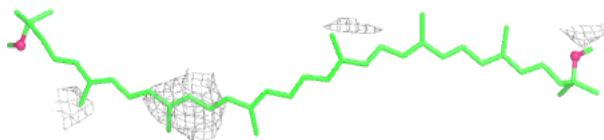


Electron density around BCL AH 103:

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

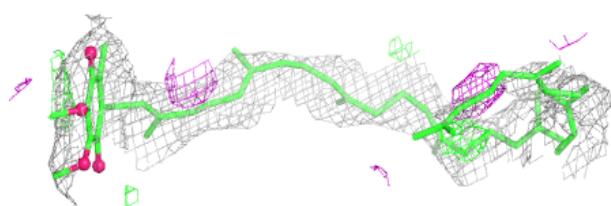
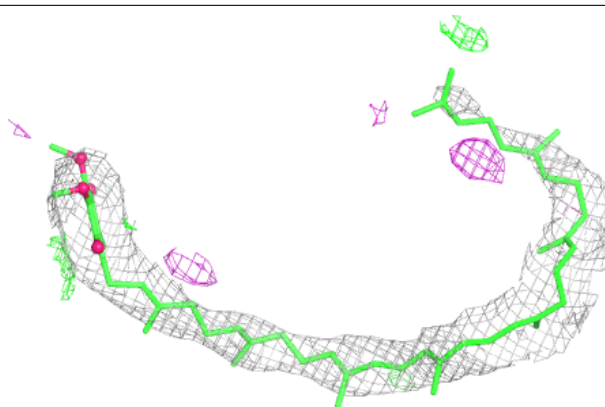
**Electron density around CRT z 101:**

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

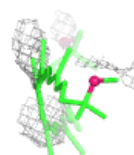
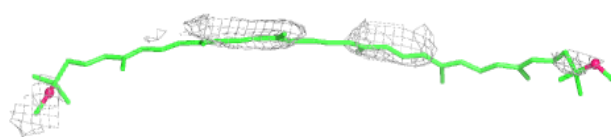


Electron density around UQ8 L 304:

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

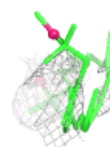
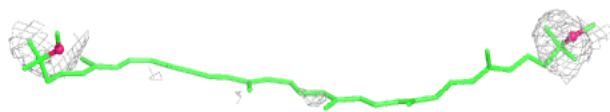
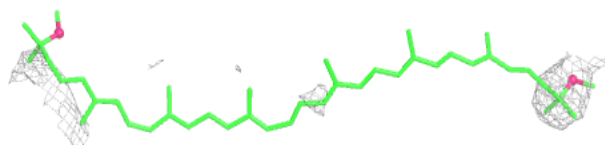
**Electron density around CRT AC 101:**

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

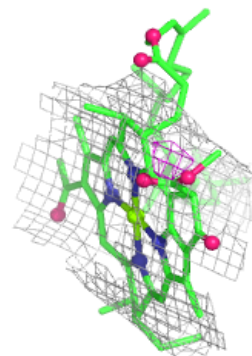
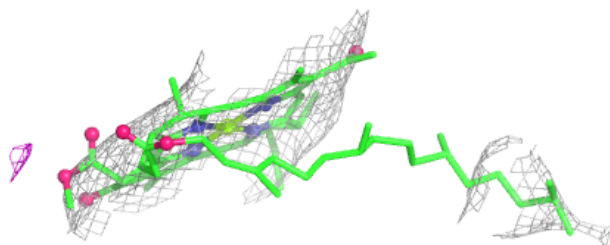
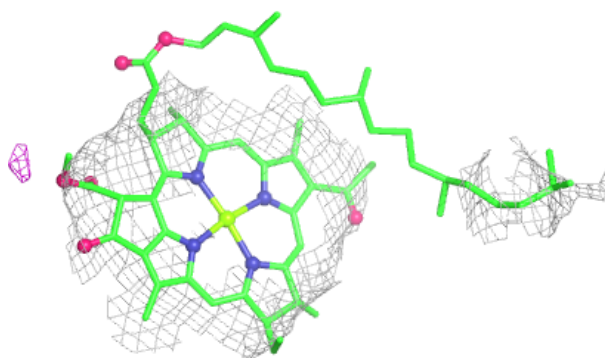


Electron density around CRT AJ 101:

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

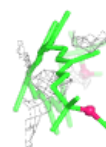
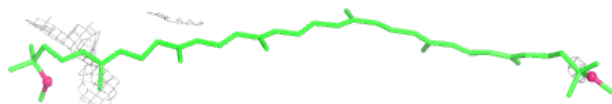
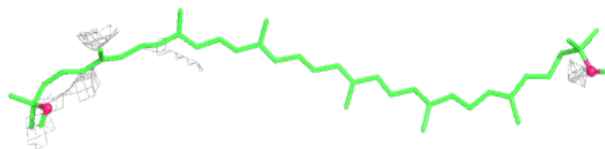
**Electron density around BCL G 102:**

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

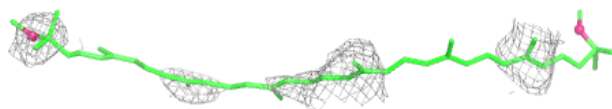
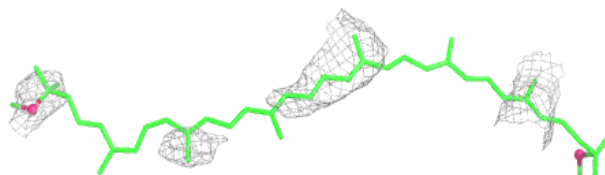


Electron density around CRT e 101:

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

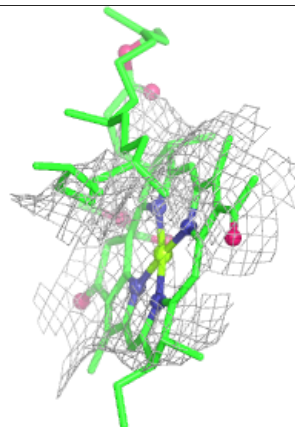
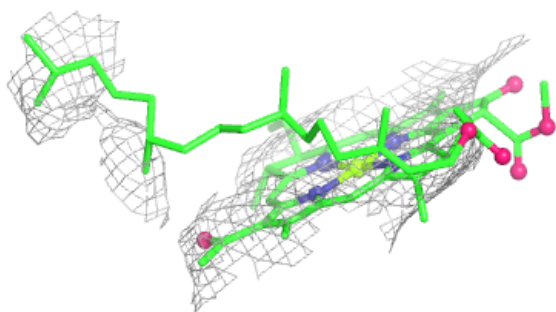
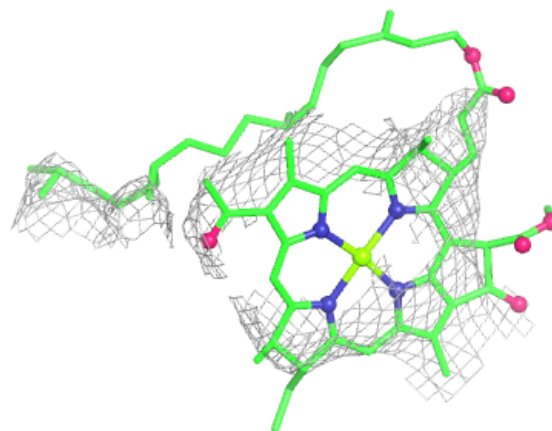
**Electron density around CRT f 102:**

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

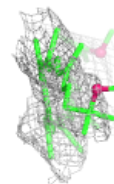
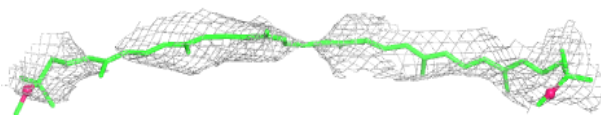
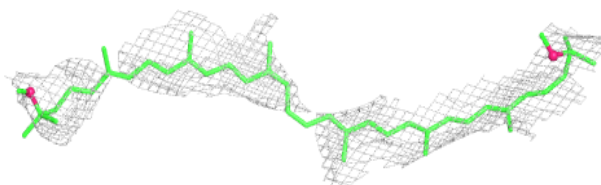


Electron density around BCL N 102:

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

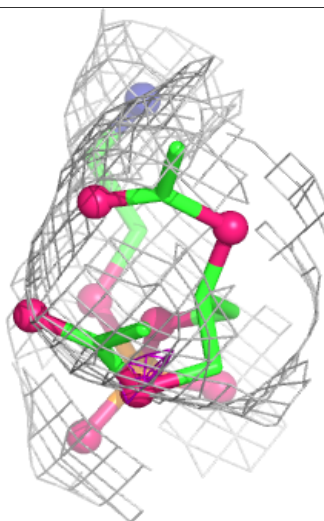
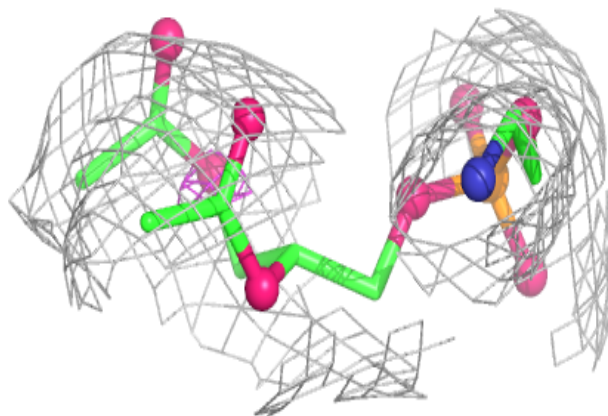
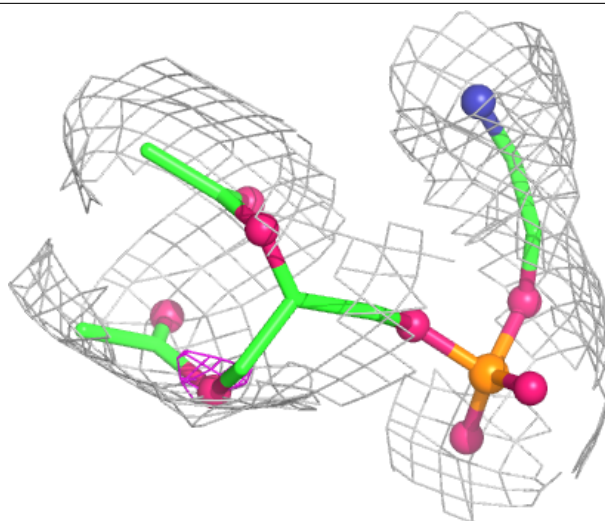
**Electron density around CRT k 101:**

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



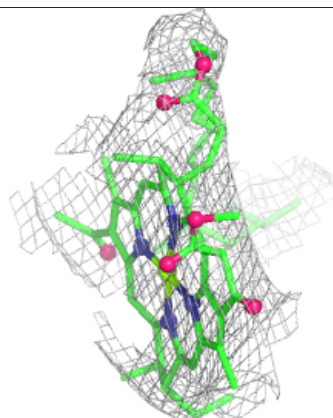
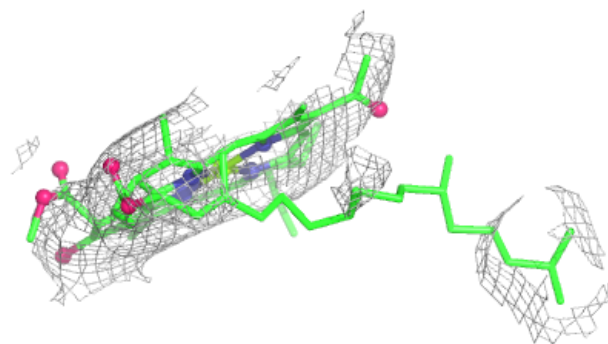
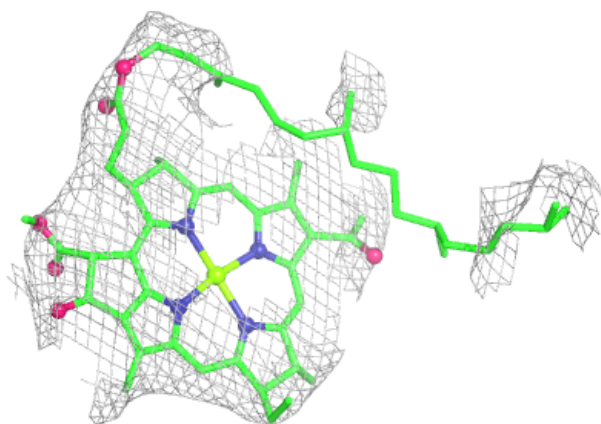
Electron density around PEF M 408:

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

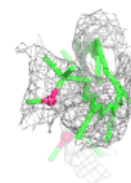
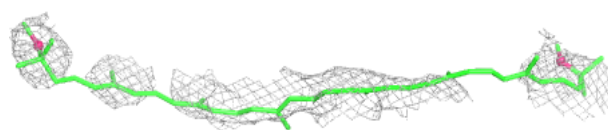
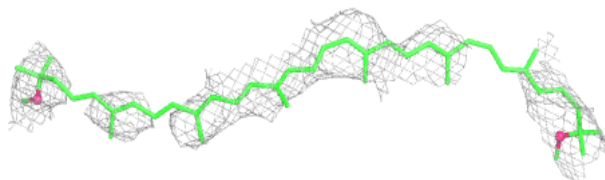


Electron density around BCL T 102:

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

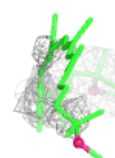
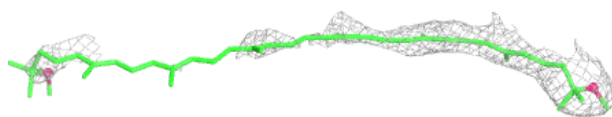
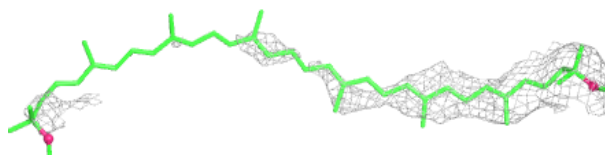
**Electron density around CRT X 101:**

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

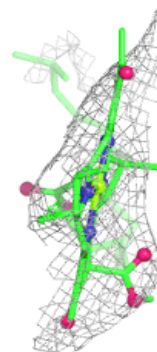
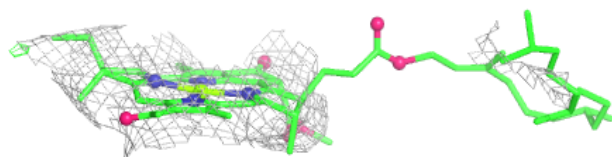
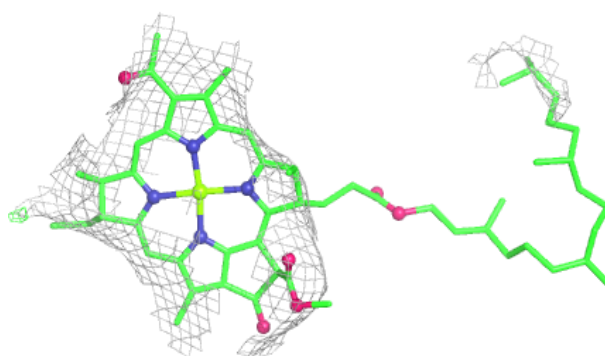


Electron density around CRT 2 101:

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

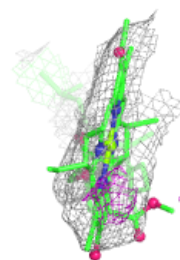
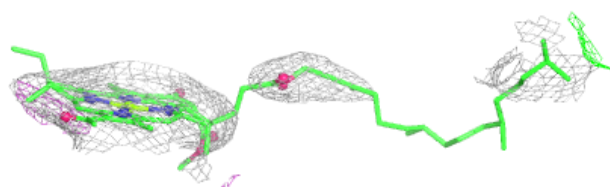
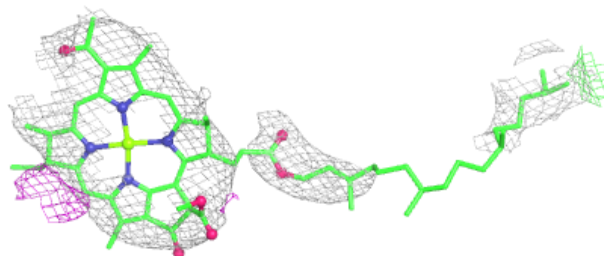
**Electron density around BCL f 101:**

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

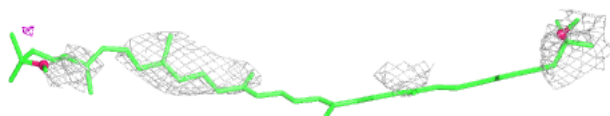
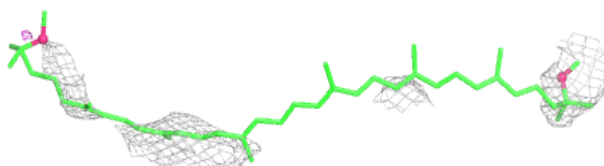


Electron density around BCL S 102:

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

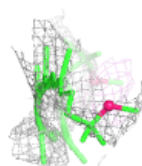
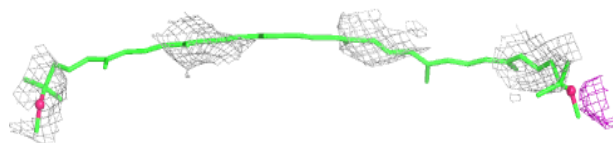
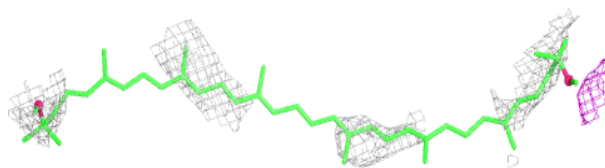
**Electron density around CRT n 101:**

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

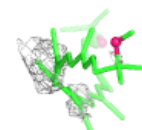
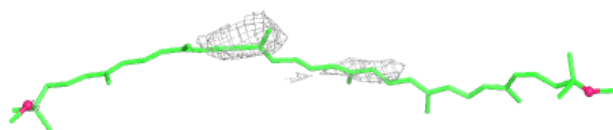
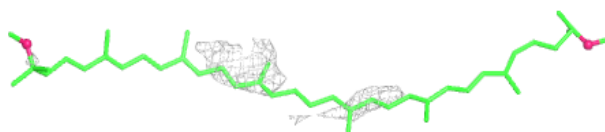


Electron density around CRT s 101:

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

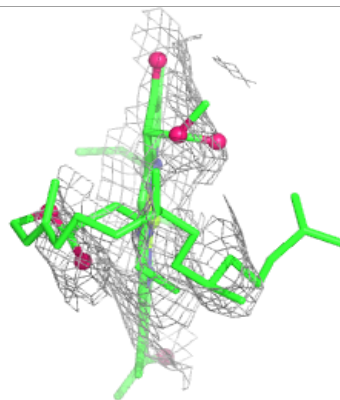
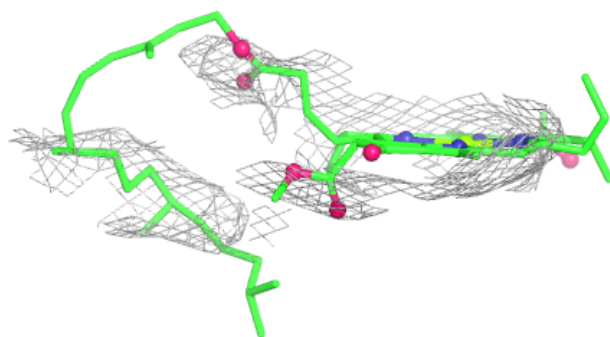
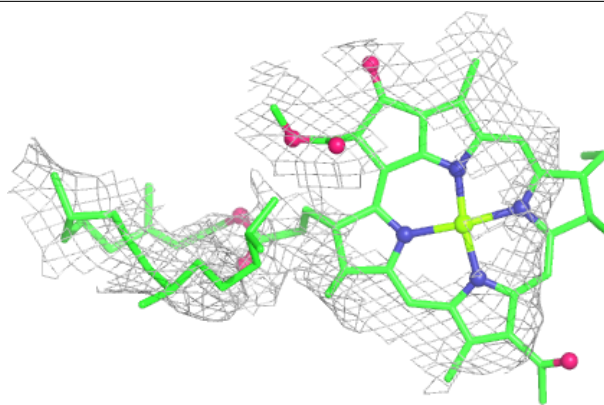
**Electron density around CRT v 101:**

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



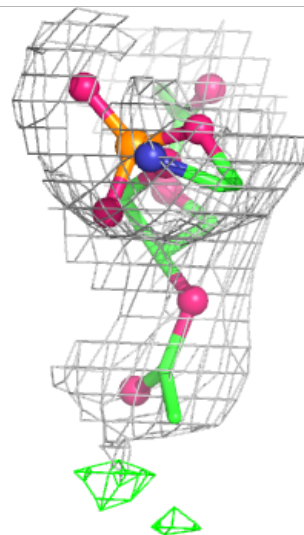
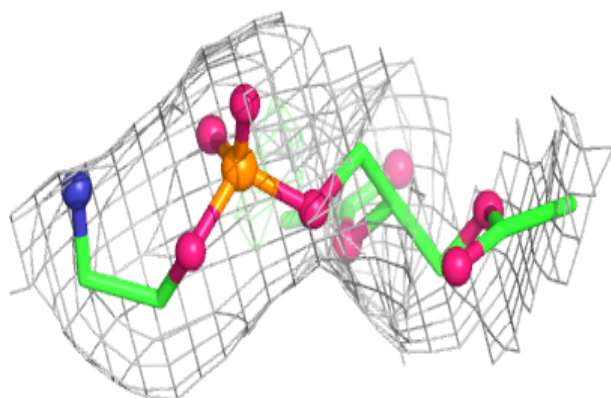
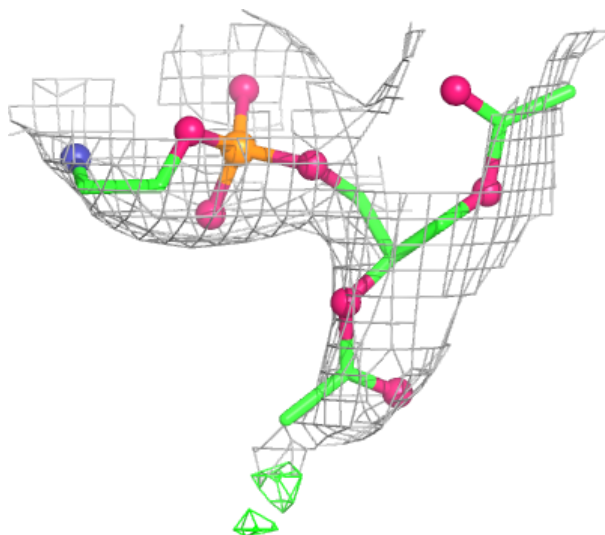
Electron density around BCL AD 101:

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



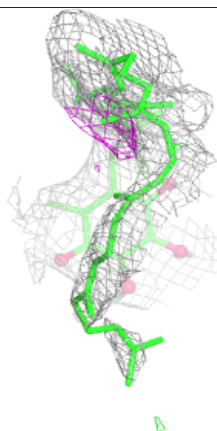
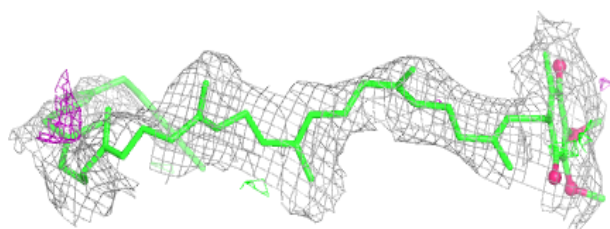
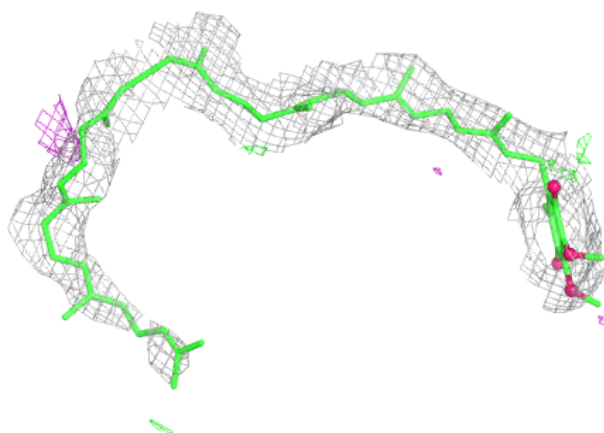
Electron density around PEF H 301:

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

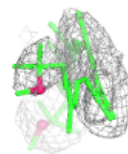
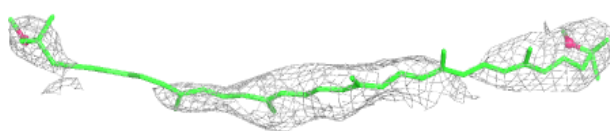
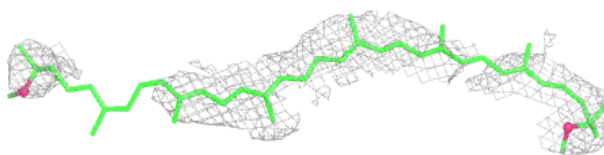


Electron density around UQ8 x 304:

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

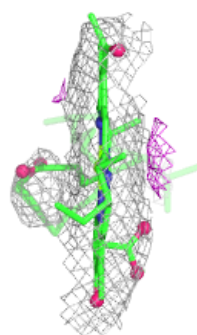
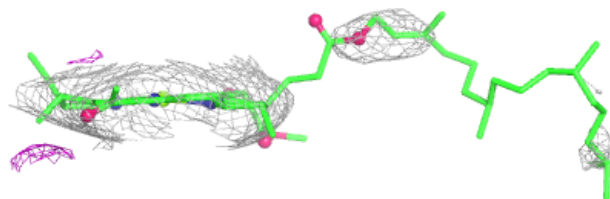
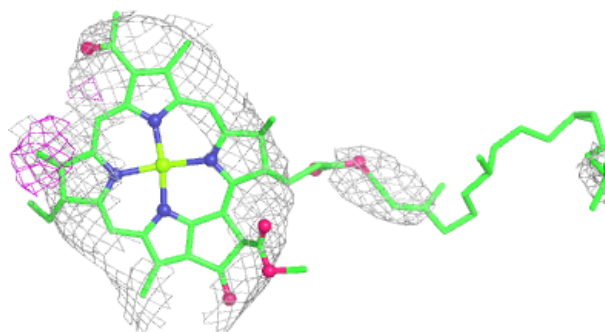
**Electron density around CRT 4 101:**

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

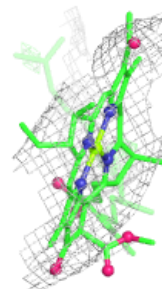
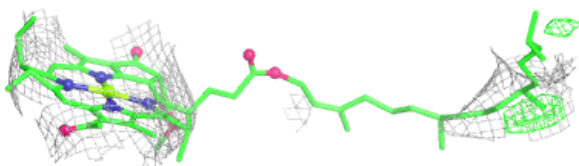
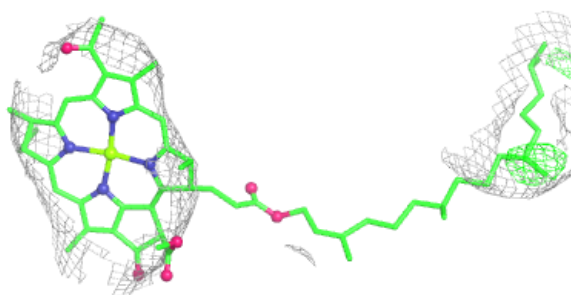


Electron density around BCL AK 101:

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

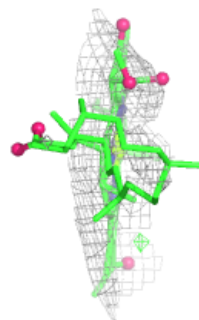
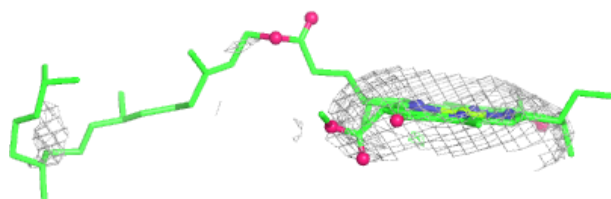
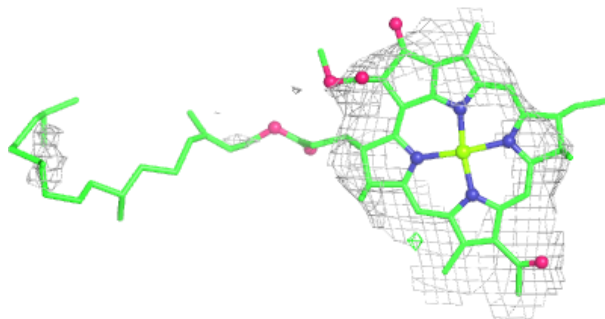
**Electron density around BCL d 101:**

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

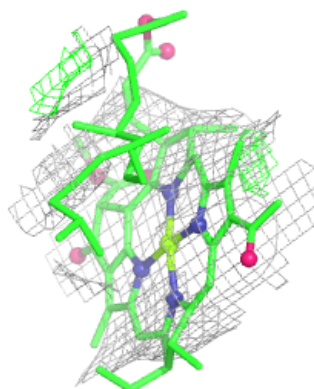
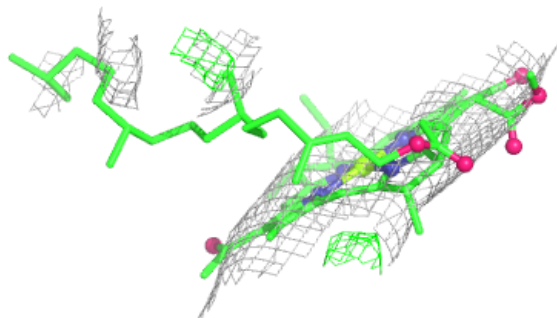
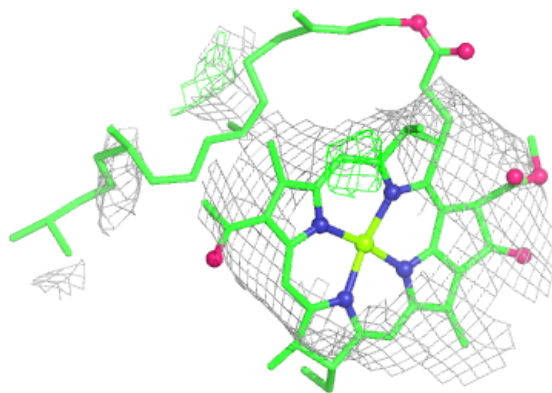


Electron density around BCL K 101:

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

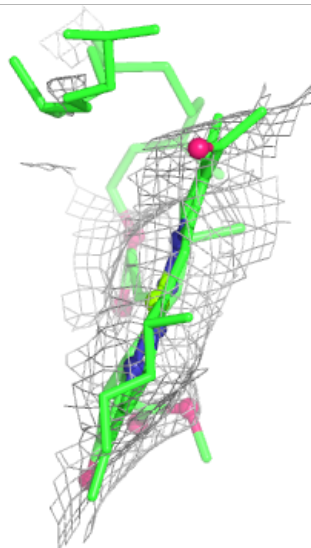
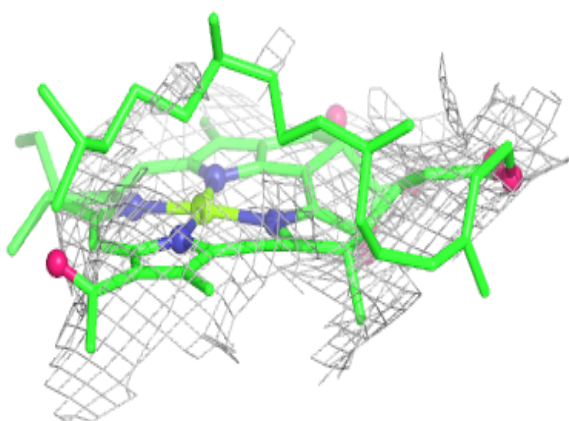
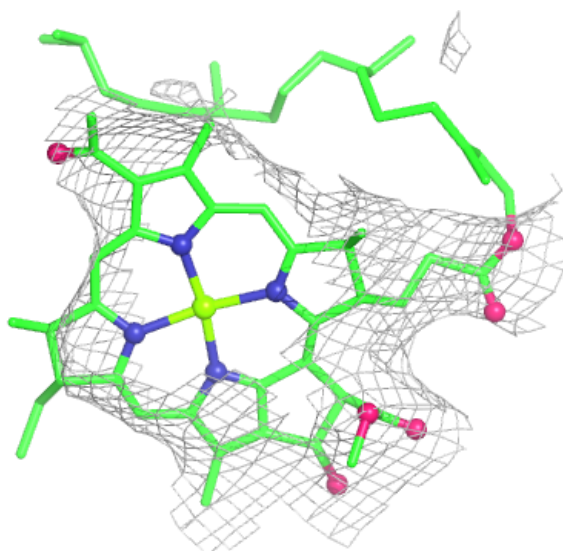
**Electron density around BCL v 102:**

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



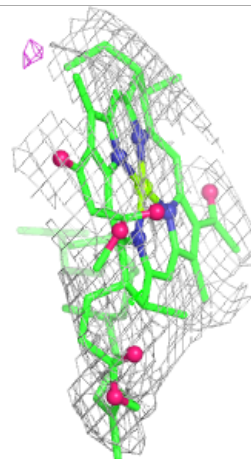
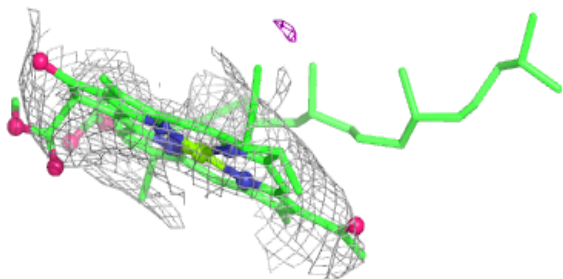
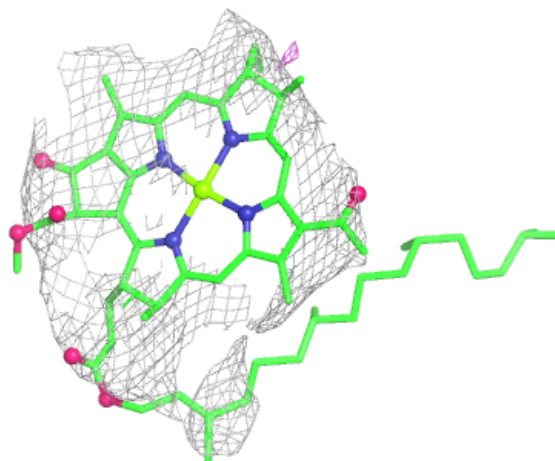
Electron density around BCL k 102:

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



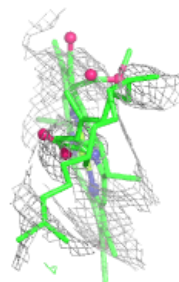
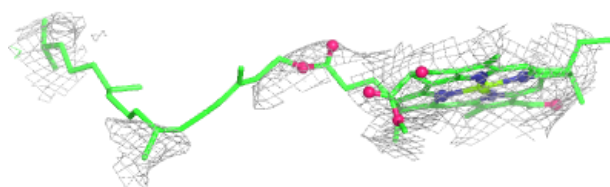
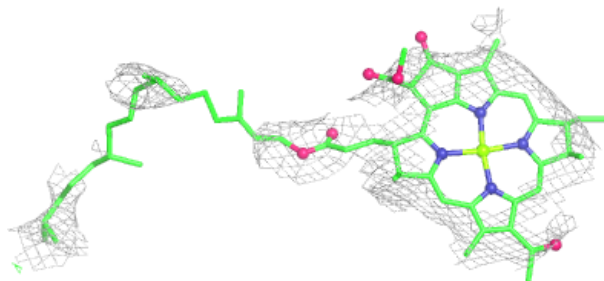
Electron density around BCL R 102:

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

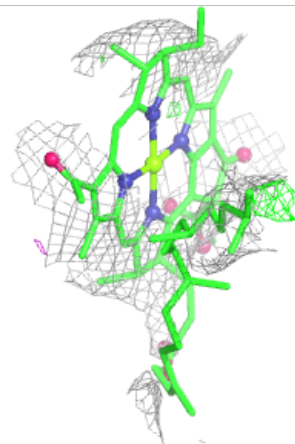
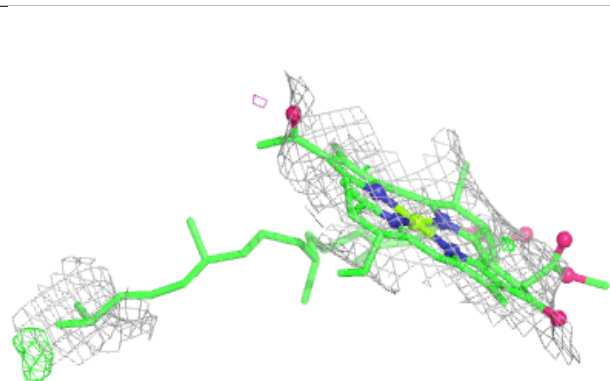
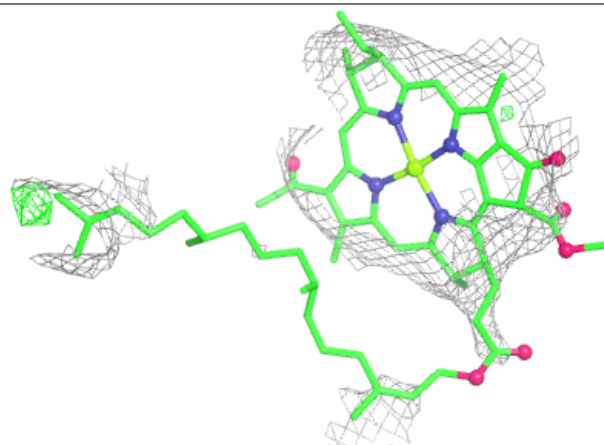


Electron density around BCL AE 102:

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

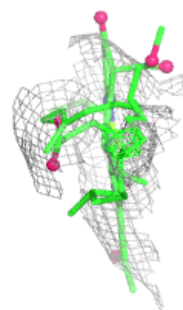
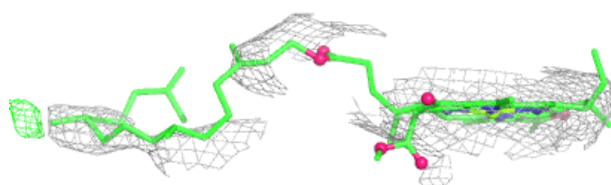
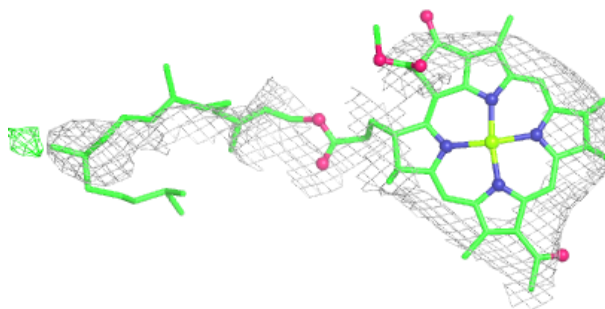
**Electron density around BCL 1 102:**

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

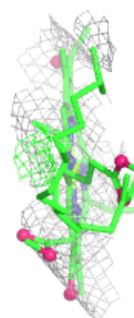
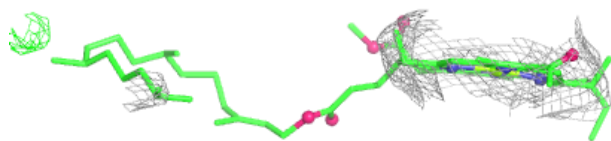
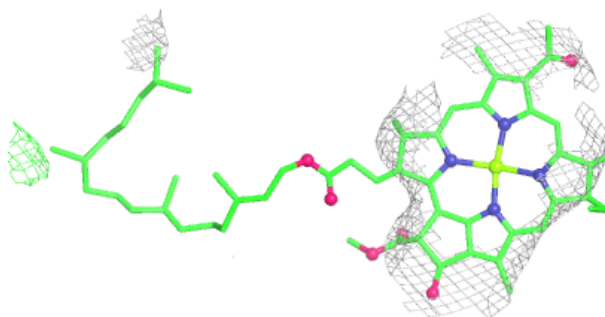


Electron density around BCL AH 101:

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

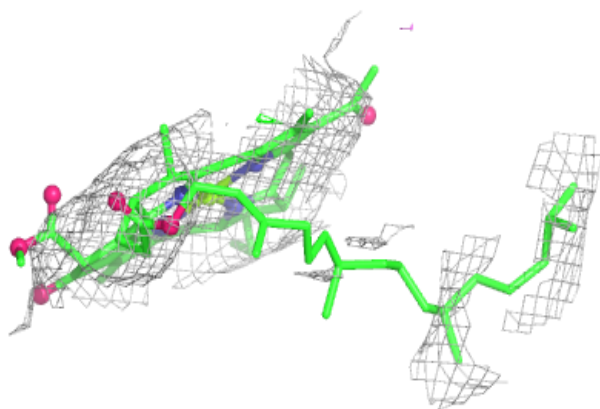
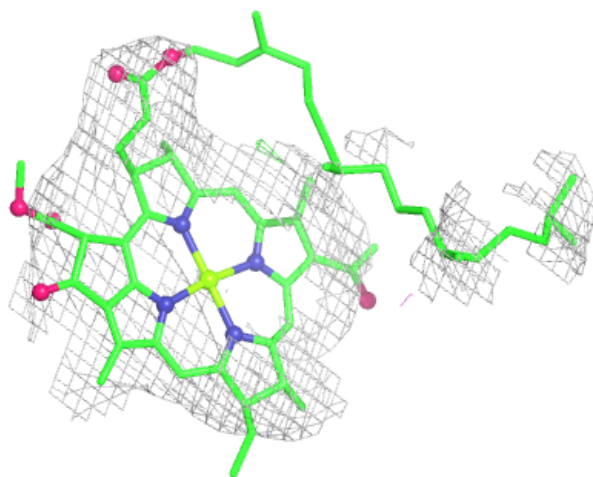
**Electron density around BCL 9 103:**

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



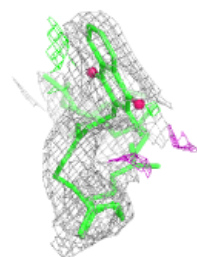
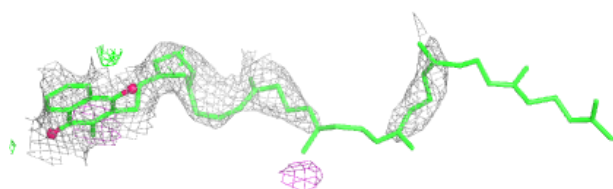
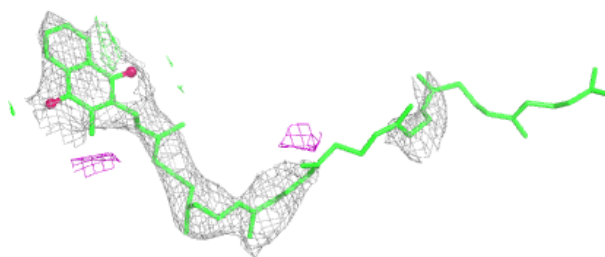
Electron density around BCL AJ 102:

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

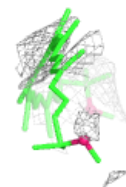
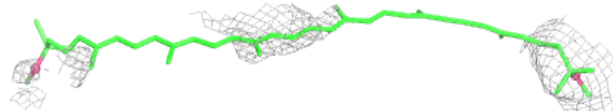
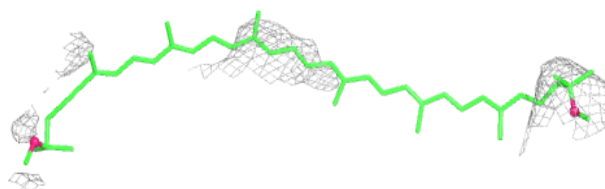


Electron density around MQ8 y 403:

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

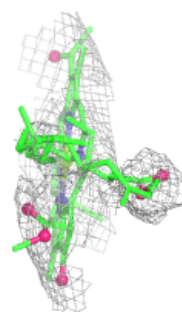
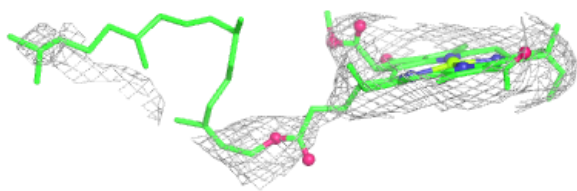
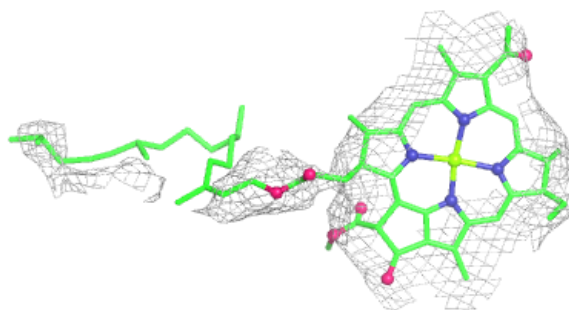
**Electron density around CRT A 103:**

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



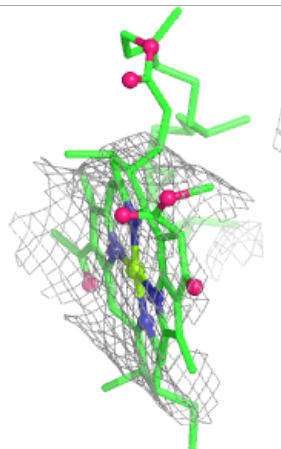
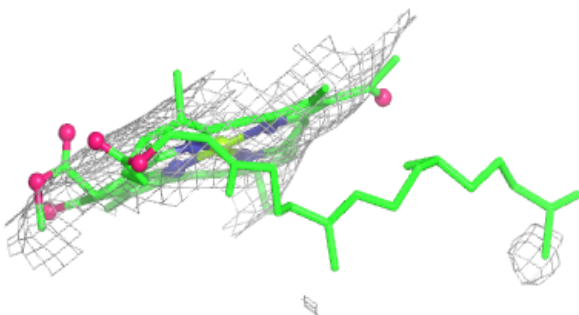
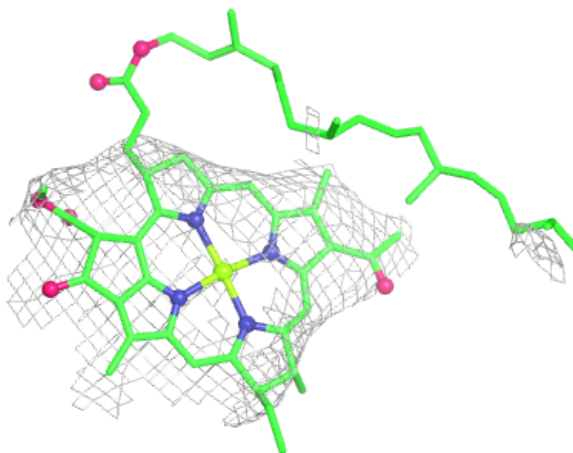
Electron density around BCL h 101:

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



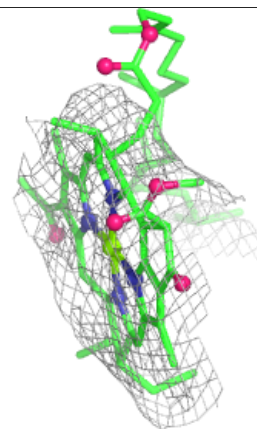
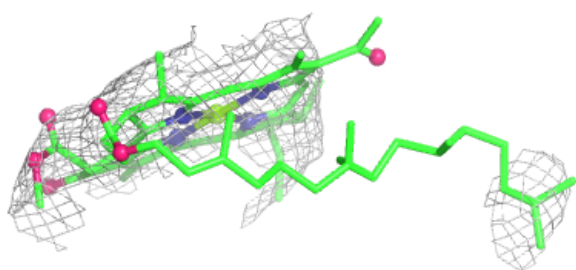
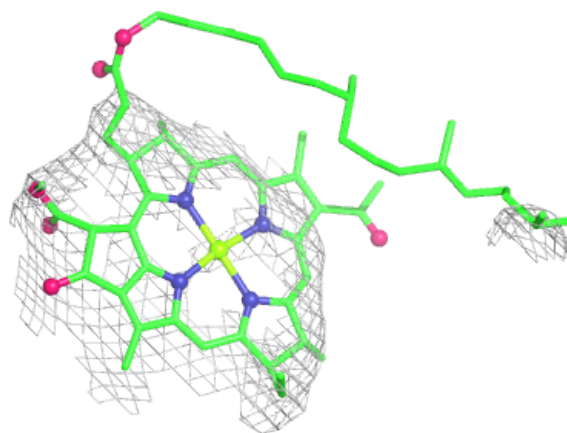
Electron density around BCL z 102:

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



Electron density around BCL 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)

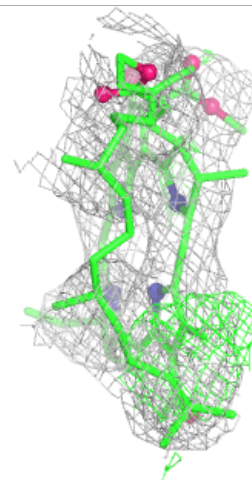
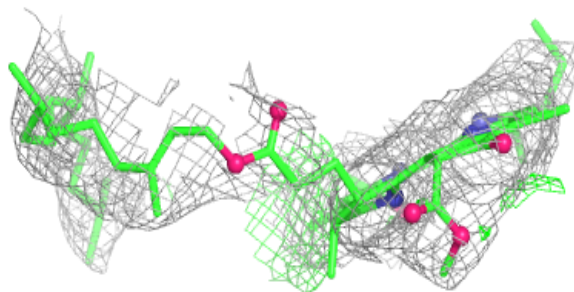
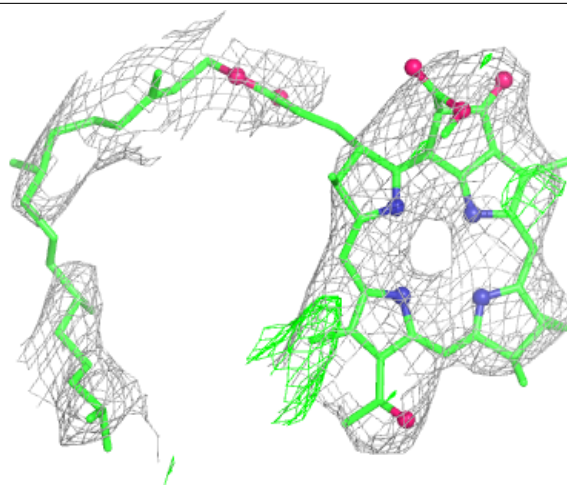
**Electron density around CRT U 102:**

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



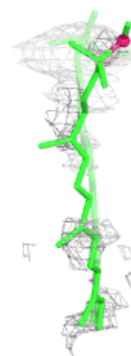
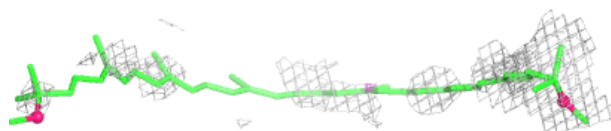
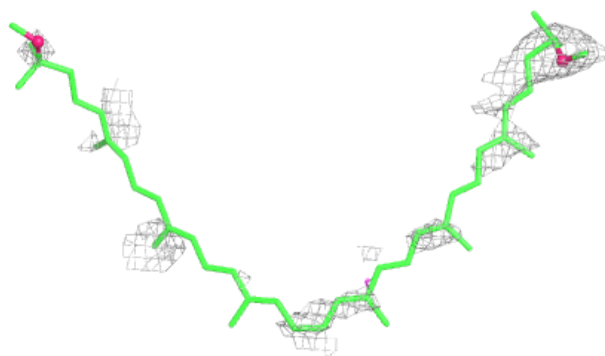
Electron density around BPH L 302:

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

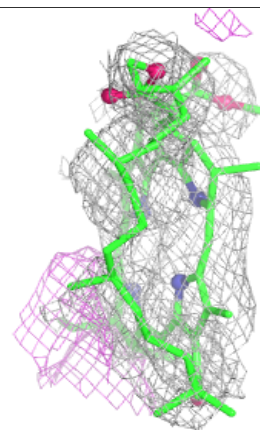
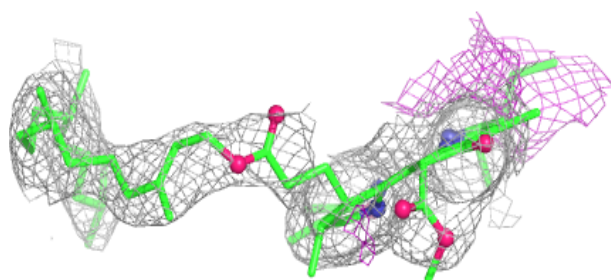
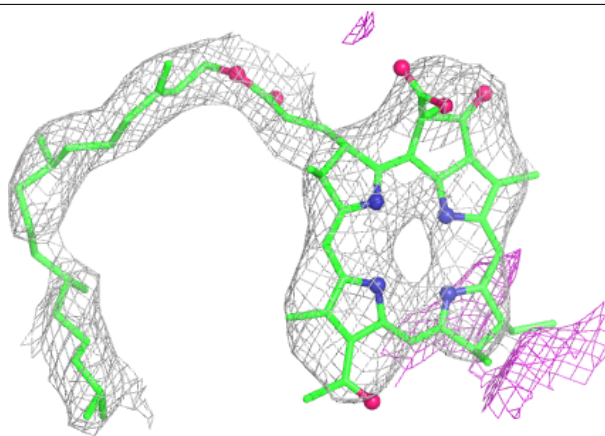


Electron density around CRT M 404:

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

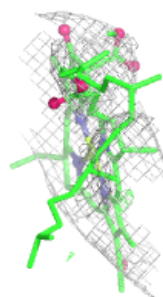
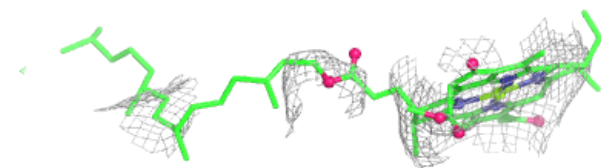
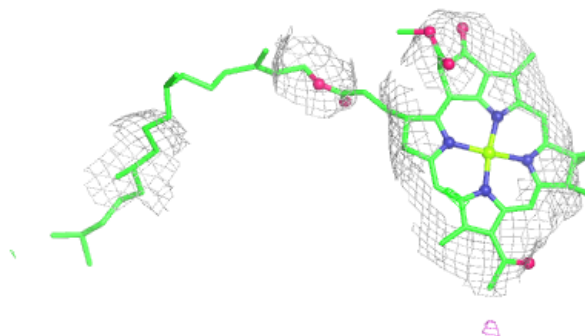
**Electron density around BPH x 302:**

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

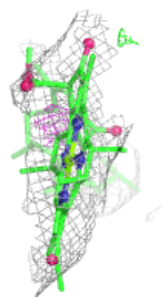
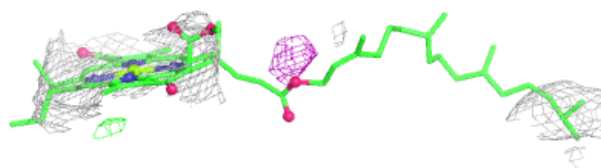
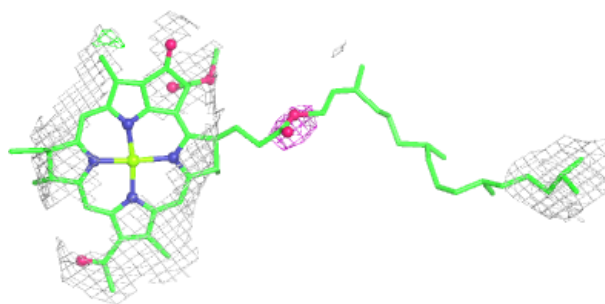


Electron density around BCL u 101:

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

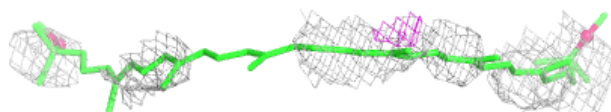
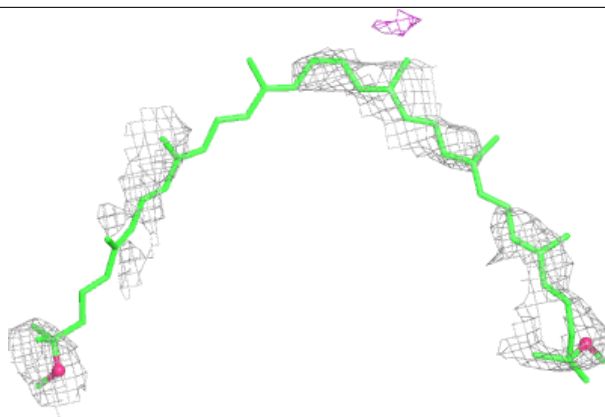
**Electron density around BCL p 102:**

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

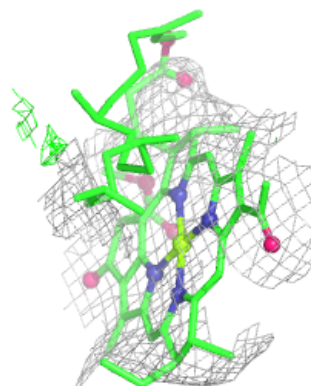
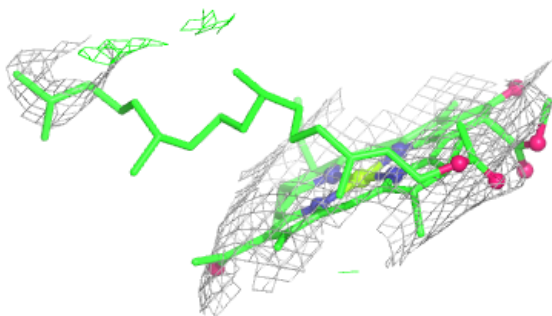
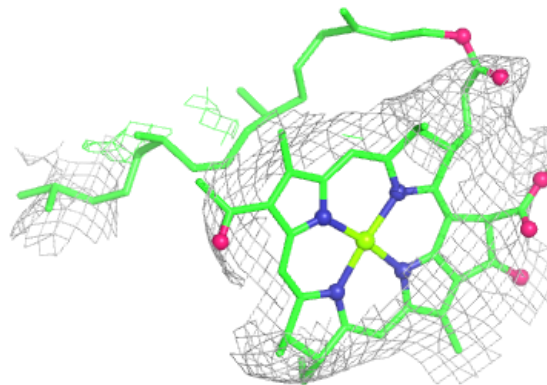


Electron density around CRT y 404:

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

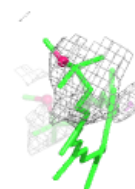
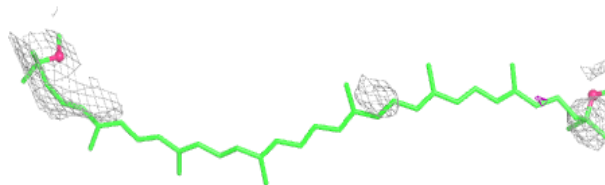
**Electron density around BCL J 102:**

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

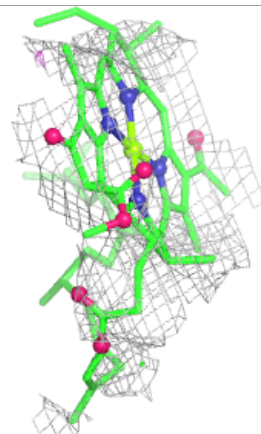
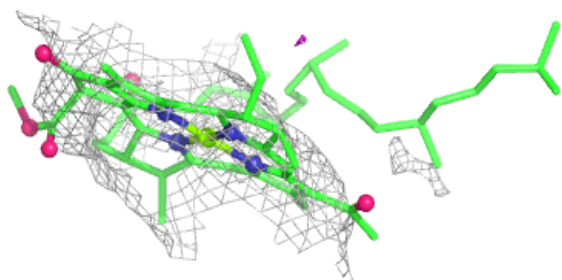
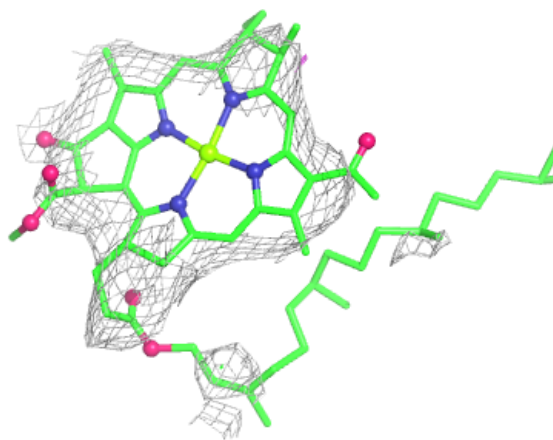


Electron density around CRT T 101:

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

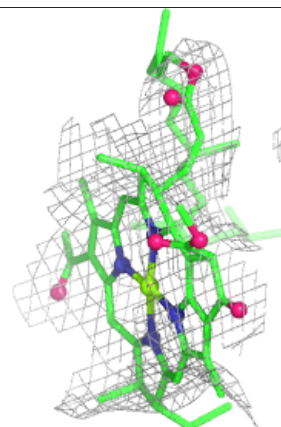
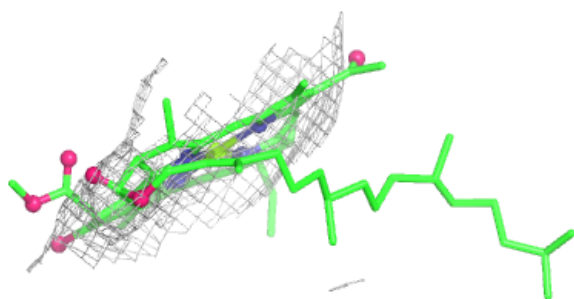
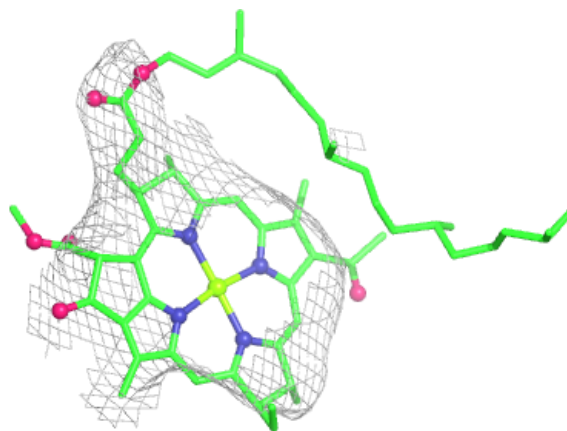
**Electron density around BCL 5 102:**

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



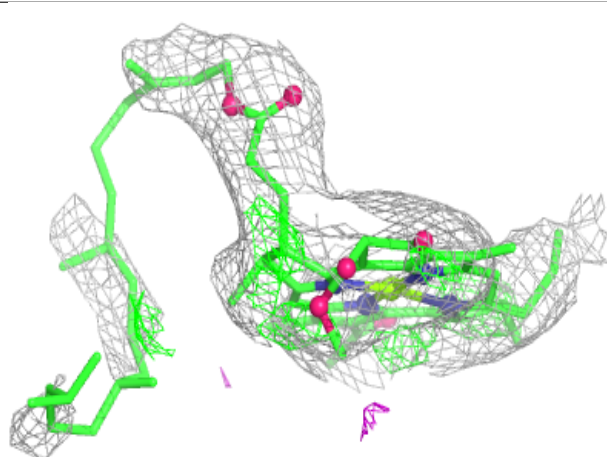
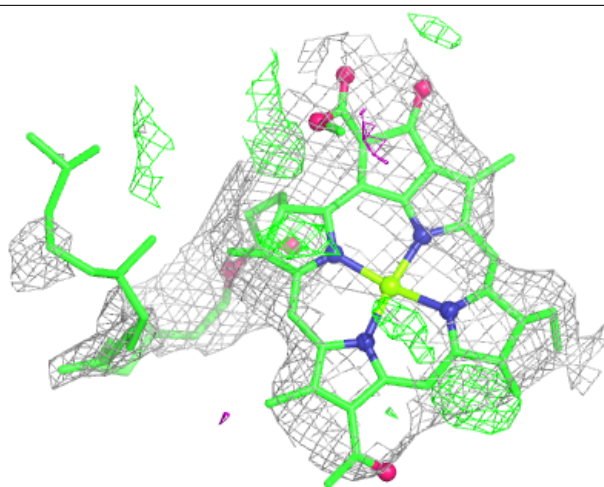
Electron density around BCL c 102:

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



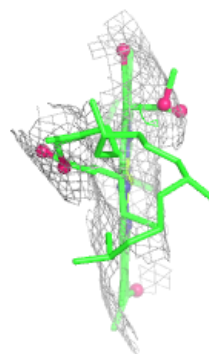
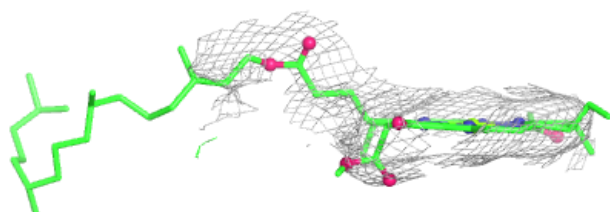
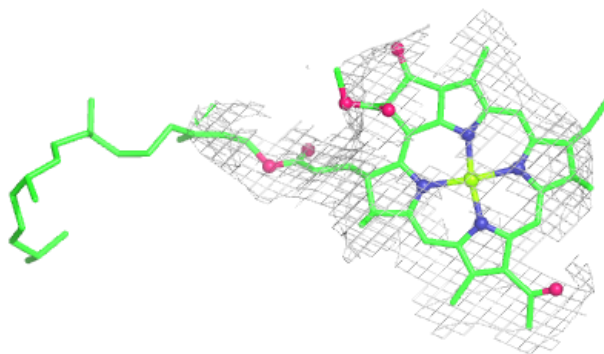
Electron density around BCL L 303:

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

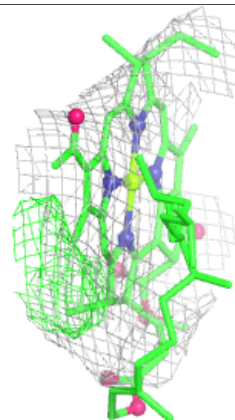
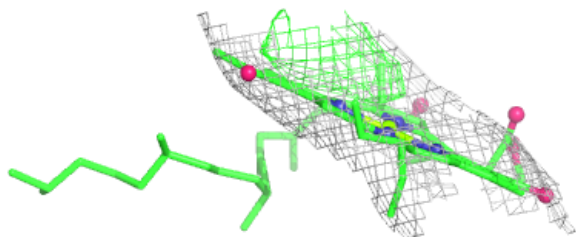
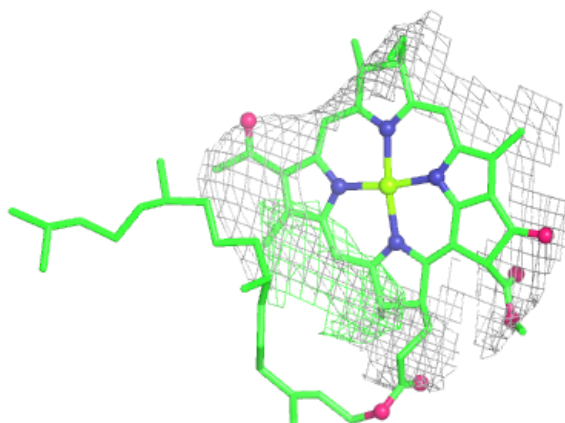


Electron density around BCL m 102:

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

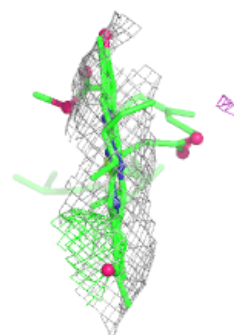
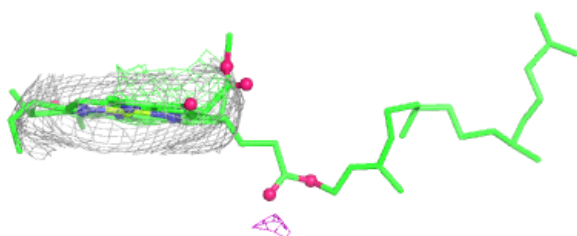
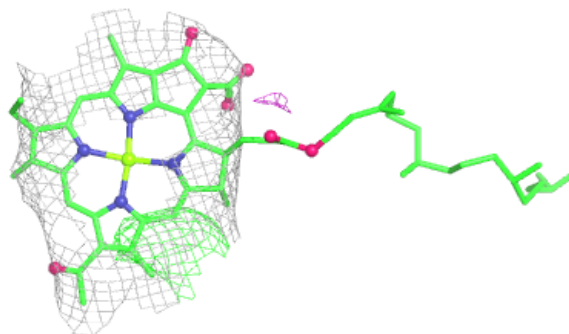
**Electron density around BCL D 102:**

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

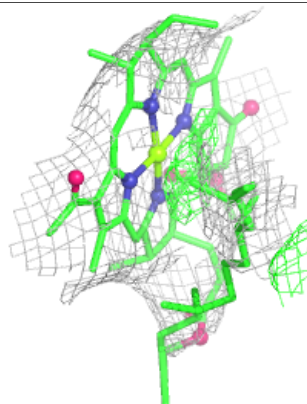
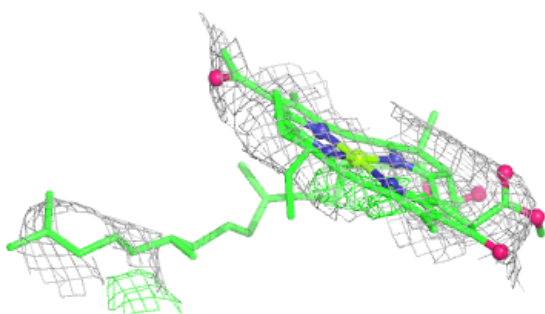
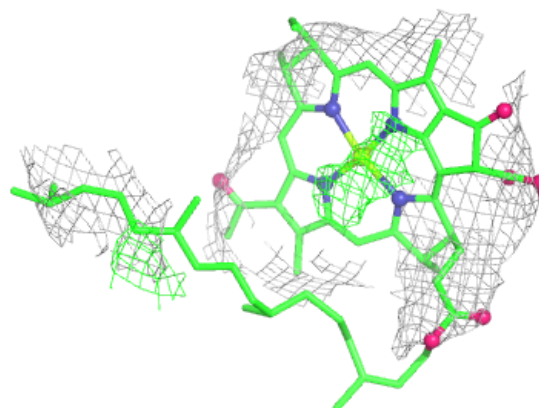


Electron density around BCL F 101:

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

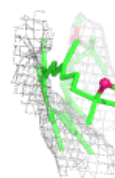
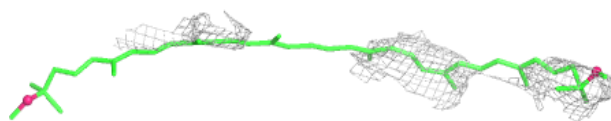
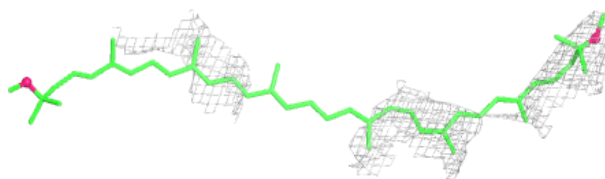
**Electron density around BCL AL 102:**

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

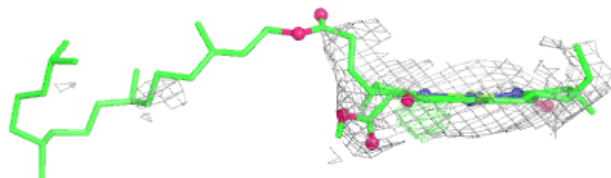
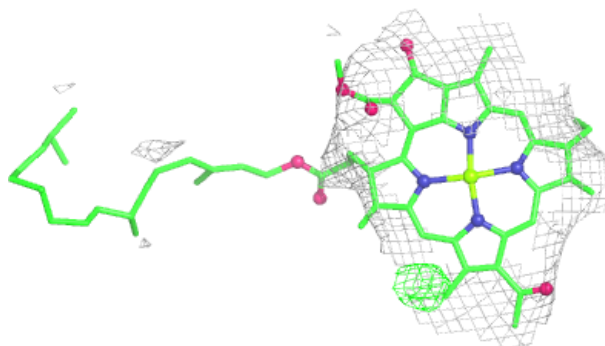


Electron density around CRT AD 102:

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

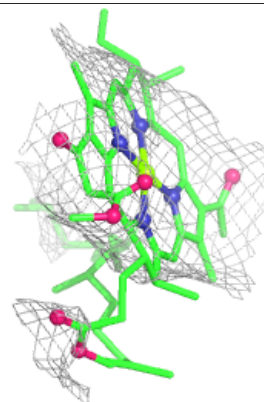
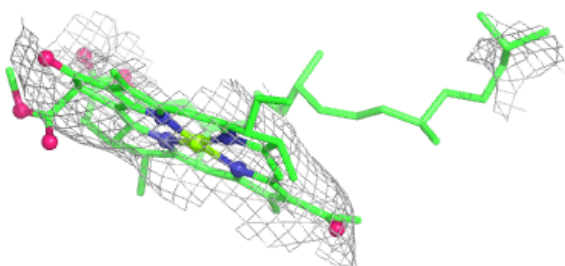
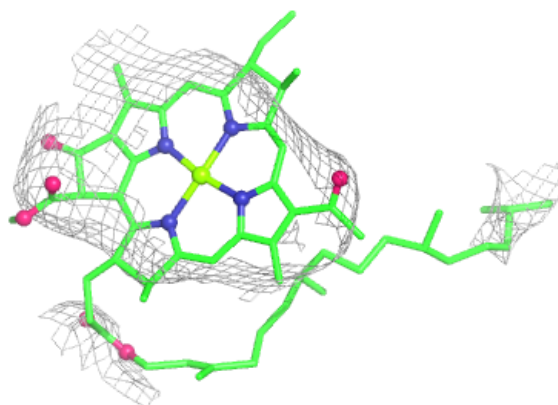
**Electron density around BCL w 101:**

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

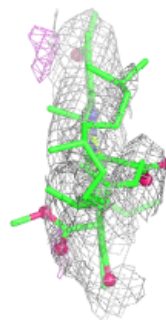
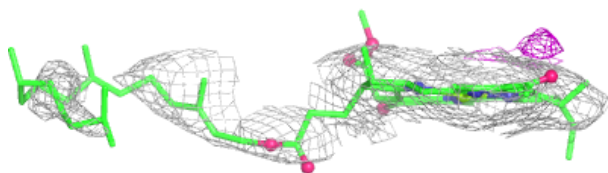
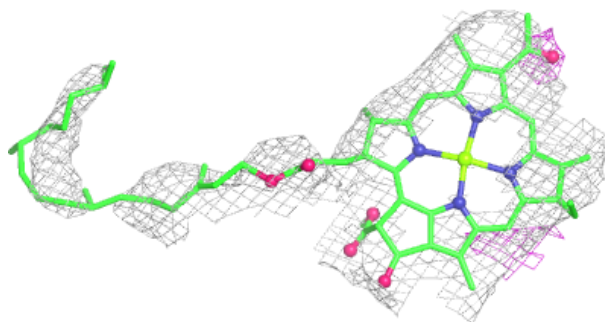


Electron density around BCL g 101:

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

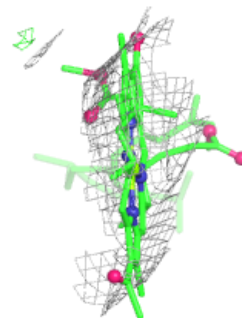
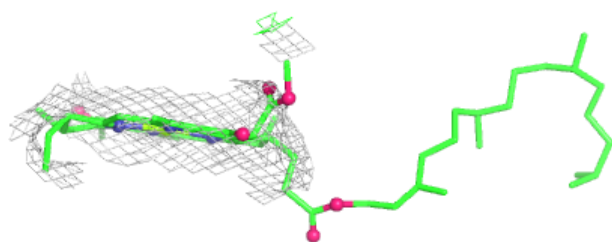
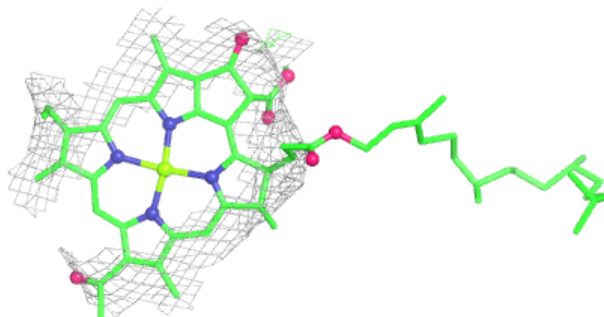
**Electron density around BCL W 101:**

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

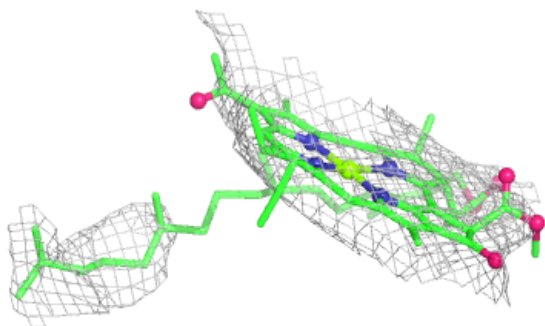
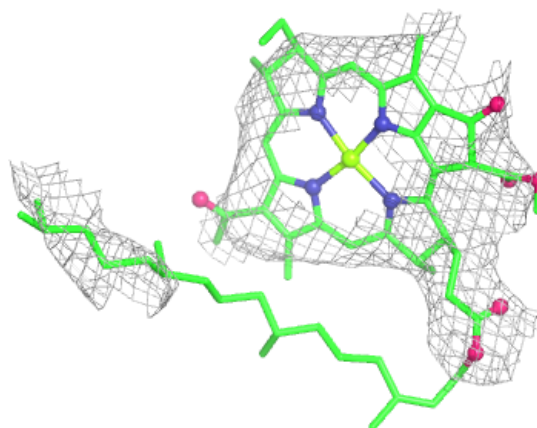


Electron density around BCL AA 101:

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

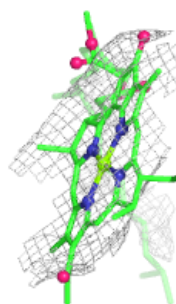
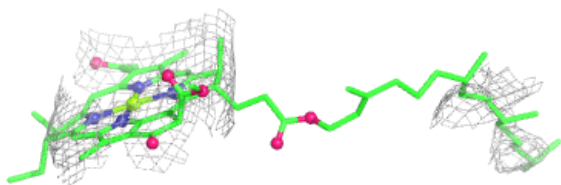
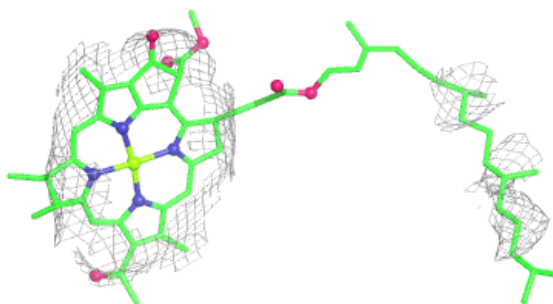
**Electron density around BCL Z 102:**

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

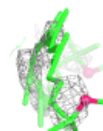
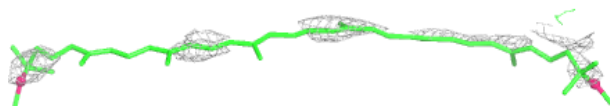
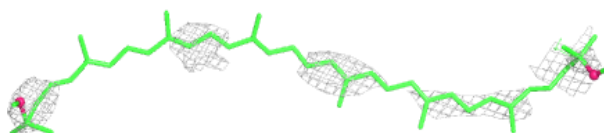


Electron density around BCL I 101:

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

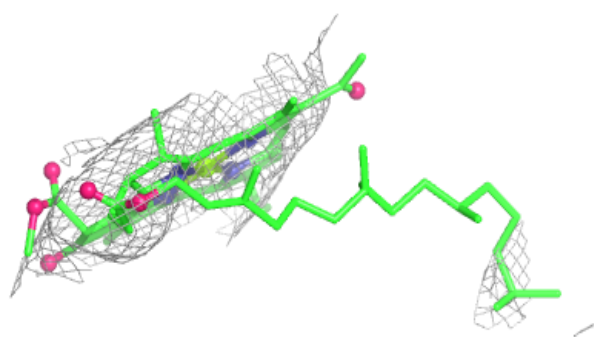
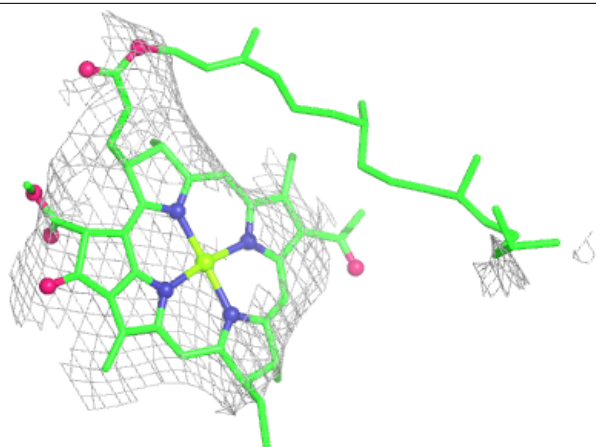
**Electron density around CRT 6 101:**

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

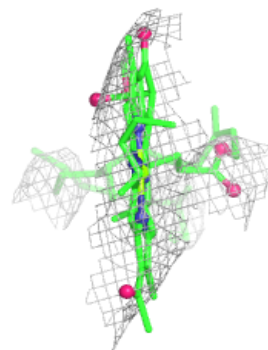
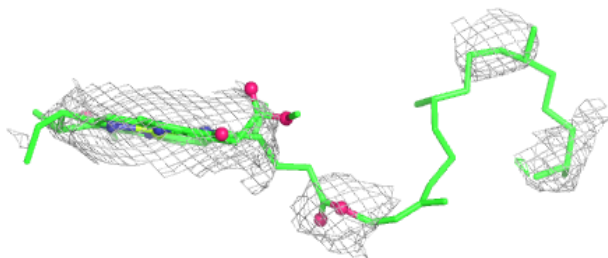
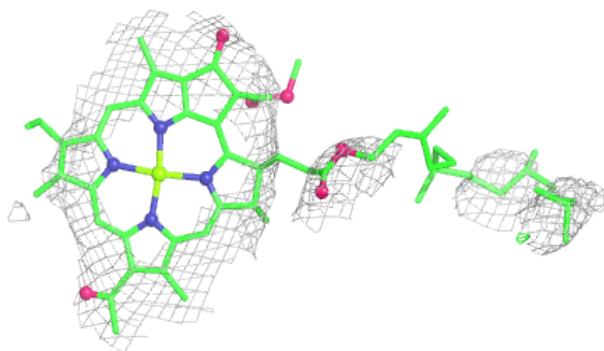


Electron density around BCL O 101:

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

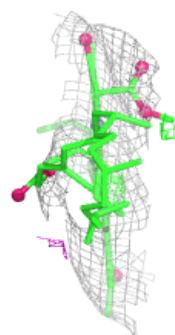
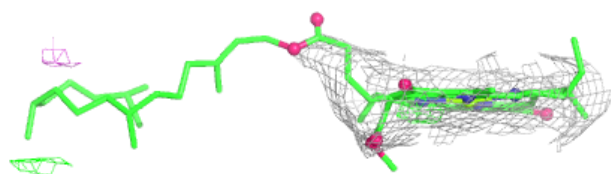
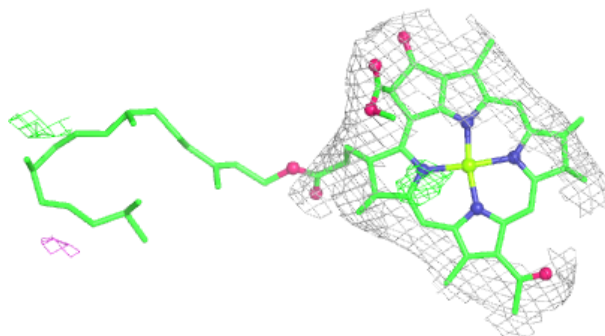
**Electron density around BCL P 101:**

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

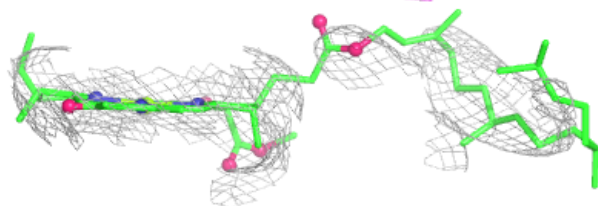
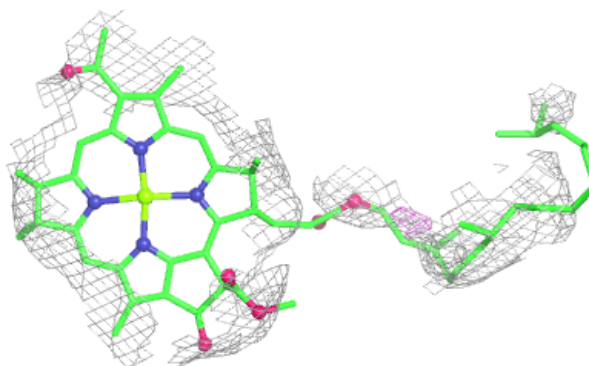


Electron density around BCL AI 101:

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

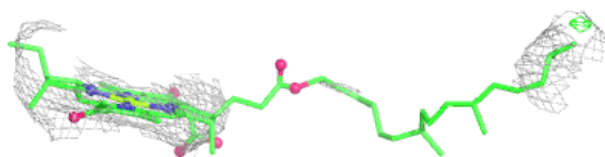
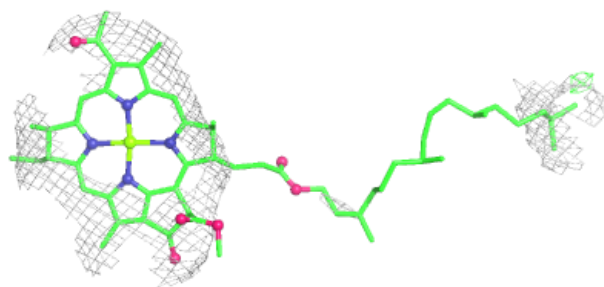
**Electron density around BCL 1 101:**

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

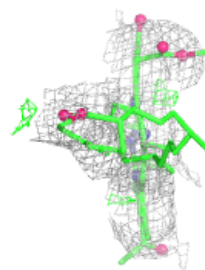
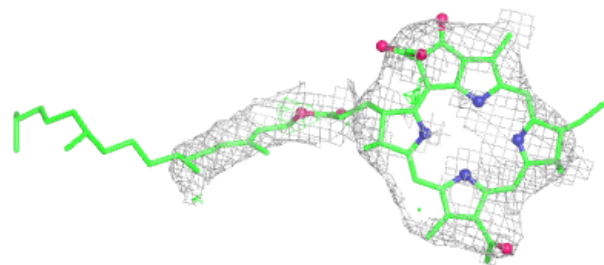


Electron density around BCL D 101:

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

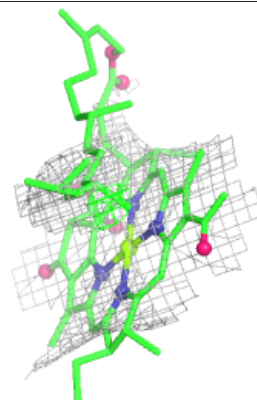
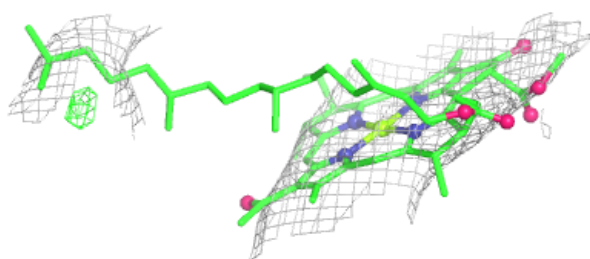
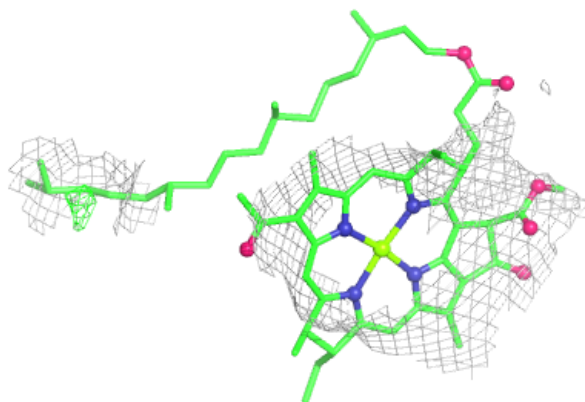
**Electron density around BPH y 402:**

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

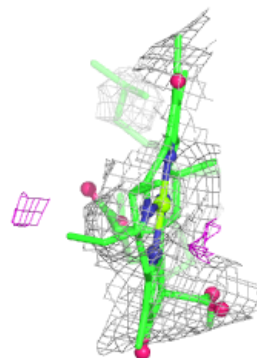
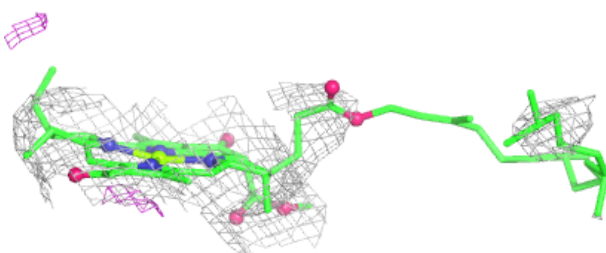
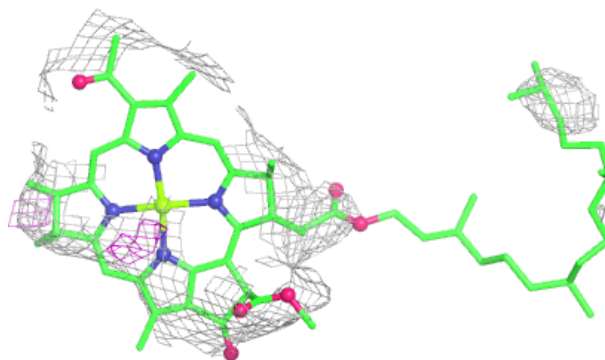


Electron density around BCL s 102:

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

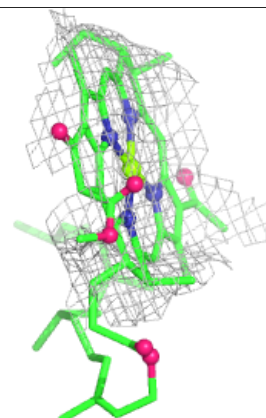
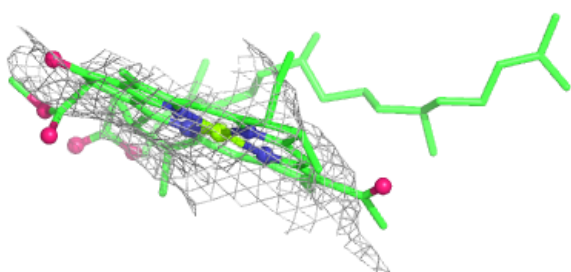
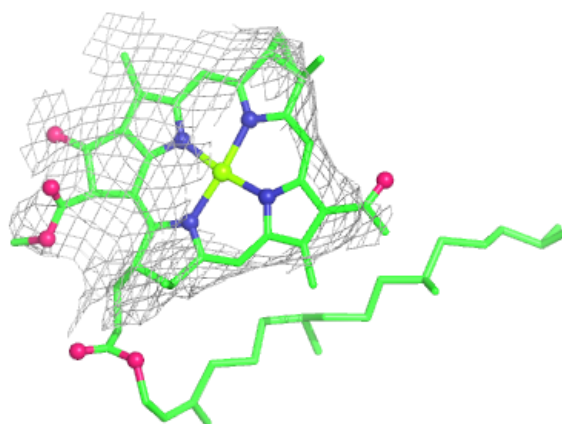
**Electron density around BCL 3 101:**

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

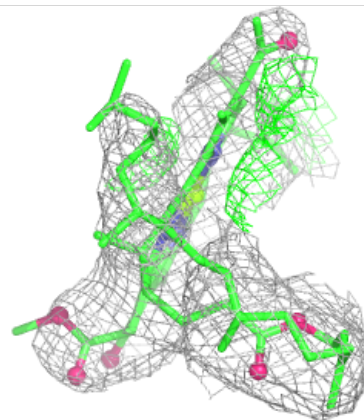
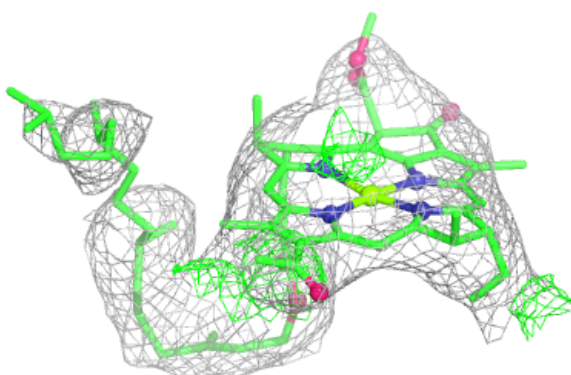
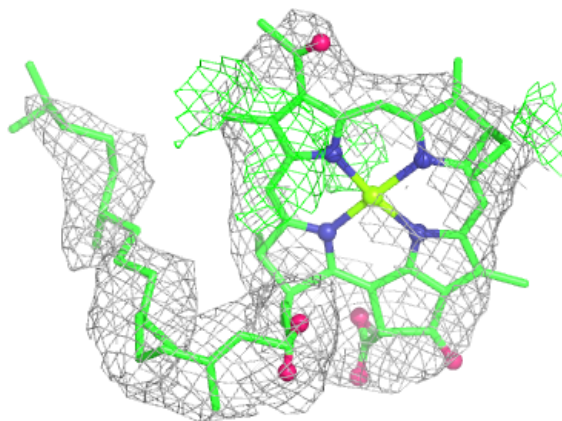


Electron density around BCL i 102:

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

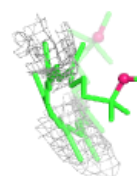
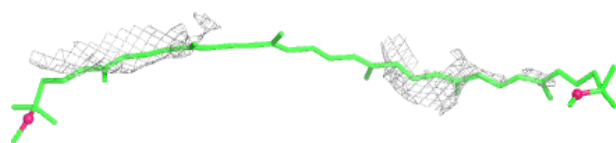
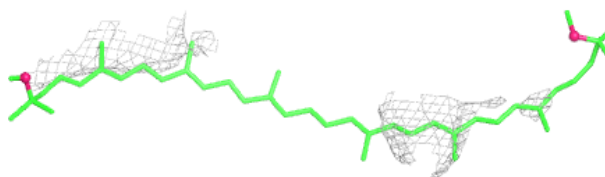
**Electron density around BCL L 305:**

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

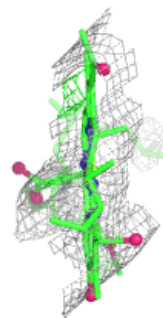
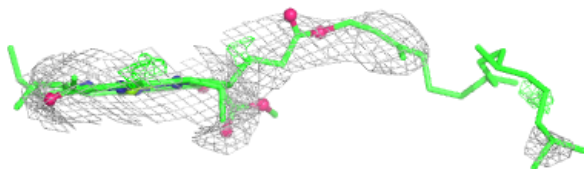
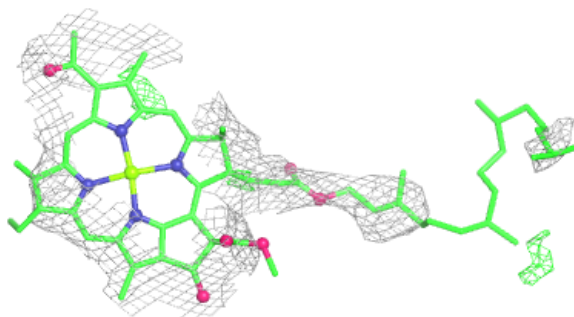


Electron density around CRT AE 103:

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

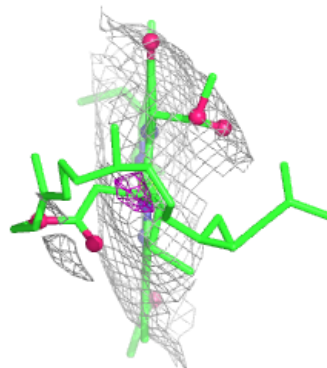
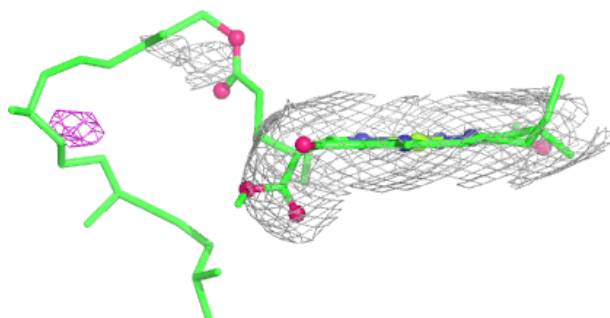
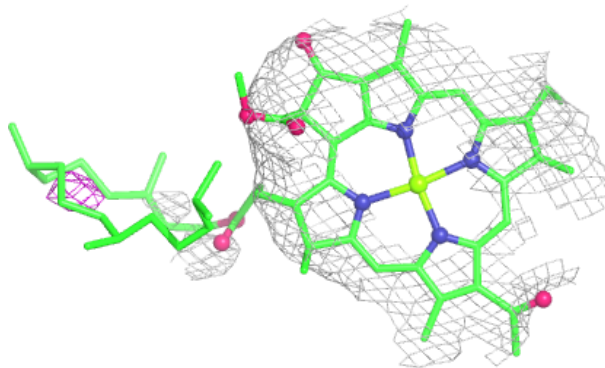
**Electron density around BCL 7 101:**

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

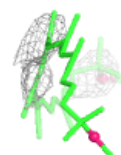
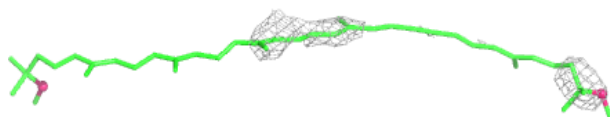
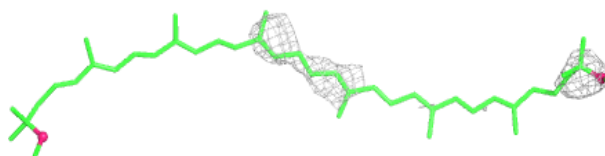


Electron density around BCL Q 101:

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

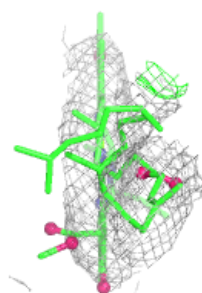
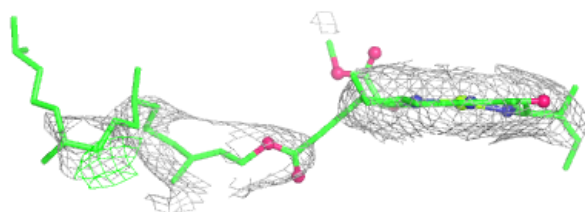
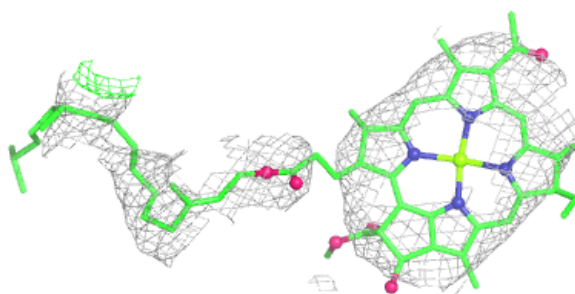
**Electron density around CRT Z 101:**

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



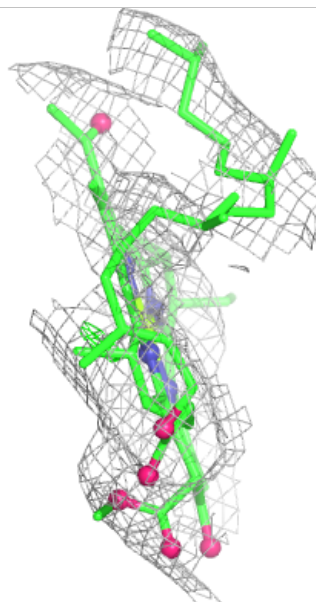
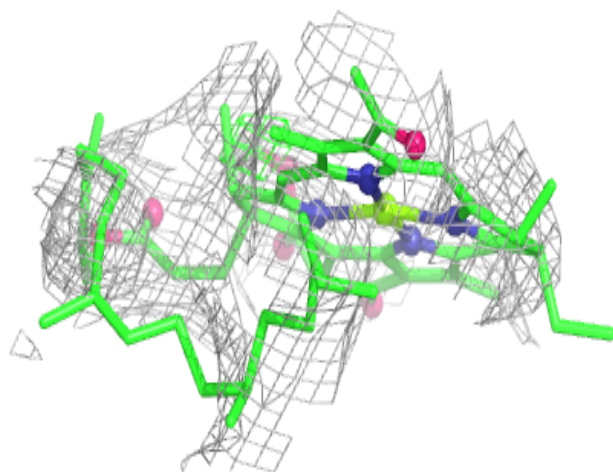
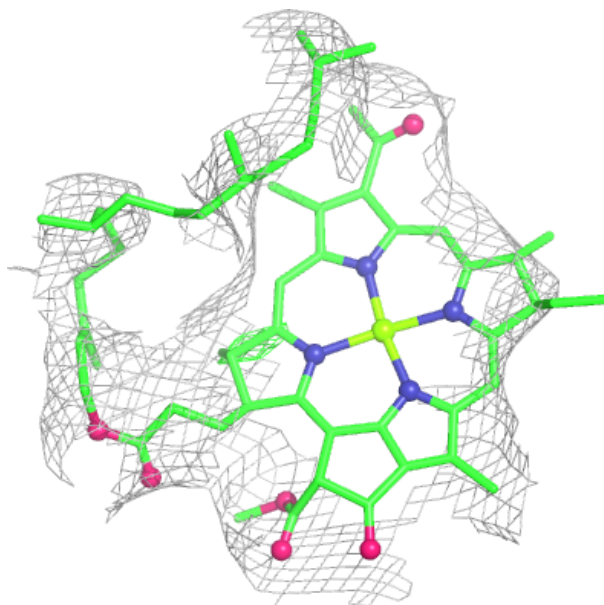
Electron density around BCL Y 101:

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



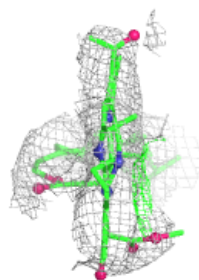
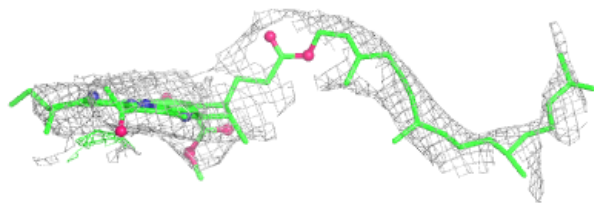
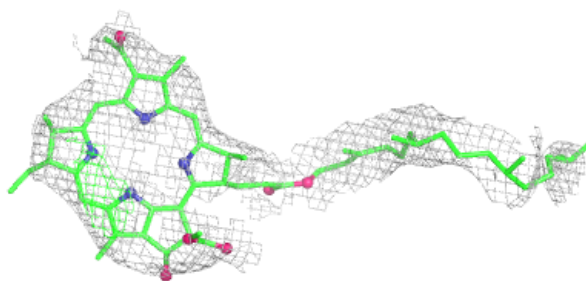
Electron density around BCL 8 102:

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

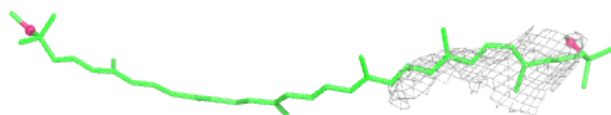
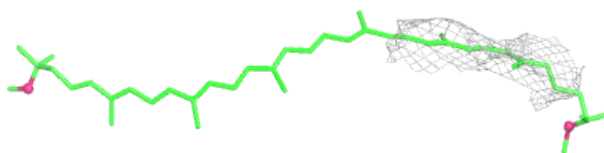


Electron density around BPH M 402:

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

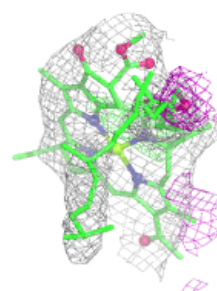
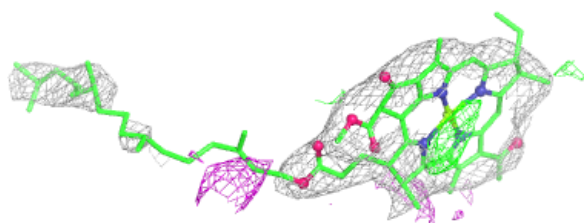
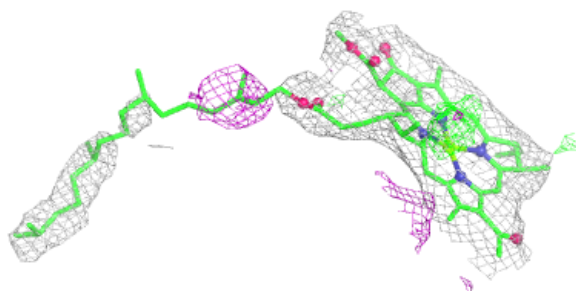
**Electron density around CRT 9 102:**

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

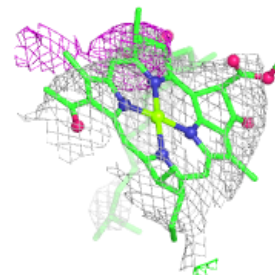
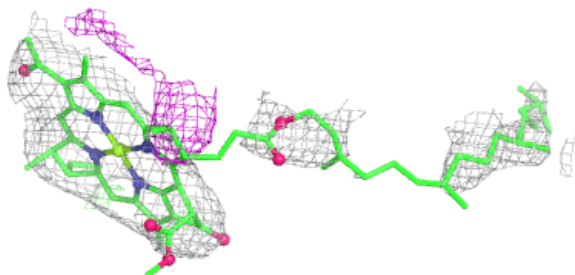
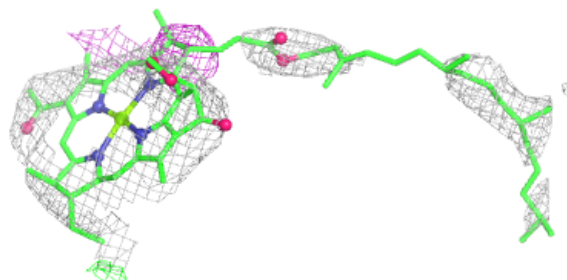


Electron density around BCL x 301:

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

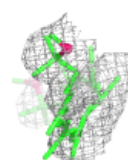
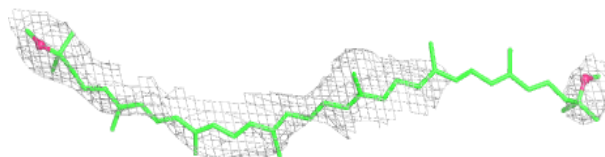
**Electron density around BCL y 401:**

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

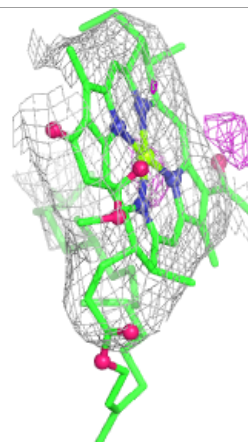
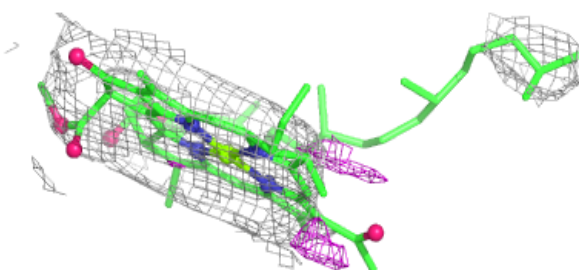
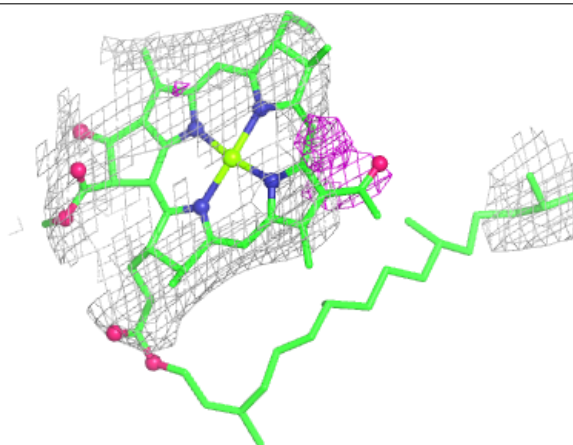


Electron density around CRT P 102:

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

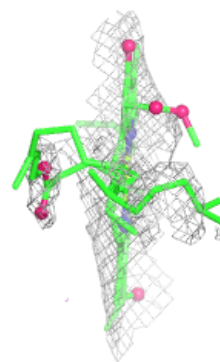
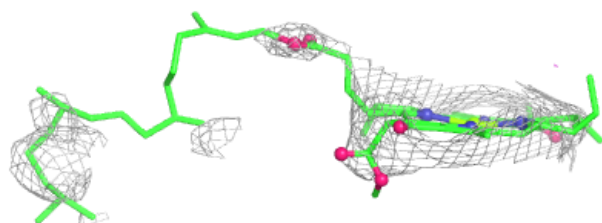
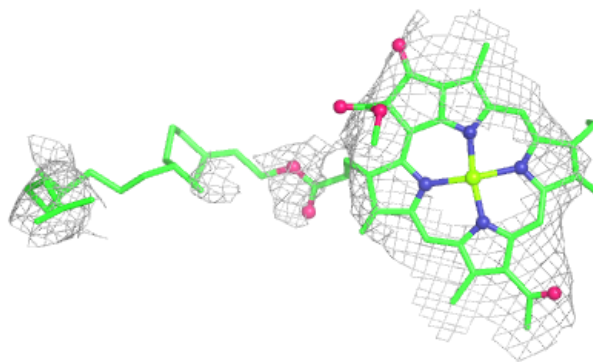
**Electron density around BCL V 101:**

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

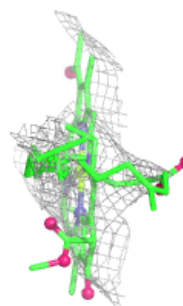
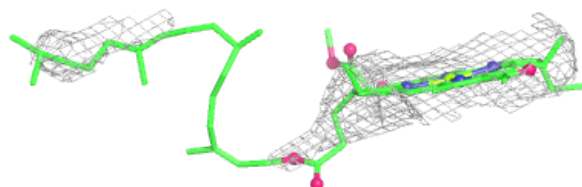
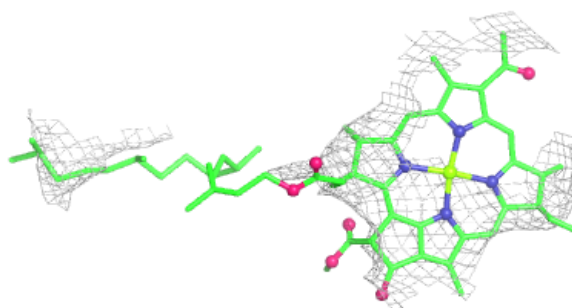


Electron density around BCL r 101:

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

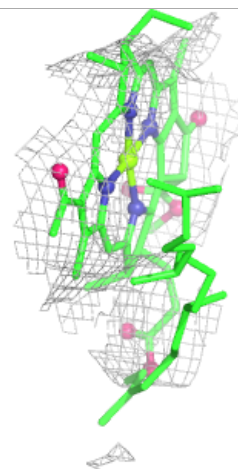
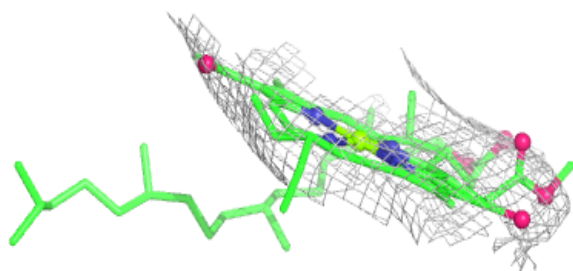
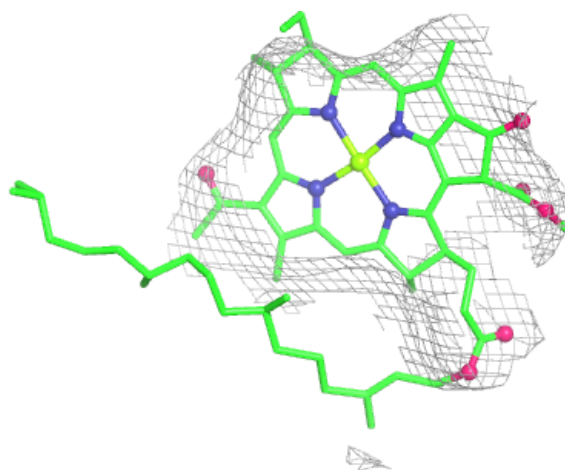
**Electron density around BCL 5 101:**

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



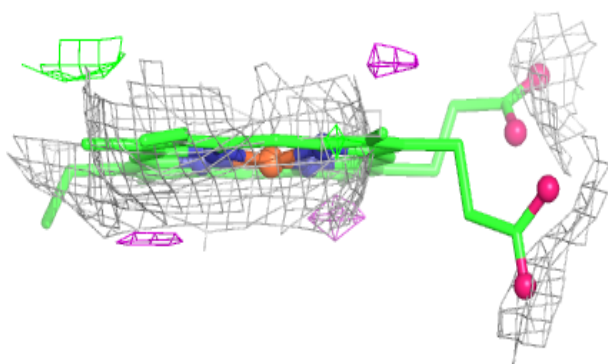
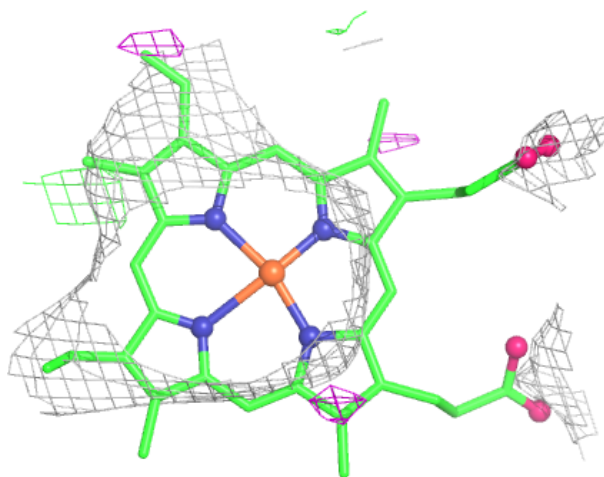
Electron density around BCL 0 101:

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



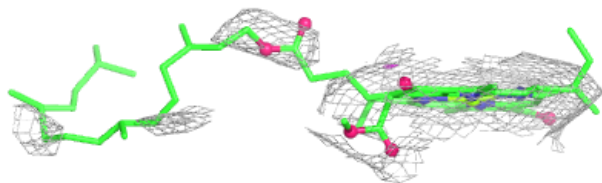
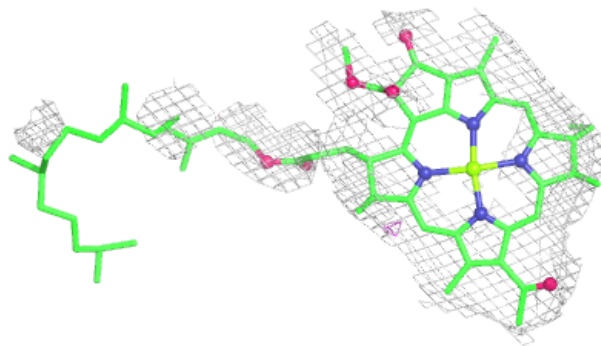
Electron density around HEM o 501:

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



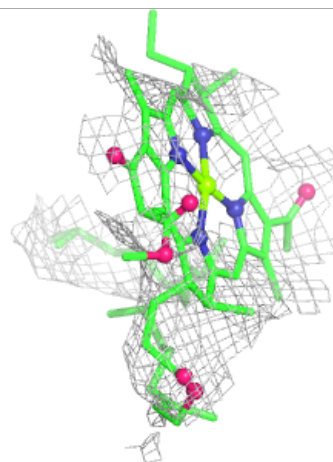
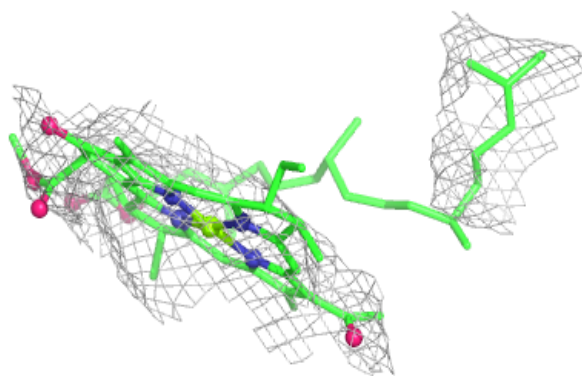
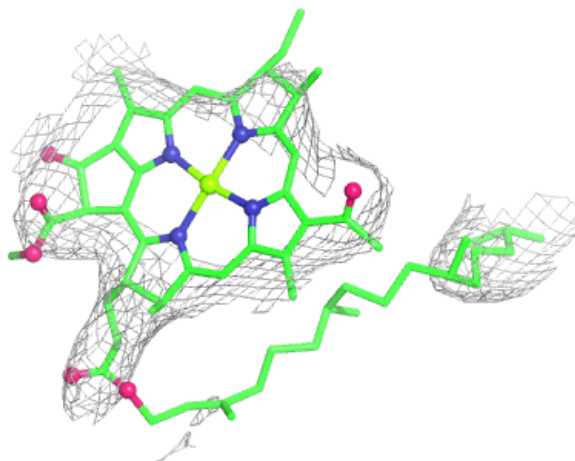
Electron density around BCL U 101:

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



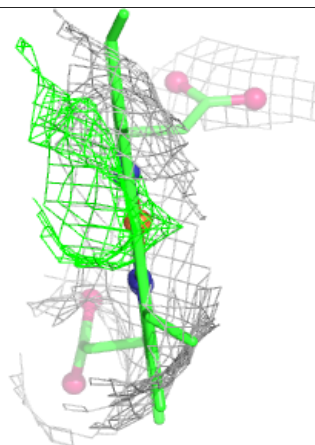
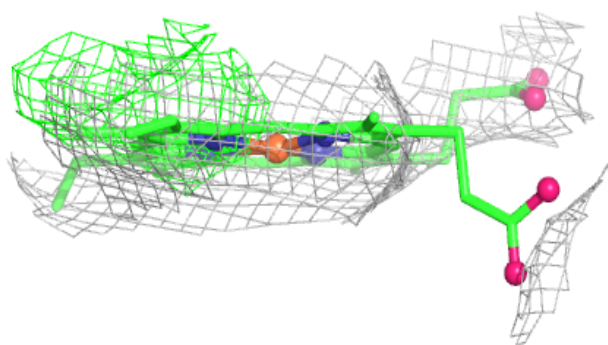
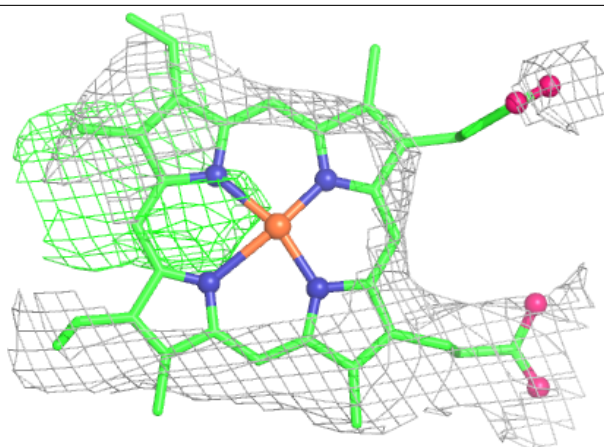
Electron density around BCL 4 102:

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



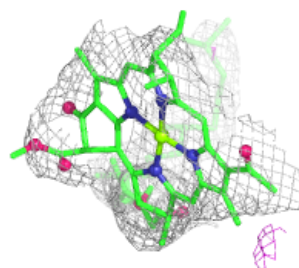
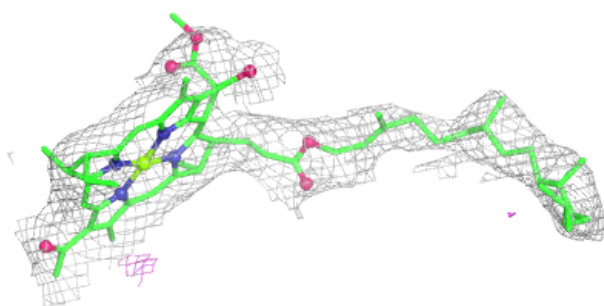
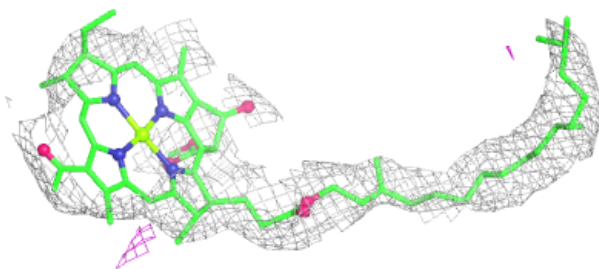
Electron density around HEM C 501:

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

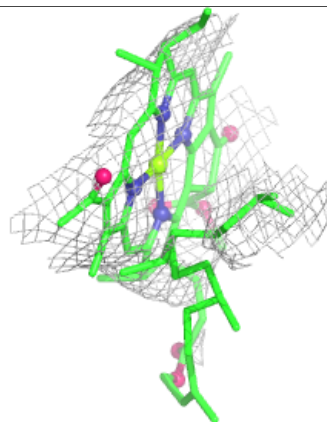
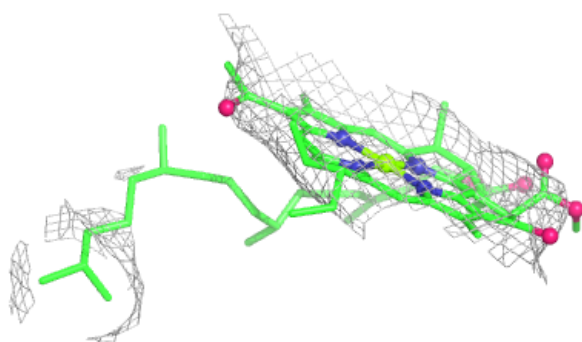
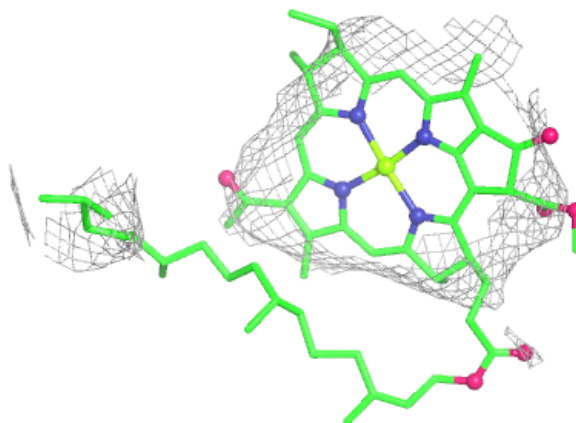


Electron density around BCL M 401:

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

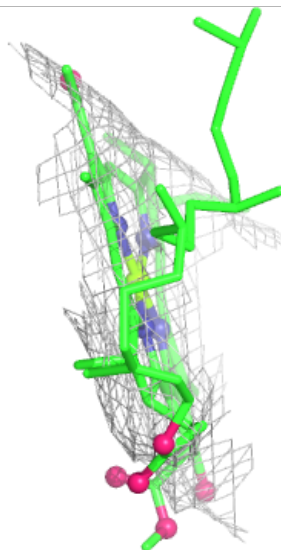
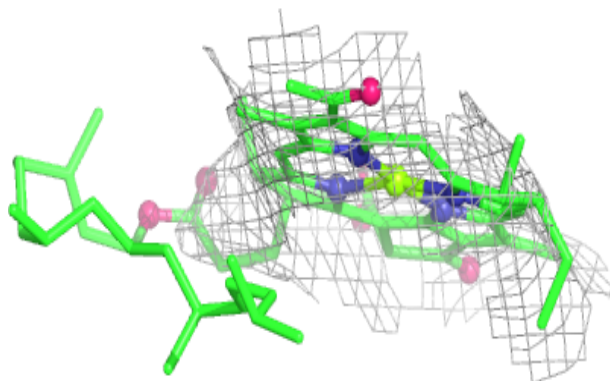
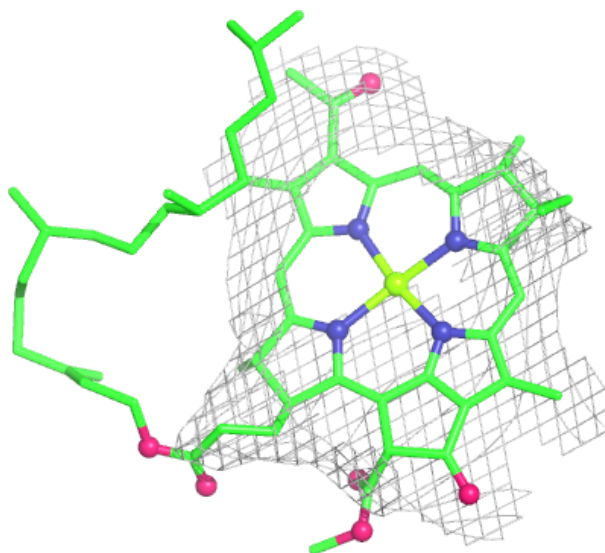
**Electron density around BCL e 102:**

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



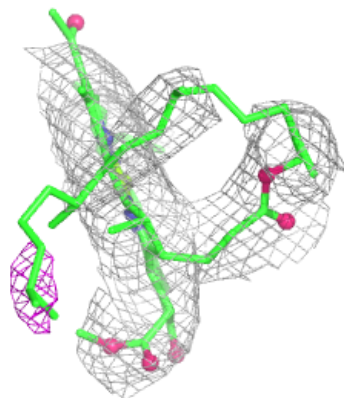
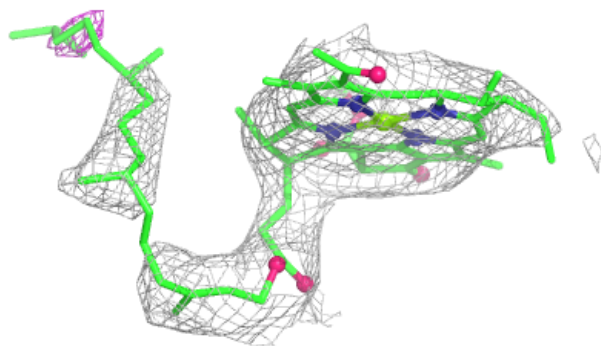
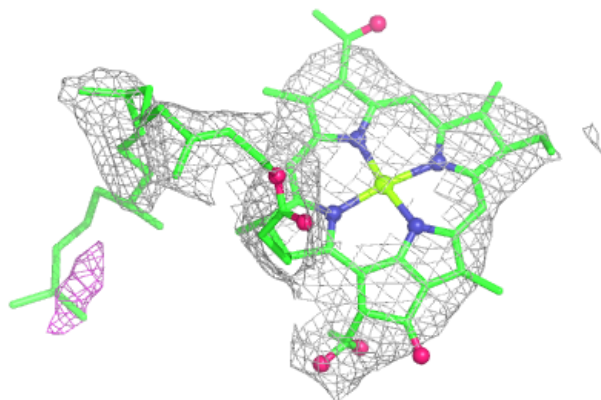
Electron density around BCL A 102:

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

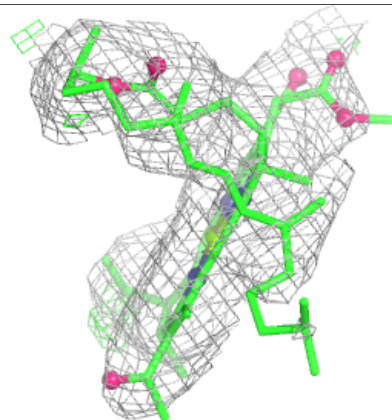
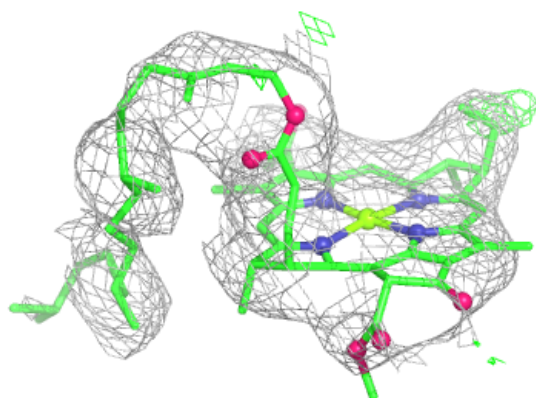
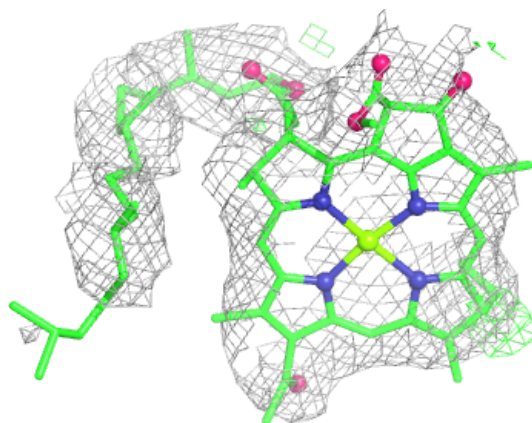


Electron density around BCL x 303:

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

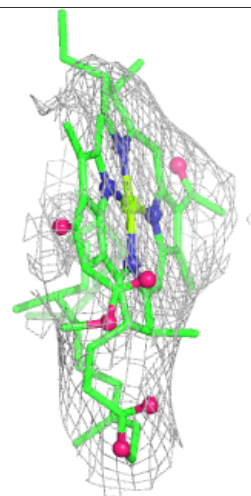
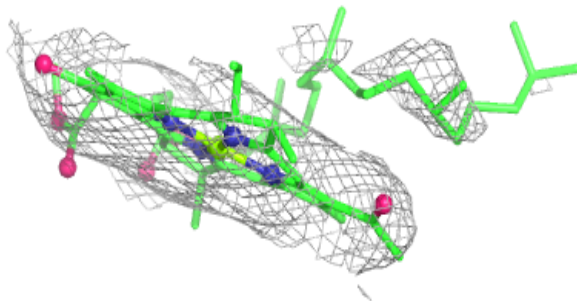
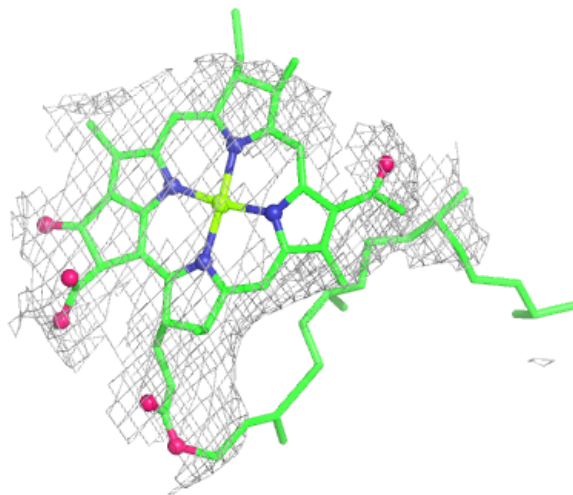
**Electron density around BCL x 305:**

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



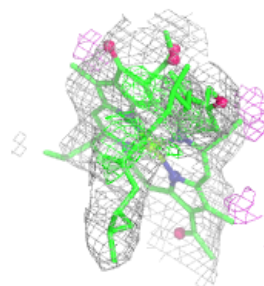
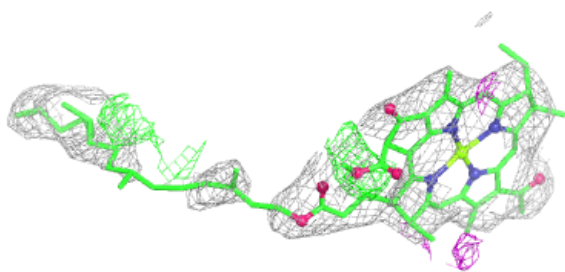
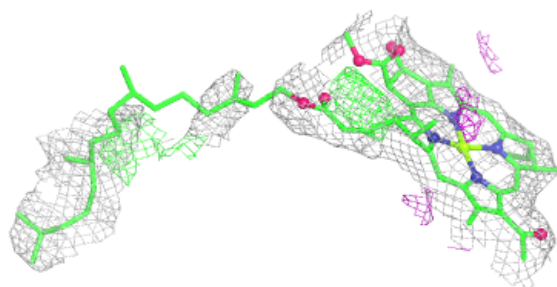
Electron density around BCL X 102:

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



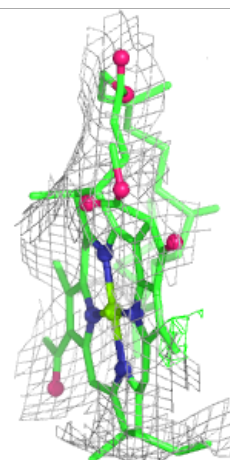
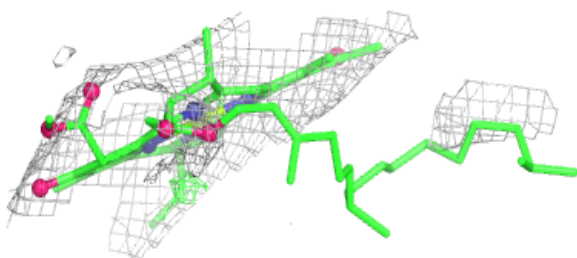
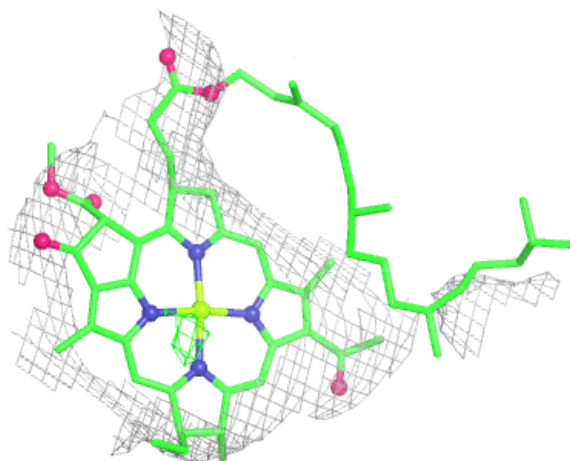
Electron density around BCL L 301:

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



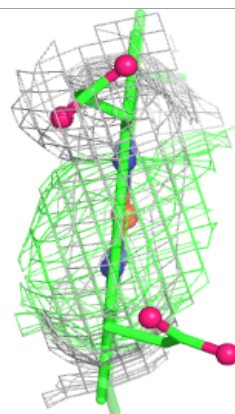
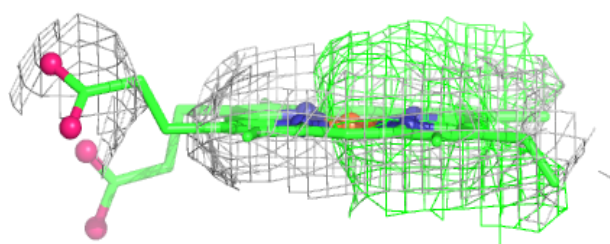
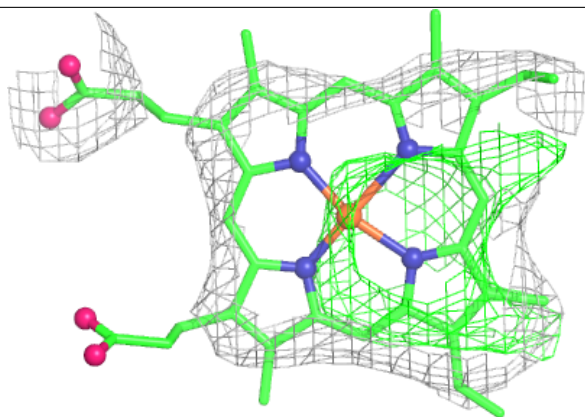
Electron density around BCL p 104:

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



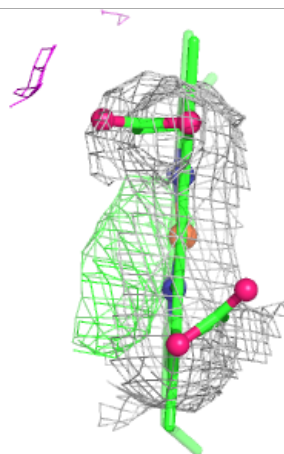
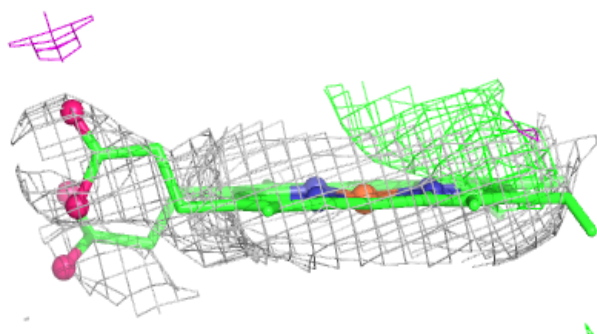
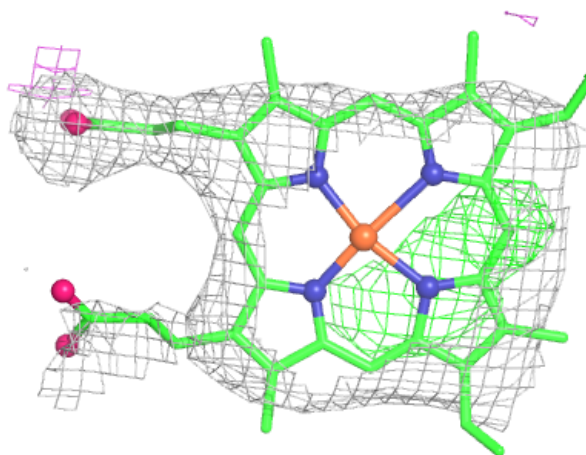
Electron density around HEM o 503:

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



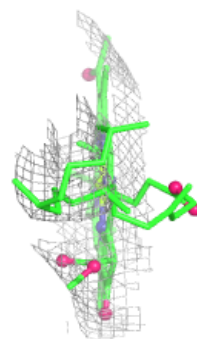
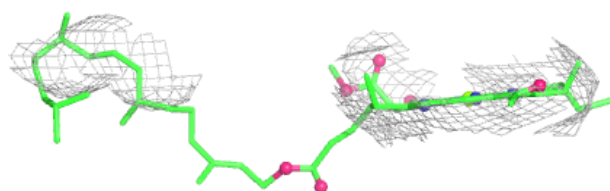
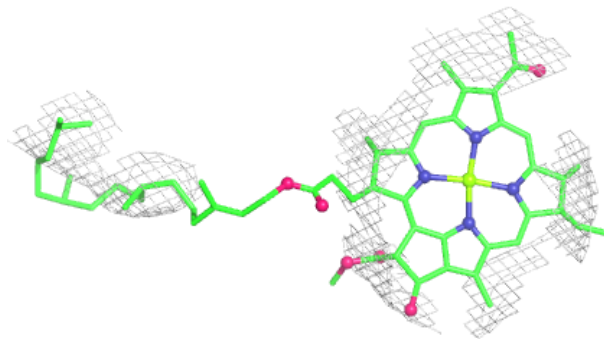
Electron density around HEM o 504:

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



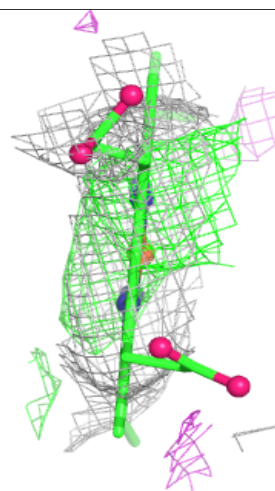
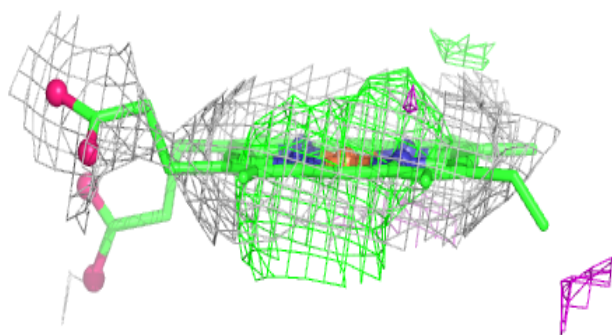
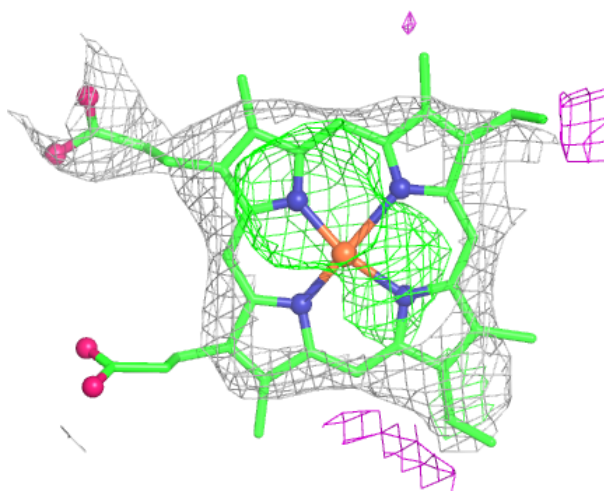
Electron density around BCL B 101:

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



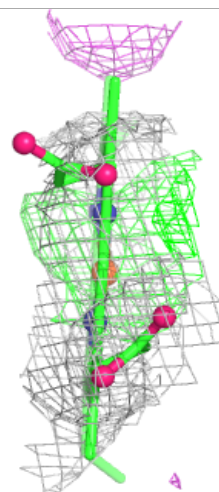
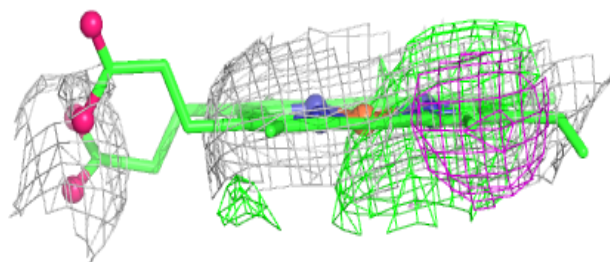
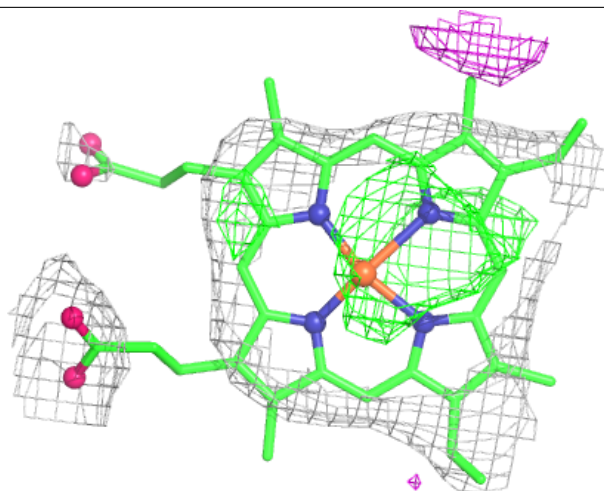
Electron density around HEM C 503:

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



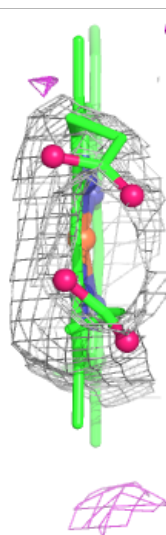
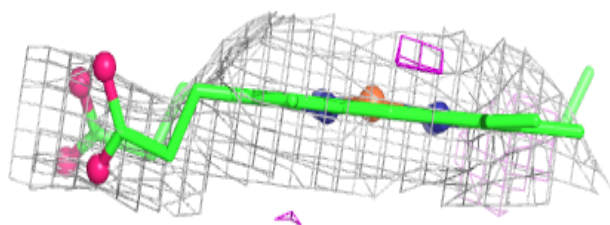
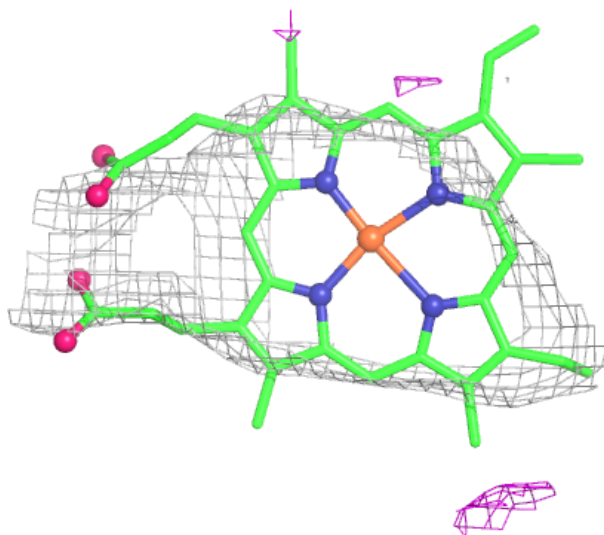
Electron density around HEM C 504:

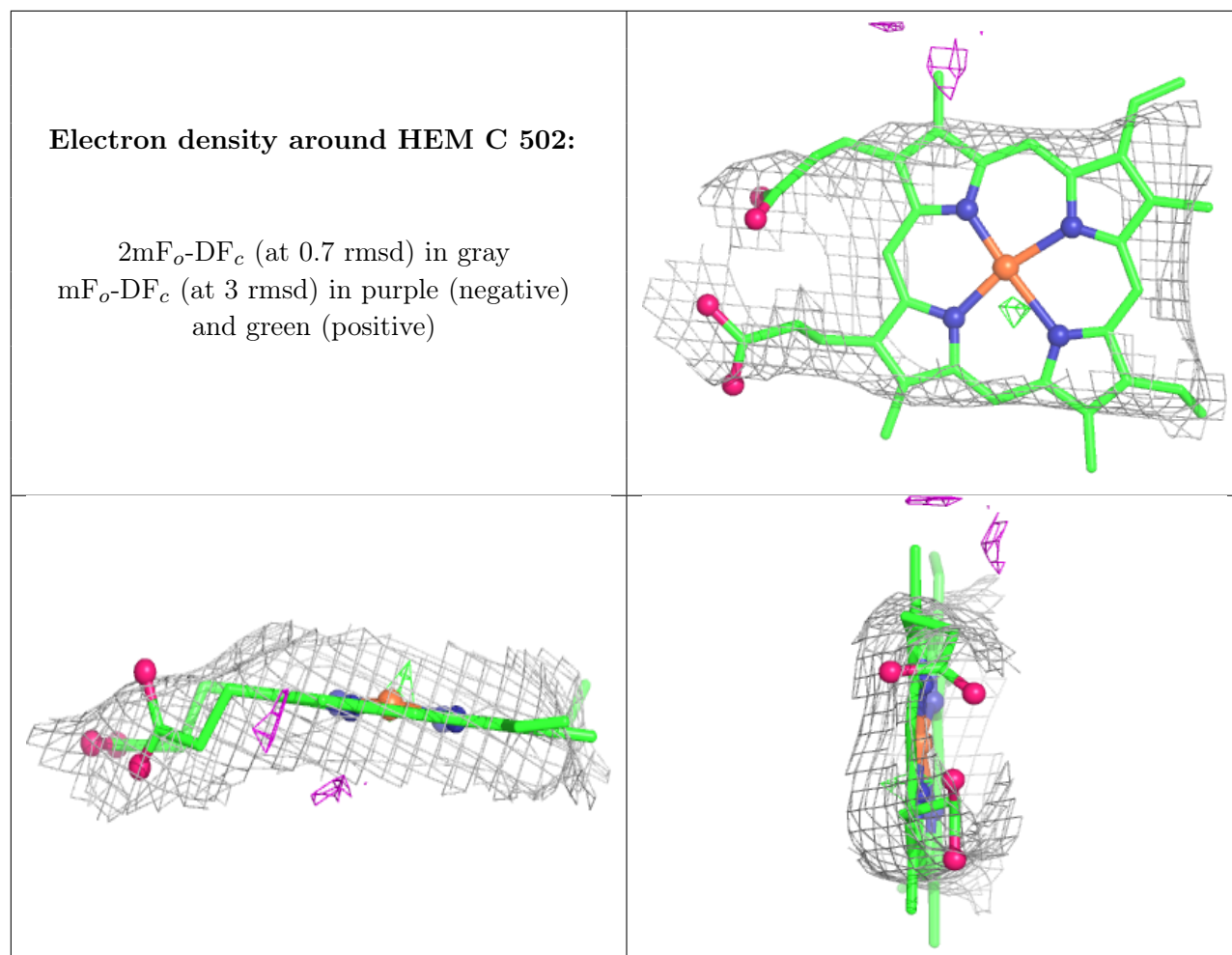
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.