



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 05:50 PM BST

PDB ID : 5B5N
Title : Crystal structure of the Ba-substituted LH1-RC complex from T_{ch}. 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

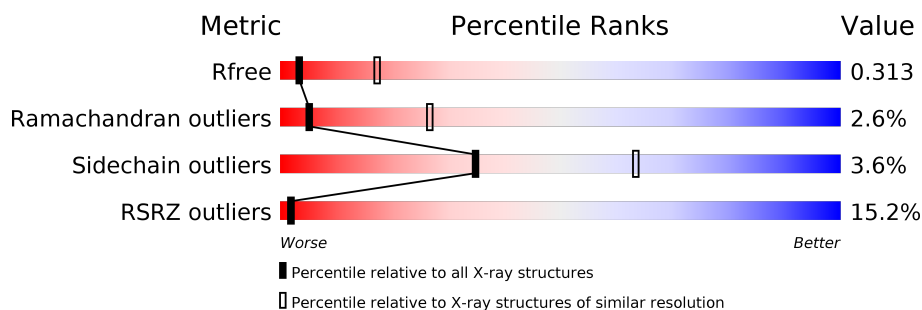
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	<div> <div>11%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	o	333	<div> <div>11%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
2	L	281	<div> <div>7%</div> <div>93%</div> <div>7%</div> </div>
2	x	281	<div> <div>4%</div> <div>90%</div> <div>10%</div> </div>
3	M	319	<div> <div>4%</div> <div>93%</div> <div>7%</div> </div>
3	y	319	<div> <div>4%</div> <div>92%</div> <div>7%</div> </div>
4	H	259	<div> <div>9%</div> <div>90%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
5	f	61	

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Mol	Chain	Length	Quality of chain
5	h	61	<div> <div>18%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
5	j	61	<div> <div>18%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
5	l	61	<div> <div>20%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
5	m	61	<div> <div>30%</div> <div>97%</div> <div>.</div> <div>.</div> </div>
5	p	61	<div> <div>26%</div> <div>93%</div> <div>.</div> <div>.</div> <div>.</div> </div>
5	r	61	<div> <div>28%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
5	u	61	<div> <div>30%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
5	w	61	<div> <div>28%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
6	0	47	<div> <div>17%</div> <div>83%</div> <div>.</div> <div>15%</div> </div>
6	2	47	<div> <div>11%</div> <div>85%</div> <div>15%</div> </div>
6	4	47	<div> <div>11%</div> <div>85%</div> <div>15%</div> </div>
6	6	47	<div> <div>11%</div> <div>85%</div> <div>15%</div> </div>
6	8	47	<div> <div>11%</div> <div>85%</div> <div>15%</div> </div>
6	AB	47	<div> <div>6%</div> <div>83%</div> <div>.</div> <div>15%</div> </div>
6	AD	47	<div> <div>21%</div> <div>85%</div> <div>15%</div> </div>
6	AF	47	<div> <div>11%</div> <div>85%</div> <div>15%</div> </div>
6	AH	47	<div> <div>21%</div> <div>83%</div> <div>.</div> <div>15%</div> </div>
6	AJ	47	<div> <div>13%</div> <div>81%</div> <div>.</div> <div>.</div> <div>15%</div> </div>
6	AL	47	<div> <div>17%</div> <div>85%</div> <div>15%</div> </div>
6	B	47	<div> <div>21%</div> <div>79%</div> <div>6%</div> <div>15%</div> </div>
6	E	47	<div> <div>13%</div> <div>83%</div> <div>.</div> <div>15%</div> </div>
6	G	47	<div> <div>28%</div> <div>83%</div> <div>.</div> <div>15%</div> </div>
6	J	47	<div> <div>11%</div> <div>85%</div> <div>15%</div> </div>
6	N	47	<div> <div>11%</div> <div>83%</div> <div>.</div> <div>15%</div> </div>
6	P	47	<div> <div>6%</div> <div>83%</div> <div>.</div> <div>15%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	PEF	A	101	-	-	-	X
12	PEF	H	304	-	-	-	X
14	MQ8	M	404	-	-	-	X
15	CRT	0	101	-	-	-	X
15	CRT	2	101	-	-	-	X
15	CRT	4	101	-	-	-	X
15	CRT	7	101	-	-	-	X
15	CRT	7	103	-	-	-	X
15	CRT	9	101	-	-	-	X
15	CRT	AC	101	-	-	-	X
15	CRT	AD	101	-	-	-	X
15	CRT	AF	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CRT	AH	102	-	-	-	X
15	CRT	AJ	101	-	-	-	X
15	CRT	AL	101	-	-	-	X
15	CRT	E	101	-	-	-	X
15	CRT	G	101	-	-	-	X
15	CRT	I	102	-	-	-	X
15	CRT	M	405	-	-	-	X
15	CRT	O	101	-	-	-	X
15	CRT	P	102	-	-	-	X
15	CRT	R	101	-	-	-	X
15	CRT	T	101	-	-	-	X
15	CRT	V	101	-	-	-	X
15	CRT	e	101	-	-	-	X
15	CRT	g	101	-	-	-	X
15	CRT	i	101	-	-	-	X
15	CRT	k	101	-	-	-	X
15	CRT	m	104	-	-	-	X
15	CRT	n	101	-	-	-	X
15	CRT	q	101	-	-	-	X
15	CRT	v	101	-	-	-	X
15	CRT	z	101	-	-	-	X
16	PO4	H	303	-	-	-	X
7	HEM	o	501	-	-	-	X
9	BCL	AB	102	-	-	-	X
9	BCL	AC	103	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

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

- Molecule 5 is a protein called LH1 alpha polypeptide.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AC	60	Total 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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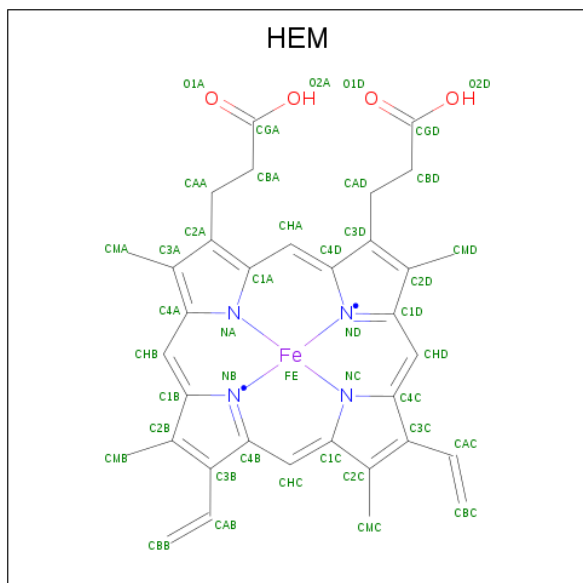
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	X	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	Z	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	2	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	4	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	6	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	8	40	Total 337	C 228	N 52	O 55	S 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 (three-letter code: 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 BARIUM ION (three-letter code: BA) (formula: Ba).

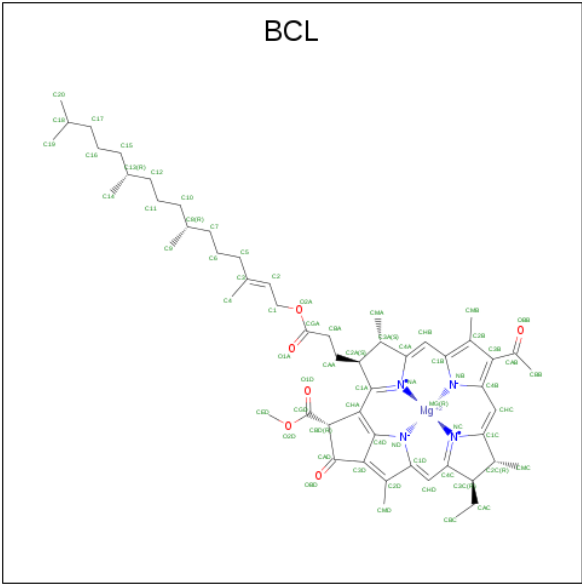
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	1	Total Ba 1 1	0	0
8	h	1	Total Ba 1 1	0	0
8	AC	1	Total Ba 1 1	0	0
8	W	1	Total Ba 1 1	0	0
8	o	1	Total Ba 1 1	0	0
8	S	1	Total Ba 1 1	0	0
8	f	1	Total Ba 1 1	0	0
8	AK	1	Total Ba 1 1	0	0
8	p	1	Total Ba 1 1	0	0
8	AE	1	Total Ba 1 1	0	0
8	w	1	Total Ba 1 1	0	0
8	A	2	Total Ba 2 2	0	0
8	5	1	Total Ba 1 1	0	0
8	x	2	Total Ba 2 2	0	0
8	AA	1	Total Ba 1 1	0	0
8	j	1	Total Ba 1 1	0	0
8	1	1	Total Ba 1 1	0	0
8	D	1	Total Ba 1 1	0	0
8	I	1	Total Ba 1 1	0	0
8	U	1	Total Ba 1 1	0	0
8	r	1	Total Ba 1 1	0	0
8	L	2	Total Ba 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	m	2	Total	Ba	0	0
			2	2		
8	AG	1	Total	Ba	0	0
			1	1		
8	Q	1	Total	Ba	0	0
			1	1		
8	d	1	Total	Ba	0	0
			1	1		
8	AI	1	Total	Ba	0	0
			1	1		
8	C	1	Total	Ba	0	0
			1	1		
8	7	1	Total	Ba	0	0
			1	1		
8	u	1	Total	Ba	0	0
			1	1		
8	O	1	Total	Ba	0	0
			1	1		
8	Y	1	Total	Ba	0	0
			1	1		
8	3	1	Total	Ba	0	0
			1	1		
8	F	1	Total	Ba	0	0
			1	1		

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

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

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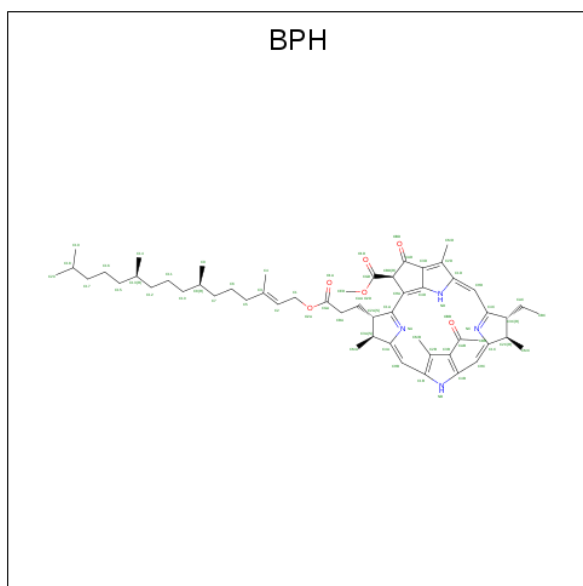
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	r	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	s	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	u	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	u	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	w	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	z	1	Total 66	C 55	Mg 1	N 4	O 6	0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

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

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



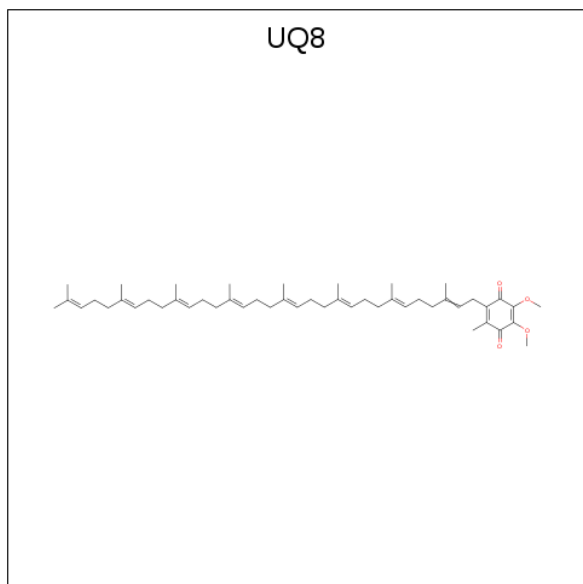
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		
10	x	1	Total	C	N	O	0	0
			65	55	4	6		

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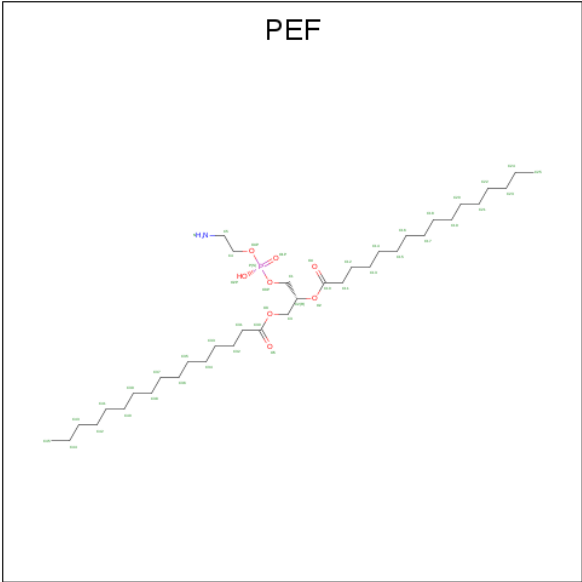
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	y	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is Ubiquinone-8 (three-letter code: UQ8) (formula: C₄₉H₇₄O₄).



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 (three-letter code: PEF) (formula: C₃₇H₇₄NO₈P).



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

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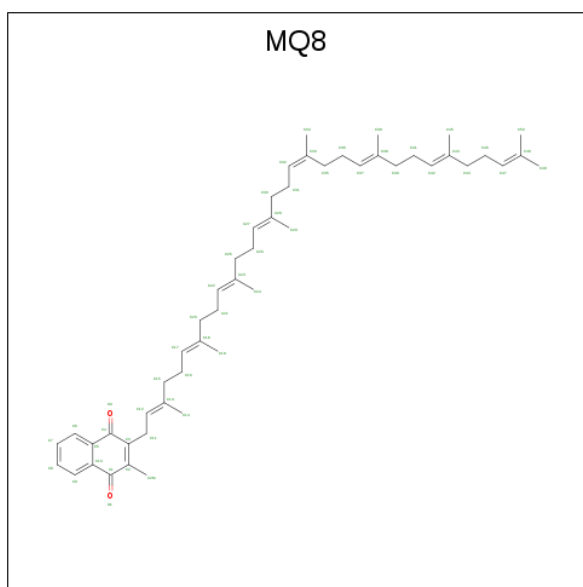
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	m	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
12	p	1	Total	C	N	O	P	0	0
			16	7	1	7	1		

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe).

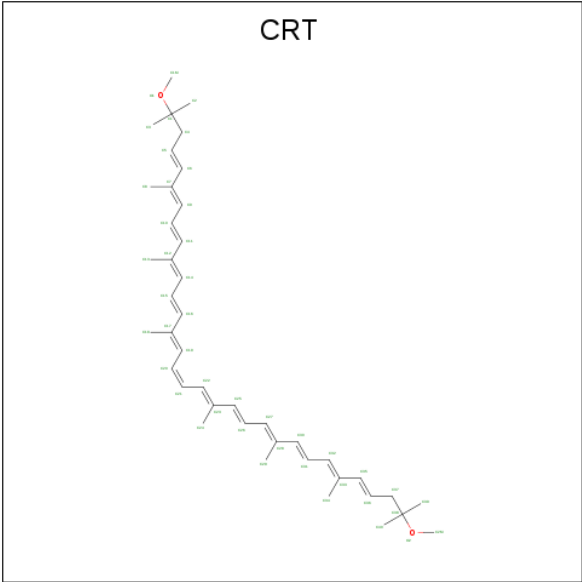
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	x	1	Total	Fe	0	0
			1	1		
13	L	1	Total	Fe	0	0
			1	1		

- Molecule 14 is MENAQUINONE 8 (three-letter code: 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 (three-letter code: CRT) (formula: C₄₂H₆₀O₂).



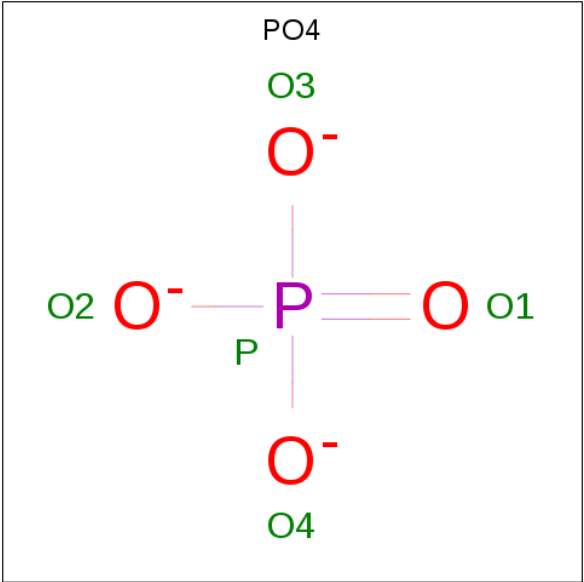
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			44	42	2		
15	E	1	Total	C	O	0	0
			44	42	2		
15	G	1	Total	C	O	0	0
			44	42	2		
15	I	1	Total	C	O	0	0
			44	42	2		
15	O	1	Total	C	O	0	0
			44	42	2		
15	P	1	Total	C	O	0	0
			44	42	2		
15	R	1	Total	C	O	0	0
			44	42	2		
15	T	1	Total	C	O	0	0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

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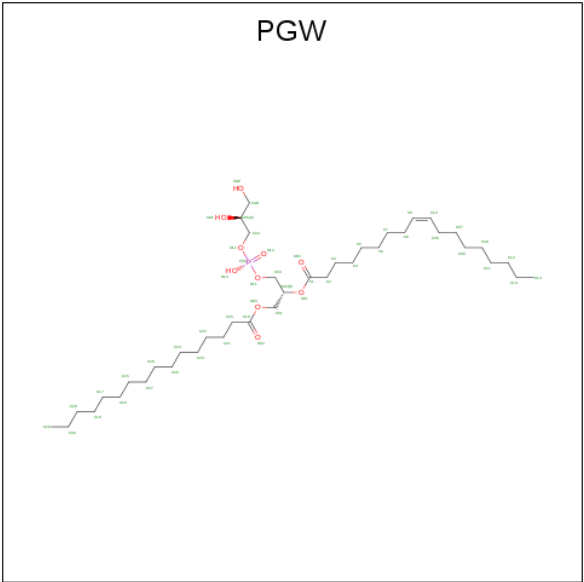
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	7	1	Total	C	O	0	0
			44	42	2		
15	9	1	Total	C	O	0	0
			44	42	2		
15	0	1	Total	C	O	0	0
			44	42	2		
15	y	1	Total	C	O	0	0
			44	42	2		
15	m	1	Total	C	O	0	0
			44	42	2		
15	n	1	Total	C	O	0	0
			44	42	2		
15	q	1	Total	C	O	0	0
			44	42	2		
15	s	1	Total	C	O	0	0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

- Molecule 16 is PHOSPHATE ION (three-letter code: 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 (three-letter code: PGW) (formula: C₄₀H₇₇O₁₀P).



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

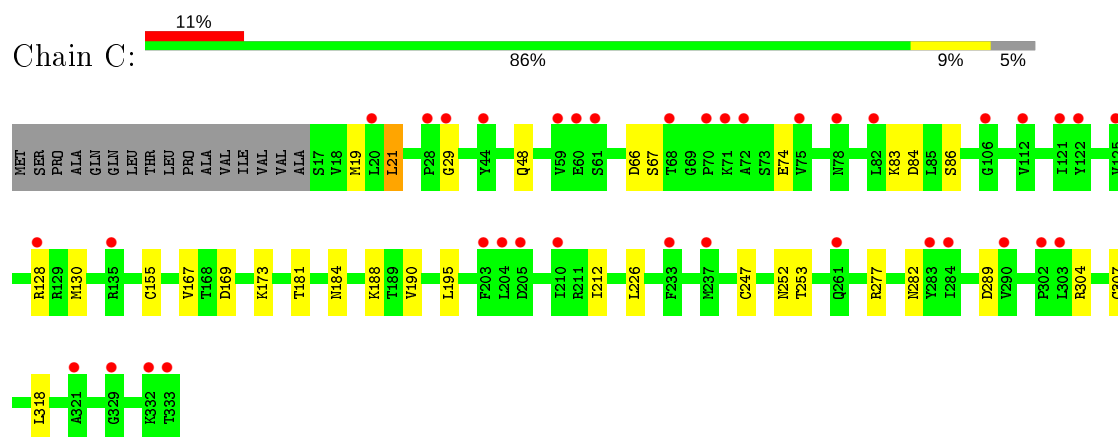
- Molecule 18 is water.

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

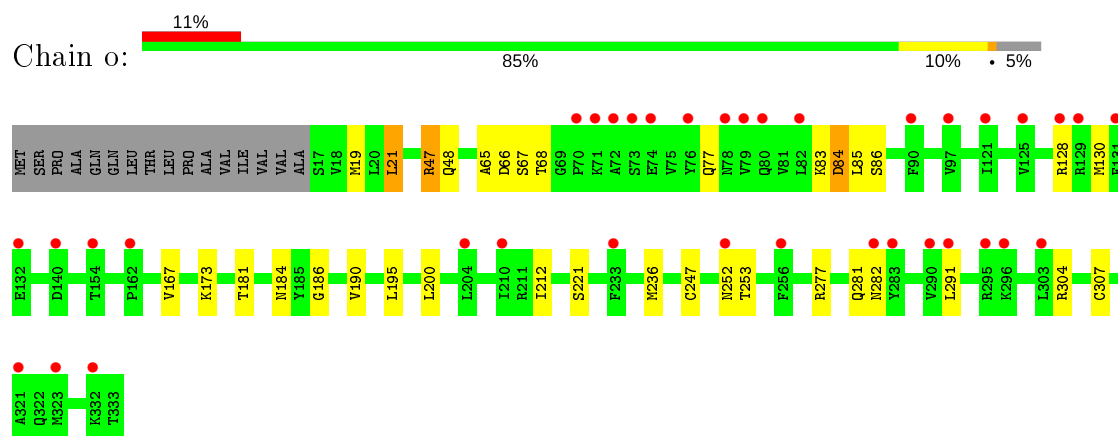
3 Residue-property plots [i](#)

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

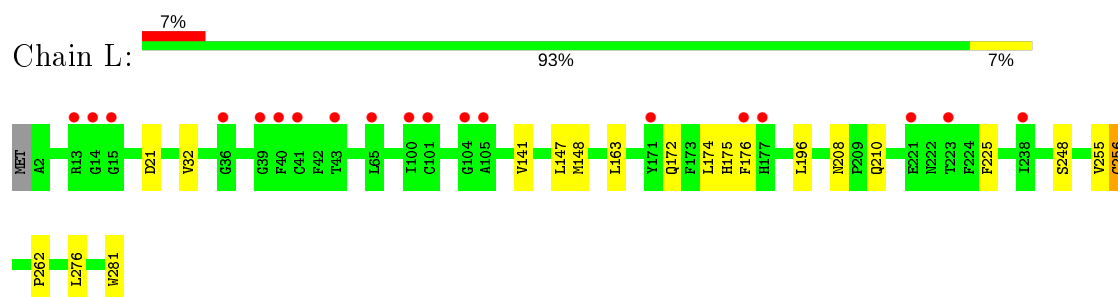
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



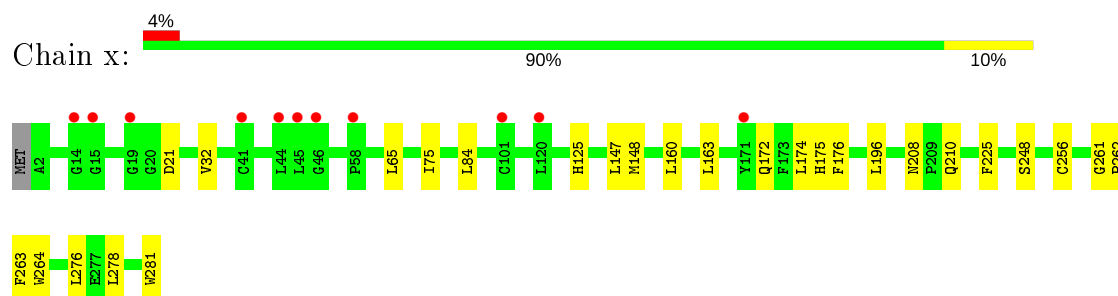
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



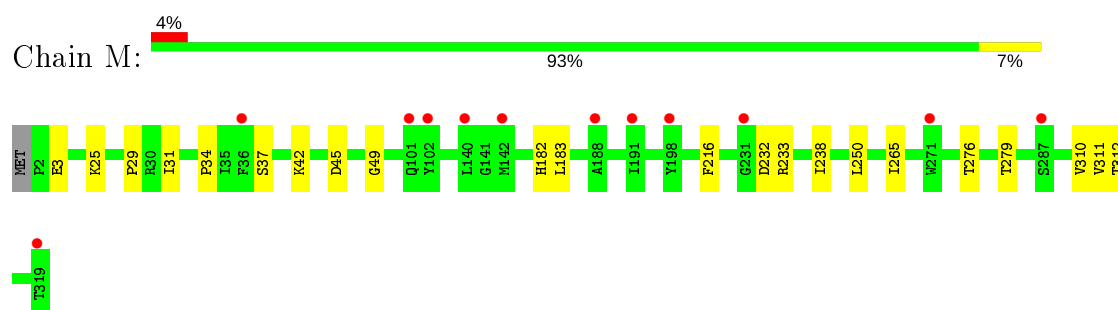
- Molecule 2: Photosynthetic reaction center L subunit



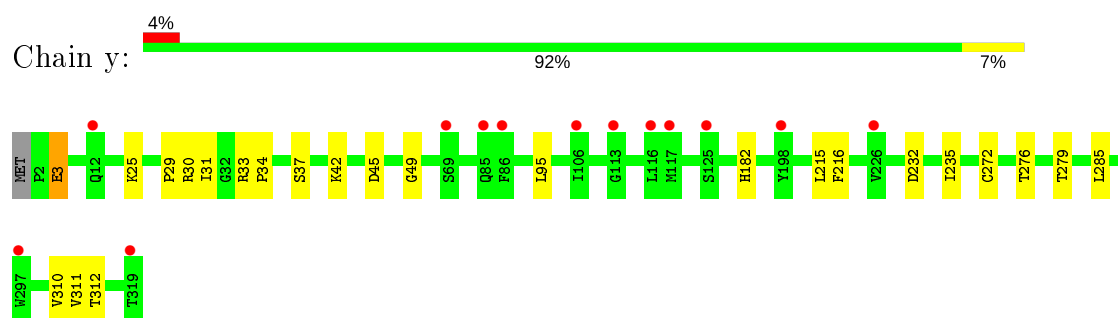
- Molecule 2: Photosynthetic reaction center L subunit



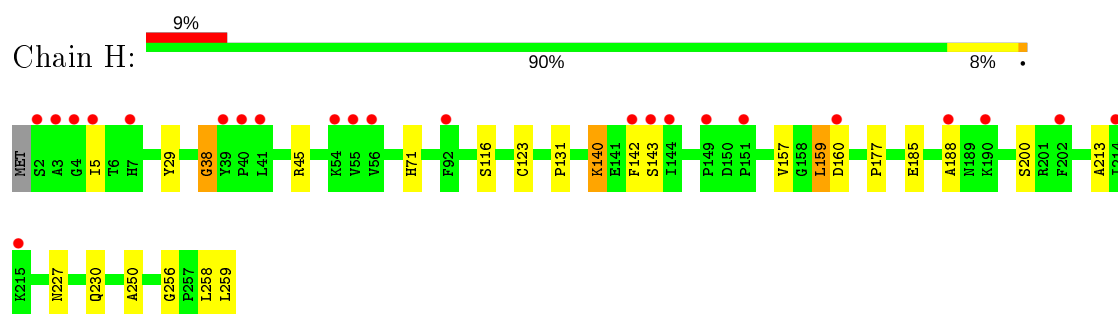
- Molecule 3: Photosynthetic reaction center M subunit



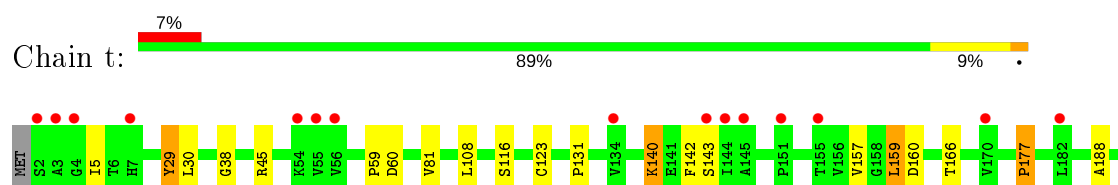
- Molecule 3: Photosynthetic reaction center M subunit



- Molecule 4: Photosynthetic reaction center H subunit

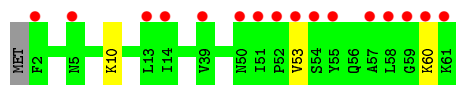
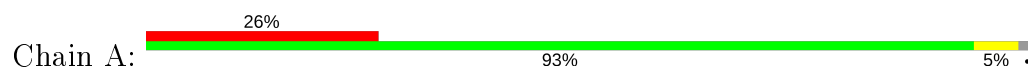


- Molecule 4: Photosynthetic reaction center H subunit

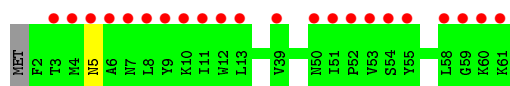




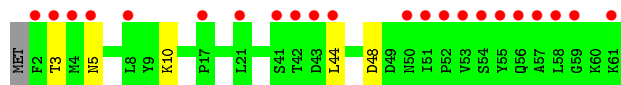
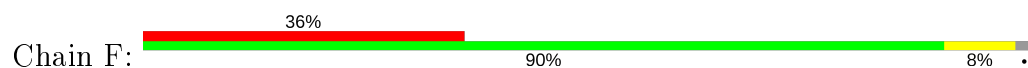
- Molecule 5: LH1 alpha polypeptide



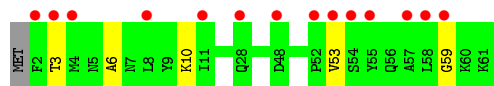
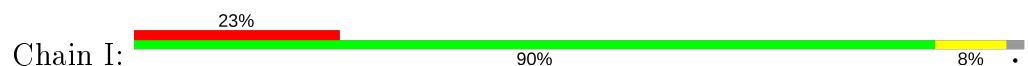
- Molecule 5: LH1 alpha polypeptide



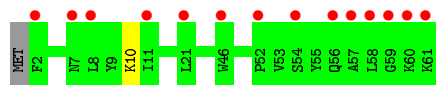
- Molecule 5: LH1 alpha polypeptide



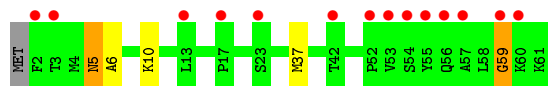
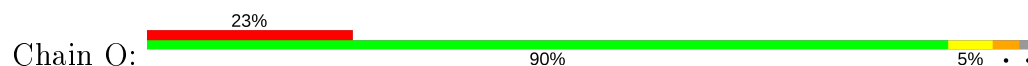
- Molecule 5: LH1 alpha polypeptide



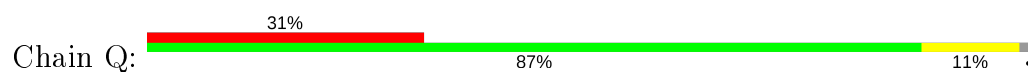
- Molecule 5: LH1 alpha polypeptide



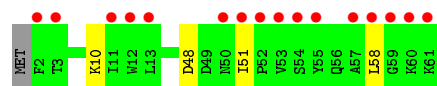
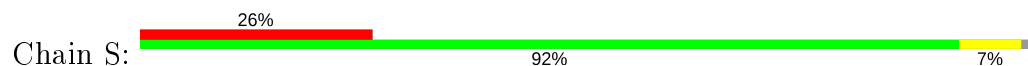
- Molecule 5: LH1 alpha polypeptide



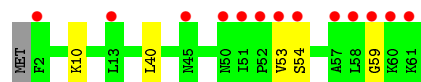
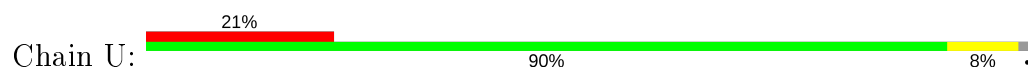
- Molecule 5: LH1 alpha polypeptide



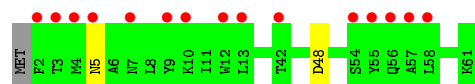
- Molecule 5: LH1 alpha polypeptide



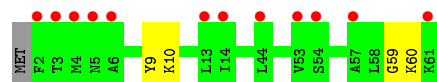
- Molecule 5: LH1 alpha polypeptide



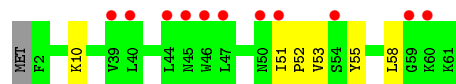
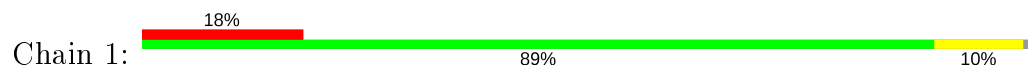
- Molecule 5: LH1 alpha polypeptide



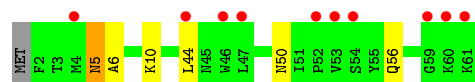
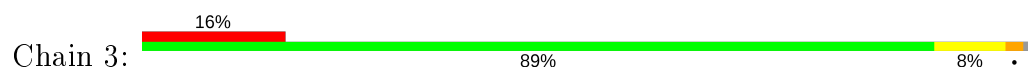
- Molecule 5: LH1 alpha polypeptide



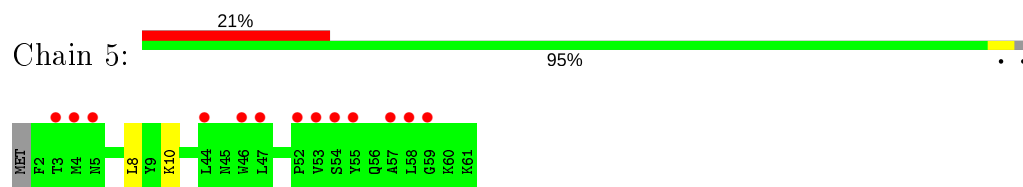
- Molecule 5: LH1 alpha polypeptide



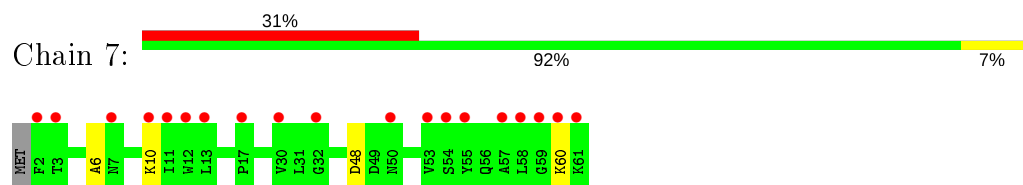
- Molecule 5: LH1 alpha polypeptide



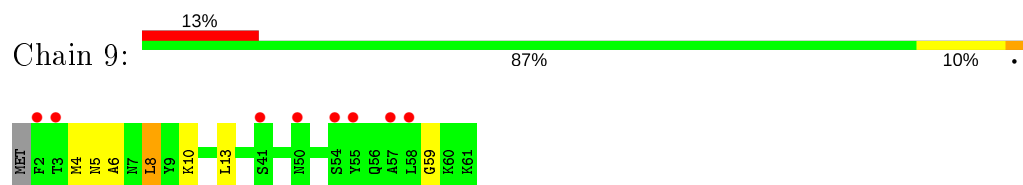
- Molecule 5: LH1 alpha polypeptide



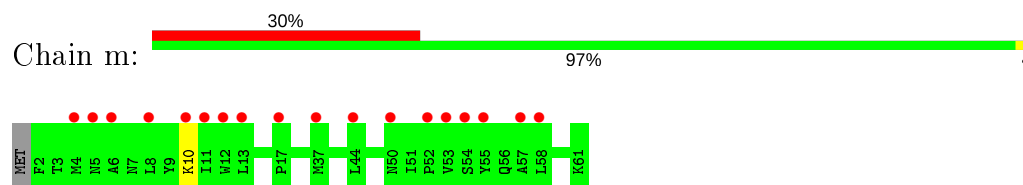
- Molecule 5: LH1 alpha polypeptide



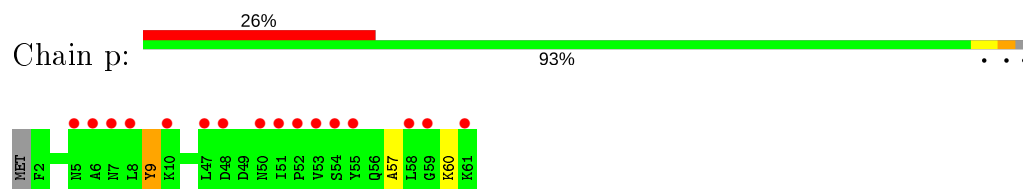
- Molecule 5: LH1 alpha polypeptide



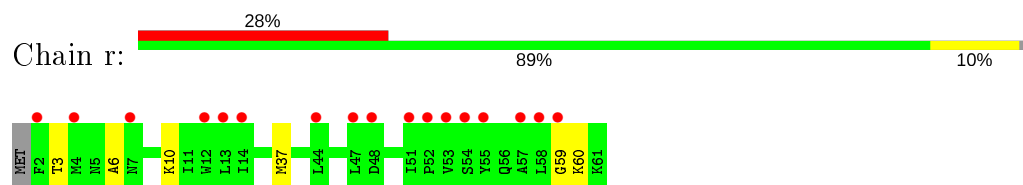
- Molecule 5: LH1 alpha polypeptide



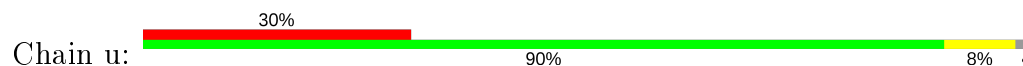
- Molecule 5: LH1 alpha polypeptide

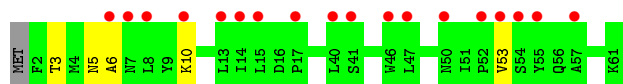


- Molecule 5: LH1 alpha polypeptide

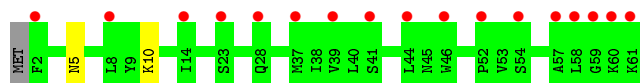


- Molecule 5: LH1 alpha polypeptide

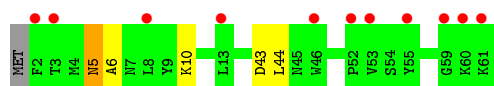
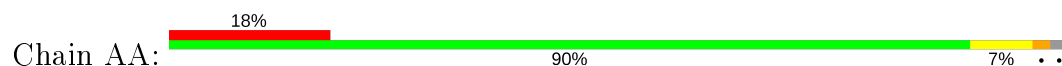




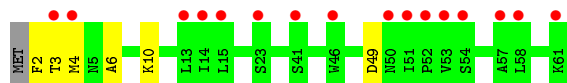
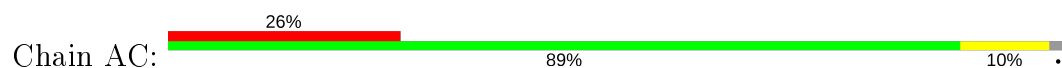
- Molecule 5: LH1 alpha polypeptide



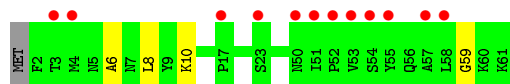
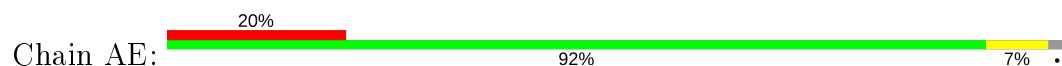
- Molecule 5: LH1 alpha polypeptide



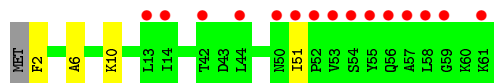
- Molecule 5: LH1 alpha polypeptide



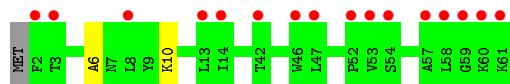
- Molecule 5: LH1 alpha polypeptide



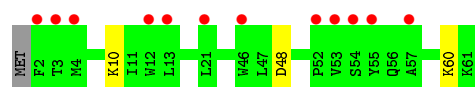
- Molecule 5: LH1 alpha polypeptide



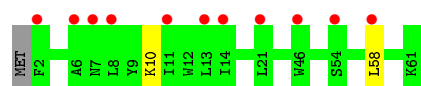
- Molecule 5: LH1 alpha polypeptide



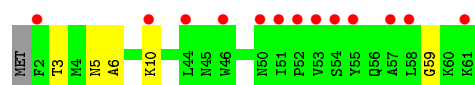
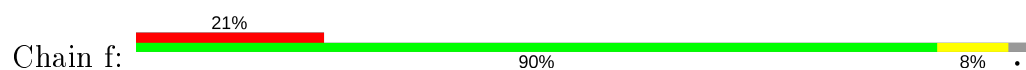
- Molecule 5: LH1 alpha polypeptide



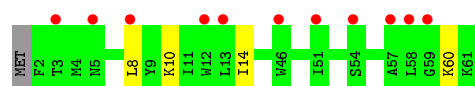
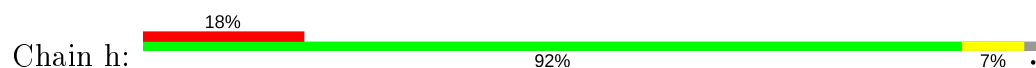
- Molecule 5: LH1 alpha polypeptide



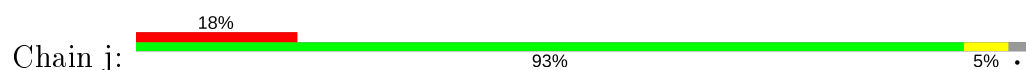
- Molecule 5: LH1 alpha polypeptide



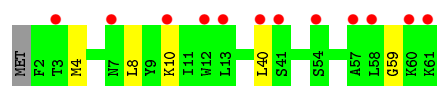
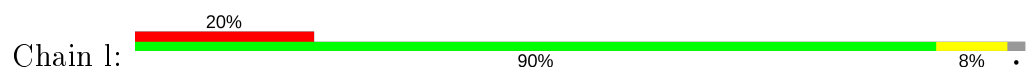
- Molecule 5: LH1 alpha polypeptide



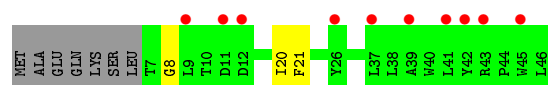
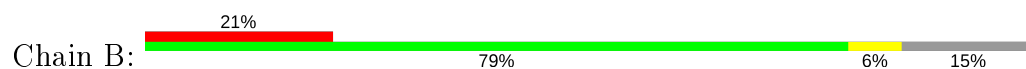
- Molecule 5: LH1 alpha polypeptide



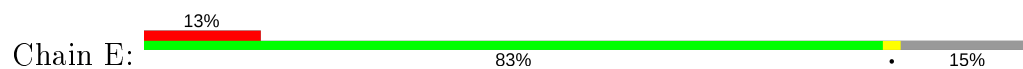
- Molecule 5: LH1 alpha polypeptide



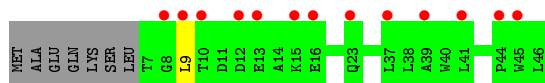
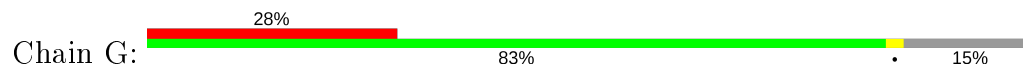
- Molecule 6: LH1 beta polypeptide



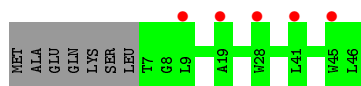
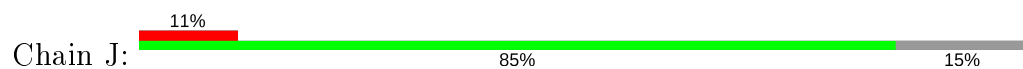
• Molecule 6: LH1 beta polypeptide



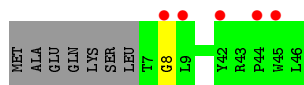
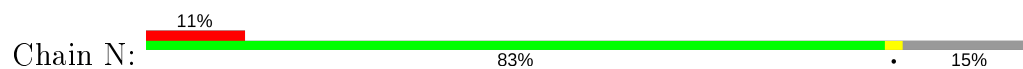
• Molecule 6: LH1 beta polypeptide



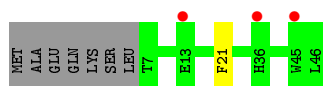
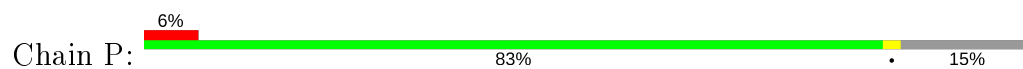
• Molecule 6: LH1 beta polypeptide



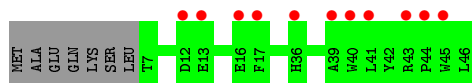
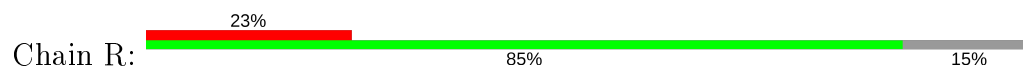
• Molecule 6: LH1 beta polypeptide



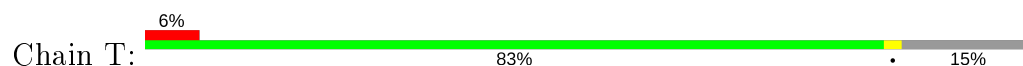
• Molecule 6: LH1 beta polypeptide

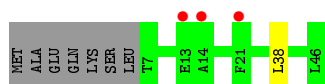


• Molecule 6: LH1 beta polypeptide

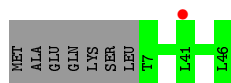
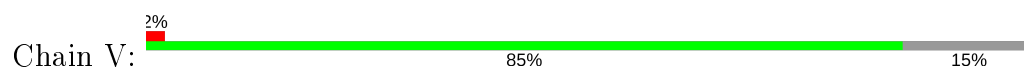


• Molecule 6: LH1 beta polypeptide

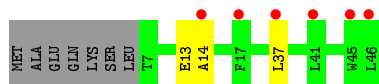
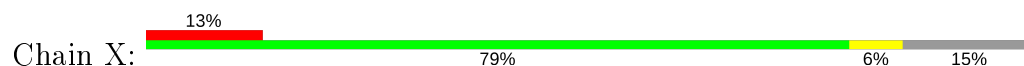




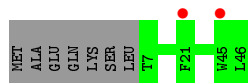
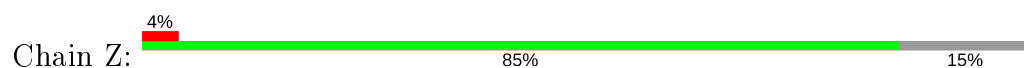
- Molecule 6: LH1 beta polypeptide



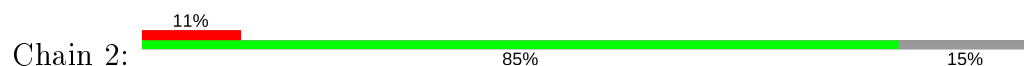
- Molecule 6: LH1 beta polypeptide



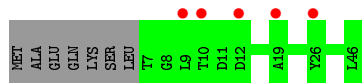
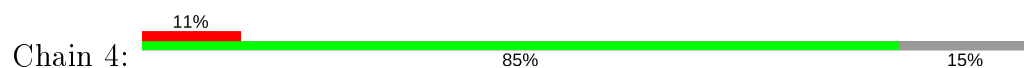
- Molecule 6: LH1 beta polypeptide



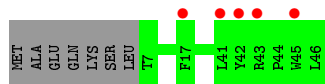
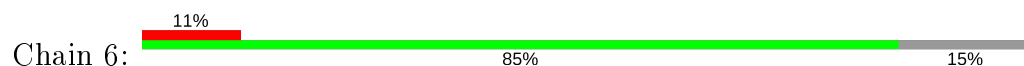
- Molecule 6: LH1 beta polypeptide



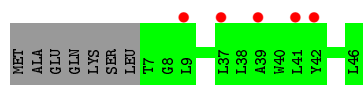
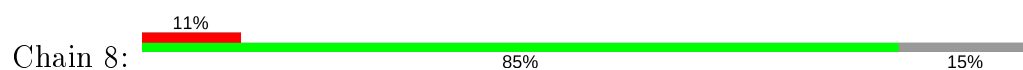
- Molecule 6: LH1 beta polypeptide



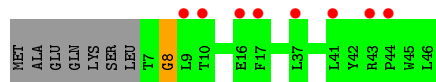
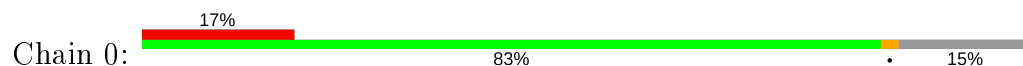
- Molecule 6: LH1 beta polypeptide



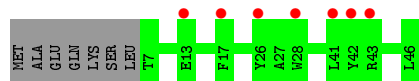
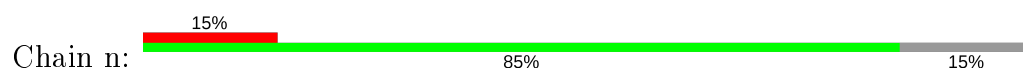
- Molecule 6: LH1 beta polypeptide



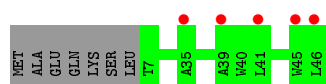
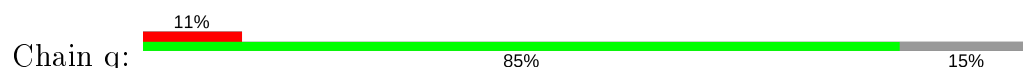
- Molecule 6: LH1 beta polypeptide



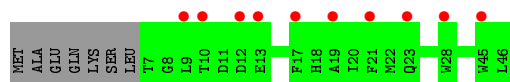
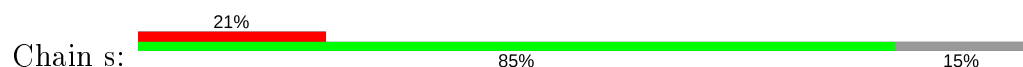
- Molecule 6: LH1 beta polypeptide



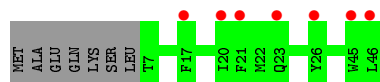
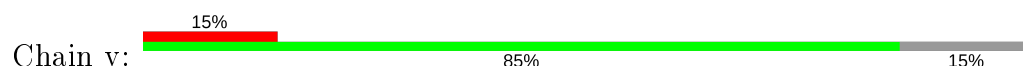
- Molecule 6: LH1 beta polypeptide



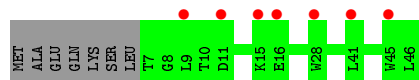
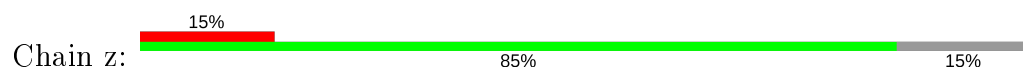
- Molecule 6: LH1 beta polypeptide



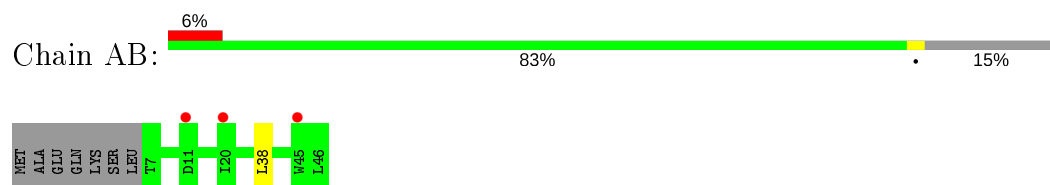
- Molecule 6: LH1 beta polypeptide



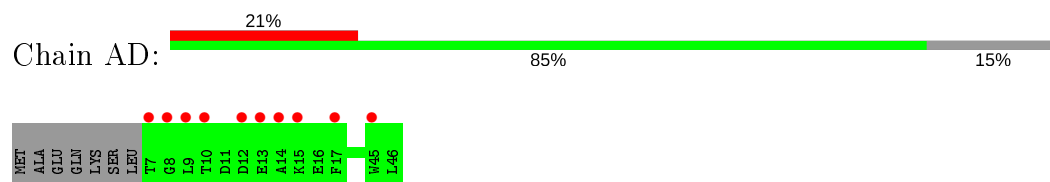
- Molecule 6: LH1 beta polypeptide



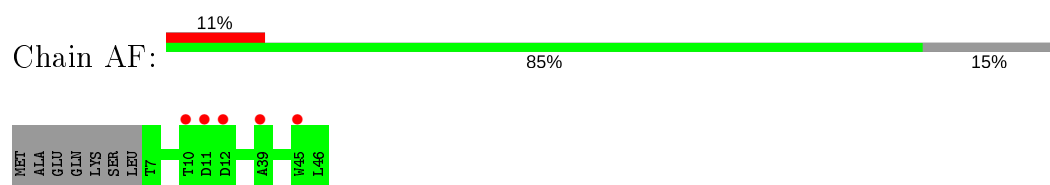
- Molecule 6: LH1 beta polypeptide



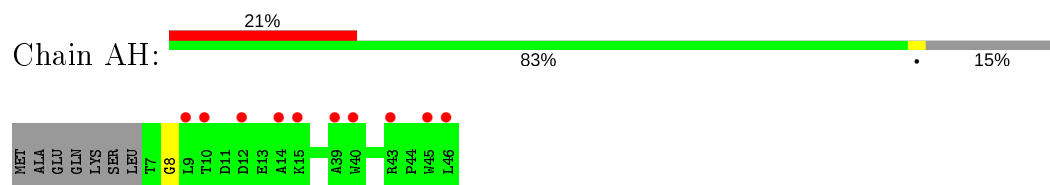
- Molecule 6: LH1 beta polypeptide



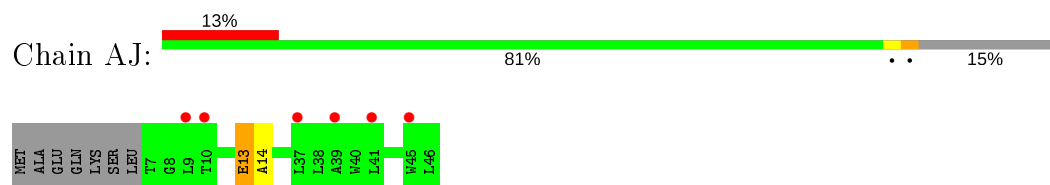
- Molecule 6: LH1 beta polypeptide



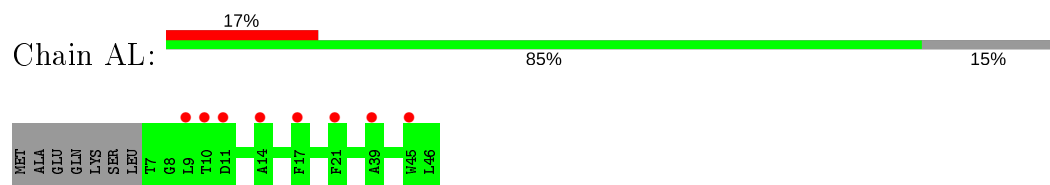
- Molecule 6: LH1 beta polypeptide



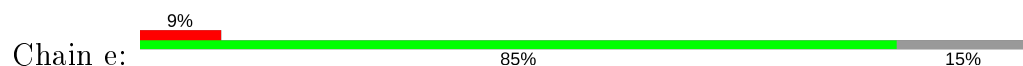
- Molecule 6: LH1 beta polypeptide

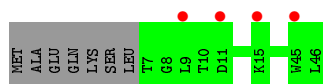


- Molecule 6: LH1 beta polypeptide

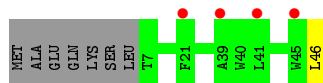
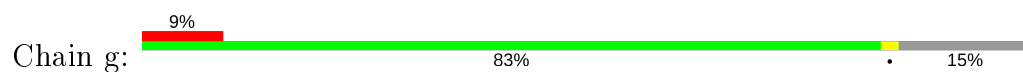


- Molecule 6: LH1 beta polypeptide

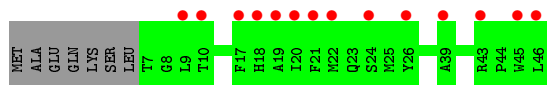
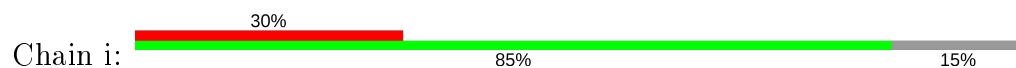




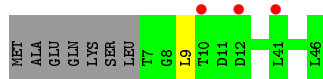
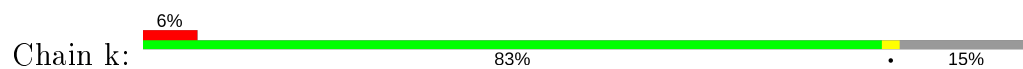
- Molecule 6: LH1 beta polypeptide



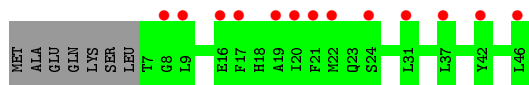
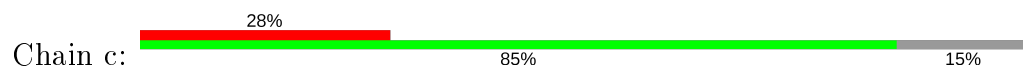
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	163.83Å 148.56Å 210.00Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	49.90 – 3.30 49.90 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (49.90-3.30) 92.6 (49.90-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.279 , 0.313 0.280 , 0.313	Depositor DCC
R_{free} test set	6658 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 86.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	51893	wwPDB-VP
Average B, all atoms (Å ²)	162.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.75	1/2528 (0.0%)	1.05	6/3451 (0.2%)
1	o	0.73	1/2528 (0.0%)	1.05	9/3451 (0.3%)
2	L	0.78	1/2318 (0.0%)	1.02	3/3167 (0.1%)
2	x	0.80	1/2318 (0.0%)	1.06	10/3167 (0.3%)
3	M	0.72	0/2646	1.02	5/3621 (0.1%)
3	y	0.71	0/2646	0.98	3/3621 (0.1%)
4	H	0.79	1/2037 (0.0%)	1.08	6/2776 (0.2%)
4	t	0.79	1/2037 (0.0%)	1.07	5/2776 (0.2%)
5	1	0.52	0/485	0.91	0/664
5	3	0.48	0/485	0.76	0/664
5	5	0.47	0/485	0.70	0/664
5	7	0.46	0/485	0.69	0/664
5	9	0.44	0/485	0.77	1/664 (0.2%)
5	A	0.46	0/485	0.78	0/664
5	AA	0.45	0/485	0.78	0/664
5	AC	0.43	0/485	0.72	0/664
5	AE	0.40	0/491	0.70	0/672
5	AG	0.47	0/485	0.76	0/664
5	AI	0.46	0/485	0.77	0/664
5	AK	0.52	0/485	0.76	0/664
5	D	0.47	0/485	0.83	0/664
5	F	0.42	0/485	0.76	1/664 (0.2%)
5	I	0.45	0/485	0.74	0/664
5	K	0.42	0/485	0.76	0/664
5	O	0.45	0/485	0.77	1/664 (0.2%)
5	Q	0.48	0/485	0.80	1/664 (0.2%)
5	S	0.47	0/491	0.74	0/672
5	U	0.51	0/485	0.81	1/664 (0.2%)
5	W	0.54	0/485	0.84	0/664
5	Y	0.55	0/485	0.83	0/664
5	d	0.48	0/485	0.77	0/664
5	f	0.55	0/485	0.84	0/664

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	h	0.50	0/485	0.83	1/664 (0.2%)
5	j	0.46	0/485	0.72	0/664
5	l	0.44	0/485	0.74	0/664
5	m	0.42	0/485	0.75	0/664
5	p	0.49	0/485	0.81	1/664 (0.2%)
5	r	0.47	0/485	0.74	0/664
5	u	0.44	0/485	0.73	0/664
5	w	0.41	0/485	0.77	0/664
6	0	0.42	0/350	0.72	1/476 (0.2%)
6	2	0.52	0/350	0.67	0/476
6	4	0.46	0/350	0.73	0/476
6	6	0.47	0/350	0.71	0/476
6	8	0.43	0/350	0.62	0/476
6	AB	0.43	0/350	0.75	1/476 (0.2%)
6	AD	0.44	0/350	0.61	0/476
6	AF	0.44	0/350	0.60	0/476
6	AH	0.39	0/350	0.62	0/476
6	AJ	0.46	0/350	0.68	0/476
6	AL	0.48	0/350	0.70	0/476
6	B	0.41	0/350	0.75	0/476
6	E	0.43	0/350	0.72	0/476
6	G	0.48	0/350	0.73	1/476 (0.2%)
6	J	0.43	0/350	0.69	0/476
6	N	0.41	0/350	0.63	0/476
6	P	0.44	0/350	0.66	0/476
6	R	0.40	0/350	0.66	0/476
6	T	0.47	0/350	0.70	1/476 (0.2%)
6	V	0.43	0/350	0.64	0/476
6	X	0.47	0/350	0.83	1/476 (0.2%)
6	Z	0.45	0/350	0.65	0/476
6	c	0.43	0/350	0.67	0/476
6	e	0.50	0/350	0.63	0/476
6	g	0.43	0/350	0.67	1/476 (0.2%)
6	i	0.43	0/350	0.66	0/476
6	k	0.42	0/350	0.61	1/476 (0.2%)
6	n	0.51	0/350	0.72	0/476
6	q	0.49	0/350	0.74	0/476
6	s	0.46	0/350	0.69	0/476
6	v	0.44	0/350	0.71	0/476
6	z	0.40	0/350	0.70	0/476
All	All	0.60	6/45790 (0.0%)	0.88	61/62526 (0.1%)

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

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

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	o	247	CYS	CB-SG	-6.19	1.71	1.82
2	L	256	CYS	CB-SG	-6.14	1.71	1.82
4	H	123	CYS	CB-SG	-5.82	1.72	1.81
1	C	155	CYS	CB-SG	-5.78	1.72	1.81
2	x	264	TRP	CB-CG	-5.42	1.40	1.50

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	o	247	CYS	CA-CB-SG	-8.94	97.92	114.00
2	L	276	LEU	CB-CG-CD2	-8.58	96.41	111.00
2	x	276	LEU	CB-CG-CD2	-7.94	97.50	111.00
1	C	247	CYS	CA-CB-SG	-7.75	100.06	114.00
1	o	47	ARG	NE-CZ-NH1	7.18	123.89	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	315/333 (95%)	274 (87%)	33 (10%)	8 (2%)	5	27
1	o	315/333 (95%)	277 (88%)	30 (10%)	8 (2%)	5	27
2	L	278/281 (99%)	248 (89%)	26 (9%)	4 (1%)	11	38
2	x	278/281 (99%)	247 (89%)	28 (10%)	3 (1%)	14	45
3	M	316/319 (99%)	282 (89%)	30 (10%)	4 (1%)	12	40
3	y	316/319 (99%)	286 (90%)	26 (8%)	4 (1%)	12	40
4	H	256/259 (99%)	216 (84%)	31 (12%)	9 (4%)	3	21
4	t	256/259 (99%)	214 (84%)	32 (12%)	10 (4%)	3	18
5	1	58/61 (95%)	44 (76%)	12 (21%)	2 (3%)	3	22
5	3	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	8
5	5	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	22
5	7	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	13
5	9	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	1	5
5	A	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	22
5	AA	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	2	13
5	AC	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	8
5	AE	59/61 (97%)	49 (83%)	7 (12%)	3 (5%)	2	13
5	AG	58/61 (95%)	53 (91%)	3 (5%)	2 (3%)	3	22
5	AI	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	22
5	AK	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	22
5	D	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	13
5	I	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	13
5	K	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	35
5	O	58/61 (95%)	46 (79%)	8 (14%)	4 (7%)	1	8
5	Q	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	8
5	S	59/61 (97%)	49 (83%)	8 (14%)	2 (3%)	3	22
5	U	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	2	13
5	W	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	35
5	Y	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2	13
5	d	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	22
5	f	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	8
5	h	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	22
5	j	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	22
5	l	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	2	13
5	m	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	9	35
5	p	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	22
5	r	58/61 (95%)	46 (79%)	7 (12%)	5 (9%)	1	5
5	u	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	13
5	w	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	35
6	0	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	5	27
6	2	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	4	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	6	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	8	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AB	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AD	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AF	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AH	38/47 (81%)	37 (97%)	0	1 (3%)	5	27
6	AJ	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AL	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	B	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	38/47 (81%)	38 (100%)	0	0	100	100
6	G	38/47 (81%)	38 (100%)	0	0	100	100
6	J	38/47 (81%)	38 (100%)	0	0	100	100
6	N	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	5	27
6	P	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	R	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	T	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	V	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	X	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	Z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	c	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	e	38/47 (81%)	38 (100%)	0	0	100	100
6	g	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	i	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	k	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	n	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	q	38/47 (81%)	38 (100%)	0	0	100	100
6	s	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	v	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
All	All	5404/5840 (92%)	4783 (88%)	483 (9%)	138 (3%)	5	27

5 of 138 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	265/278 (95%)	247 (93%)	18 (7%)	16	44
1	o	265/278 (95%)	245 (92%)	20 (8%)	13	39
2	L	228/229 (100%)	215 (94%)	13 (6%)	20	51
2	x	228/229 (100%)	215 (94%)	13 (6%)	20	51
3	M	256/257 (100%)	244 (95%)	12 (5%)	26	57
3	y	256/257 (100%)	240 (94%)	16 (6%)	18	47
4	H	210/211 (100%)	198 (94%)	12 (6%)	20	51
4	t	210/211 (100%)	194 (92%)	16 (8%)	13	39
5	1	52/56 (93%)	49 (94%)	3 (6%)	20	50
5	3	52/56 (93%)	49 (94%)	3 (6%)	20	50
5	5	52/56 (93%)	52 (100%)	0	100	100
5	7	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	9	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	A	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	AA	52/56 (93%)	49 (94%)	3 (6%)	20	50
5	AC	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	AE	53/56 (95%)	52 (98%)	1 (2%)	57	77
5	AG	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	AI	52/56 (93%)	52 (100%)	0	100	100
5	AK	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	D	52/56 (93%)	52 (100%)	0	100	100
5	F	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	I	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	K	52/56 (93%)	52 (100%)	0	100	100
5	O	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	Q	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	S	53/56 (95%)	51 (96%)	2 (4%)	33	62
5	U	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	W	52/56 (93%)	51 (98%)	1 (2%)	57	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Y	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	d	52/56 (93%)	52 (100%)	0	100	100
5	f	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	h	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	j	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	l	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	m	52/56 (93%)	52 (100%)	0	100	100
5	p	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	r	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	u	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	w	52/56 (93%)	51 (98%)	1 (2%)	57	77
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%)	41	68
6	AL	33/39 (85%)	33 (100%)	0	100	100
6	B	33/39 (85%)	31 (94%)	2 (6%)	18	48
6	E	33/39 (85%)	32 (97%)	1 (3%)	41	68
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%)	41	68
6	R	33/39 (85%)	33 (100%)	0	100	100
6	T	33/39 (85%)	33 (100%)	0	100	100
6	V	33/39 (85%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	X	33/39 (85%)	32 (97%)	1 (3%)	41	68
6	Z	33/39 (85%)	33 (100%)	0	100	100
6	c	33/39 (85%)	33 (100%)	0	100	100
6	e	33/39 (85%)	33 (100%)	0	100	100
6	g	33/39 (85%)	33 (100%)	0	100	100
6	i	33/39 (85%)	33 (100%)	0	100	100
6	k	33/39 (85%)	33 (100%)	0	100	100
6	n	33/39 (85%)	33 (100%)	0	100	100
6	q	33/39 (85%)	33 (100%)	0	100	100
6	s	33/39 (85%)	33 (100%)	0	100	100
6	v	33/39 (85%)	33 (100%)	0	100	100
6	z	33/39 (85%)	33 (100%)	0	100	100
All	All	4640/4990 (93%)	4473 (96%)	167 (4%)	35	63

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	1	55	TYR
1	o	181	THR
5	AA	44	LEU
5	3	44	LEU
1	o	47	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
5	Y	36	HIS
1	o	183	GLN
5	r	56	GLN
5	K	56	GLN
5	f	5	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 40 are monoatomic - leaving 144 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	CRT	AC	101	-	41,43,43	0.80	0	50,54,54	2.04	16 (32%)
15	CRT	7	103	-	41,43,43	0.95	1 (2%)	50,54,54	3.62	11 (22%)
9	BCL	AB	101	-	58,74,74	1.59	9 (15%)	69,115,115	2.18	24 (34%)
15	CRT	G	101	-	41,43,43	0.71	0	50,54,54	3.76	15 (30%)
9	BCL	4	102	-	58,74,74	1.59	9 (15%)	69,115,115	2.26	24 (34%)
9	BCL	u	102	-	58,74,74	1.60	11 (18%)	69,115,115	2.27	24 (34%)
9	BCL	q	102	-	58,74,74	1.60	9 (15%)	69,115,115	2.29	24 (34%)
9	BCL	AI	101	-	58,74,74	1.57	9 (15%)	69,115,115	2.36	26 (37%)
12	PEF	M	407	-	15,15,46	1.06	1 (6%)	17,19,51	1.12	1 (5%)
11	UQ8	x	304	-	53,53,53	1.54	4 (7%)	64,67,67	1.99	20 (31%)
15	CRT	P	102	-	41,43,43	0.70	0	50,54,54	1.77	13 (26%)
9	BCL	g	102	-	58,74,74	1.61	8 (13%)	69,115,115	2.26	24 (34%)
15	CRT	m	104	-	41,43,43	0.73	0	50,54,54	3.51	20 (40%)
9	BCL	Y	101	-	58,74,74	1.62	11 (18%)	69,115,115	2.21	23 (33%)
9	BCL	AH	101	-	58,74,74	1.65	12 (20%)	69,115,115	2.17	21 (30%)
9	BCL	AF	101	-	58,74,74	1.63	10 (17%)	69,115,115	2.15	26 (37%)
12	PEF	t	303	-	18,18,46	1.43	2 (11%)	21,23,51	2.20	7 (33%)
9	BCL	s	102	-	58,74,74	1.60	11 (18%)	69,115,115	2.29	27 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CRT	AL	101	-	41,43,43	0.80	0	50,54,54	1.75	13 (26%)
12	PEF	x	306	-	18,18,46	1.72	2 (11%)	21,23,51	1.32	3 (14%)
9	BCL	X	102	-	58,74,74	1.60	10 (17%)	69,115,115	2.29	27 (39%)
9	BCL	AK	101	-	58,74,74	1.58	9 (15%)	69,115,115	2.20	25 (36%)
15	CRT	q	101	-	41,43,43	0.74	0	50,54,54	3.69	13 (26%)
15	CRT	AD	101	-	41,43,43	0.82	0	50,54,54	3.60	19 (38%)
9	BCL	r	101	-	58,74,74	1.62	10 (17%)	69,115,115	2.10	22 (31%)
9	BCL	e	102	-	58,74,74	1.54	10 (17%)	69,115,115	2.23	25 (36%)
15	CRT	O	101	-	41,43,43	0.74	0	50,54,54	3.86	17 (34%)
9	BCL	AC	102	-	58,74,74	1.65	11 (18%)	69,115,115	2.18	27 (39%)
12	PEF	y	407	-	18,18,46	1.64	2 (11%)	21,23,51	1.24	3 (14%)
11	UQ8	L	304	-	53,53,53	1.50	4 (7%)	64,67,67	1.73	16 (25%)
16	PO4	H	303	-	4,4,4	0.62	0	6,6,6	0.73	0
9	BCL	O	102	-	58,74,74	1.59	8 (13%)	69,115,115	2.24	27 (39%)
15	CRT	2	101	-	41,43,43	0.80	0	50,54,54	1.66	14 (28%)
12	PEF	y	408	-	18,18,46	1.70	2 (11%)	21,23,51	2.35	6 (28%)
7	HEM	C	503	1	27,50,50	1.07	1 (3%)	17,82,82	1.88	4 (23%)
9	BCL	U	101	-	58,74,74	1.60	11 (18%)	69,115,115	2.23	24 (34%)
9	BCL	A	103	-	58,74,74	1.64	9 (15%)	69,115,115	2.17	23 (33%)
15	CRT	Z	101	-	41,43,43	0.86	0	50,54,54	1.92	17 (34%)
7	HEM	C	502	1	27,50,50	1.28	2 (7%)	17,82,82	2.23	6 (35%)
9	BCL	S	102	-	58,74,74	1.62	11 (18%)	69,115,115	2.25	25 (36%)
12	PEF	L	305	-	10,11,46	0.74	0	11,14,51	1.21	1 (9%)
15	CRT	7	101	-	41,43,43	0.79	0	50,54,54	3.53	17 (34%)
9	BCL	N	101	-	58,74,74	1.59	9 (15%)	69,115,115	2.23	22 (31%)
9	BCL	j	101	-	58,74,74	1.62	8 (13%)	69,115,115	2.07	21 (30%)
15	CRT	I	102	-	41,43,43	0.76	0	50,54,54	3.67	14 (28%)
9	BCL	F	101	-	58,74,74	1.55	8 (13%)	69,115,115	2.19	22 (31%)
9	BCL	D	101	-	58,74,74	1.60	9 (15%)	69,115,115	2.17	23 (33%)
9	BCL	l	101	-	58,74,74	1.64	11 (18%)	69,115,115	2.17	19 (27%)
7	HEM	o	502	1	27,50,50	1.27	2 (7%)	17,82,82	2.22	6 (35%)
16	PO4	M	406	-	4,4,4	0.49	0	6,6,6	1.02	0
15	CRT	n	101	-	41,43,43	0.78	0	50,54,54	3.99	20 (40%)
12	PEF	A	101	-	18,18,46	1.43	2 (11%)	21,23,51	1.91	4 (19%)
15	CRT	0	101	-	41,43,43	0.80	0	50,54,54	3.66	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	I	101	-	58,74,74	1.63	10 (17%)	69,115,115	2.22	28 (40%)
9	BCL	AL	102	-	58,74,74	1.58	8 (13%)	69,115,115	2.12	23 (33%)
12	PEF	H	301	-	18,18,46	1.43	2 (11%)	21,23,51	1.61	3 (14%)
9	BCL	x	303	-	58,74,74	1.64	11 (18%)	69,115,115	2.23	24 (34%)
14	MQ8	y	403	-	54,54,54	1.07	5 (9%)	66,69,69	1.62	17 (25%)
9	BCL	h	101	-	58,74,74	1.64	11 (18%)	69,115,115	2.08	24 (34%)
9	BCL	f	101	-	58,74,74	1.63	9 (15%)	69,115,115	2.33	24 (34%)
15	CRT	AH	102	-	41,43,43	0.76	0	50,54,54	3.42	14 (28%)
9	BCL	z	102	-	58,74,74	1.60	8 (13%)	69,115,115	2.09	22 (31%)
9	BCL	0	102	-	58,74,74	1.64	12 (20%)	69,115,115	2.26	27 (39%)
10	BPH	x	302	-	64,70,70	1.05	5 (7%)	76,101,101	1.91	20 (26%)
15	CRT	R	101	-	41,43,43	0.81	0	50,54,54	3.44	15 (30%)
9	BCL	W	101	-	58,74,74	1.62	10 (17%)	69,115,115	2.14	24 (34%)
15	CRT	V	101	-	41,43,43	0.77	0	50,54,54	3.43	16 (32%)
9	BCL	AC	103	-	58,74,74	1.55	9 (15%)	69,115,115	2.16	24 (34%)
9	BCL	x	301	-	58,74,74	1.64	10 (17%)	69,115,115	2.53	26 (37%)
12	PEF	y	406	-	18,18,46	1.52	2 (11%)	21,23,51	2.04	4 (19%)
12	PEF	m	101	-	18,18,46	1.53	2 (11%)	21,23,51	1.59	3 (14%)
9	BCL	c	101	-	58,74,74	1.58	8 (13%)	69,115,115	2.19	23 (33%)
15	CRT	AF	102	-	41,43,43	0.74	0	50,54,54	3.67	14 (28%)
12	PEF	H	304	-	18,18,46	1.62	2 (11%)	21,23,51	1.56	2 (9%)
9	BCL	G	102	-	58,74,74	1.59	9 (15%)	69,115,115	2.18	22 (31%)
7	HEM	C	504	1	27,50,50	1.02	2 (7%)	17,82,82	2.07	6 (35%)
16	PO4	t	302	-	4,4,4	0.87	0	6,6,6	1.03	0
10	BPH	L	302	-	64,70,70	0.81	4 (6%)	76,101,101	1.99	18 (23%)
7	HEM	o	504	1	27,50,50	0.91	2 (7%)	17,82,82	1.59	3 (17%)
9	BCL	V	102	-	58,74,74	1.62	9 (15%)	69,115,115	2.22	28 (40%)
12	PEF	H	302	-	18,18,46	1.53	2 (11%)	21,23,51	1.77	2 (9%)
9	BCL	M	401	-	58,74,74	1.57	10 (17%)	69,115,115	2.40	23 (33%)
9	BCL	i	102	-	58,74,74	1.57	9 (15%)	69,115,115	2.20	29 (42%)
12	PEF	t	301	-	18,18,46	1.57	2 (11%)	21,23,51	1.27	2 (9%)
10	BPH	y	402	-	64,70,70	0.95	6 (9%)	76,101,101	1.91	17 (22%)
9	BCL	u	101	-	58,74,74	1.61	10 (17%)	69,115,115	2.18	24 (34%)
15	CRT	E	101	-	41,43,43	0.82	0	50,54,54	3.29	14 (28%)
15	CRT	g	101	-	41,43,43	0.81	0	50,54,54	3.86	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	T	102	-	58,74,74	1.62	11 (18%)	69,115,115	2.28	30 (43%)
12	PEF	p	101	-	15,15,46	0.92	1 (6%)	17,19,51	0.96	1 (5%)
15	CRT	z	101	-	41,43,43	0.76	0	50,54,54	3.72	19 (38%)
9	BCL	AE	102	-	58,74,74	1.56	9 (15%)	69,115,115	2.15	26 (37%)
9	BCL	d	101	-	58,74,74	1.67	11 (18%)	69,115,115	2.30	25 (36%)
15	CRT	e	101	-	41,43,43	0.77	0	50,54,54	1.80	14 (28%)
9	BCL	L	303	-	58,74,74	1.60	10 (17%)	69,115,115	2.28	22 (31%)
9	BCL	K	101	-	58,74,74	1.58	10 (17%)	69,115,115	2.14	24 (34%)
9	BCL	2	102	-	58,74,74	1.62	11 (18%)	69,115,115	2.33	27 (39%)
16	PO4	y	405	-	4,4,4	0.74	0	6,6,6	1.10	0
9	BCL	l	101	-	58,74,74	1.57	9 (15%)	69,115,115	2.20	23 (33%)
9	BCL	5	101	-	58,74,74	1.63	11 (18%)	69,115,115	2.25	24 (34%)
15	CRT	AJ	101	-	41,43,43	0.78	0	50,54,54	1.97	14 (28%)
9	BCL	x	305	-	58,74,74	1.78	12 (20%)	69,115,115	2.41	27 (39%)
17	PGW	S	101	-	20,20,50	1.02	1 (5%)	23,26,56	1.28	1 (4%)
9	BCL	m	102	-	58,74,74	1.65	11 (18%)	69,115,115	2.14	24 (34%)
9	BCL	P	101	-	58,74,74	1.61	11 (18%)	69,115,115	2.17	24 (34%)
9	BCL	D	102	-	58,74,74	1.58	7 (12%)	69,115,115	2.33	30 (43%)
9	BCL	AB	102	-	58,74,74	1.65	10 (17%)	69,115,115	2.10	27 (39%)
15	CRT	v	101	-	41,43,43	0.76	0	50,54,54	3.75	18 (36%)
9	BCL	M	402	-	58,74,74	1.62	11 (18%)	69,115,115	2.53	29 (42%)
9	BCL	9	102	-	58,74,74	1.61	10 (17%)	69,115,115	2.03	18 (26%)
9	BCL	p	102	-	58,74,74	1.56	11 (18%)	69,115,115	2.24	21 (30%)
12	PEF	H	305	-	18,18,46	1.45	2 (11%)	21,23,51	1.51	3 (14%)
15	CRT	M	405	-	41,43,43	0.77	0	50,54,54	3.91	14 (28%)
9	BCL	L	301	-	58,74,74	1.59	9 (15%)	69,115,115	2.40	35 (50%)
15	CRT	k	101	-	41,43,43	0.76	0	50,54,54	3.71	15 (30%)
7	HEM	o	501	1	27,50,50	1.30	3 (11%)	17,82,82	2.83	7 (41%)
15	CRT	y	404	-	41,43,43	0.87	1 (2%)	50,54,54	3.59	13 (26%)
9	BCL	A	102	-	58,74,74	1.60	8 (13%)	69,115,115	2.11	20 (28%)
9	BCL	Z	102	-	58,74,74	1.53	9 (15%)	69,115,115	2.39	26 (37%)
15	CRT	9	101	-	41,43,43	0.75	0	50,54,54	3.59	18 (36%)
7	HEM	o	503	1	27,50,50	1.25	2 (7%)	17,82,82	2.05	4 (23%)
9	BCL	8	101	-	58,74,74	1.58	11 (18%)	69,115,115	2.24	22 (31%)
14	MQ8	M	404	-	54,54,54	1.01	5 (9%)	66,69,69	1.51	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BPH	M	403	-	64,70,70	0.86	3 (4%)	76,101,101	1.95	14 (18%)
15	CRT	i	101	-	41,43,43	0.77	0	50,54,54	3.47	16 (32%)
9	BCL	y	401	-	58,74,74	1.63	8 (13%)	69,115,115	2.30	26 (37%)
15	CRT	T	101	-	41,43,43	0.72	0	50,54,54	3.90	13 (26%)
9	BCL	Q	101	-	58,74,74	1.61	11 (18%)	69,115,115	2.21	25 (36%)
9	BCL	7	102	-	58,74,74	1.58	10 (17%)	69,115,115	2.04	25 (36%)
15	CRT	s	101	-	41,43,43	0.79	0	50,54,54	3.29	17 (34%)
15	CRT	4	101	-	41,43,43	0.84	0	50,54,54	4.08	21 (42%)
9	BCL	m	103	-	58,74,74	1.60	9 (15%)	69,115,115	2.21	27 (39%)
17	PGW	AE	101	-	20,20,50	0.97	1 (5%)	23,26,56	1.34	2 (8%)
9	BCL	3	101	-	58,74,74	1.58	9 (15%)	69,115,115	2.11	19 (27%)
15	CRT	X	101	-	41,43,43	0.90	0	50,54,54	1.79	11 (22%)
9	BCL	R	102	-	58,74,74	1.61	11 (18%)	69,115,115	2.18	27 (39%)
7	HEM	C	501	1	27,50,50	1.32	4 (14%)	17,82,82	3.50	8 (47%)
9	BCL	AG	101	-	58,74,74	1.64	11 (18%)	69,115,115	2.28	29 (42%)
9	BCL	6	101	-	58,74,74	1.61	10 (17%)	69,115,115	2.28	27 (39%)
12	PEF	M	408	-	18,18,46	1.75	2 (11%)	21,23,51	1.58	2 (9%)
9	BCL	AI	102	-	58,74,74	1.59	9 (15%)	69,115,115	2.21	23 (33%)
9	BCL	k	102	-	58,74,74	1.66	10 (17%)	69,115,115	2.23	24 (34%)
9	BCL	I	103	-	58,74,74	1.59	8 (13%)	69,115,115	2.15	22 (31%)
9	BCL	w	101	-	58,74,74	1.62	9 (15%)	69,115,115	2.21	26 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	AC	101	-	-	10/51/51/51	-
15	CRT	7	103	-	-	6/51/51/51	-
9	BCL	AB	101	-	-	14/37/137/137	-
15	CRT	G	101	-	-	12/51/51/51	-
9	BCL	4	102	-	-	16/37/137/137	-
9	BCL	u	102	-	-	10/37/137/137	-
9	BCL	q	102	-	-	18/37/137/137	-
9	BCL	AI	101	-	-	14/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEF	M	407	-	-	4/16/16/50	-
11	UQ8	x	304	-	-	15/51/75/75	0/1/1/1
15	CRT	P	102	-	-	7/51/51/51	-
9	BCL	g	102	-	-	17/37/137/137	-
15	CRT	m	104	-	-	3/51/51/51	-
9	BCL	Y	101	-	-	14/37/137/137	-
9	BCL	AH	101	-	-	21/37/137/137	-
9	BCL	AF	101	-	-	13/37/137/137	-
12	PEF	t	303	-	-	9/20/20/50	-
9	BCL	s	102	-	-	16/37/137/137	-
15	CRT	AL	101	-	-	10/51/51/51	-
12	PEF	x	306	-	-	10/20/20/50	-
9	BCL	X	102	-	-	22/37/137/137	-
9	BCL	AK	101	-	-	15/37/137/137	-
15	CRT	q	101	-	-	7/51/51/51	-
15	CRT	AD	101	-	-	8/51/51/51	-
9	BCL	r	101	-	-	18/37/137/137	-
9	BCL	e	102	-	-	15/37/137/137	-
15	CRT	O	101	-	-	8/51/51/51	-
9	BCL	AC	102	-	-	24/37/137/137	-
12	PEF	y	407	-	-	6/20/20/50	-
11	UQ8	L	304	-	-	10/51/75/75	0/1/1/1
9	BCL	O	102	-	-	15/37/137/137	-
15	CRT	2	101	-	-	4/51/51/51	-
12	PEF	y	408	-	-	7/20/20/50	-
7	HEM	C	503	1	-	0/6/54/54	-
9	BCL	U	101	-	-	17/37/137/137	-
9	BCL	A	103	-	-	12/37/137/137	-
15	CRT	Z	101	-	-	9/51/51/51	-
7	HEM	C	502	1	-	1/6/54/54	-
9	BCL	S	102	-	-	15/37/137/137	-
12	PEF	L	305	-	-	5/11/11/50	-
15	CRT	7	101	-	-	8/51/51/51	-
9	BCL	N	101	-	-	15/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	j	101	-	-	20/37/137/137	-
15	CRT	I	102	-	-	7/51/51/51	-
9	BCL	F	101	-	-	18/37/137/137	-
9	BCL	D	101	-	-	8/37/137/137	-
9	BCL	l	101	-	-	16/37/137/137	-
7	HEM	o	502	1	-	1/6/54/54	-
15	CRT	n	101	-	-	14/51/51/51	-
12	PEF	A	101	-	-	8/20/20/50	-
15	CRT	0	101	-	-	9/51/51/51	-
9	BCL	I	101	-	-	9/37/137/137	-
9	BCL	AL	102	-	-	16/37/137/137	-
12	PEF	H	301	-	-	8/20/20/50	-
9	BCL	x	303	-	-	17/37/137/137	-
14	MQ8	y	403	-	-	24/47/67/67	0/2/2/2
9	BCL	h	101	-	-	8/37/137/137	-
9	BCL	f	101	-	-	16/37/137/137	-
15	CRT	AH	102	-	-	12/51/51/51	-
9	BCL	z	102	-	-	18/37/137/137	-
9	BCL	0	102	-	-	17/37/137/137	-
10	BPH	x	302	-	-	20/54/105/105	0/5/6/6
15	CRT	R	101	-	-	15/51/51/51	-
9	BCL	W	101	-	-	20/37/137/137	-
15	CRT	V	101	-	-	16/51/51/51	-
9	BCL	AC	103	-	-	16/37/137/137	-
9	BCL	x	301	-	-	12/37/137/137	-
12	PEF	y	406	-	-	7/20/20/50	-
12	PEF	m	101	-	-	9/20/20/50	-
9	BCL	c	101	-	-	18/37/137/137	-
15	CRT	AF	102	-	-	5/51/51/51	-
12	PEF	H	304	-	-	13/20/20/50	-
9	BCL	G	102	-	-	16/37/137/137	-
7	HEM	C	504	1	-	2/6/54/54	-
10	BPH	L	302	-	-	22/54/105/105	0/5/6/6
7	HEM	o	504	1	-	2/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	V	102	-	-	15/37/137/137	-
12	PEF	H	302	-	-	8/20/20/50	-
9	BCL	M	401	-	-	15/37/137/137	-
9	BCL	i	102	-	-	19/37/137/137	-
12	PEF	t	301	-	-	6/20/20/50	-
10	BPH	y	402	-	-	21/54/105/105	0/5/6/6
9	BCL	u	101	-	-	21/37/137/137	-
15	CRT	E	101	-	-	9/51/51/51	-
15	CRT	g	101	-	-	5/51/51/51	-
9	BCL	T	102	-	-	17/37/137/137	-
12	PEF	p	101	-	-	3/16/16/50	-
15	CRT	z	101	-	-	2/51/51/51	-
9	BCL	AE	102	-	-	14/37/137/137	-
9	BCL	d	101	-	-	12/37/137/137	-
15	CRT	e	101	-	-	13/51/51/51	-
9	BCL	L	303	-	-	18/37/137/137	-
9	BCL	K	101	-	-	13/37/137/137	-
9	BCL	2	102	-	-	13/37/137/137	-
9	BCL	l	101	-	-	16/37/137/137	-
9	BCL	5	101	-	-	8/37/137/137	-
15	CRT	AJ	101	-	-	12/51/51/51	-
9	BCL	x	305	-	-	13/37/137/137	-
17	PGW	S	101	-	-	12/23/23/55	-
9	BCL	m	102	-	-	13/37/137/137	-
9	BCL	P	101	-	-	13/37/137/137	-
9	BCL	D	102	-	-	15/37/137/137	-
9	BCL	AB	102	-	-	16/37/137/137	-
15	CRT	v	101	-	-	7/51/51/51	-
9	BCL	M	402	-	-	15/37/137/137	-
9	BCL	9	102	-	-	11/37/137/137	-
9	BCL	p	102	-	-	12/37/137/137	-
12	PEF	H	305	-	-	11/20/20/50	-
15	CRT	M	405	-	-	13/51/51/51	-
9	BCL	L	301	-	-	11/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	k	101	-	-	8/51/51/51	-
7	HEM	o	501	1	-	1/6/54/54	-
15	CRT	y	404	-	-	14/51/51/51	-
9	BCL	A	102	-	-	13/37/137/137	-
9	BCL	Z	102	-	-	14/37/137/137	-
15	CRT	9	101	-	-	12/51/51/51	-
7	HEM	o	503	1	-	0/6/54/54	-
9	BCL	8	101	-	-	23/37/137/137	-
14	MQ8	M	404	-	-	20/47/67/67	0/2/2/2
10	BPH	M	403	-	-	21/54/105/105	0/5/6/6
15	CRT	i	101	-	-	8/51/51/51	-
9	BCL	y	401	-	-	13/37/137/137	-
15	CRT	T	101	-	-	6/51/51/51	-
9	BCL	Q	101	-	-	15/37/137/137	-
9	BCL	7	102	-	-	19/37/137/137	-
15	CRT	s	101	-	-	9/51/51/51	-
15	CRT	4	101	-	-	17/51/51/51	-
9	BCL	m	103	-	-	18/37/137/137	-
17	PGW	AE	101	-	-	12/23/23/55	-
9	BCL	3	101	-	-	14/37/137/137	-
15	CRT	X	101	-	-	14/51/51/51	-
9	BCL	R	102	-	-	17/37/137/137	-
7	HEM	C	501	1	-	0/6/54/54	-
9	BCL	AG	101	-	-	19/37/137/137	-
9	BCL	6	101	-	-	13/37/137/137	-
12	PEF	M	408	-	-	11/20/20/50	-
9	BCL	AI	102	-	-	17/37/137/137	-
9	BCL	k	102	-	-	21/37/137/137	-
9	BCL	I	103	-	-	13/37/137/137	-
9	BCL	w	101	-	-	14/37/137/137	-

The worst 5 of 789 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	304	UQ8	C6-C1	8.18	1.50	1.35
11	x	304	UQ8	C6-C1	8.11	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AF	101	BCL	OBD-CAD	6.56	1.31	1.22
9	Y	101	BCL	OBD-CAD	6.55	1.31	1.22
9	W	101	BCL	OBD-CAD	6.46	1.31	1.22

The worst 5 of 2532 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	405	CRT	C2-C1-C4	-19.64	80.71	110.86
15	0	101	CRT	C2-C1-C4	-19.23	81.33	110.86
15	T	101	CRT	C3-C1-C4	-18.63	82.26	110.86
15	G	101	CRT	C2-C1-C4	-18.42	82.58	110.86
15	y	404	CRT	C3-C1-C4	-17.75	83.61	110.86

There are no chirality outliers.

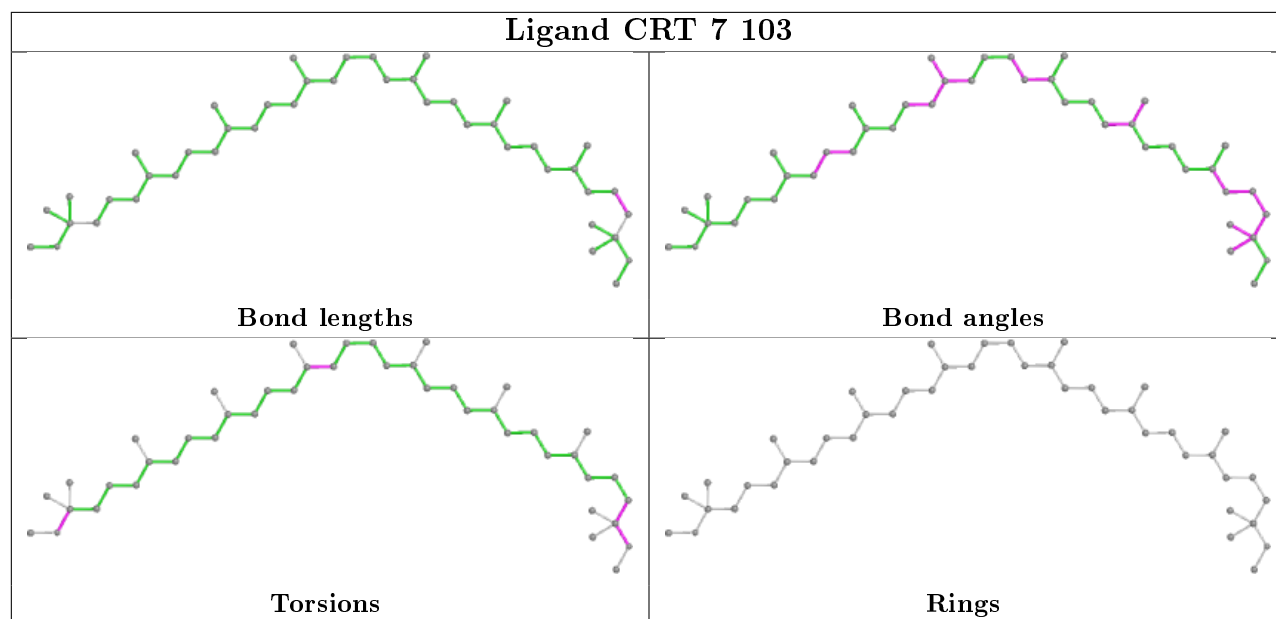
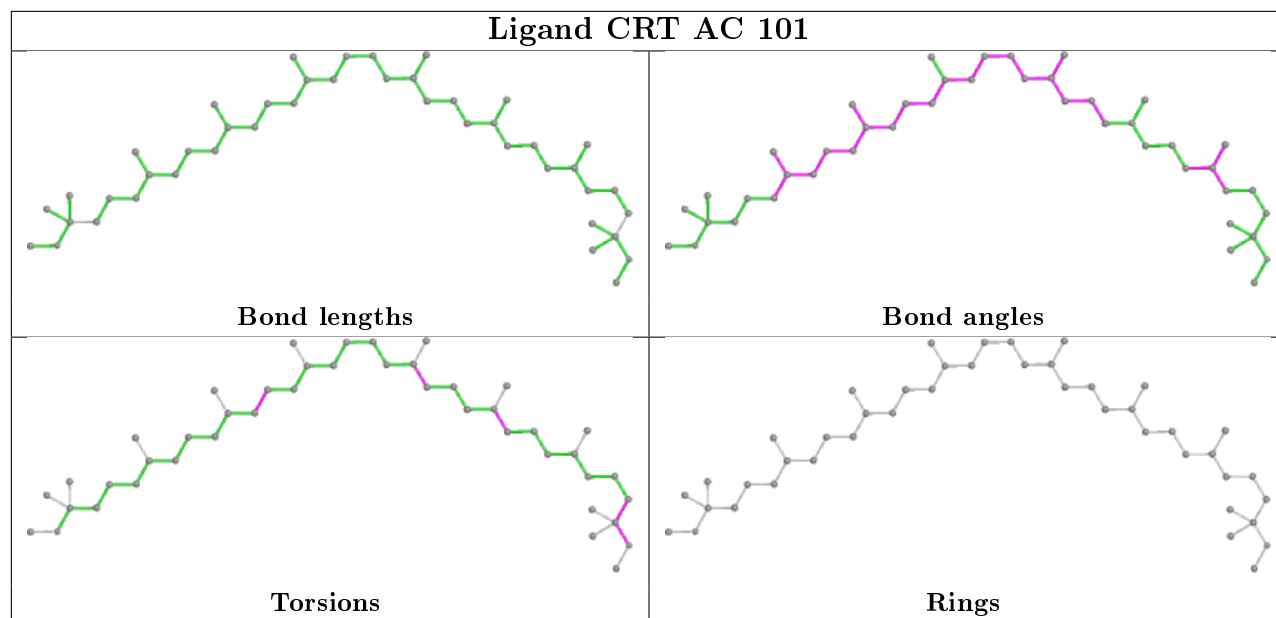
5 of 1737 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	AC	101	CRT	C2-C1-C4-C5
15	AC	101	CRT	C15-C16-C17-C18
15	7	103	CRT	C2-C1-C4-C5
15	7	103	CRT	C3-C1-C4-C5
9	AB	101	BCL	C2-C3-C5-C6

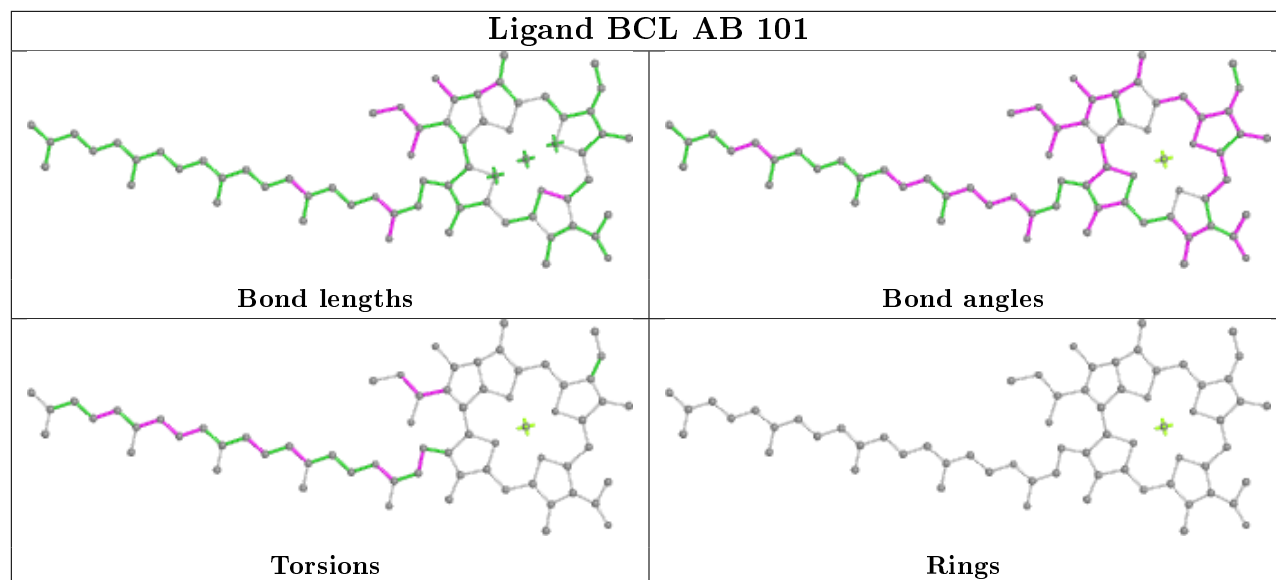
There are no ring outliers.

No monomer is involved in short contacts.

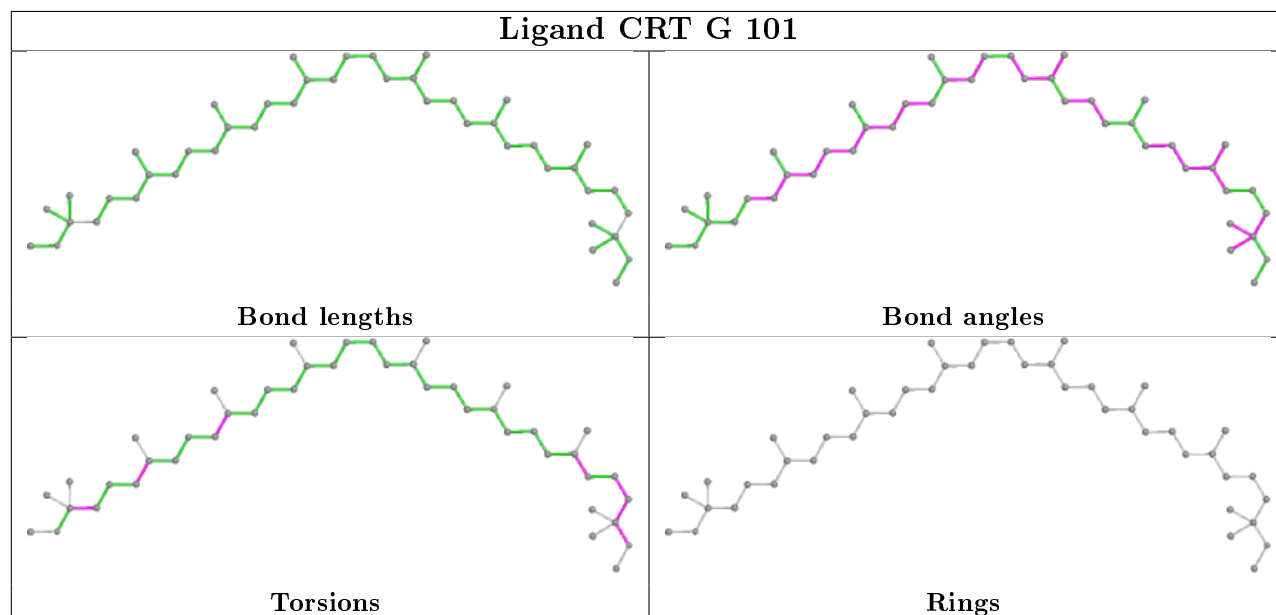
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



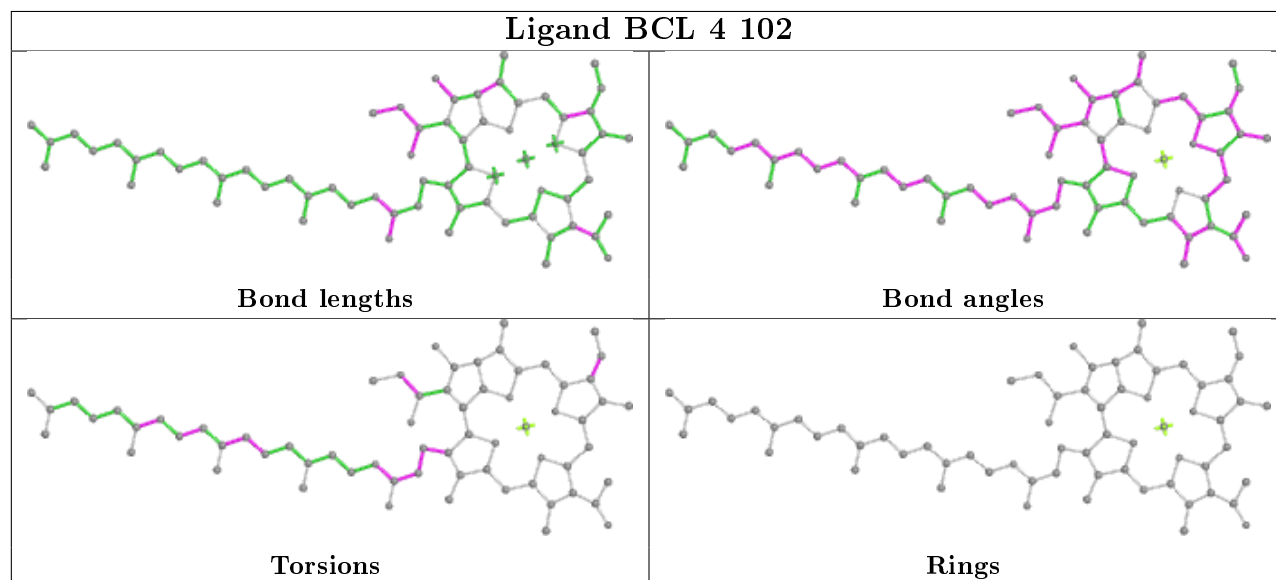
Ligand BCL AB 101

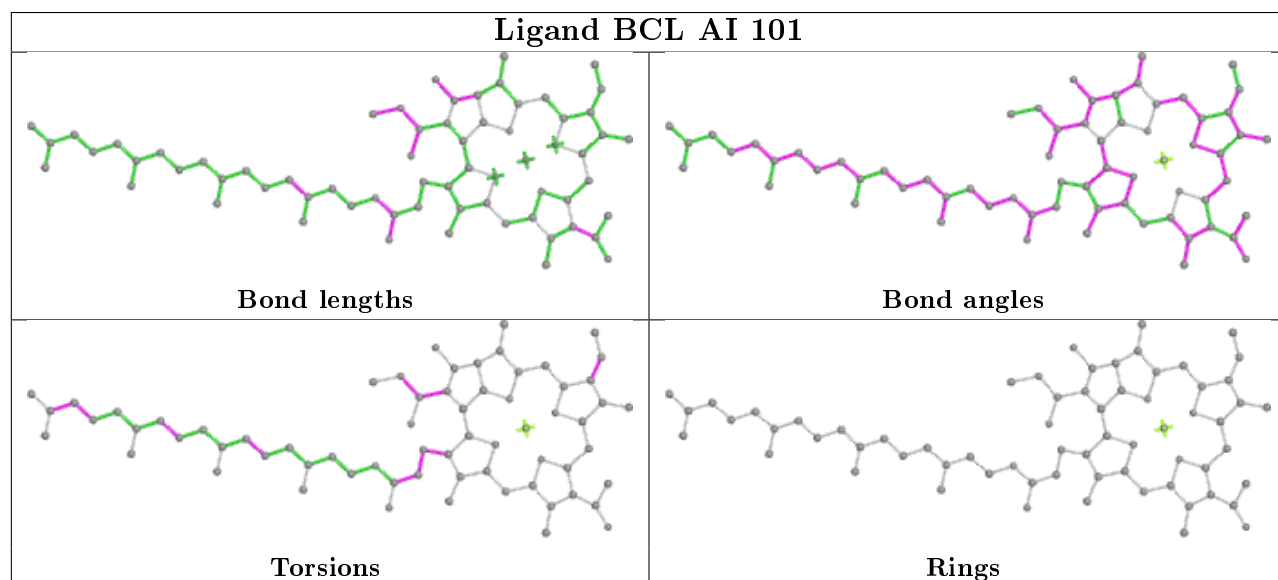
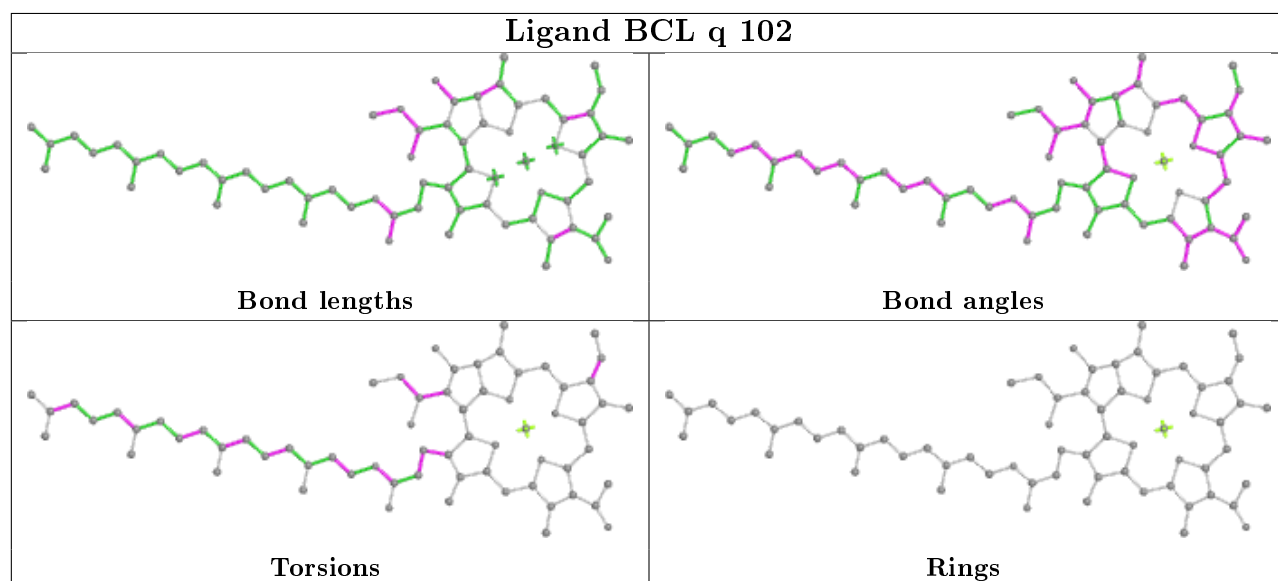
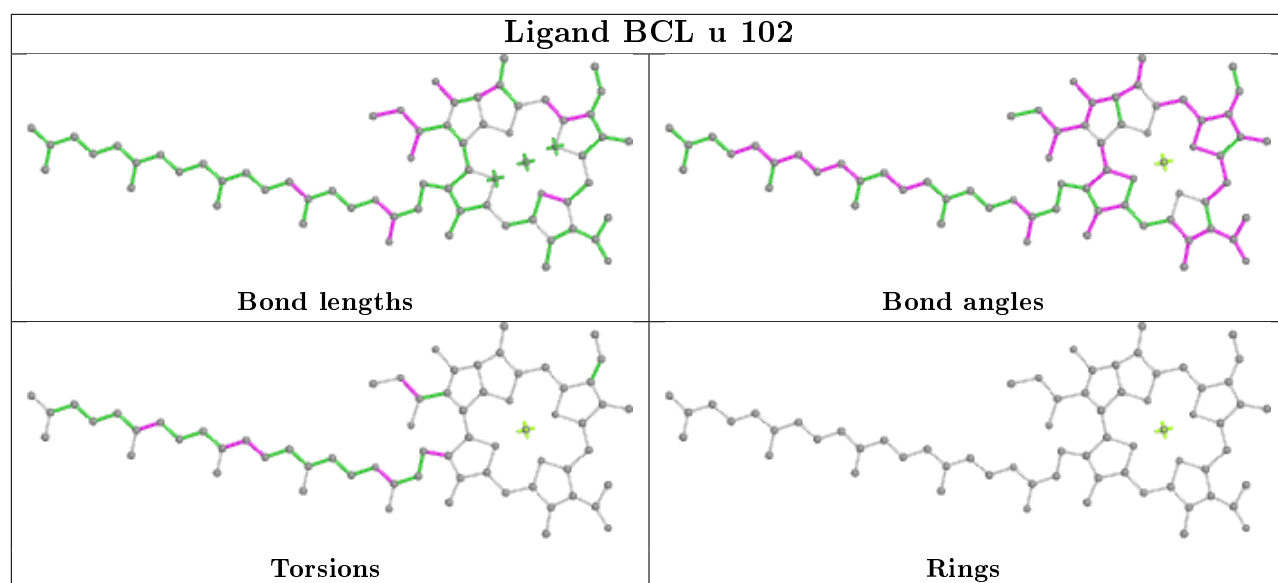


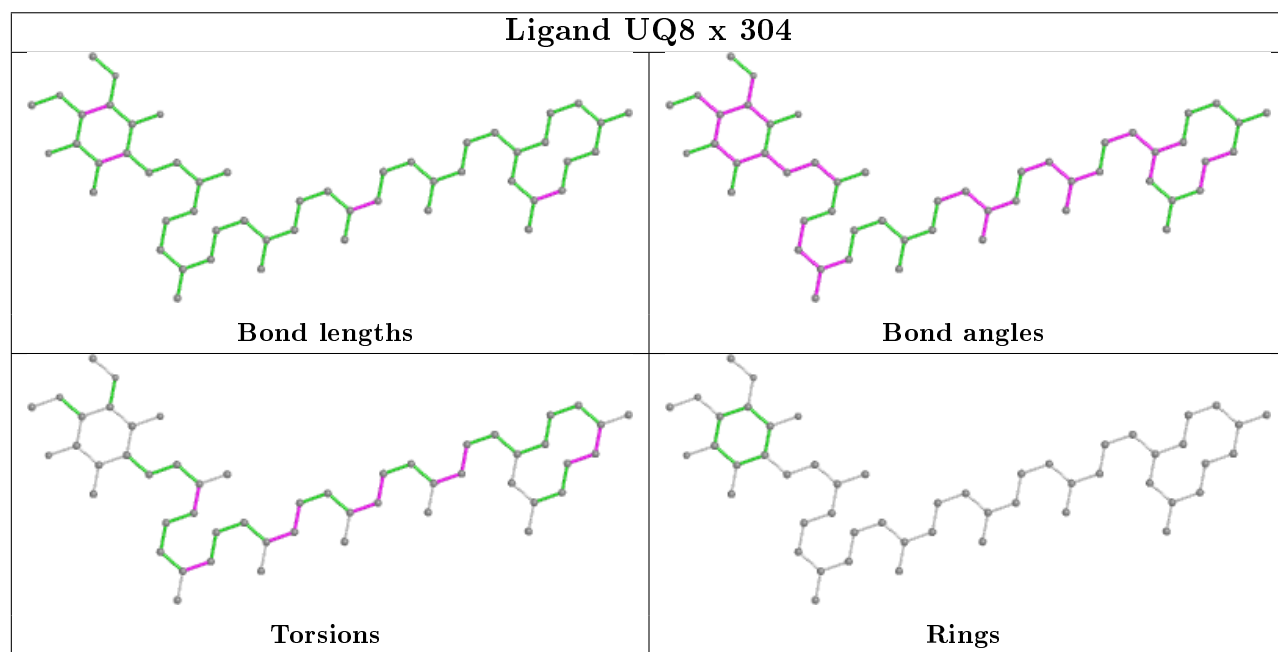
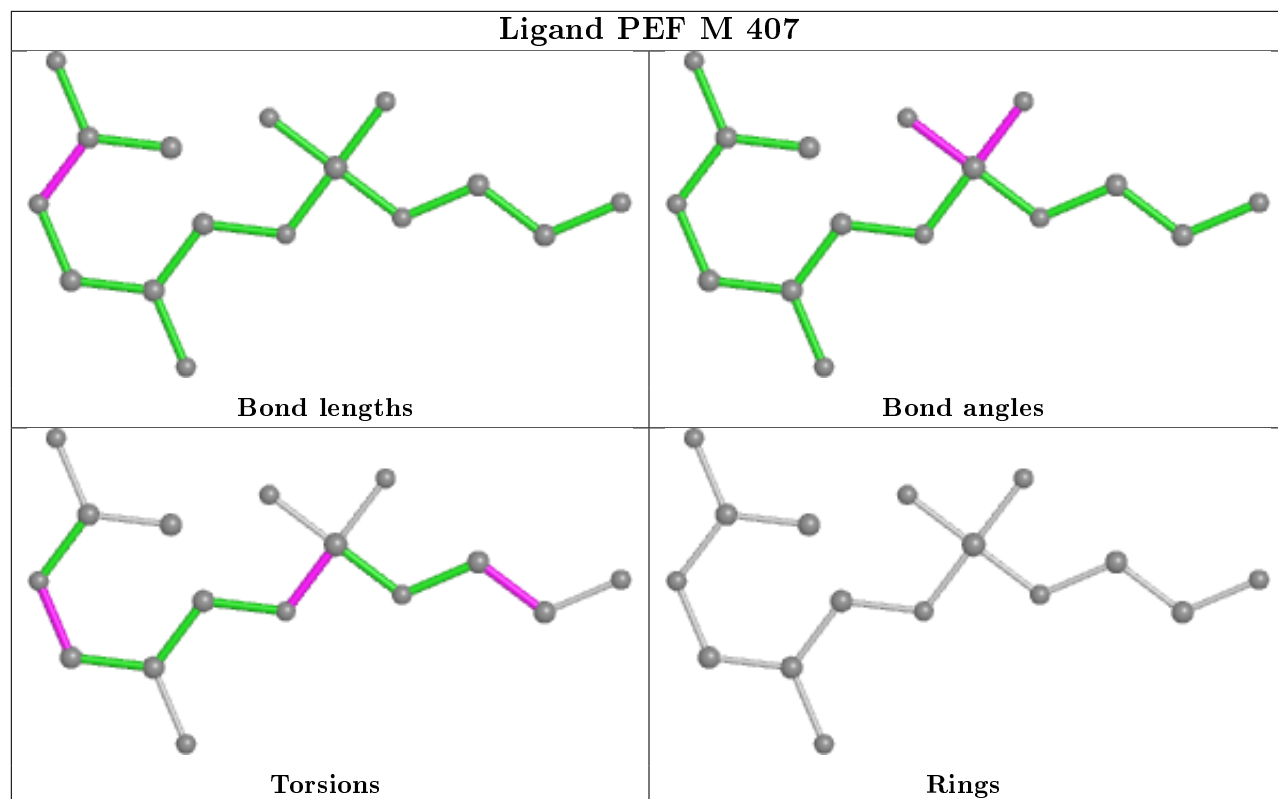
Ligand CRT G 101

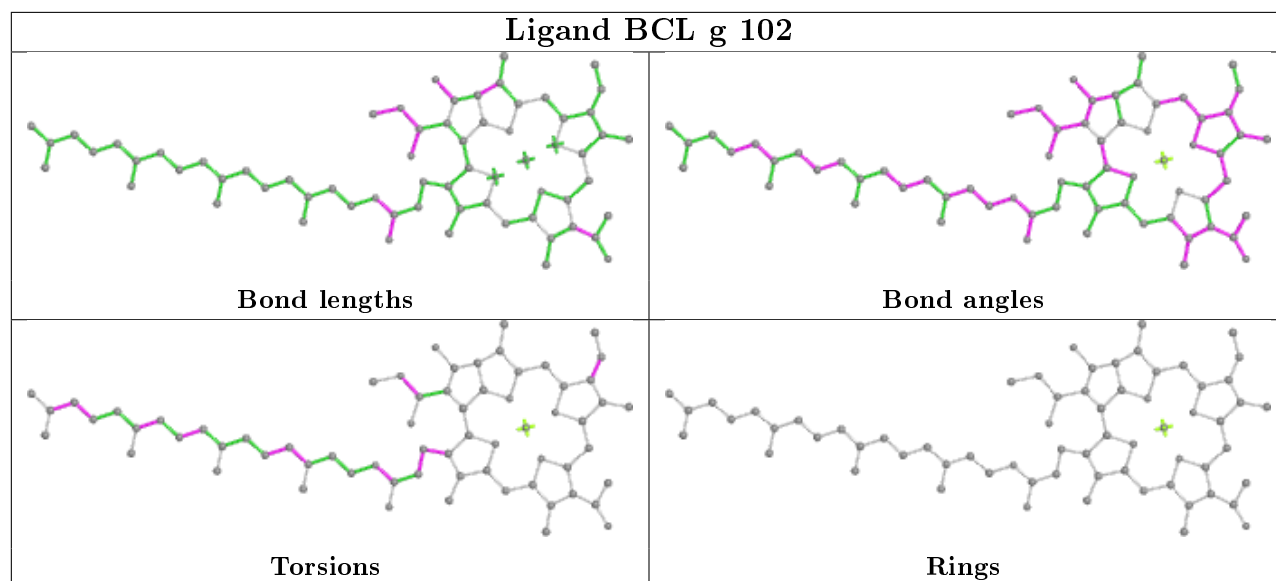
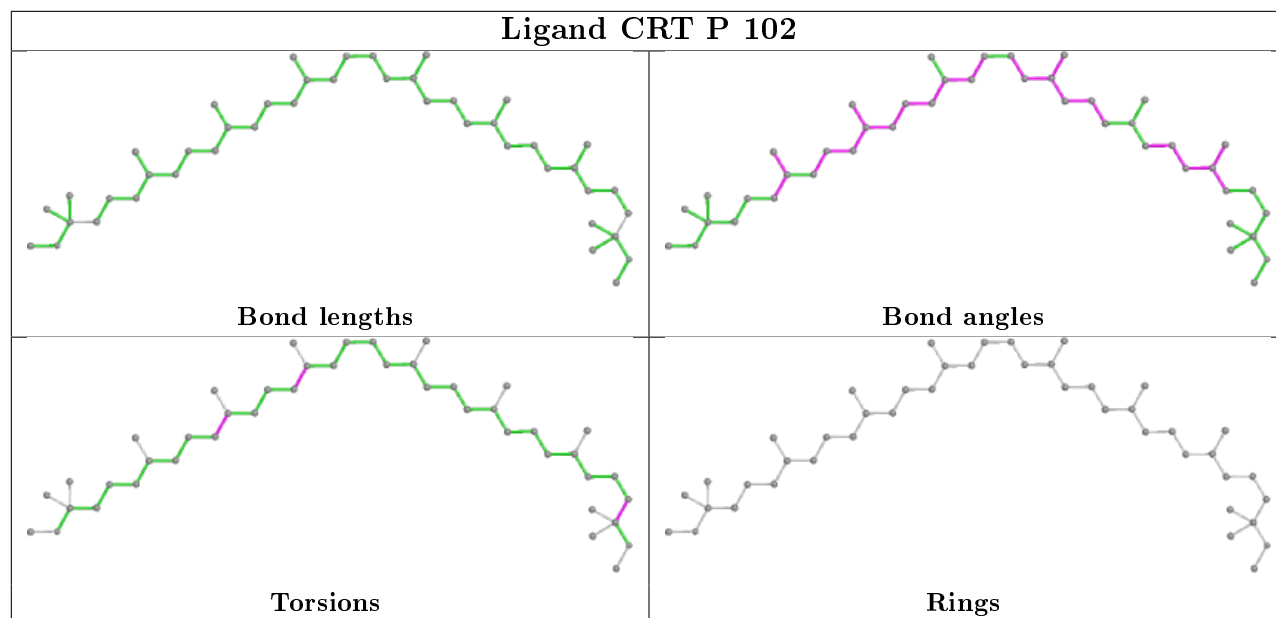


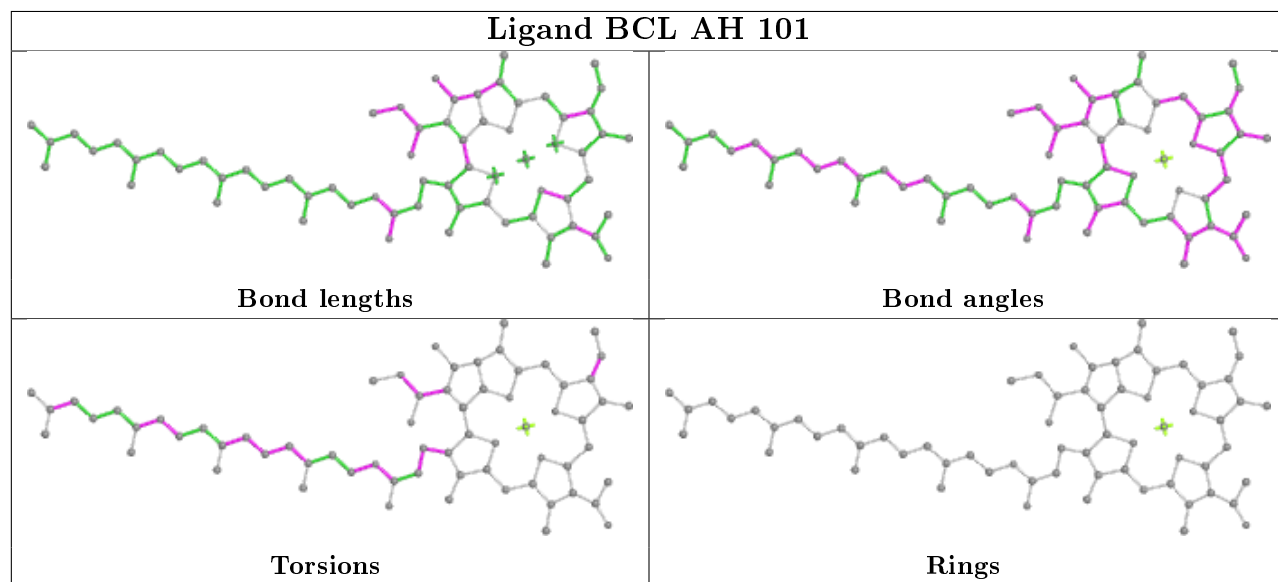
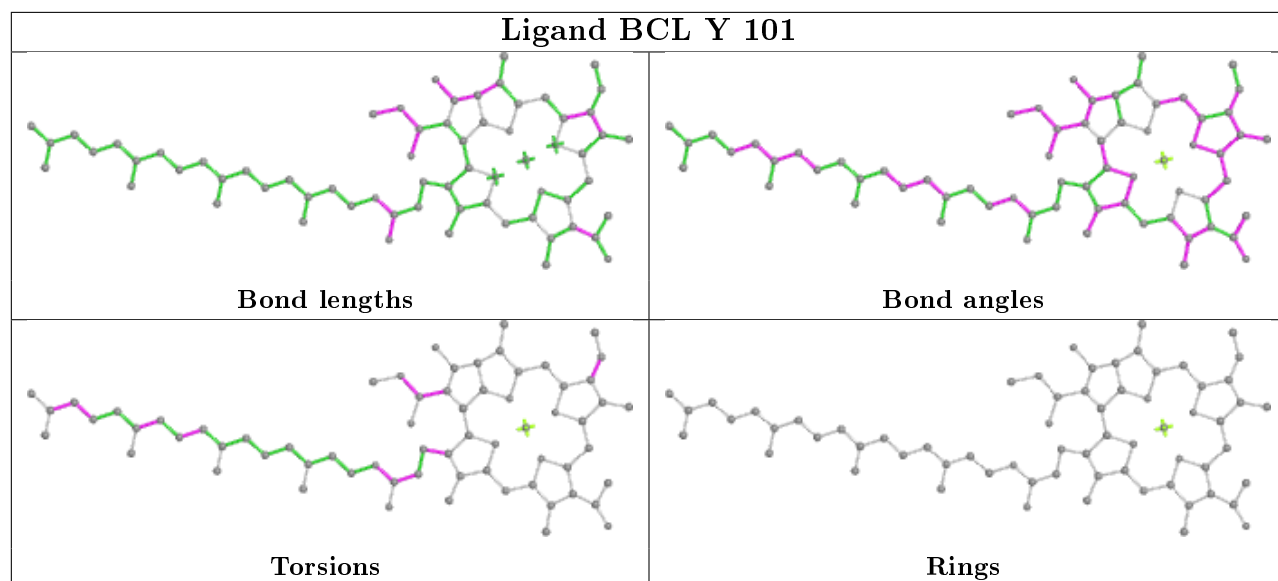
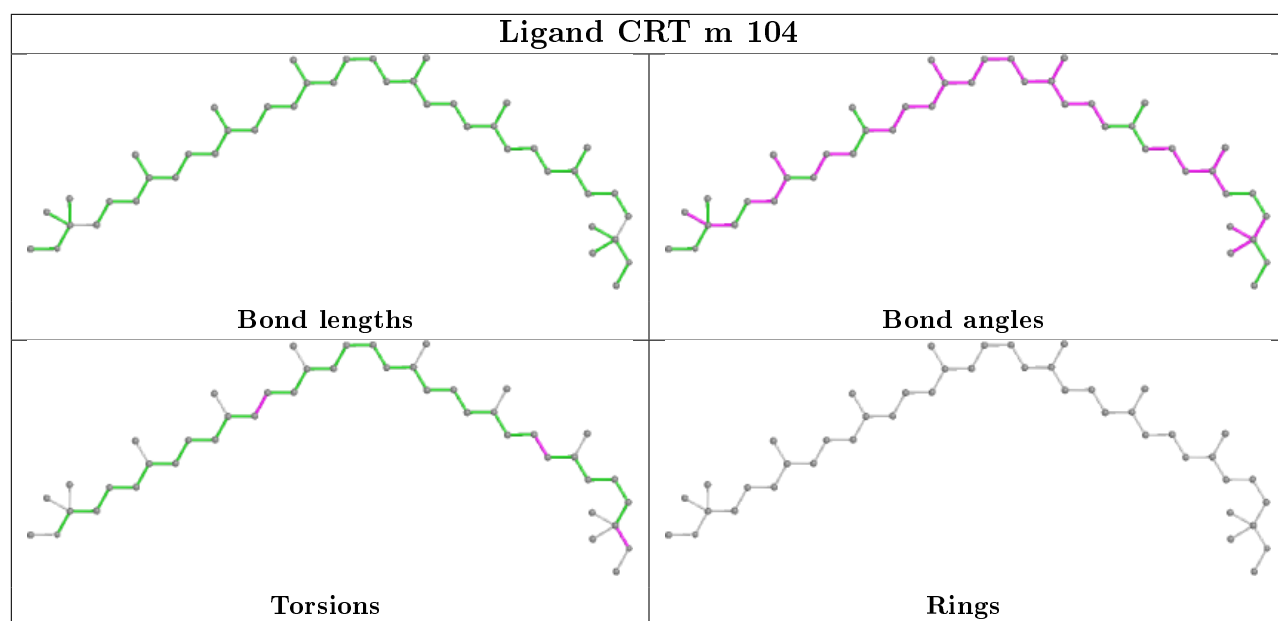
Ligand BCL 4 102

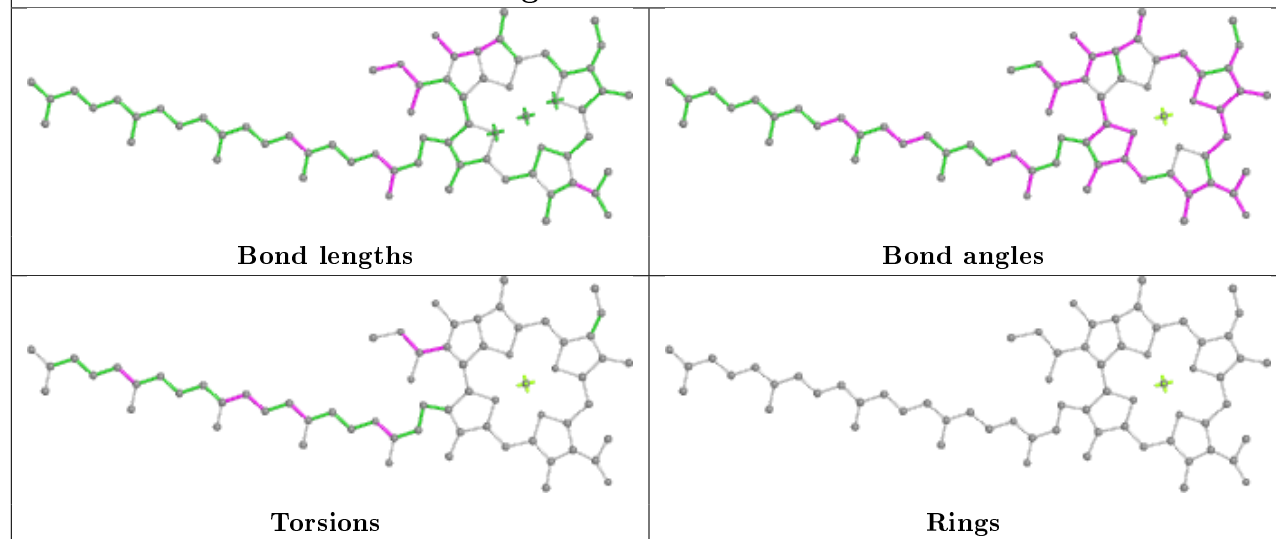
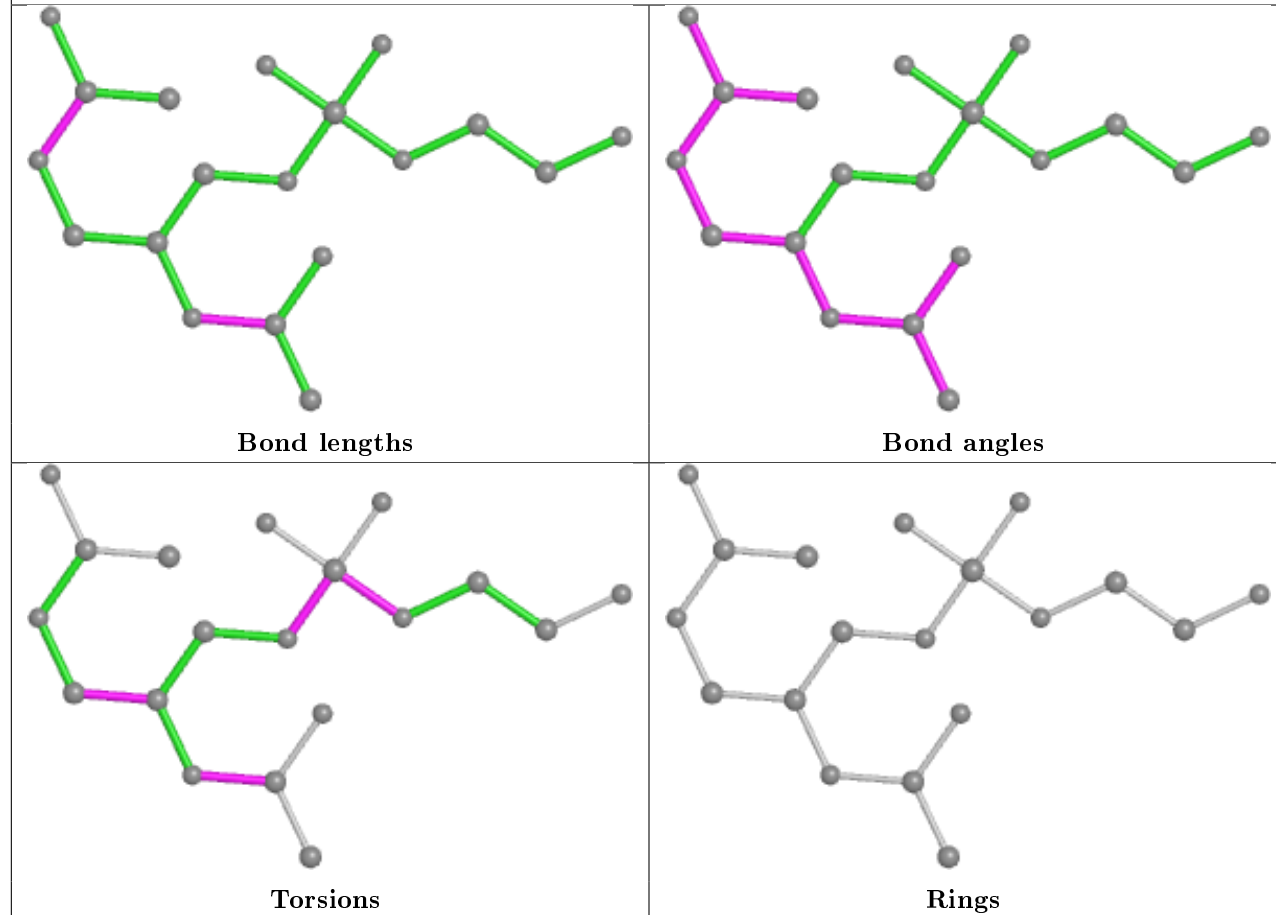


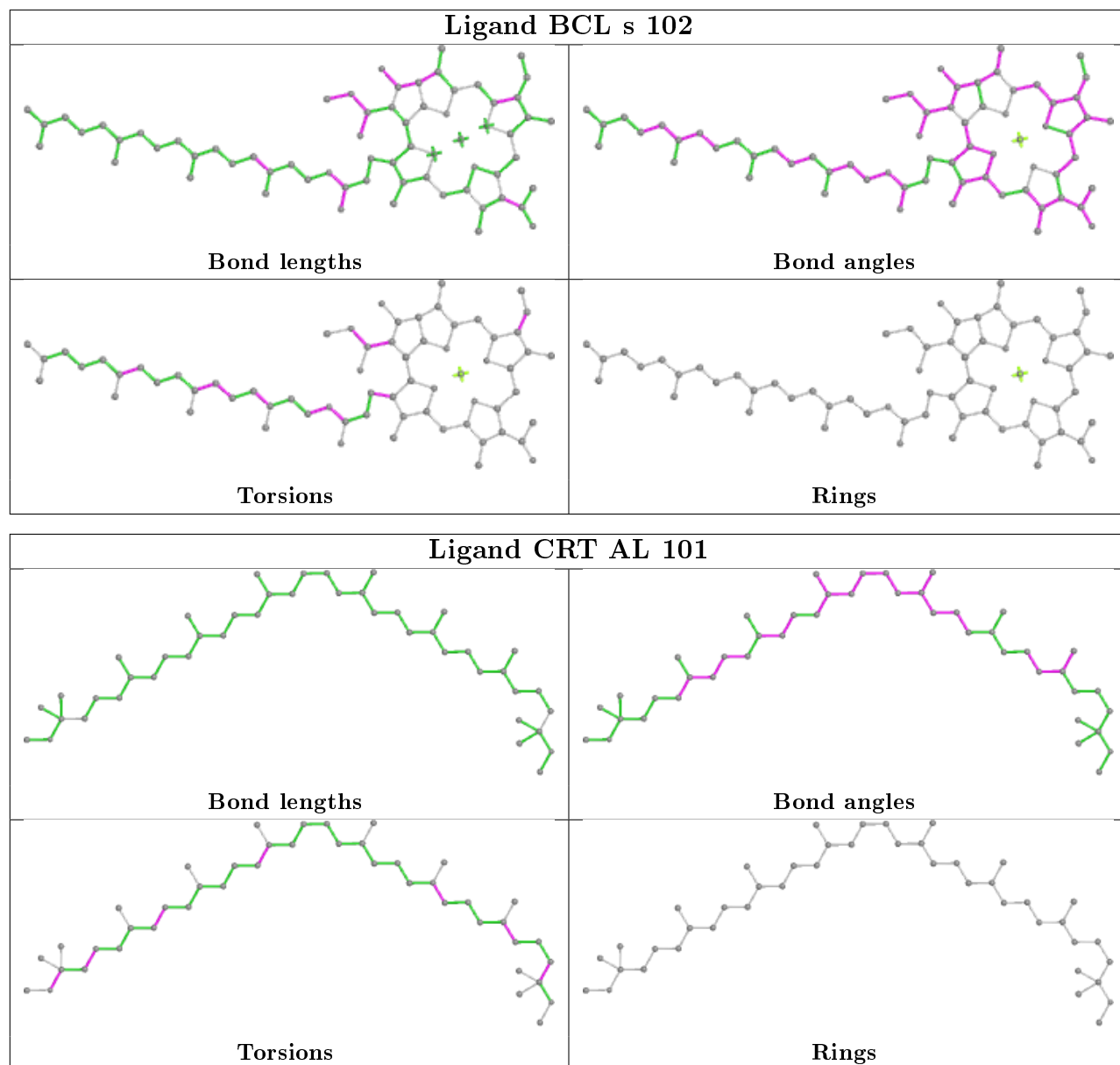


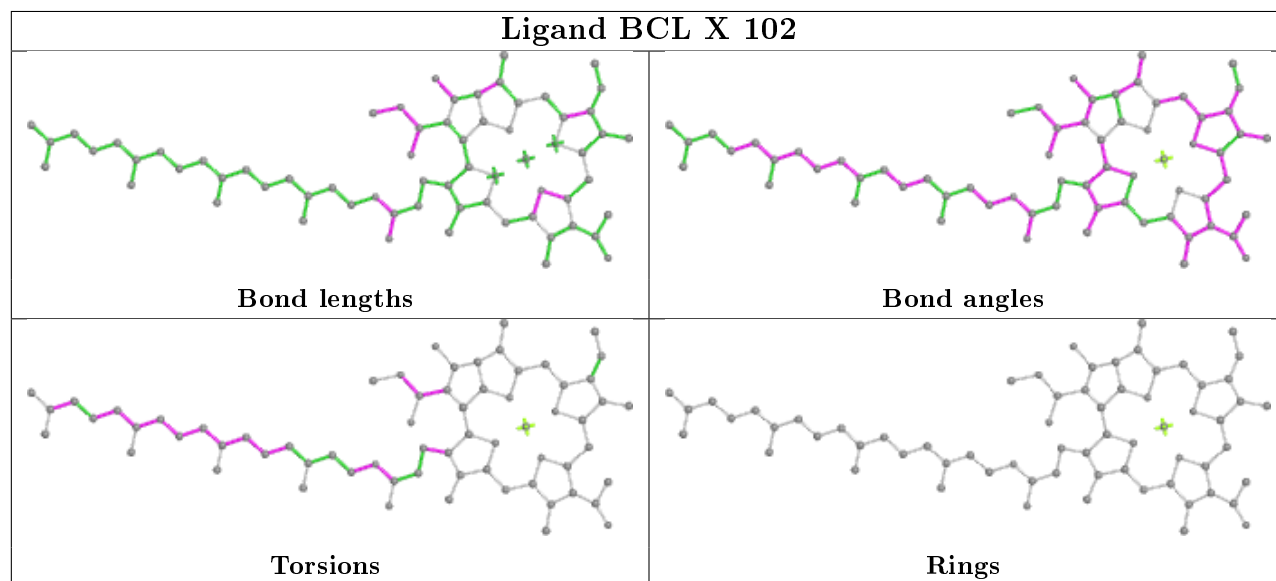
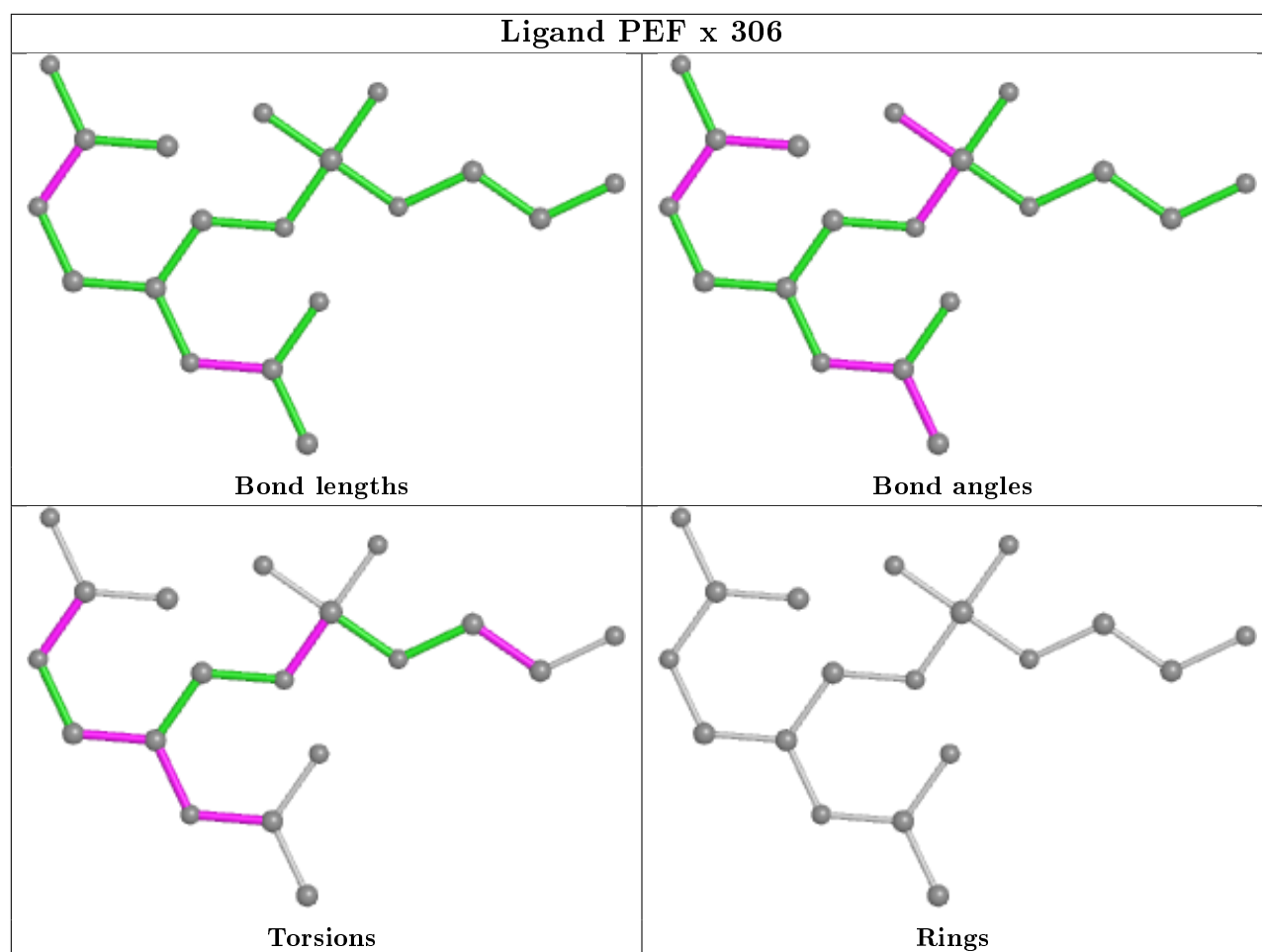


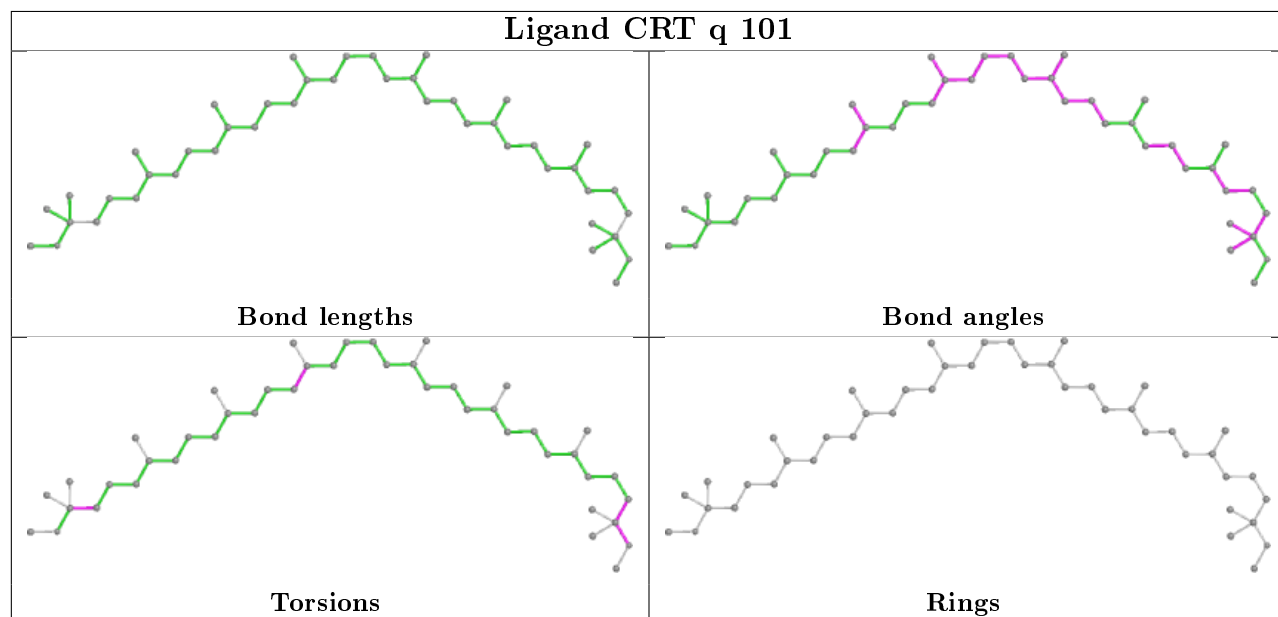
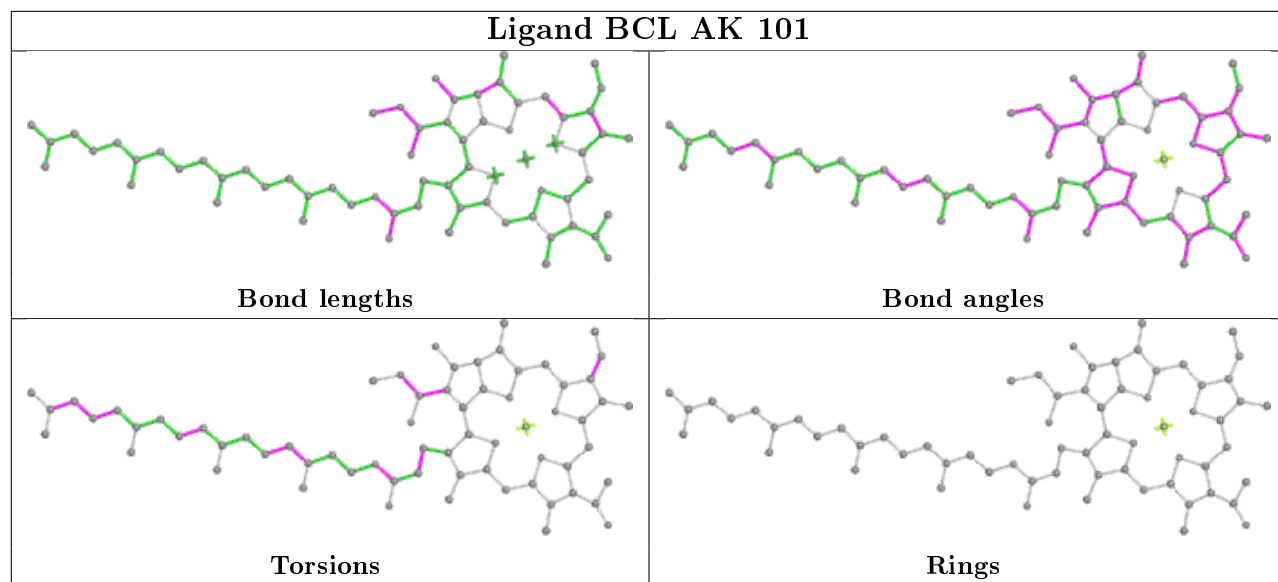


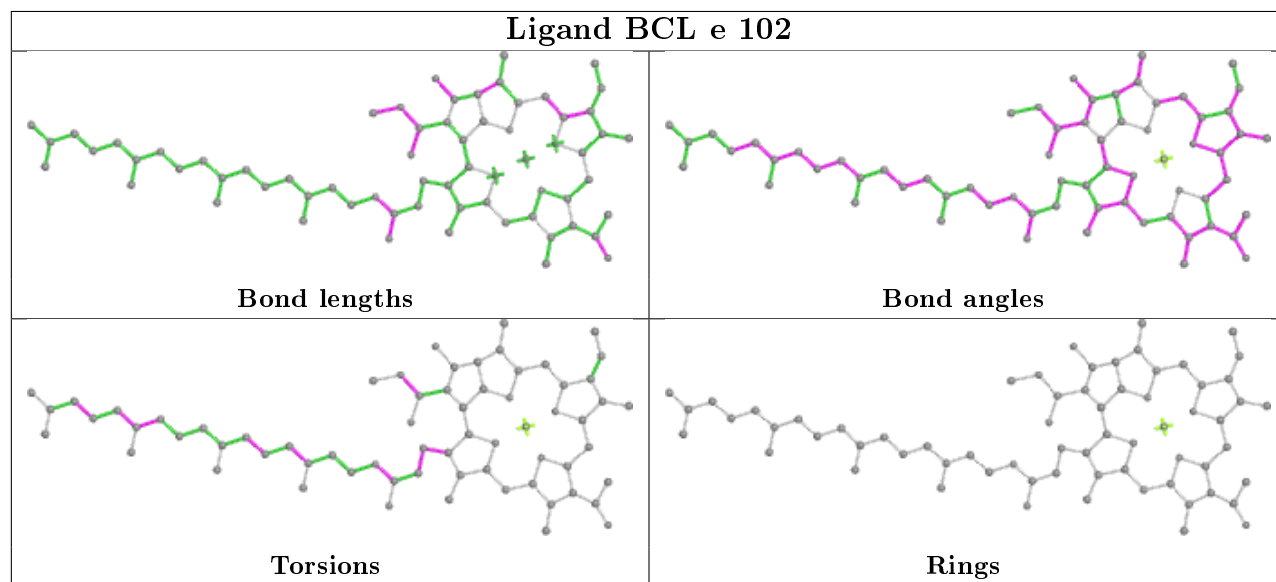
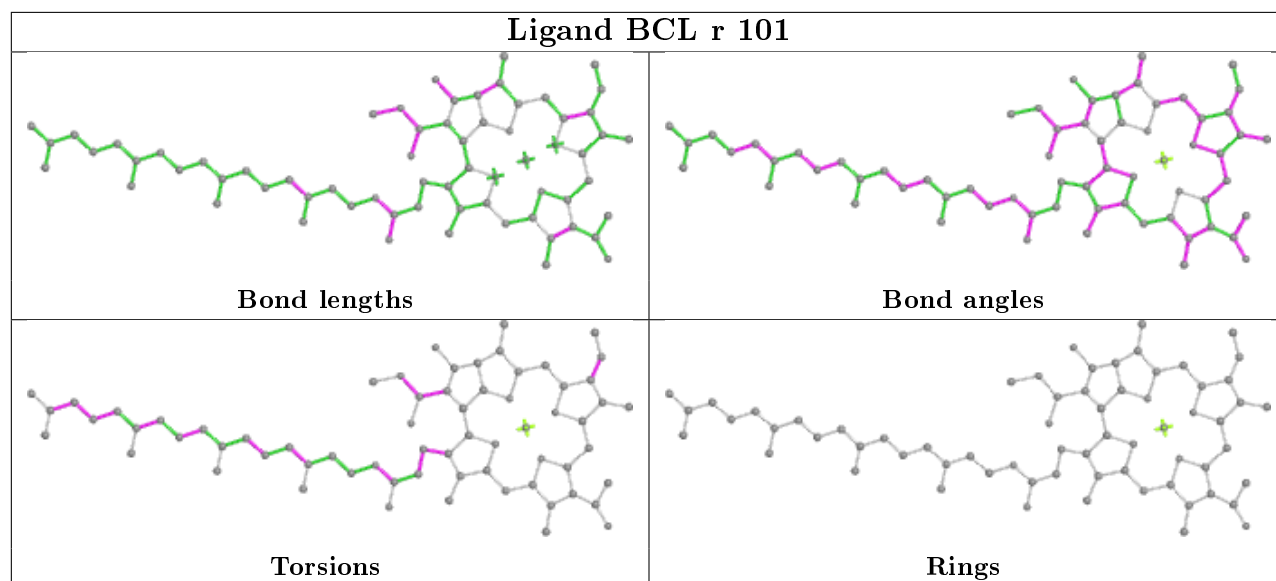
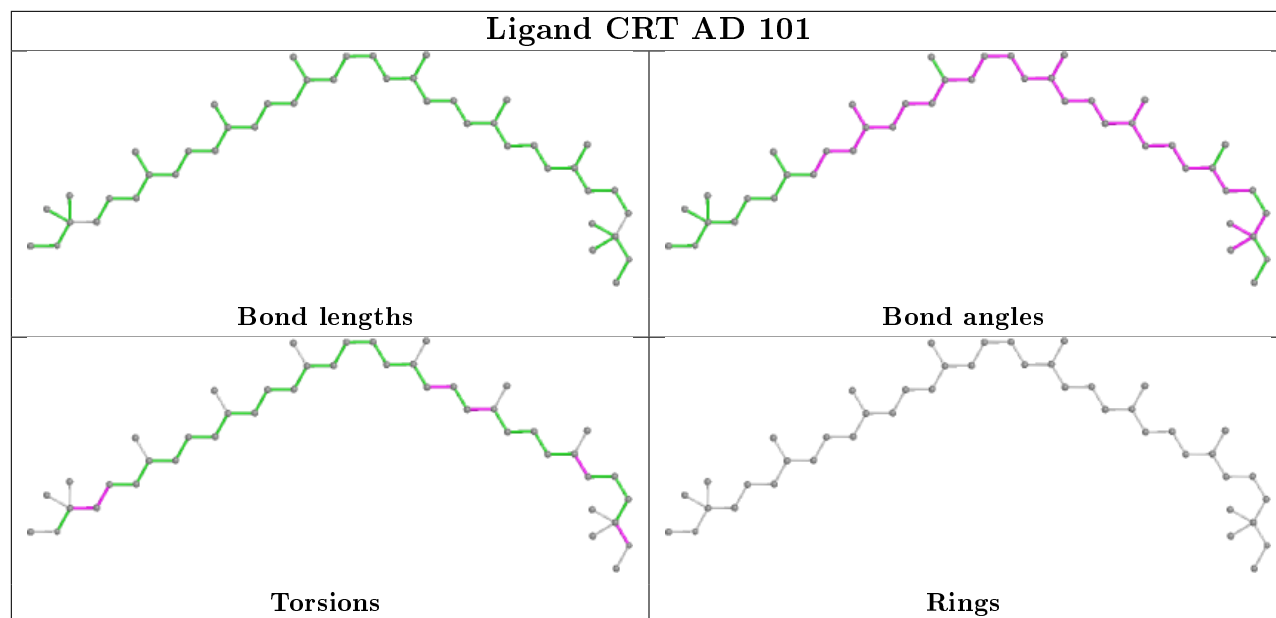


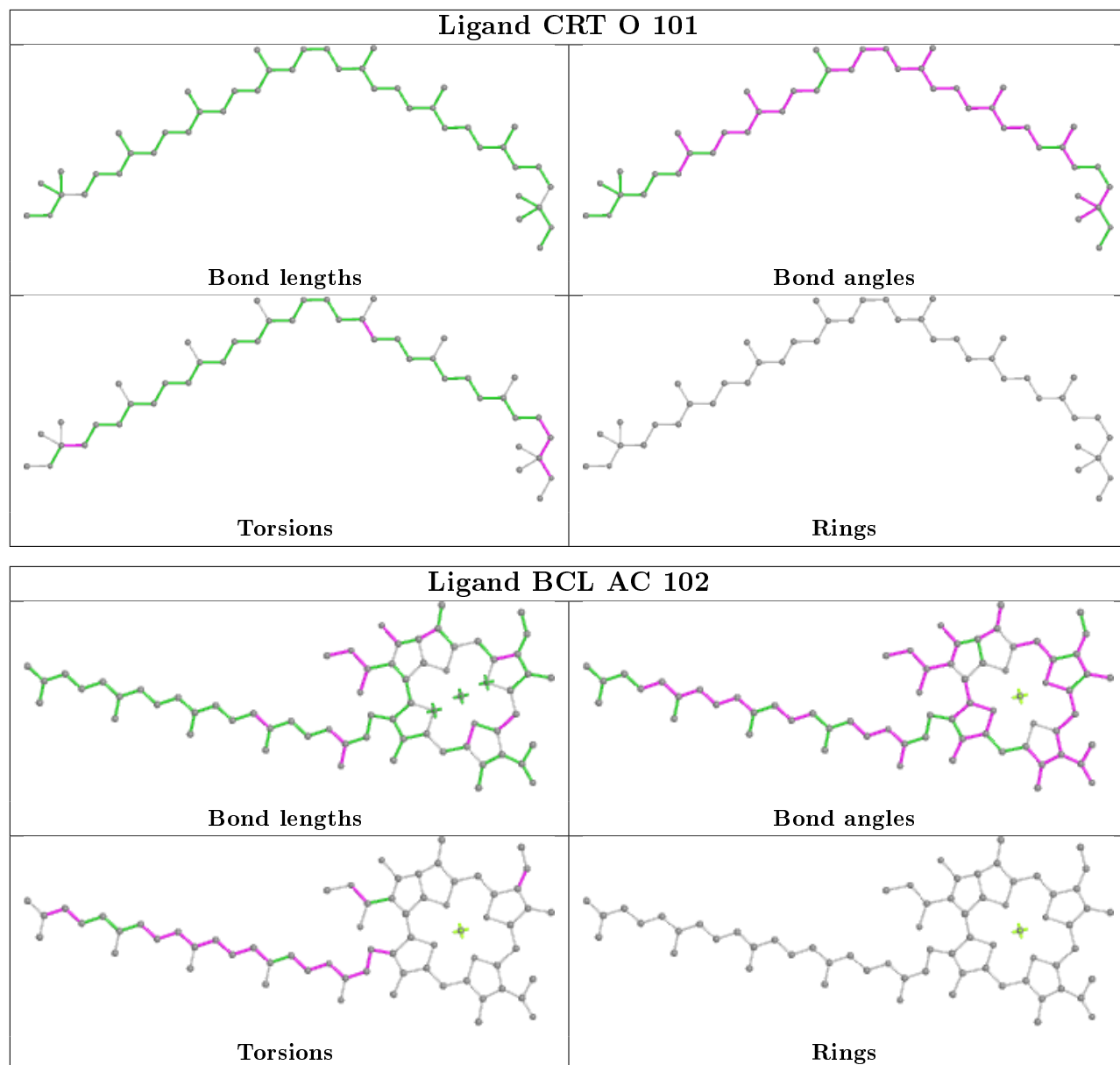
Ligand BCL AF 101**Ligand PEF t 303**

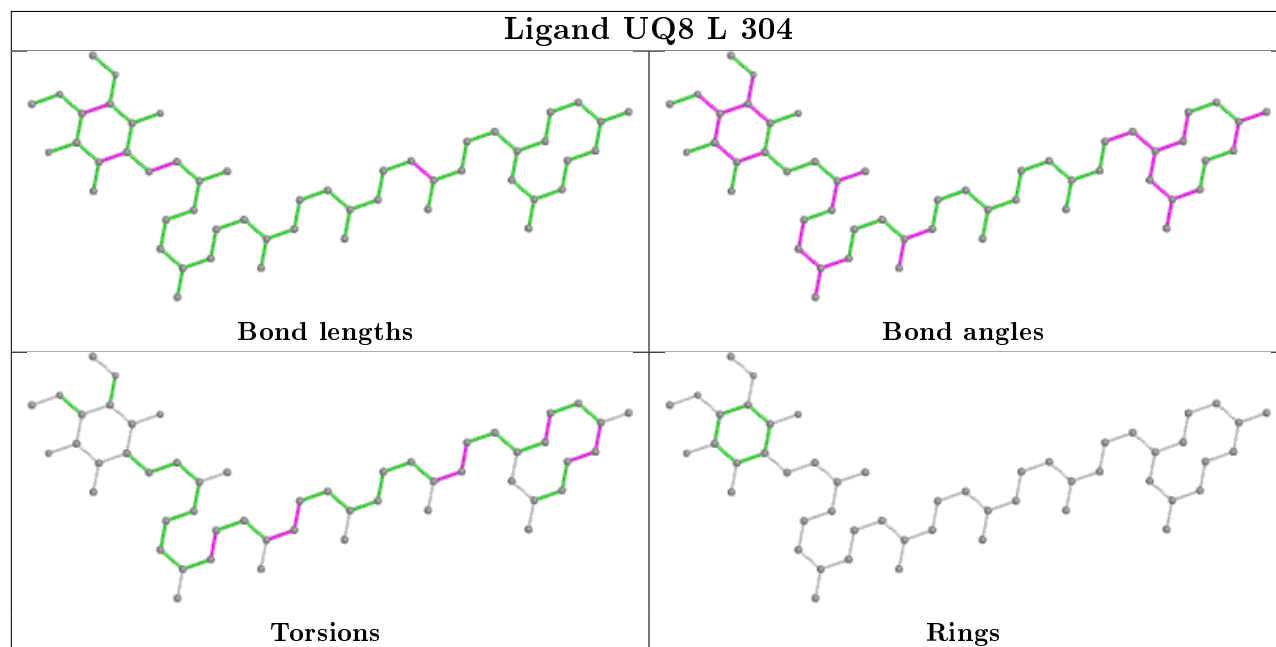
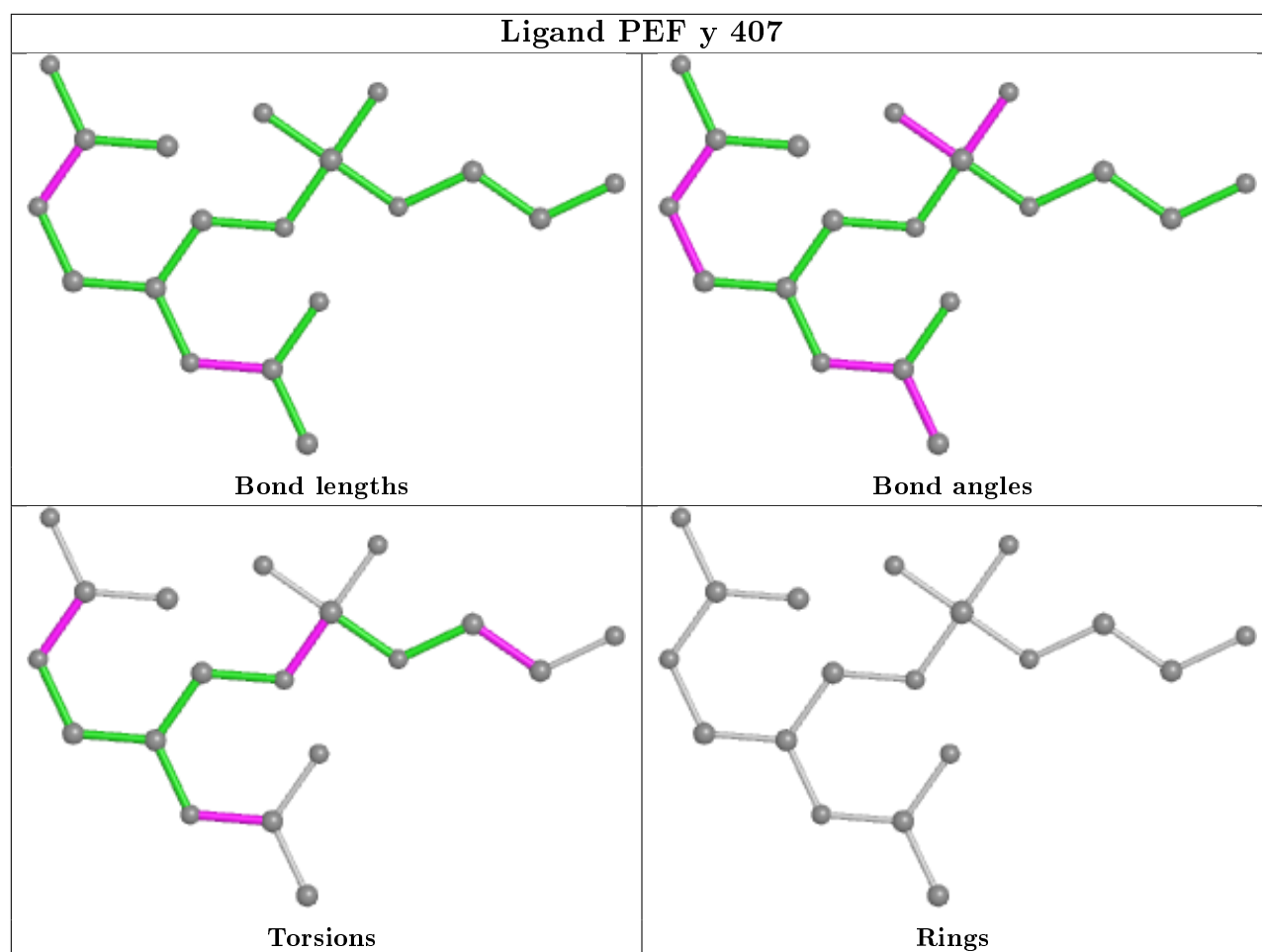


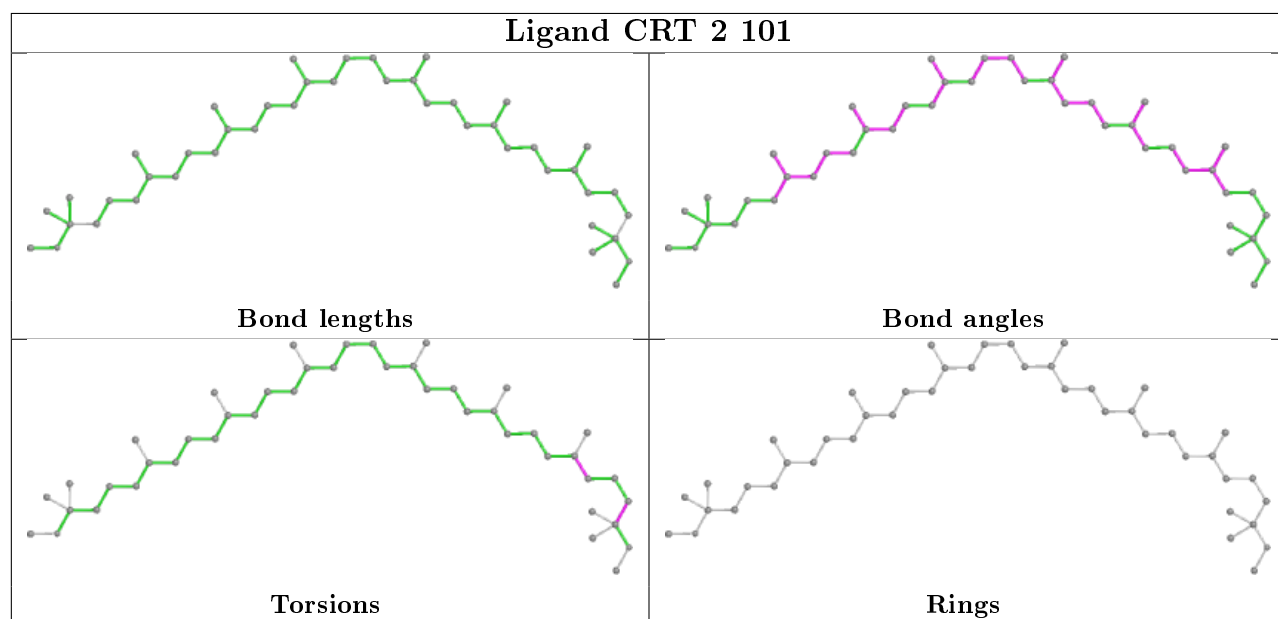
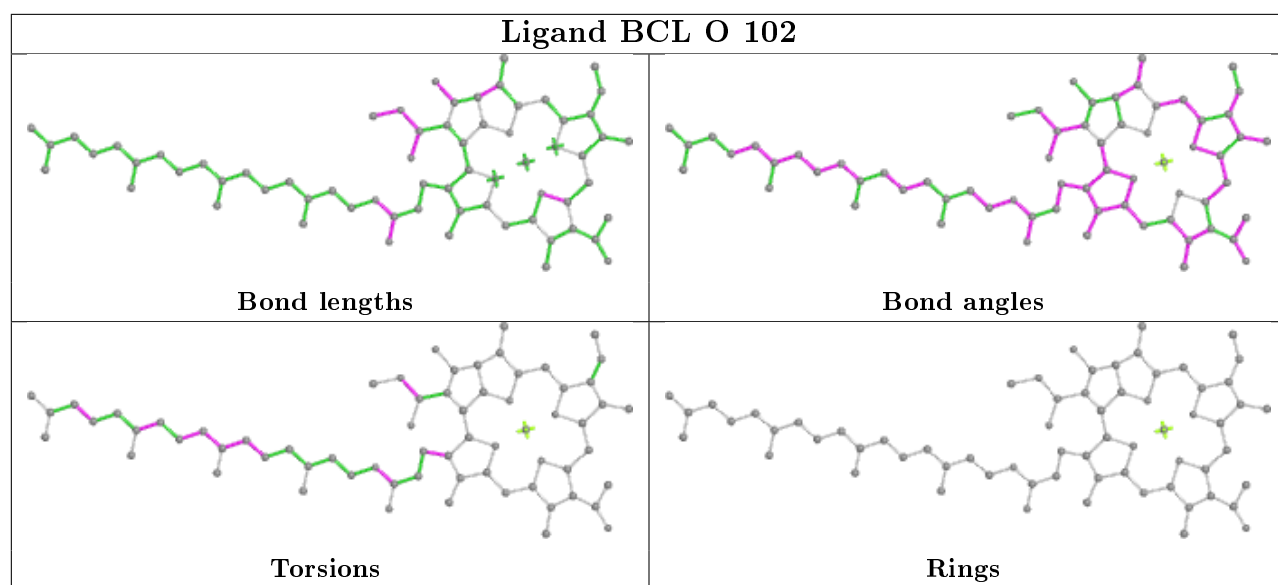


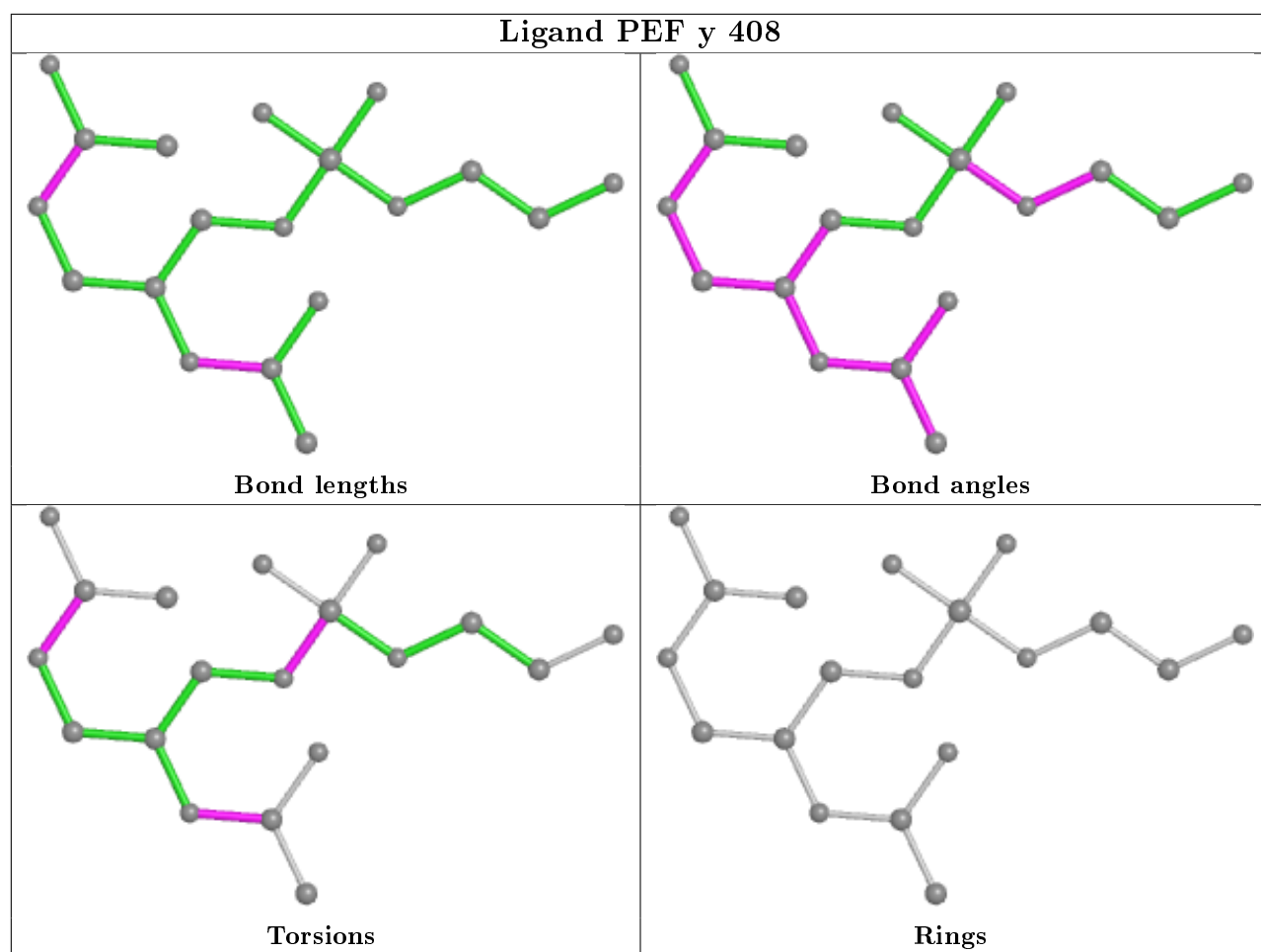


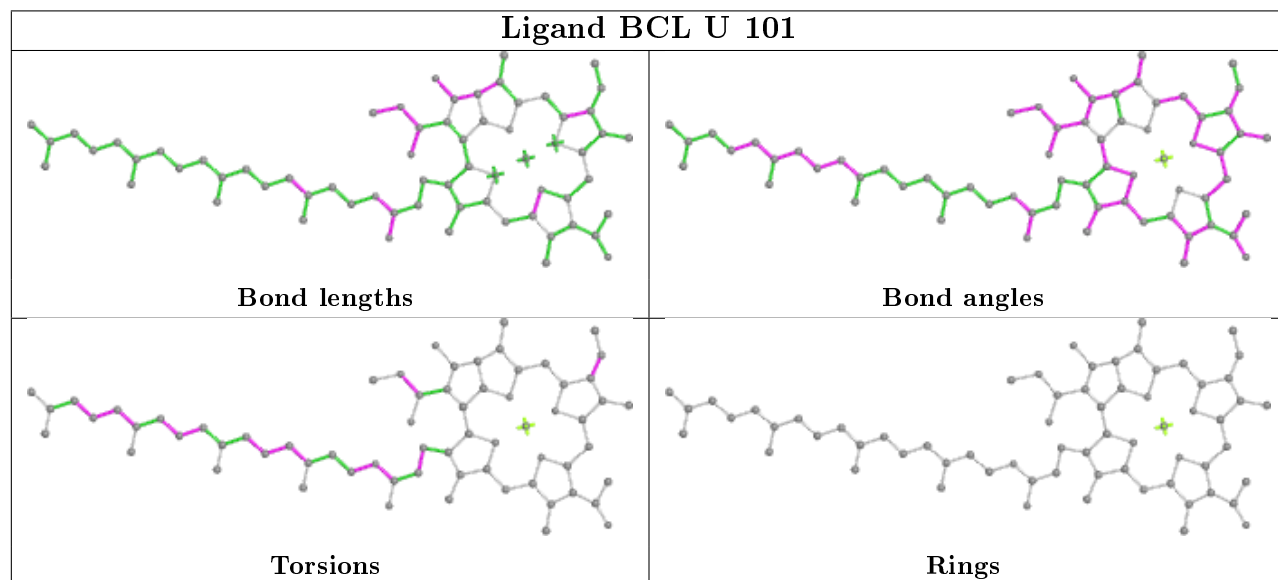
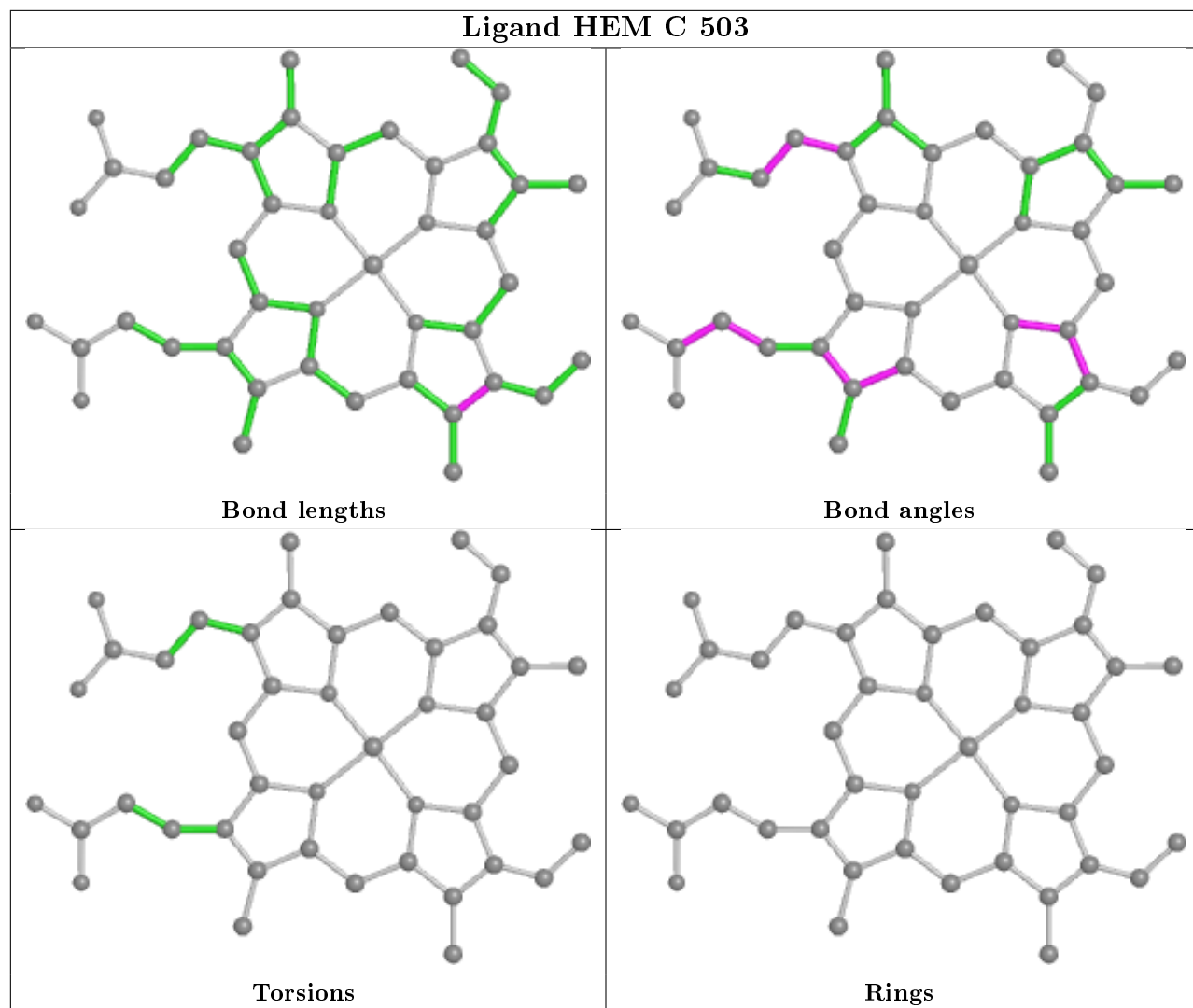


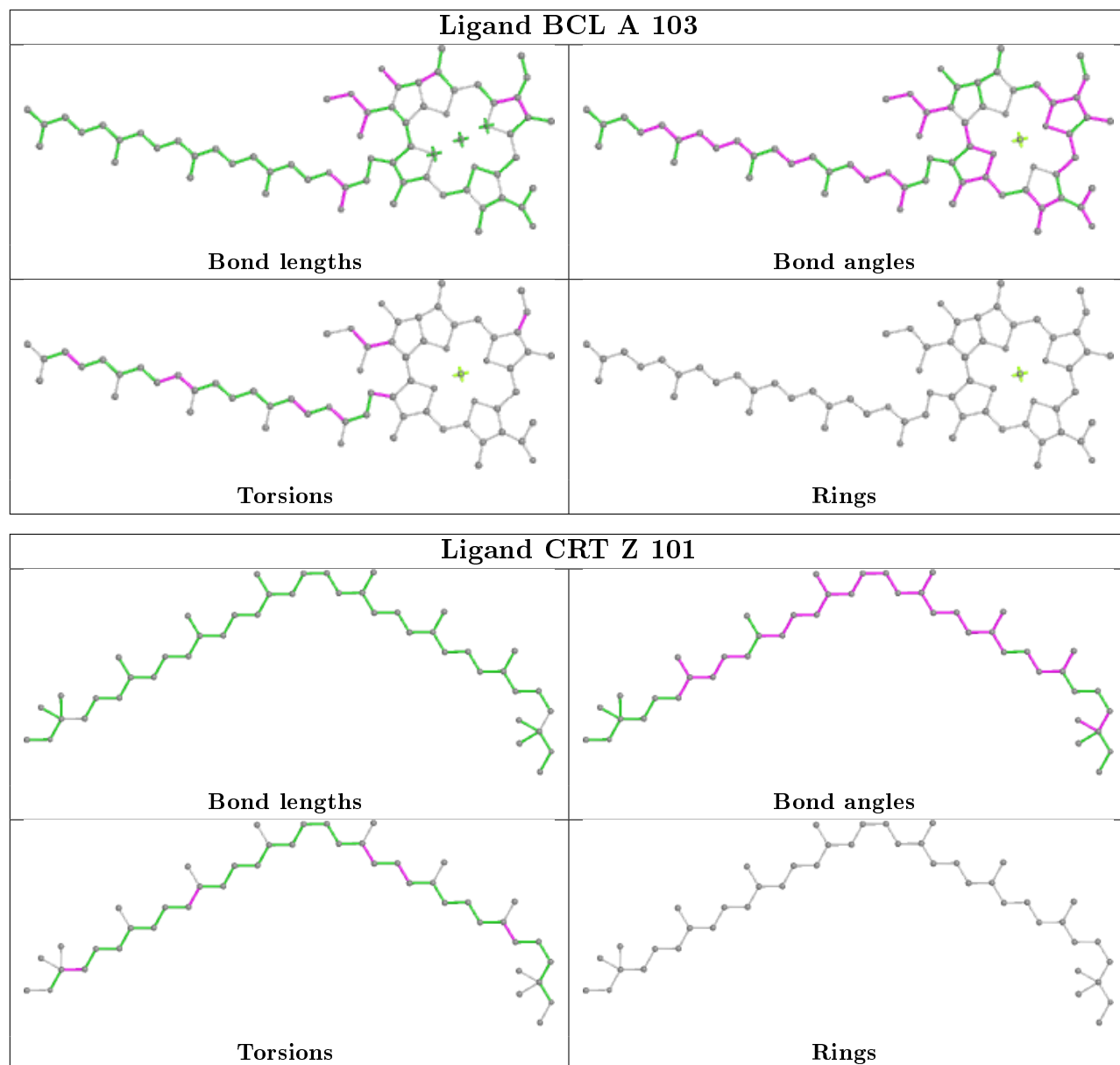


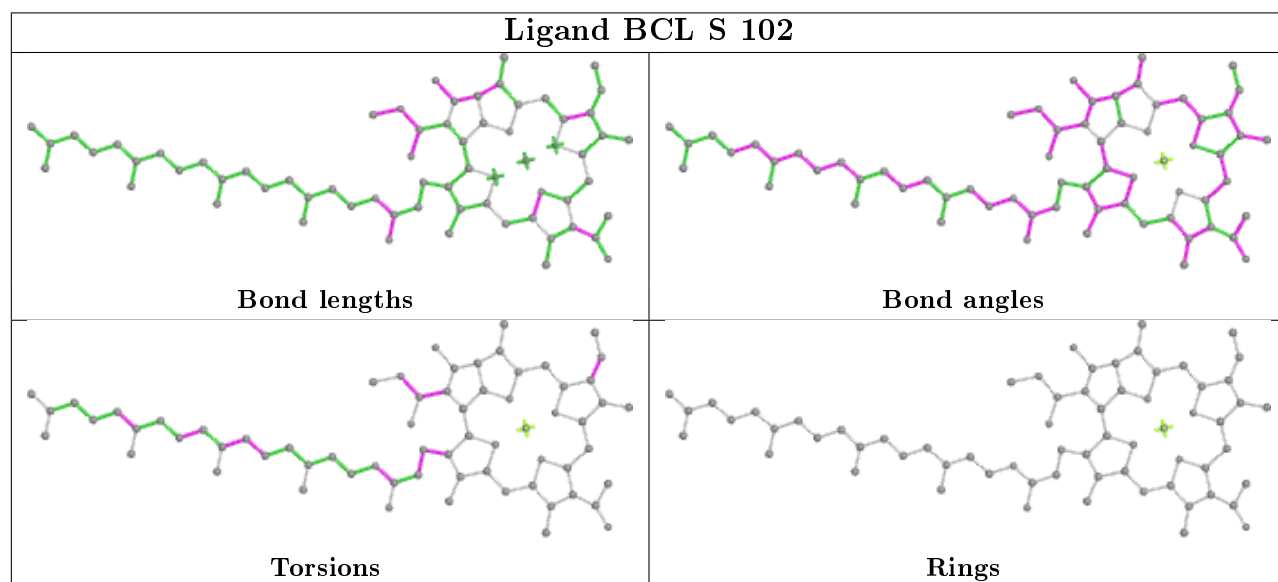
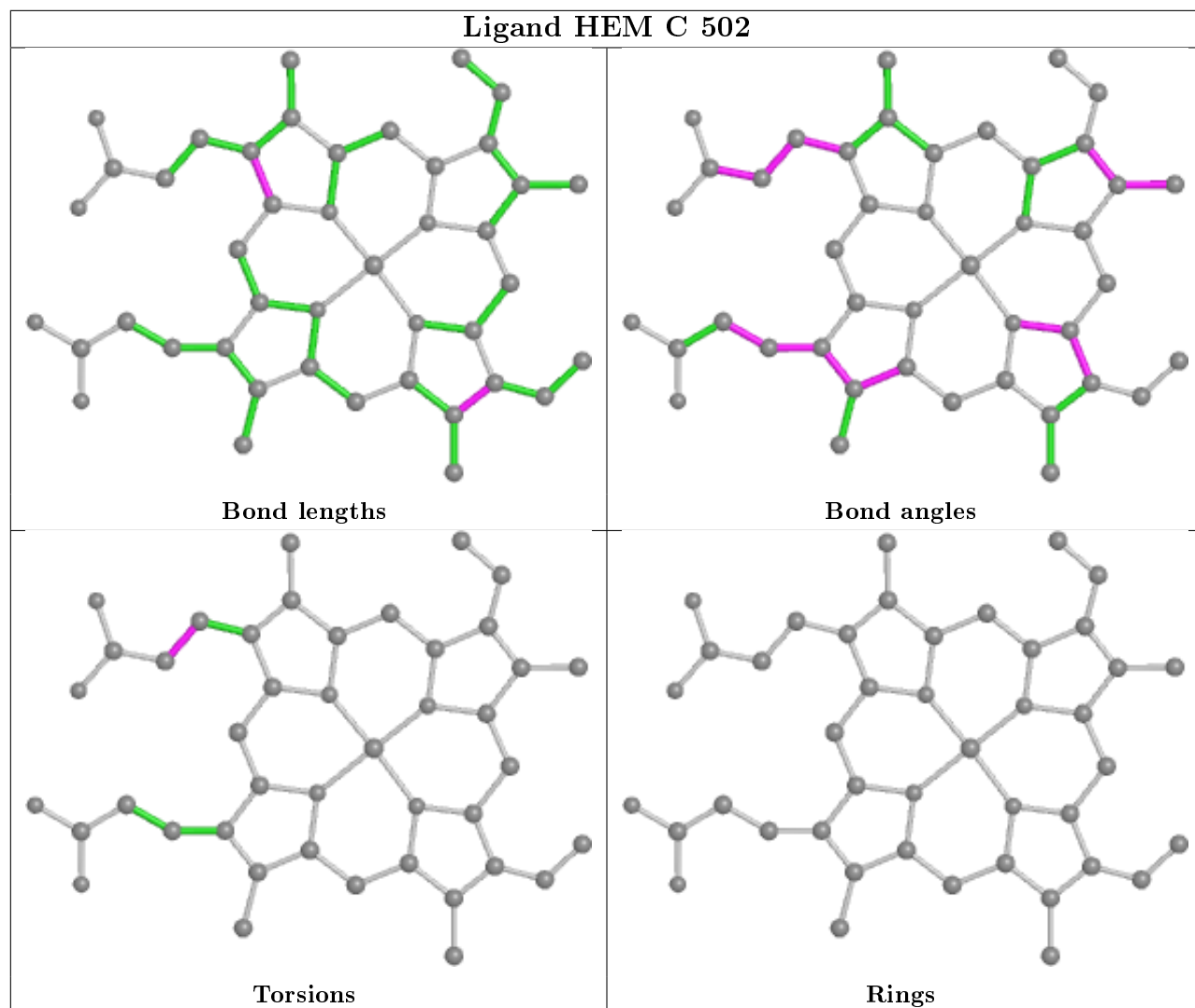




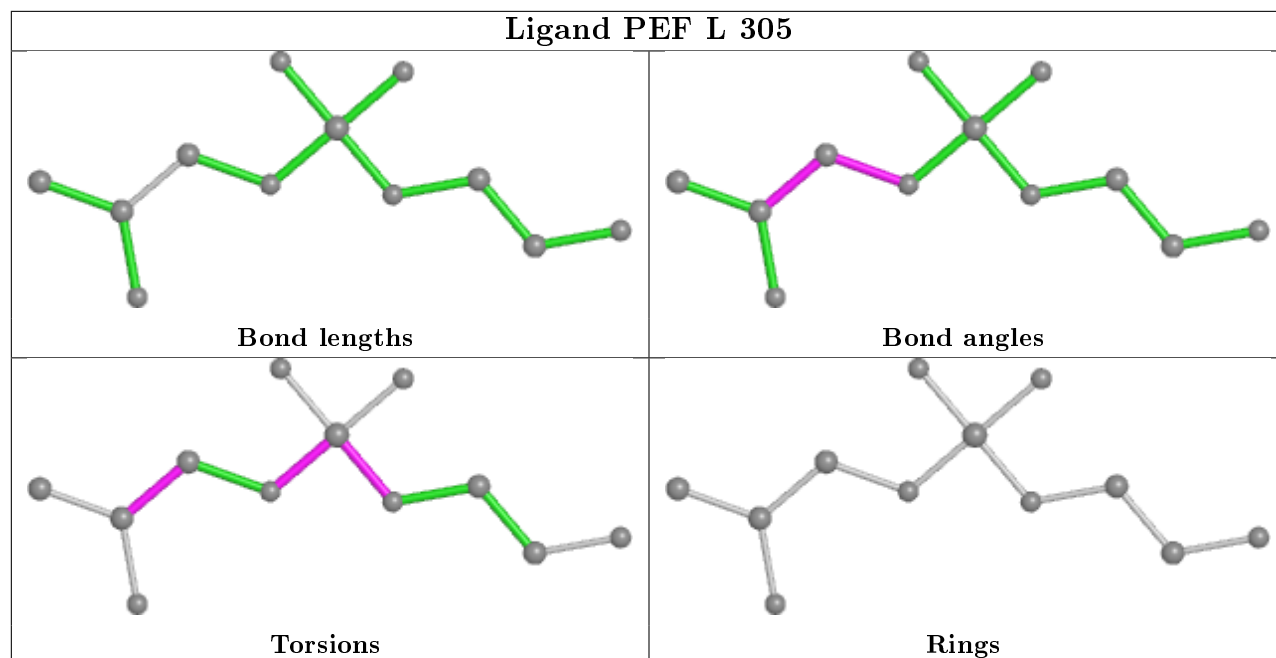




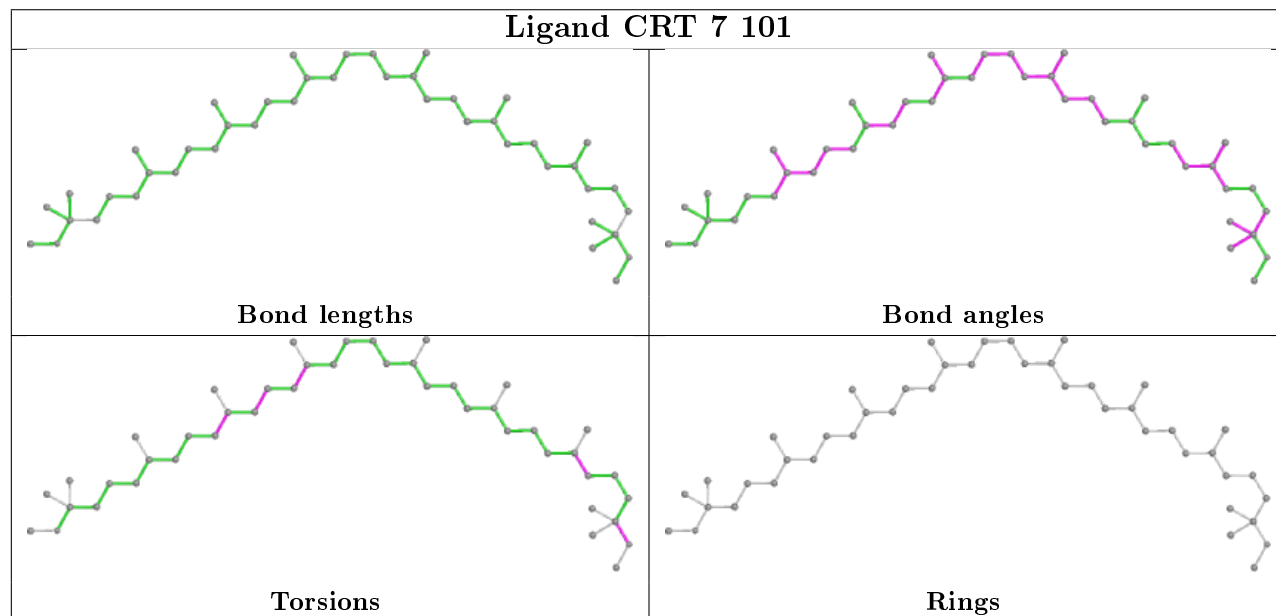


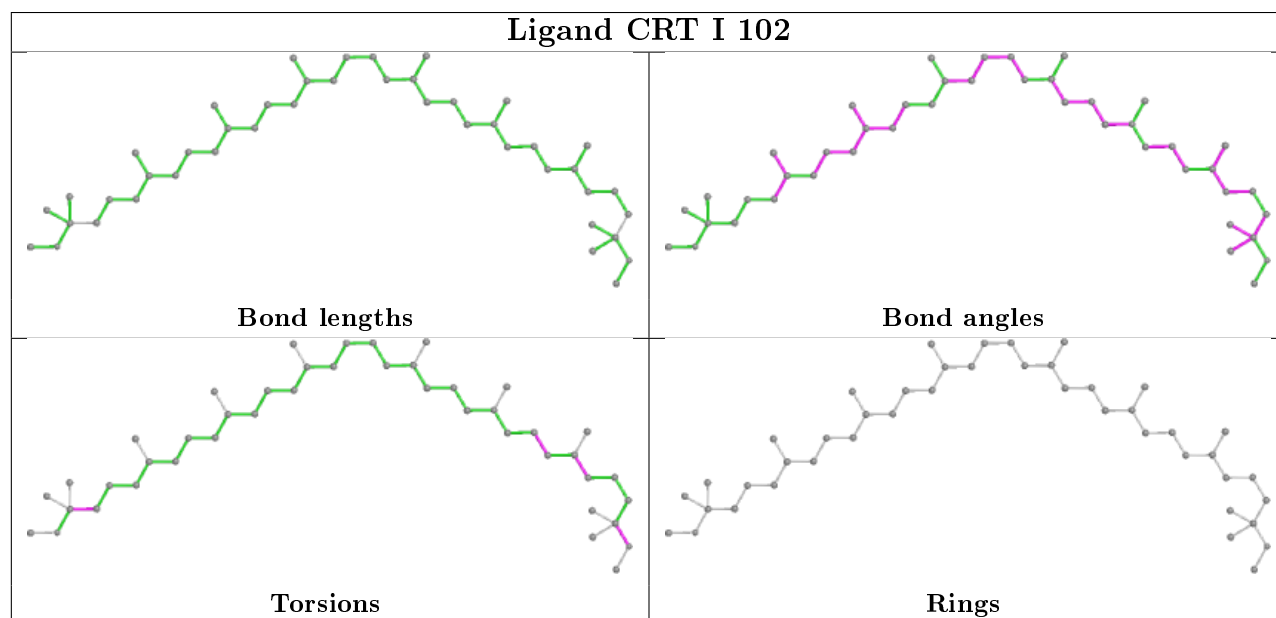
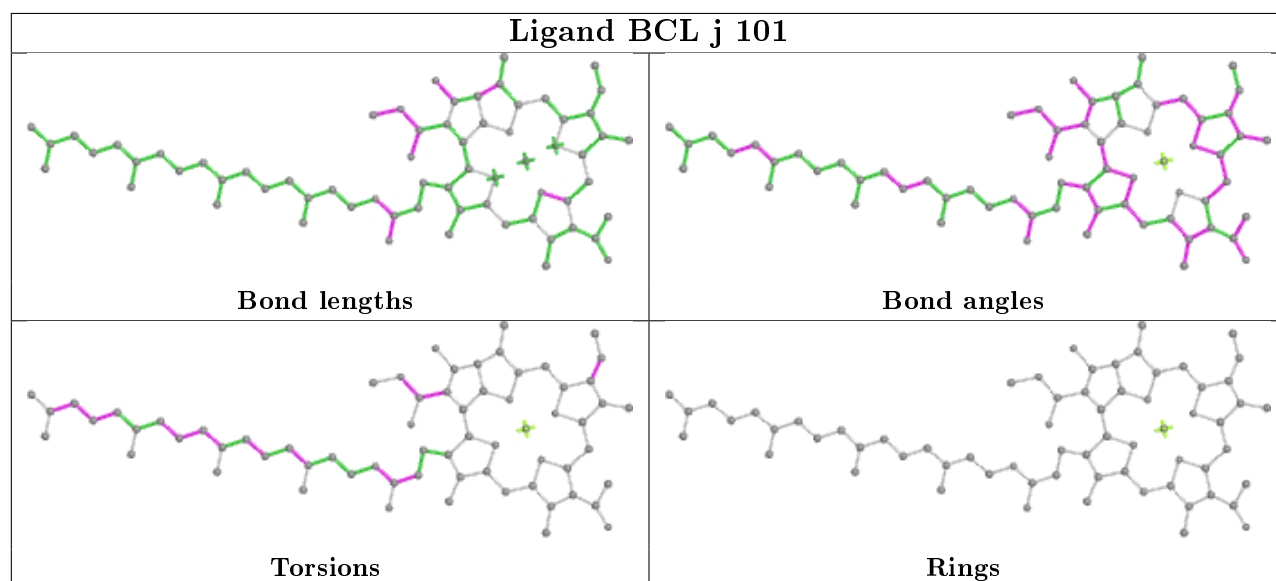
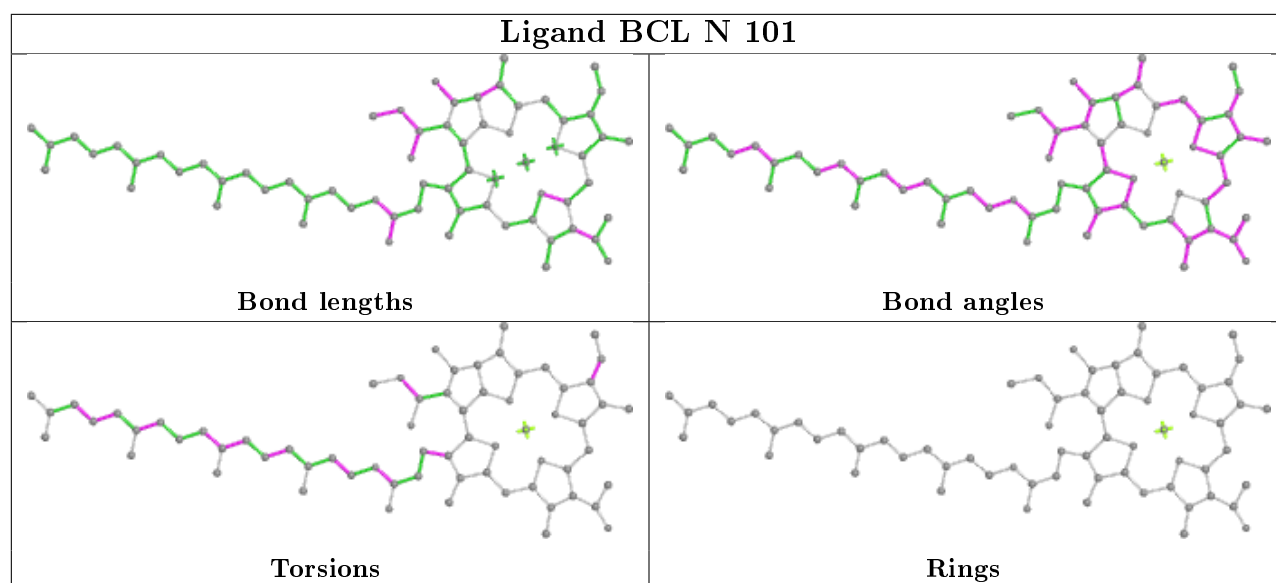


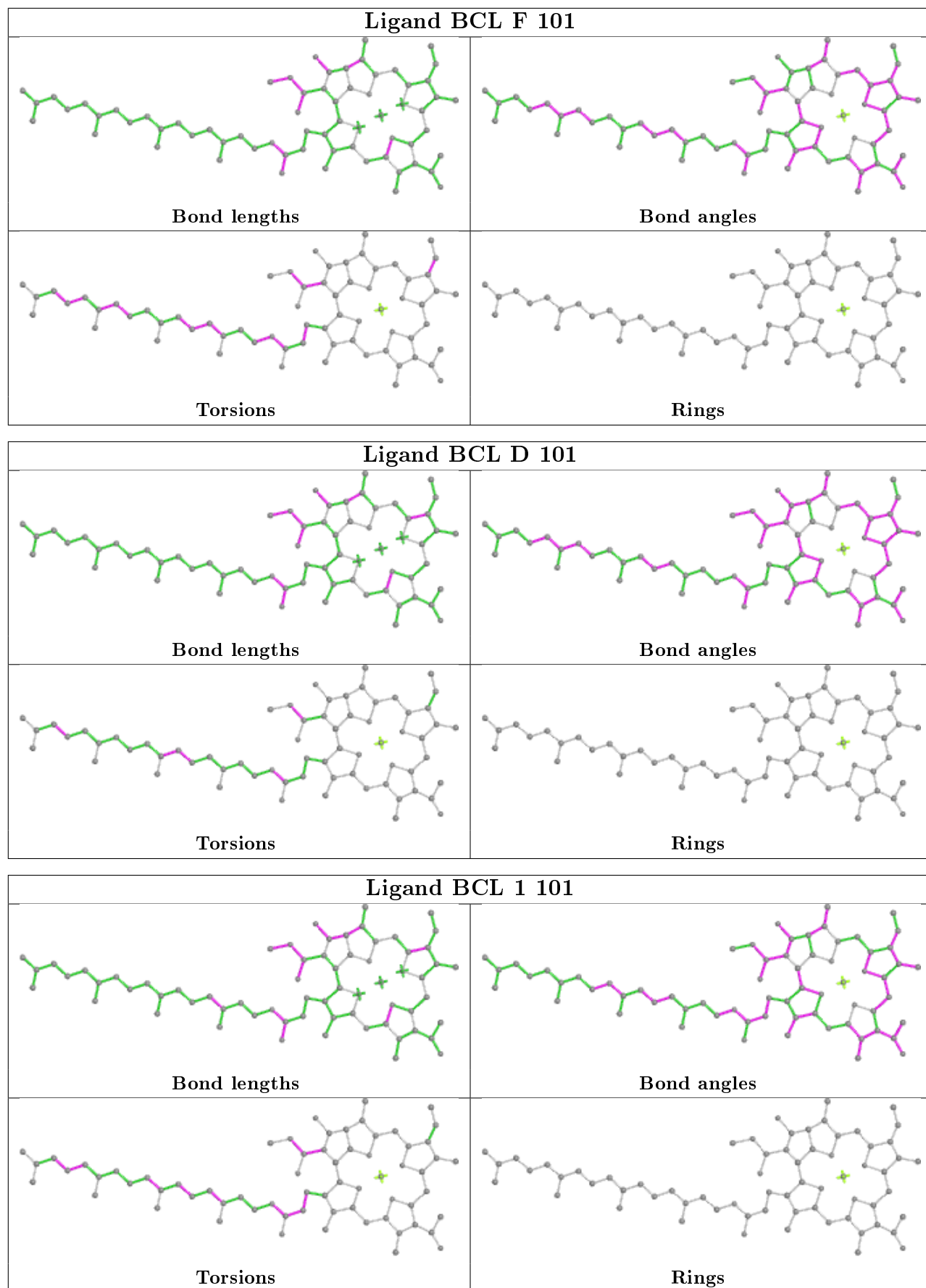
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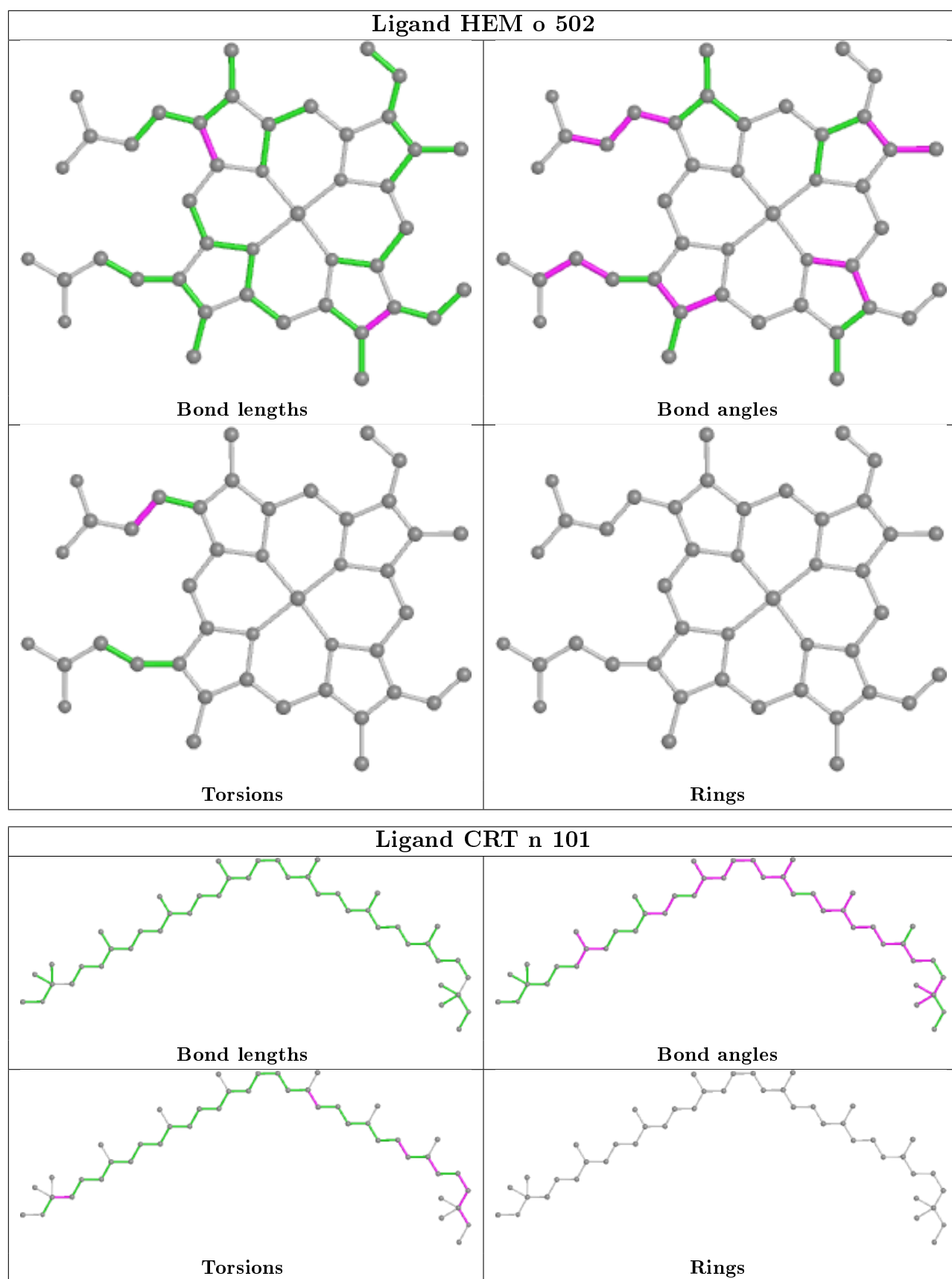


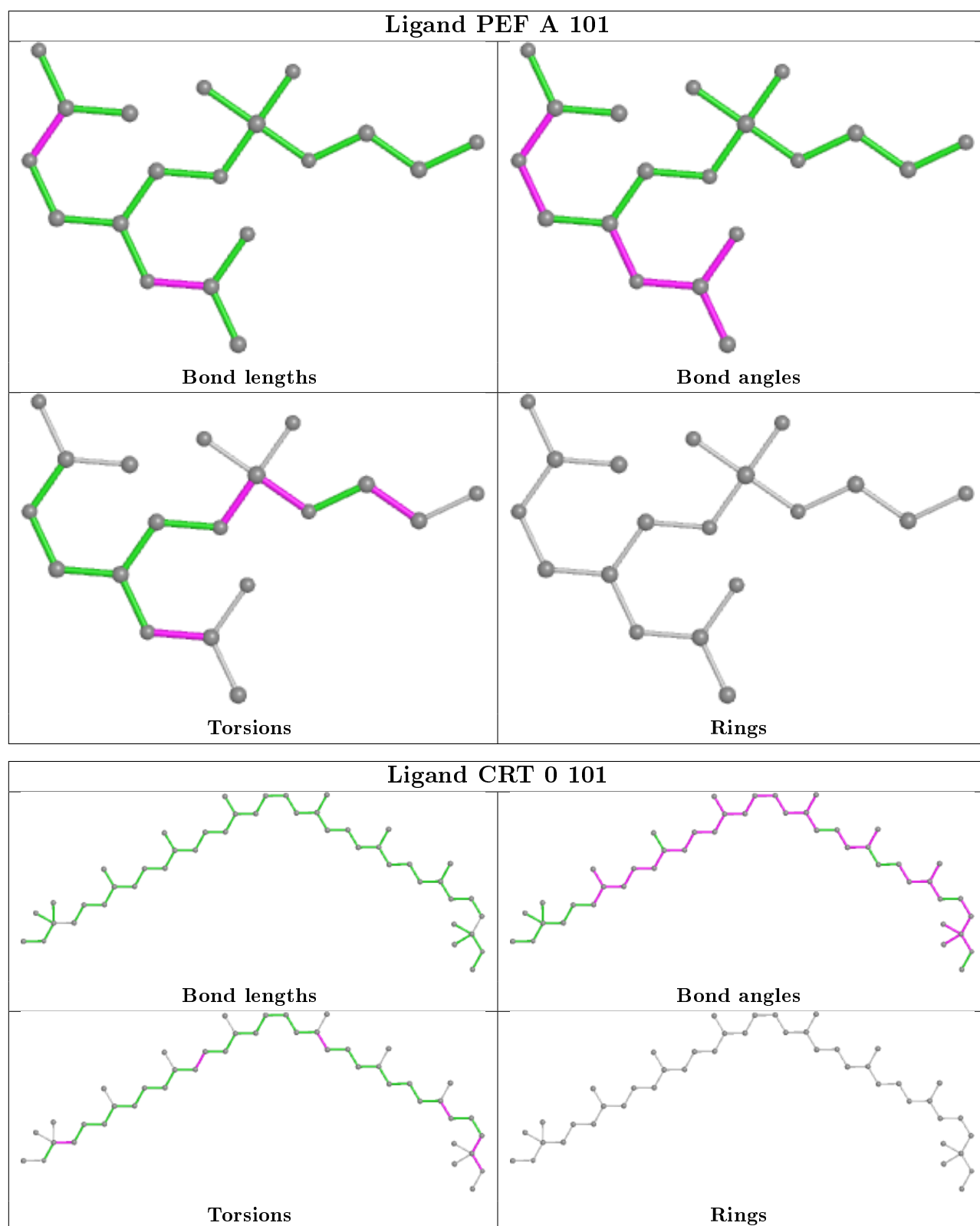
Ligand CRT 7 101

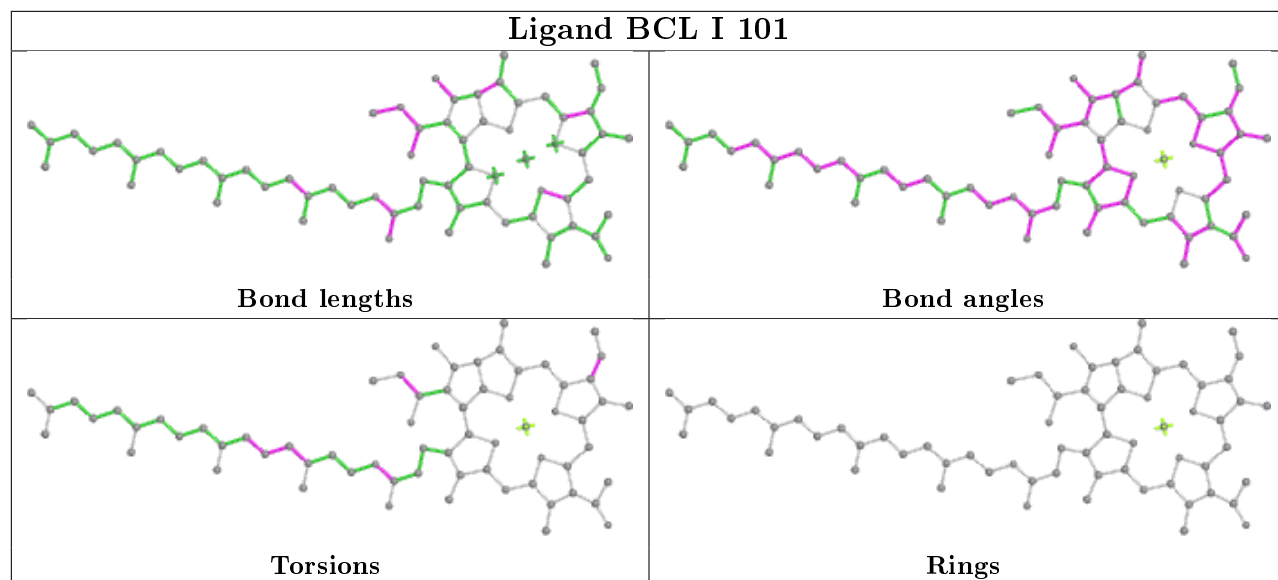
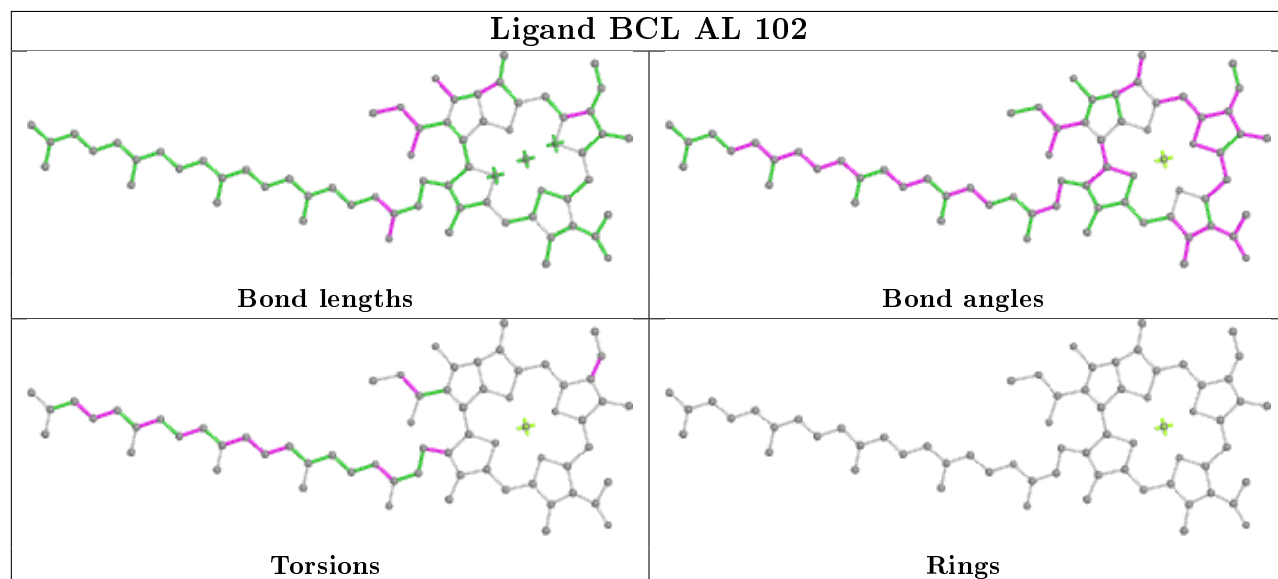


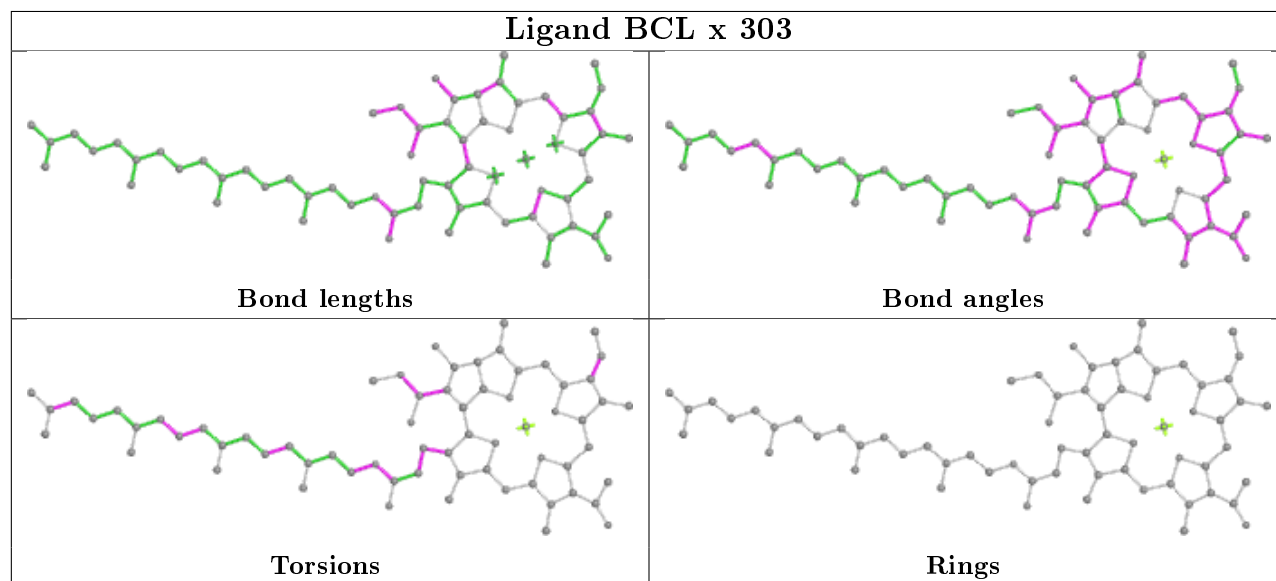
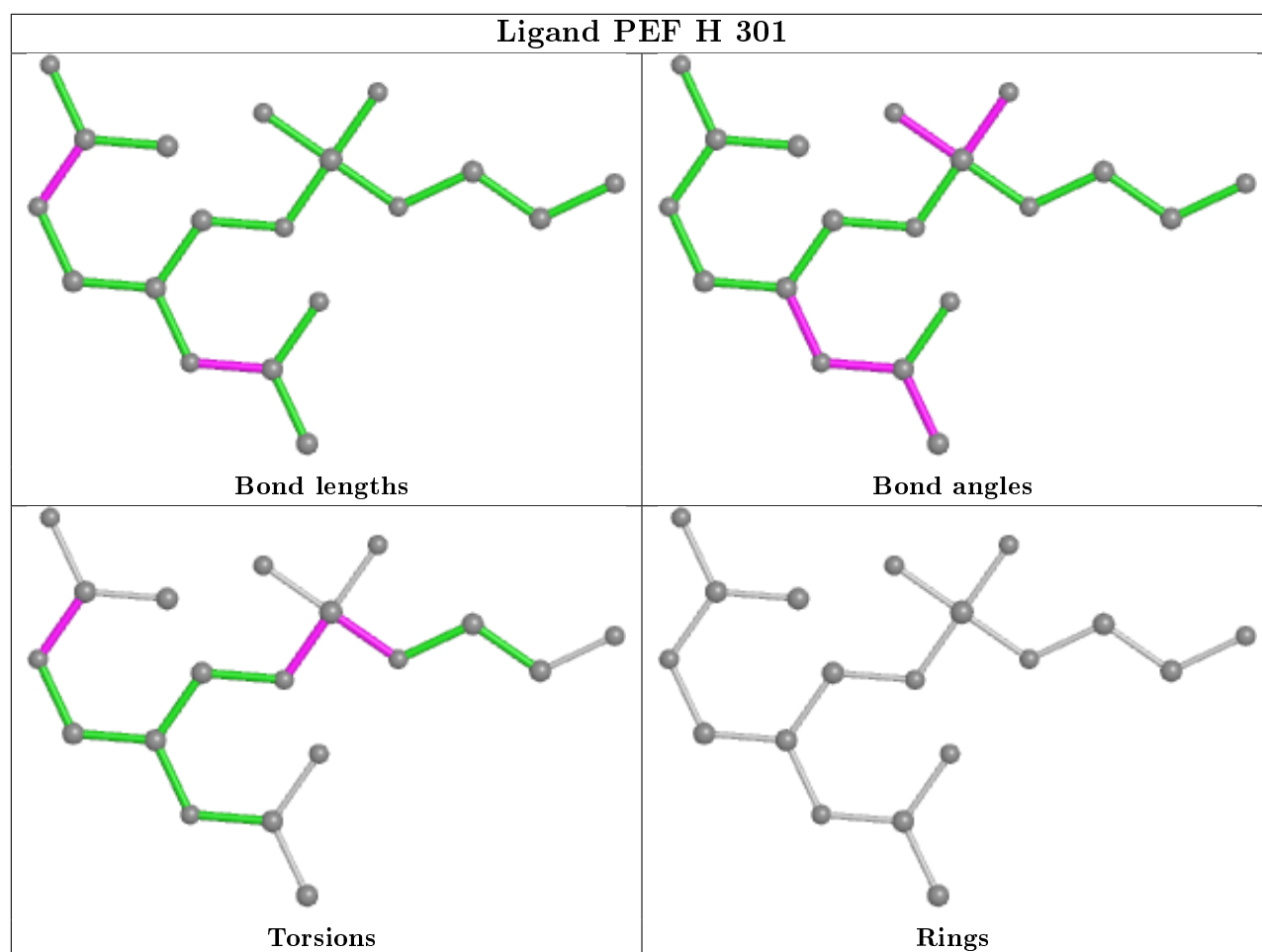


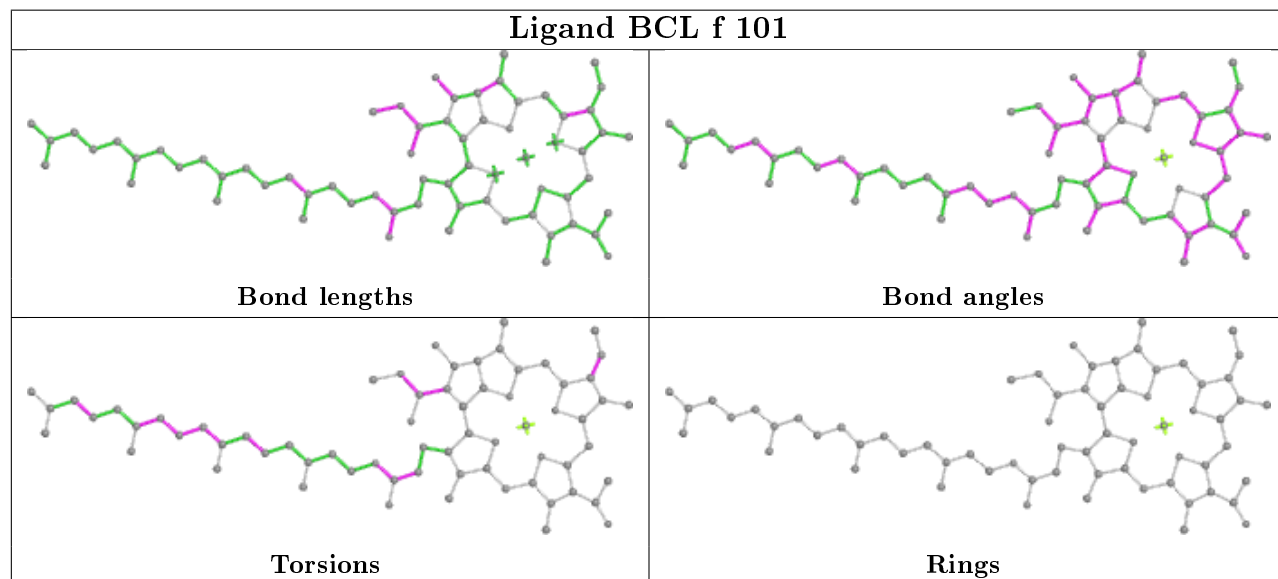
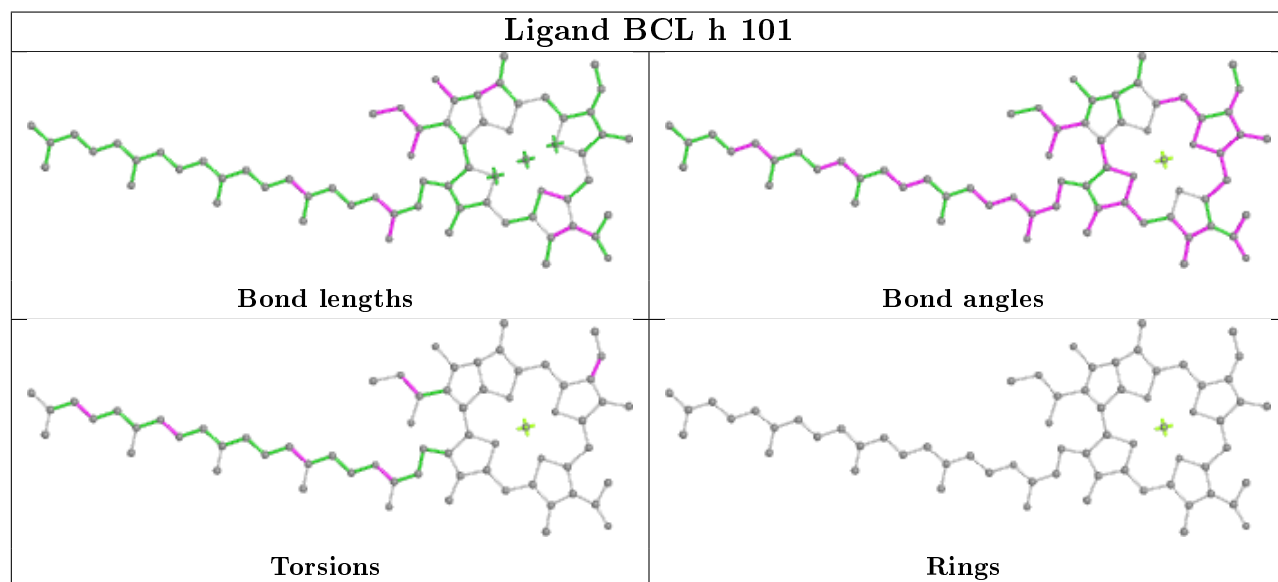
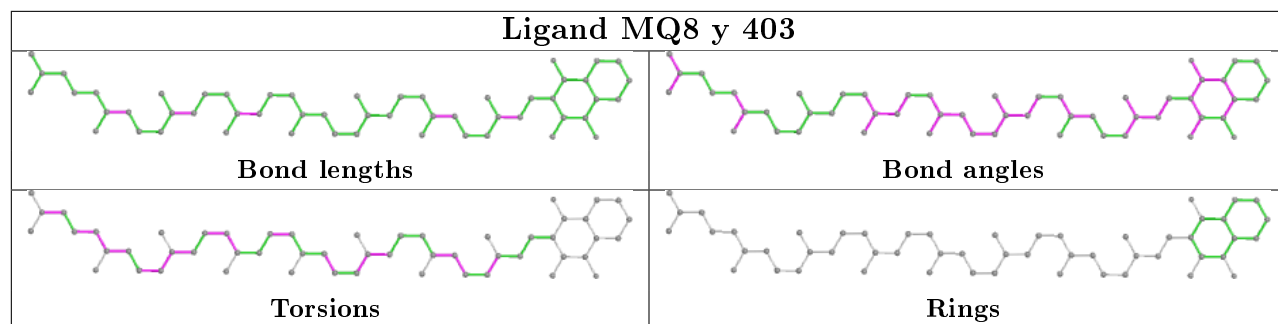


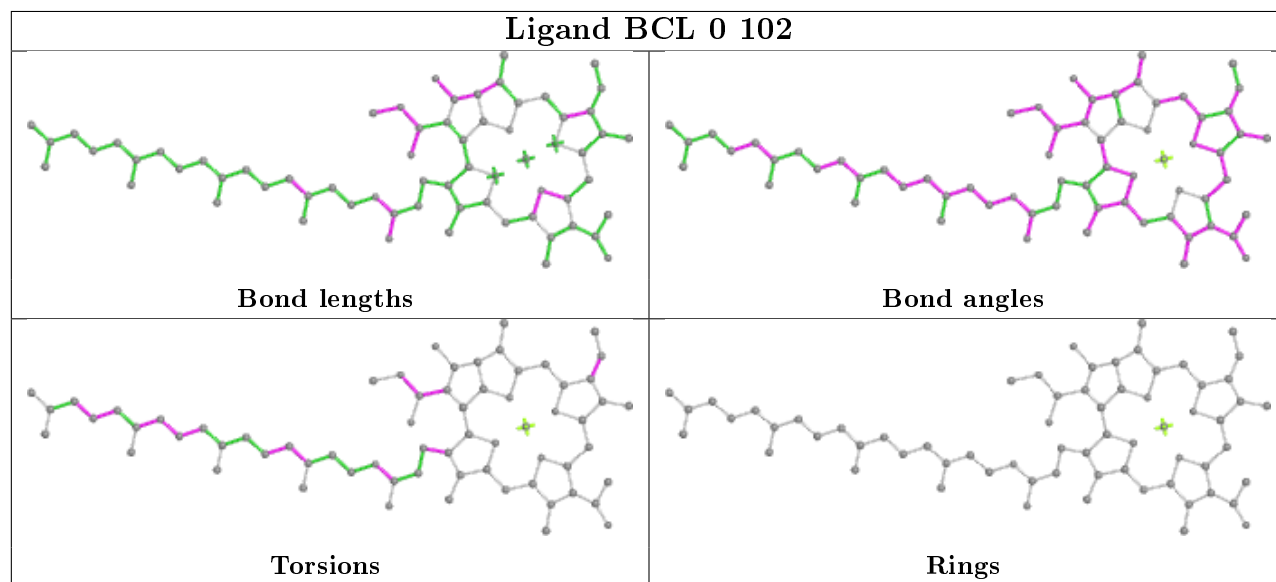
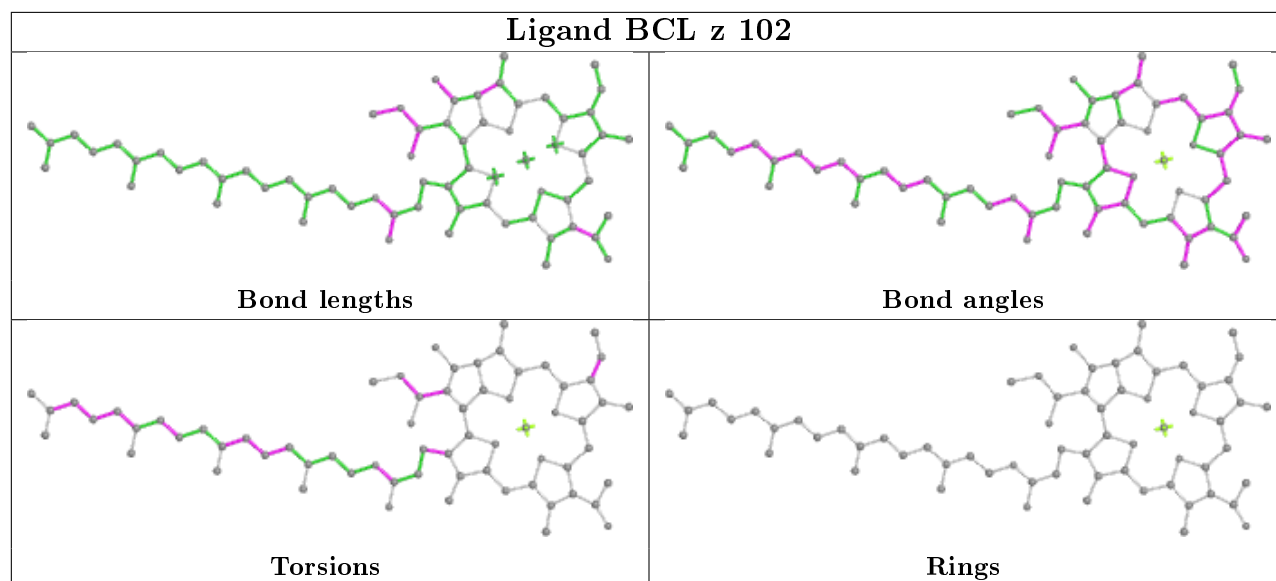
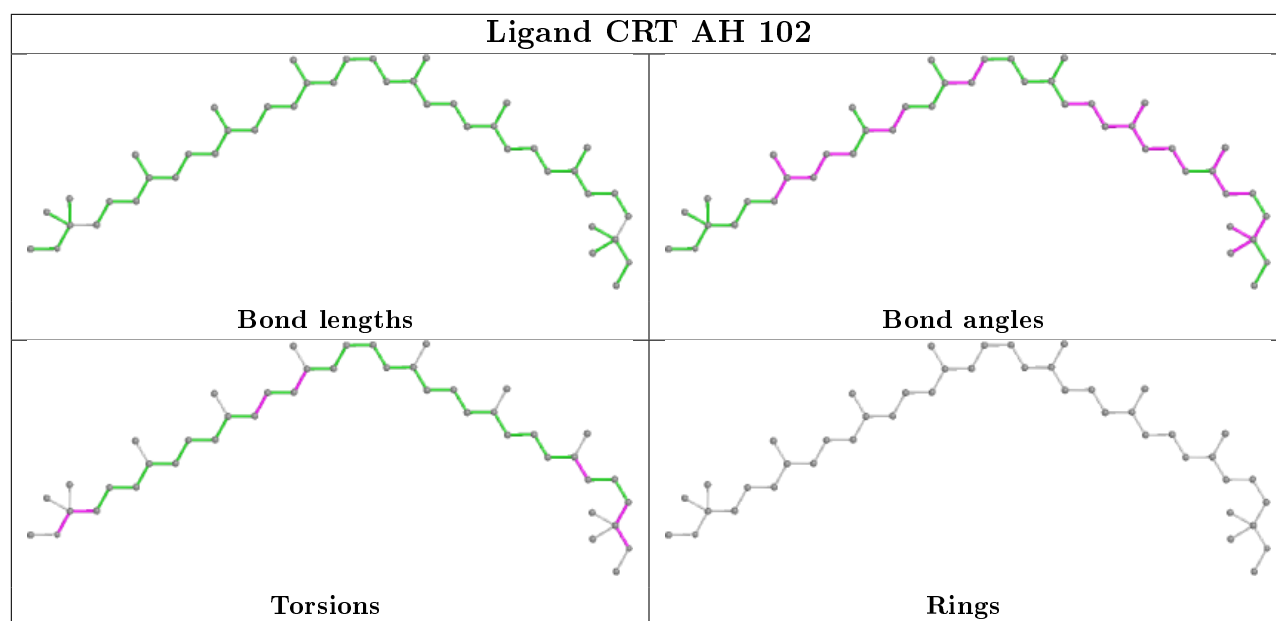


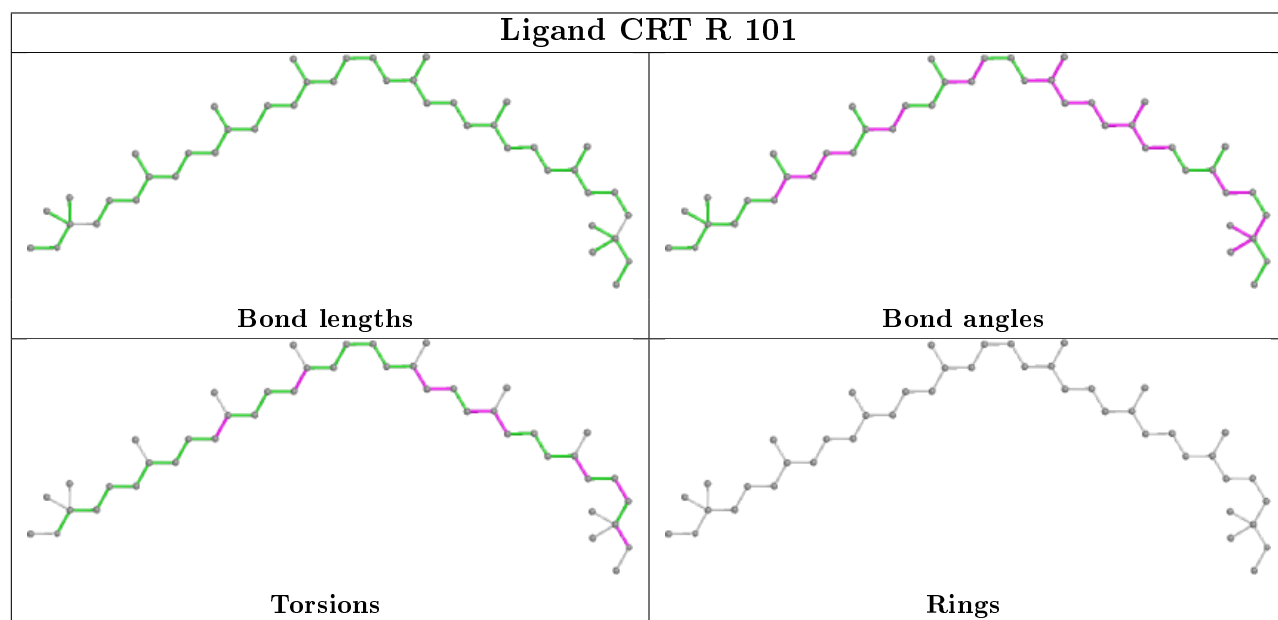
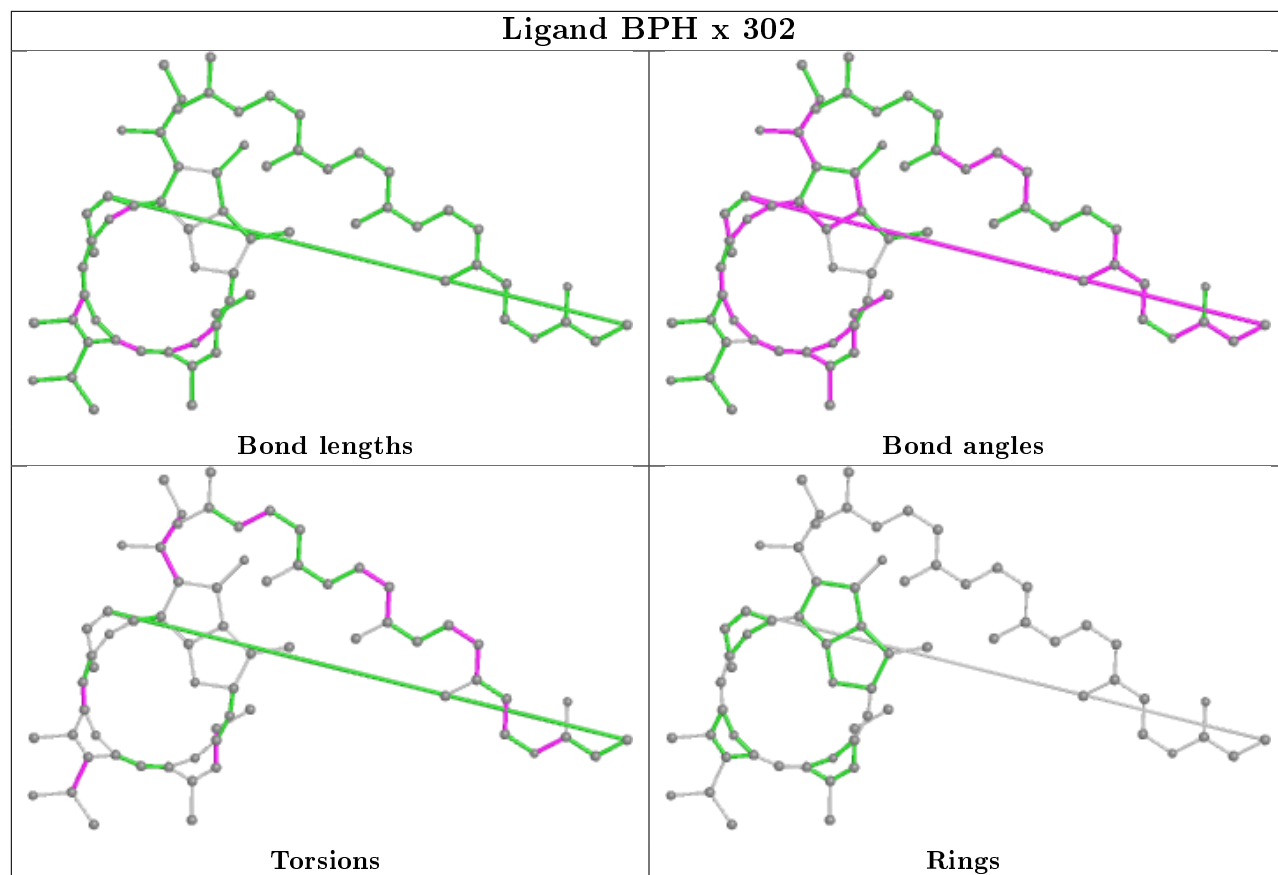


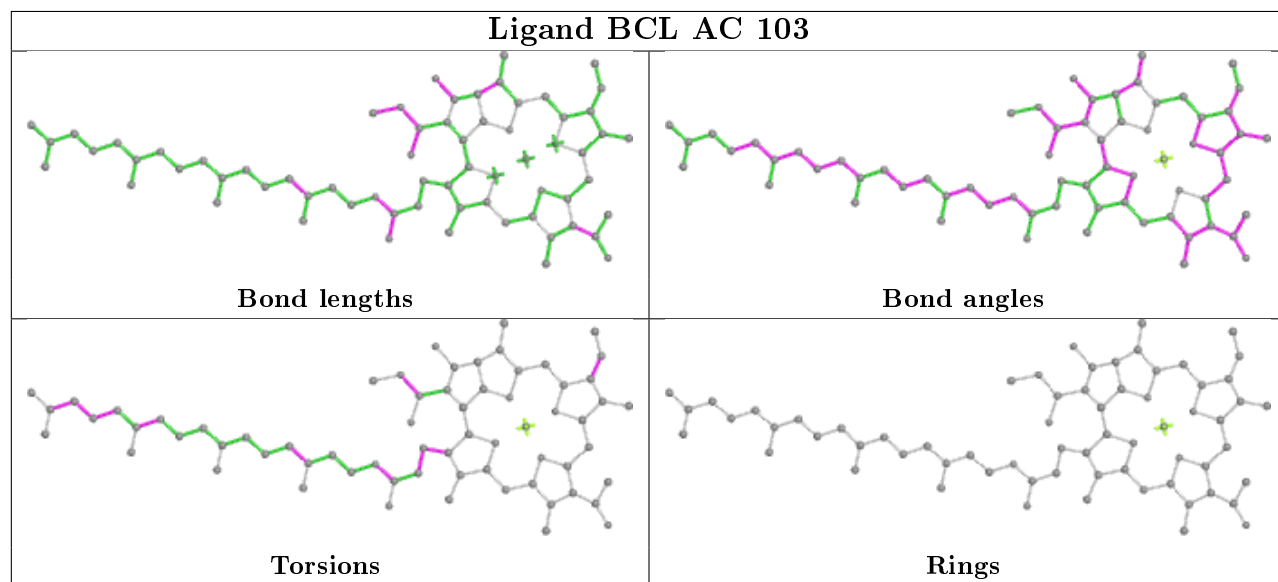
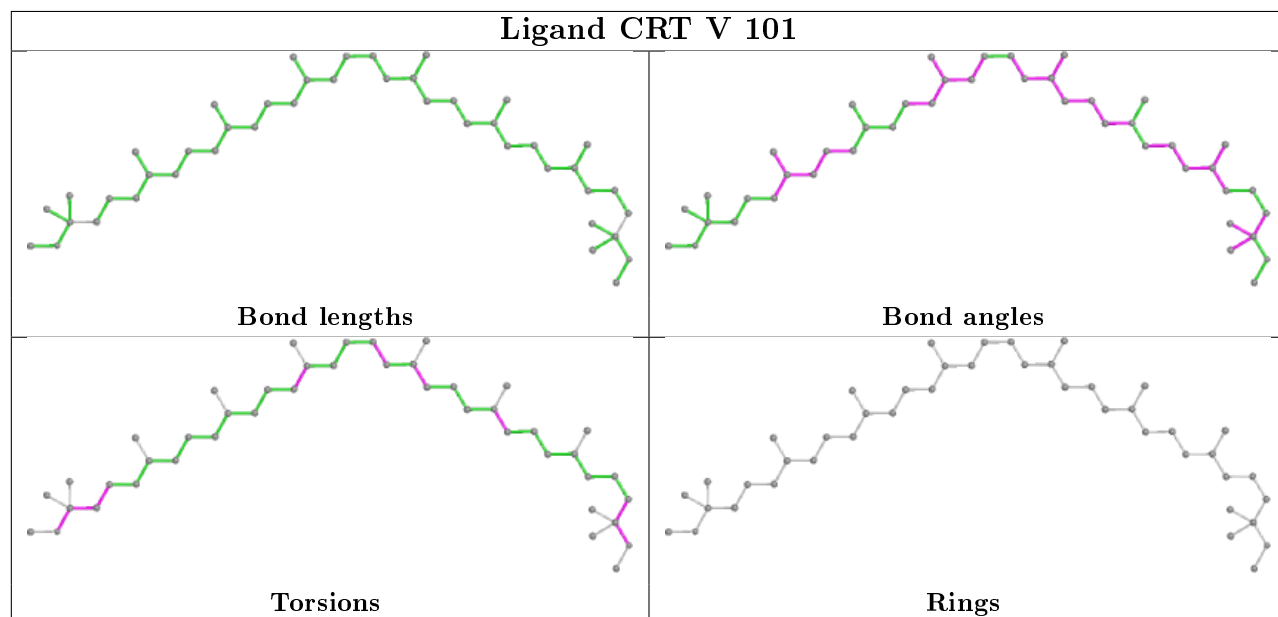
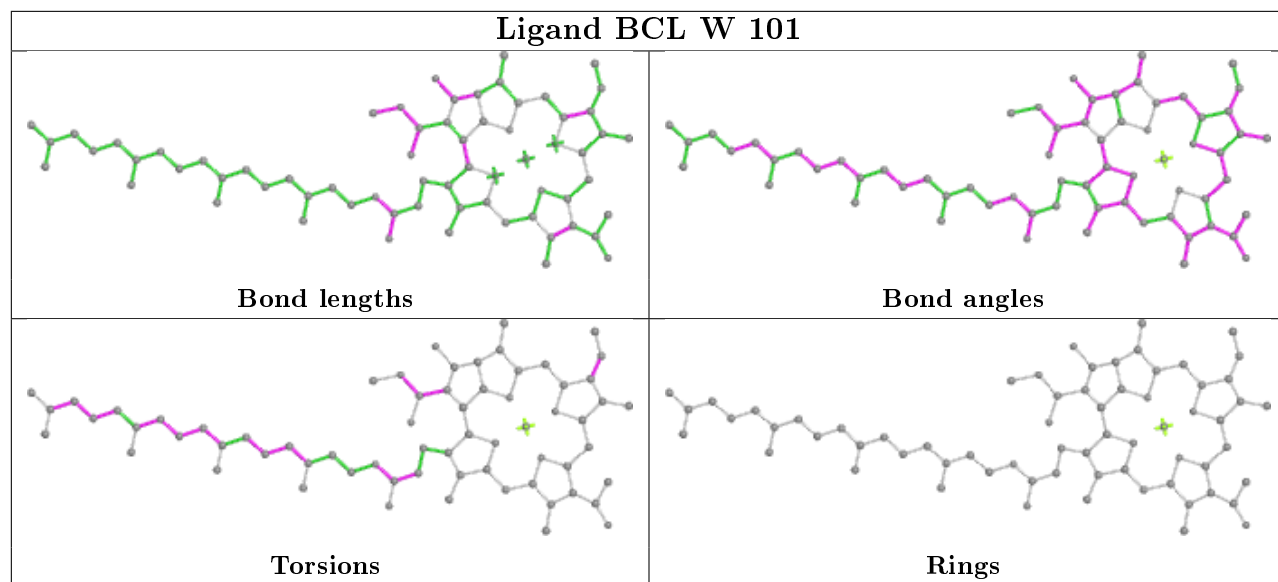
Ligand BCL I 101**Ligand BCL AL 102**



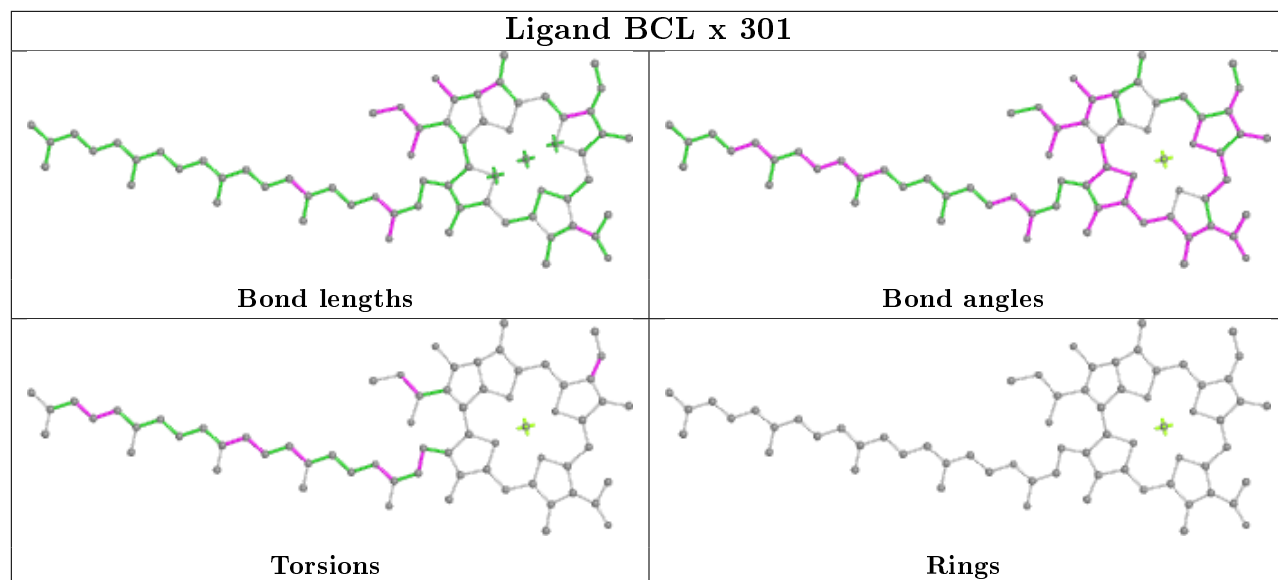




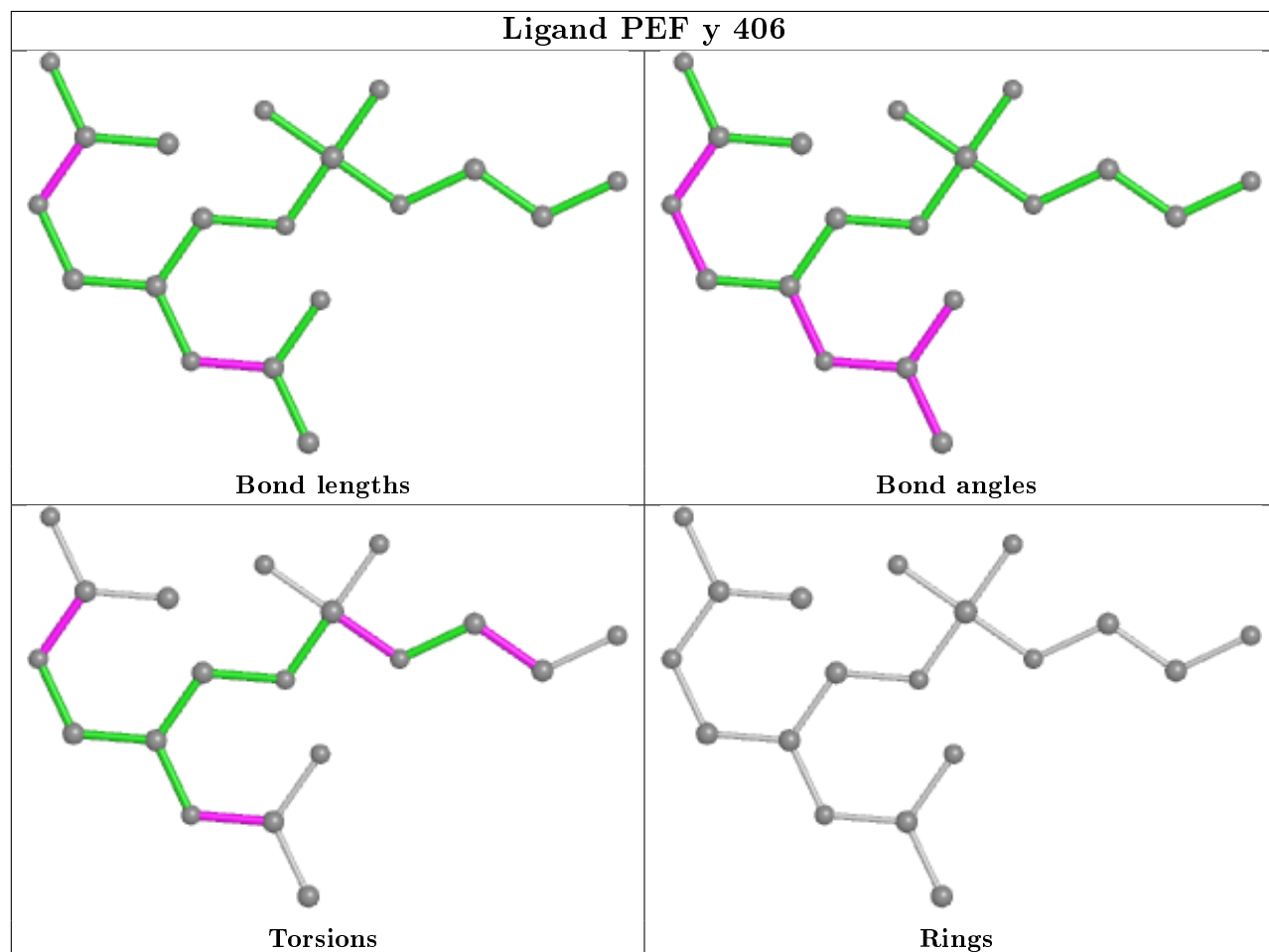


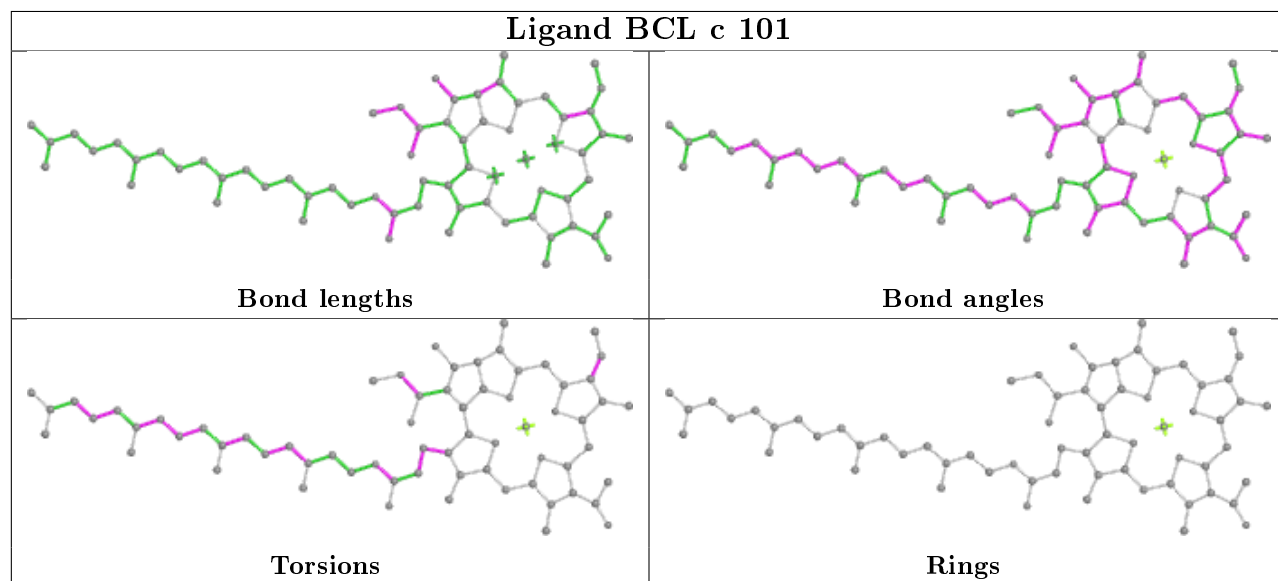
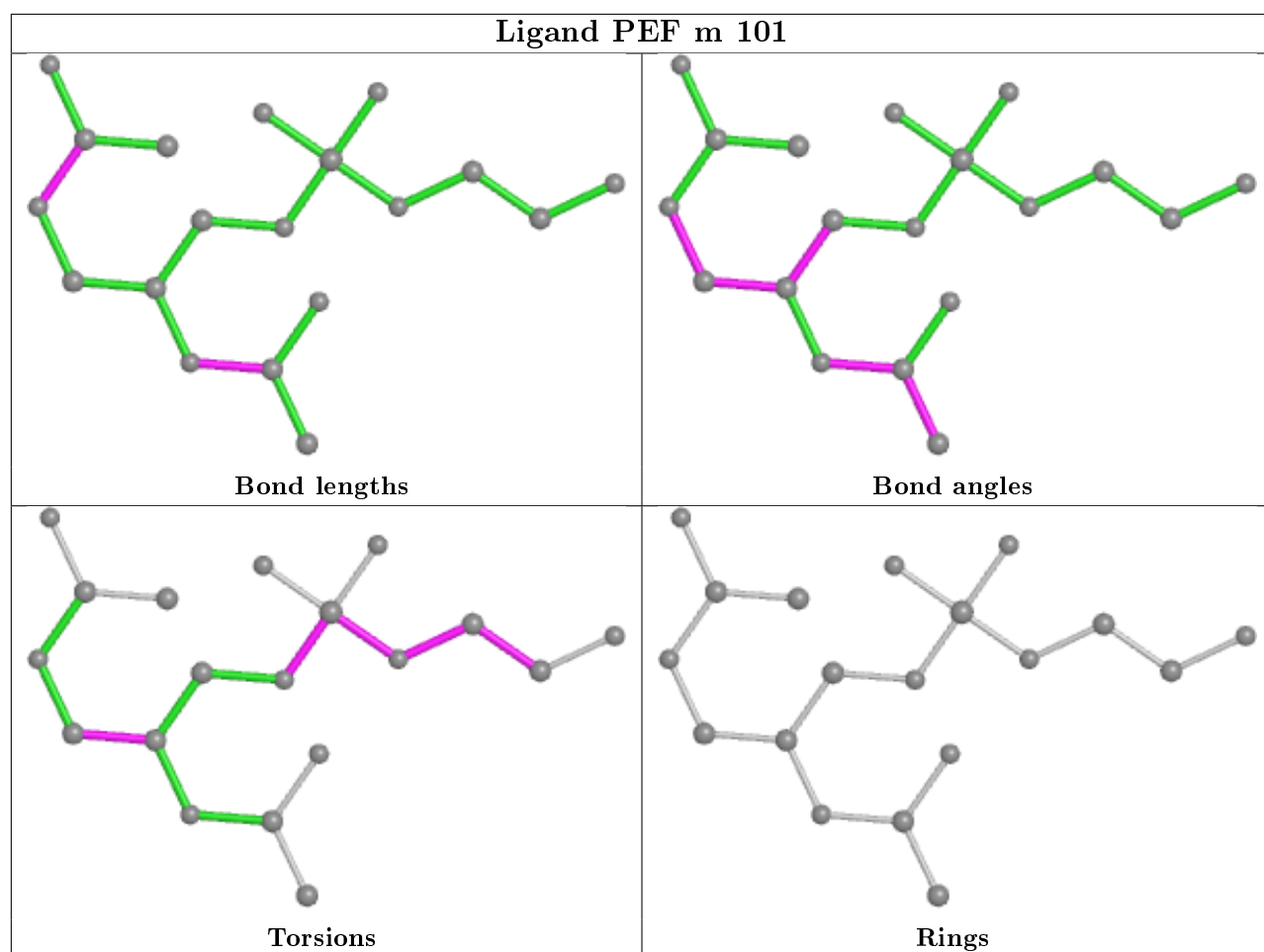


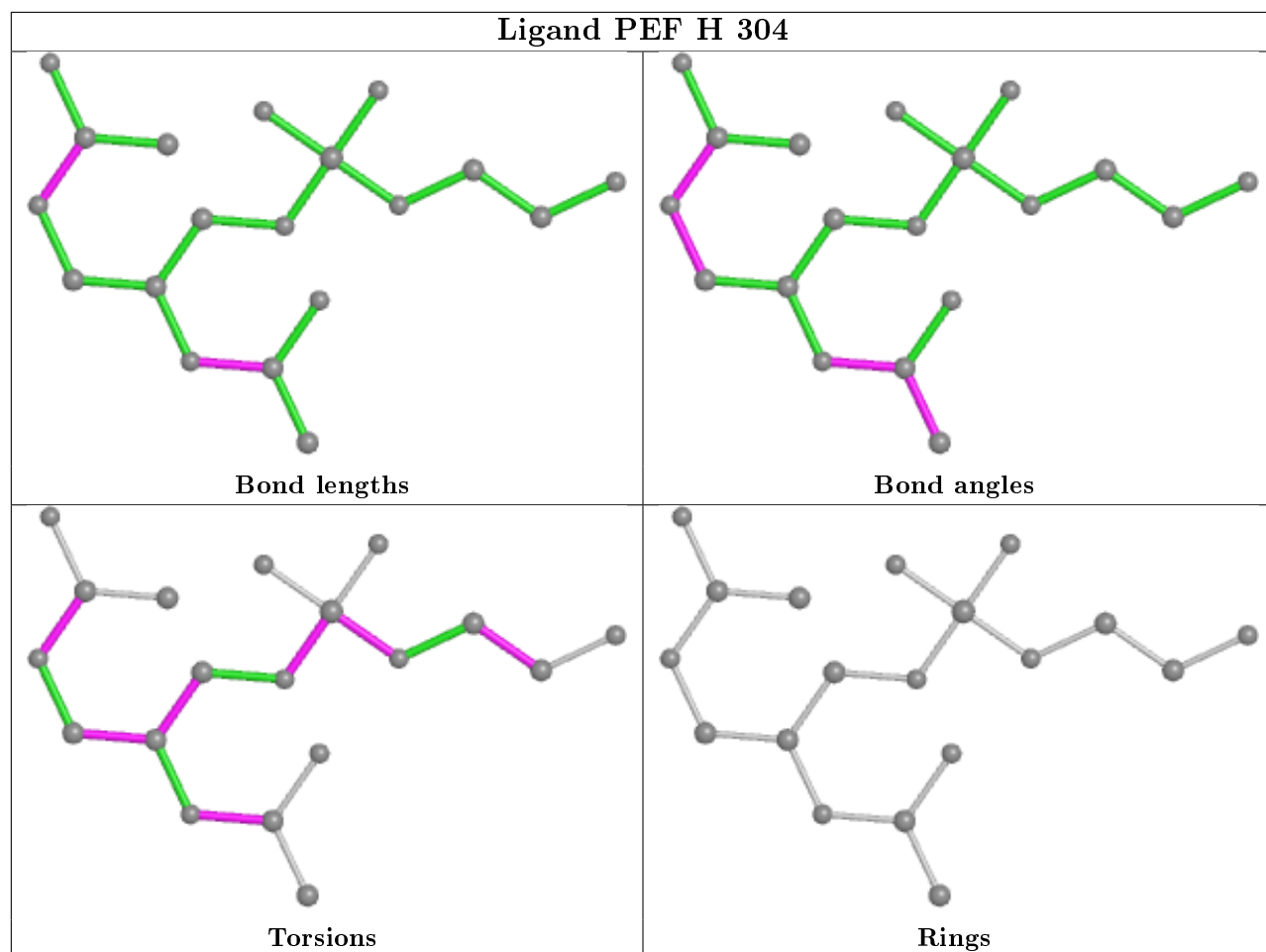
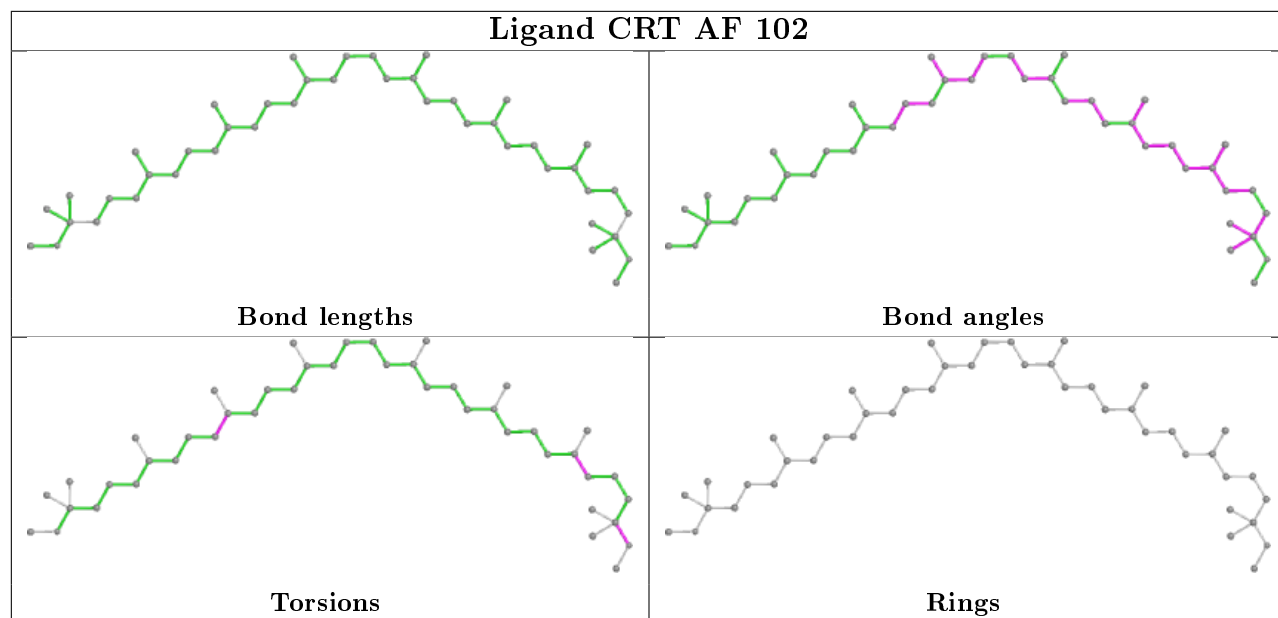
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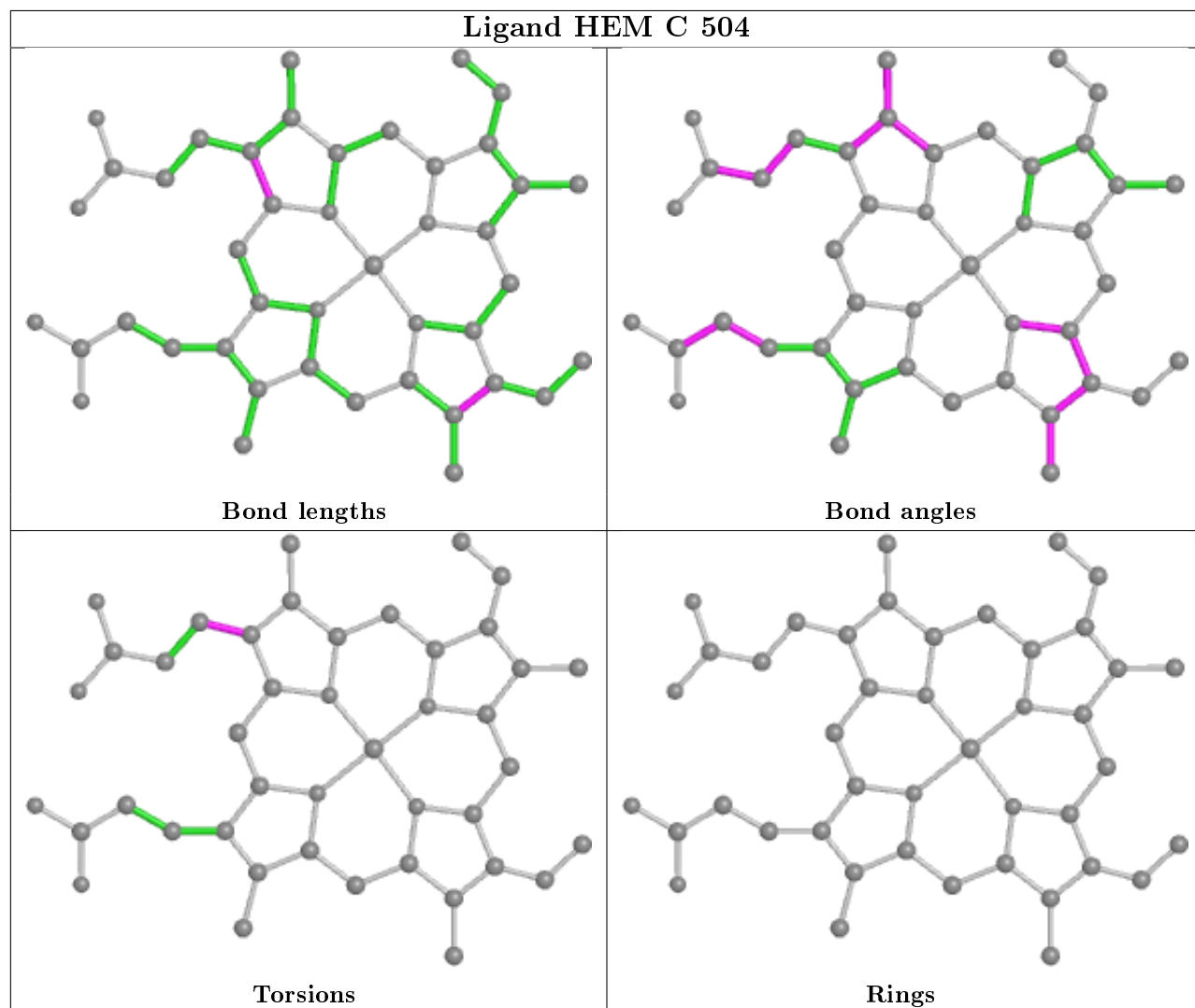
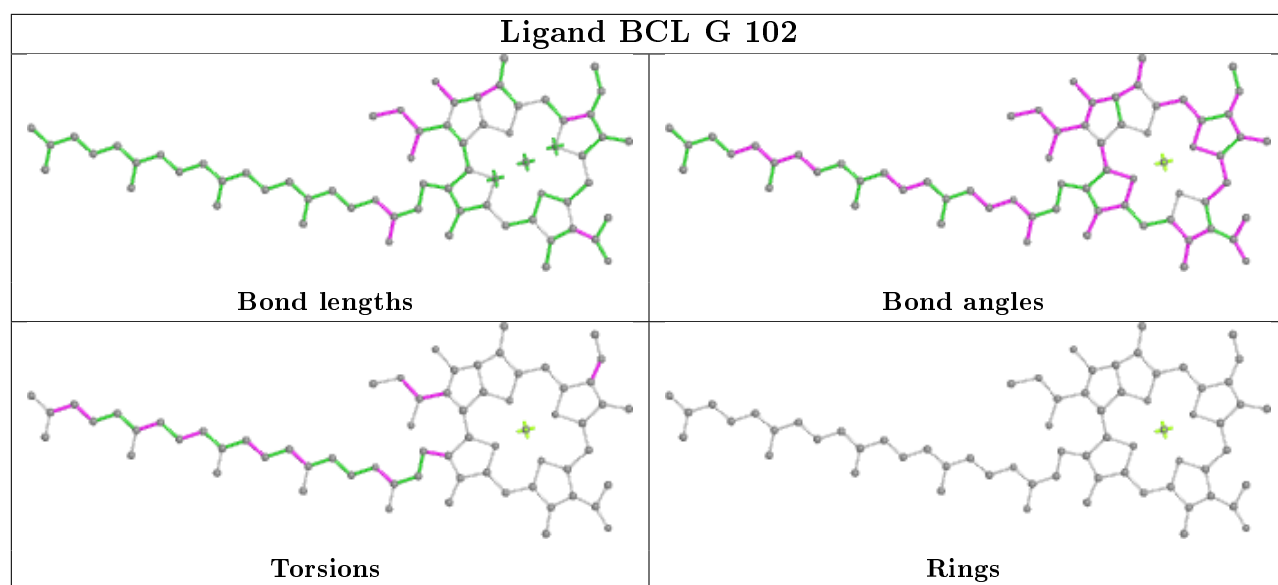


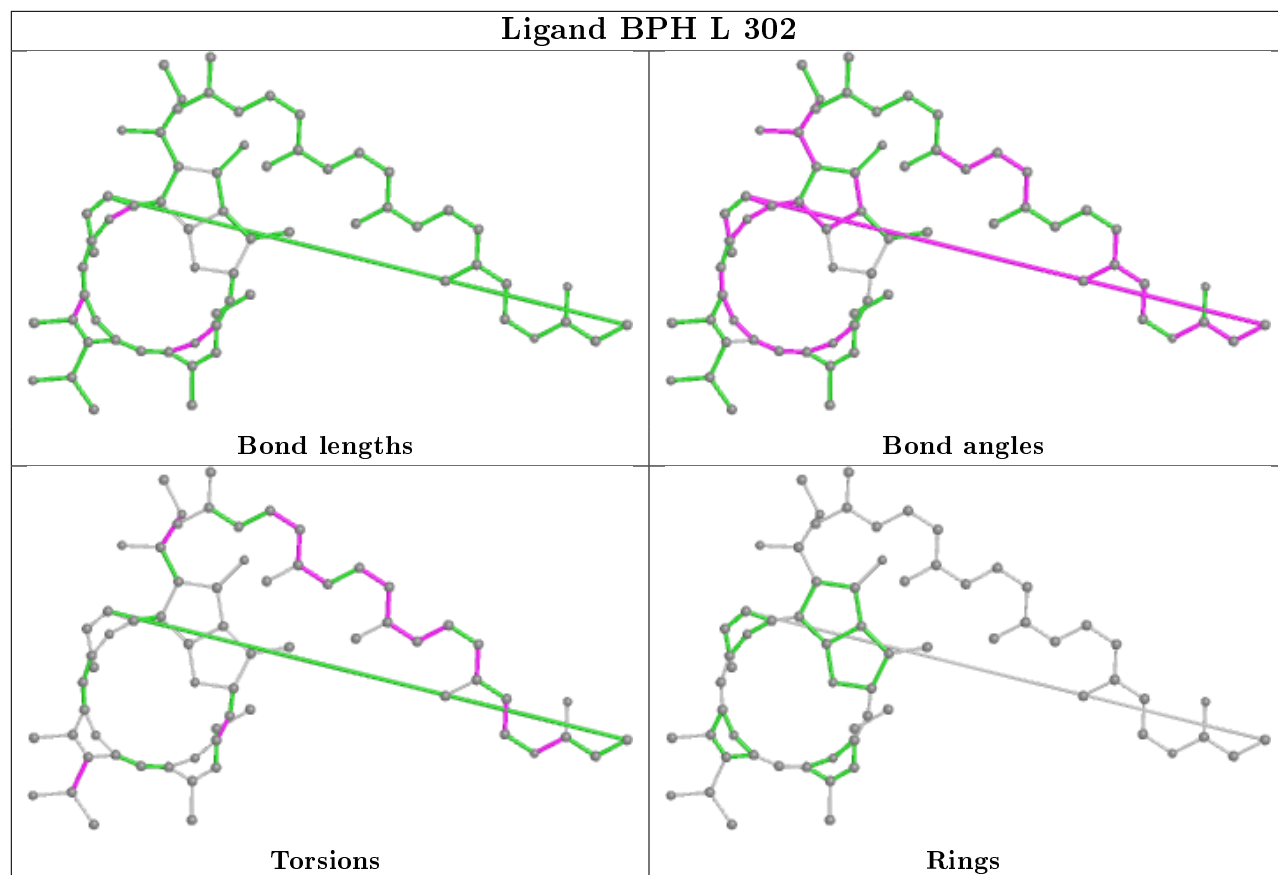
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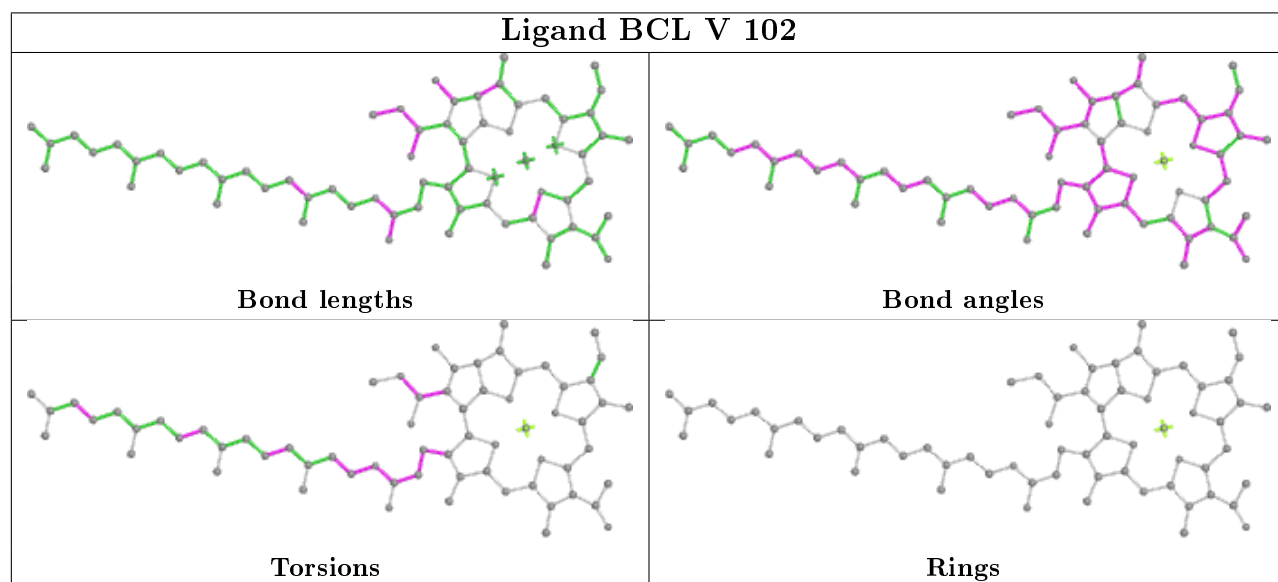
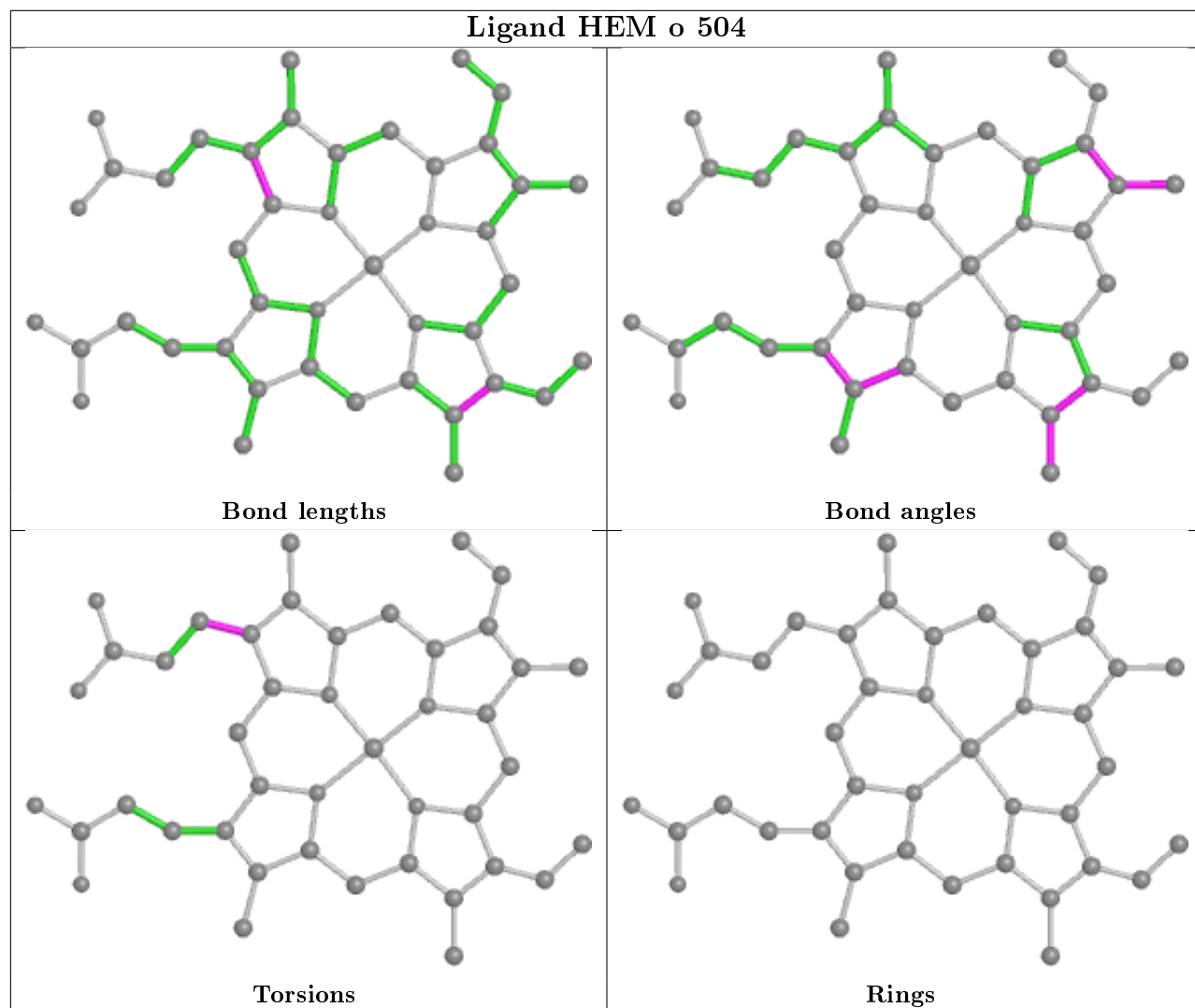




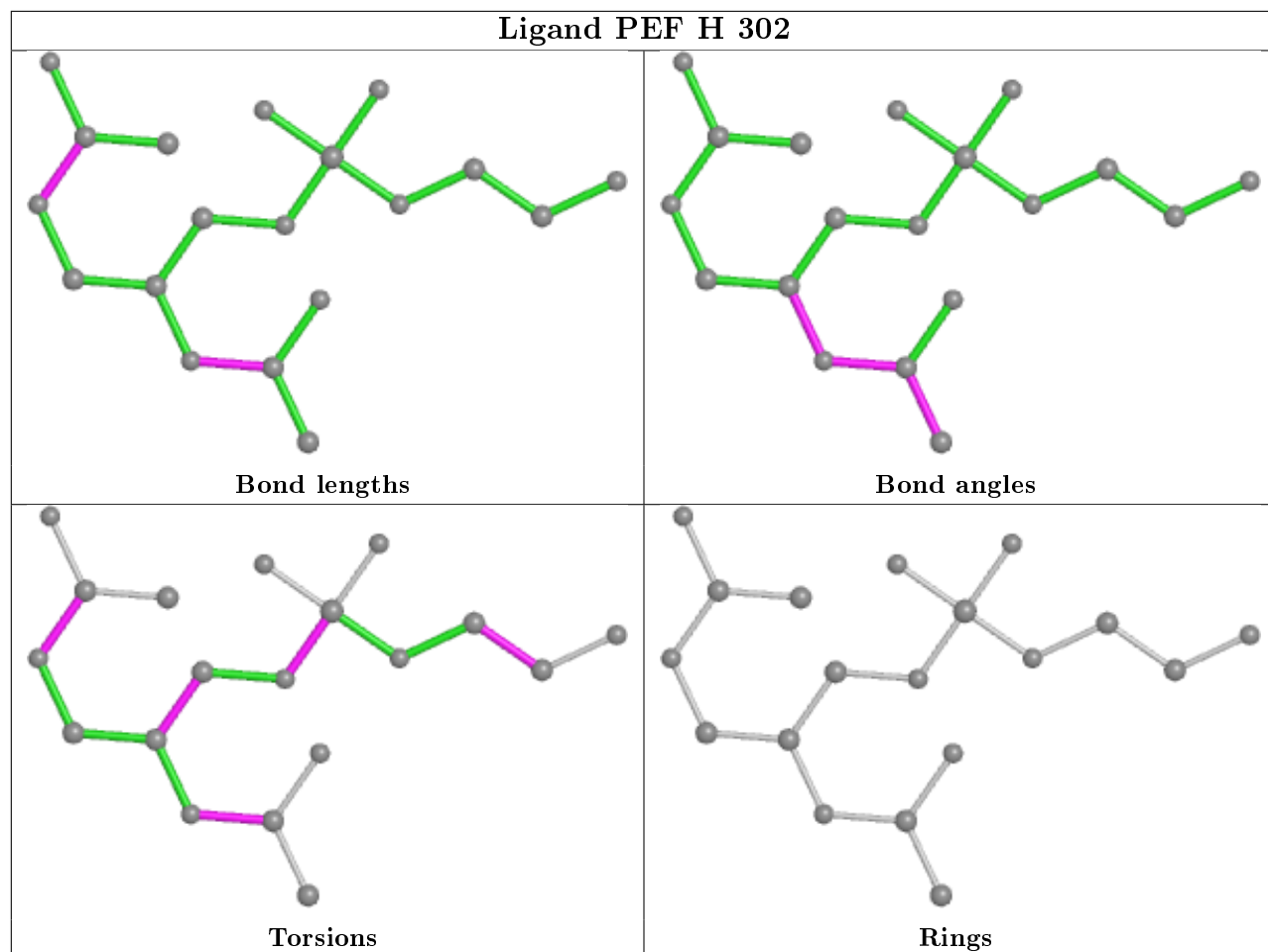




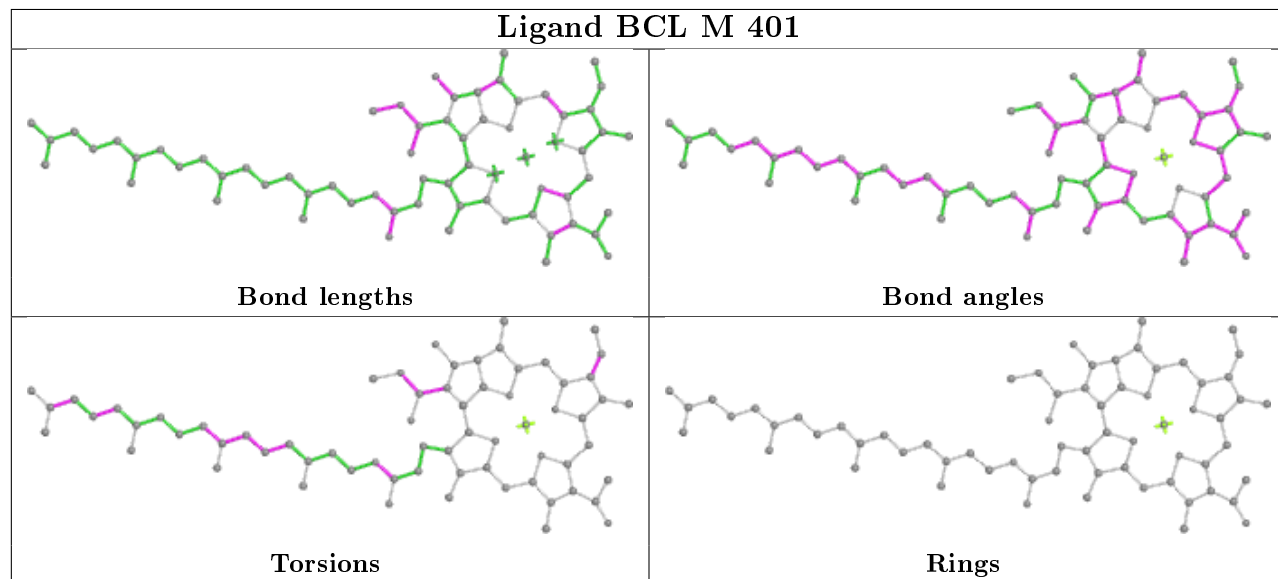




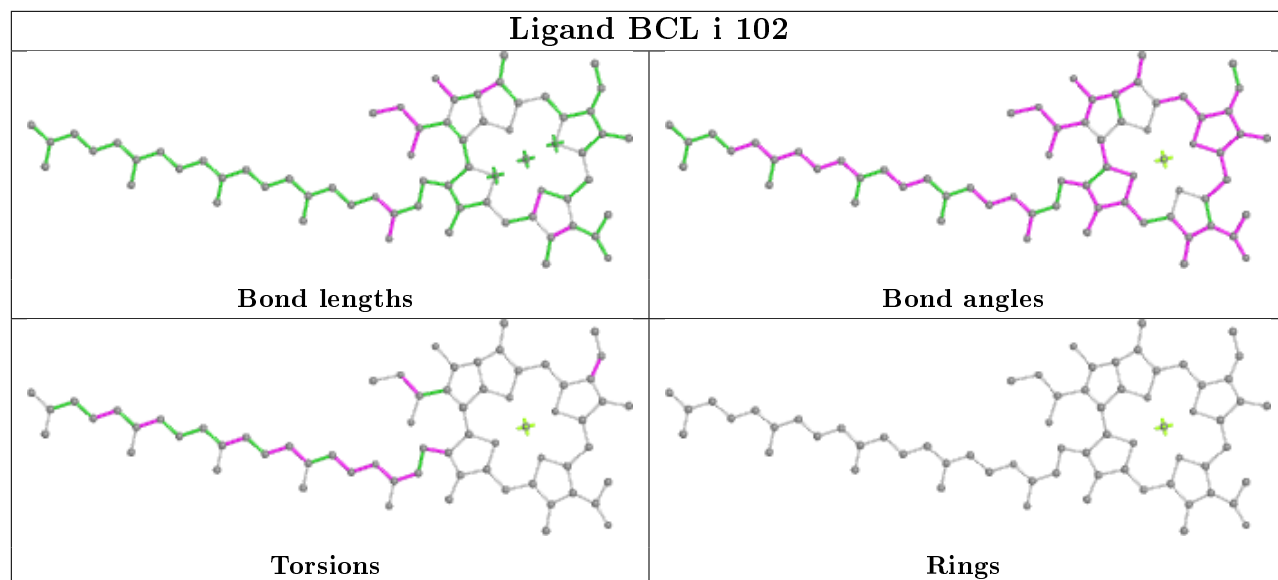
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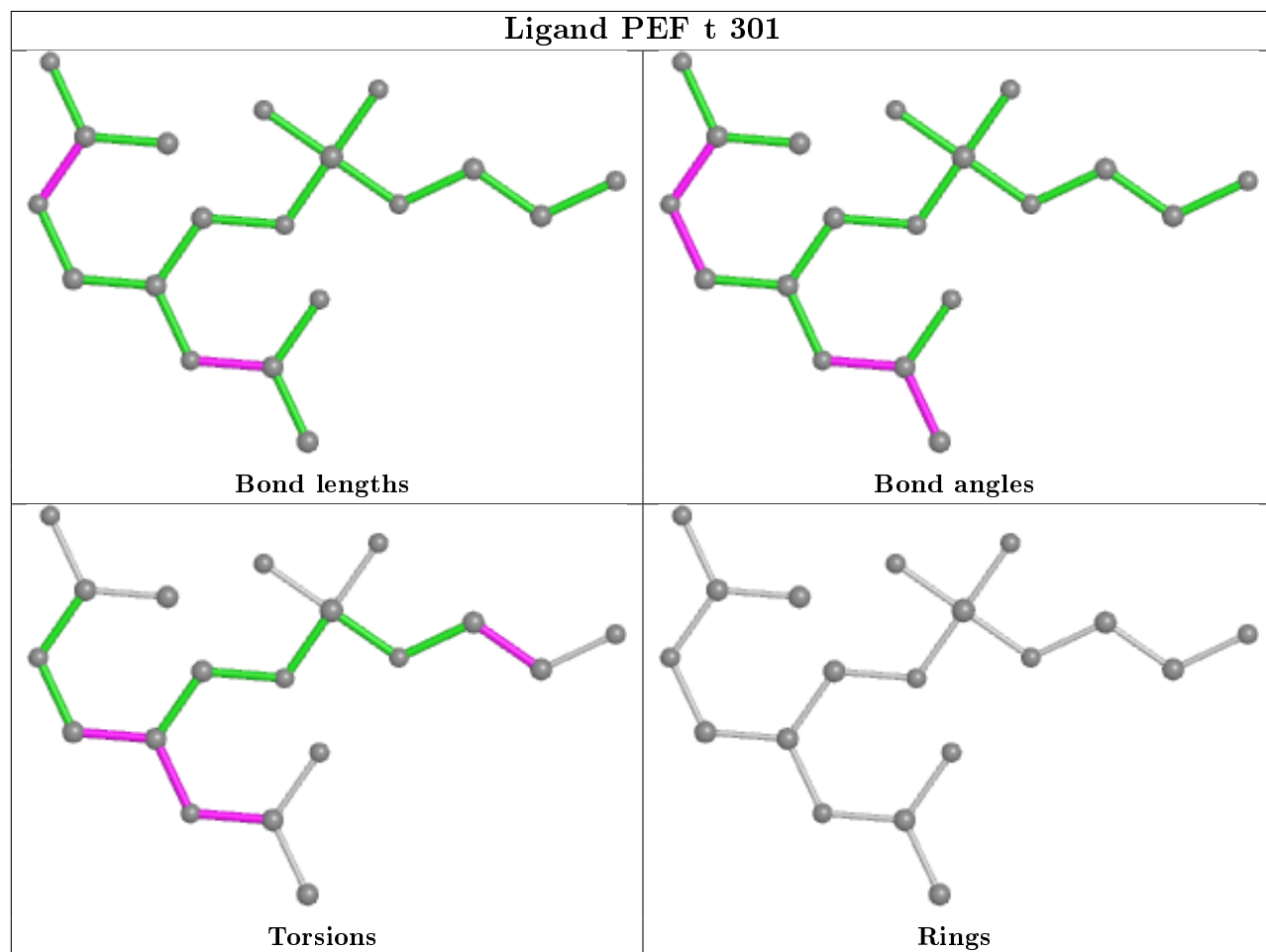
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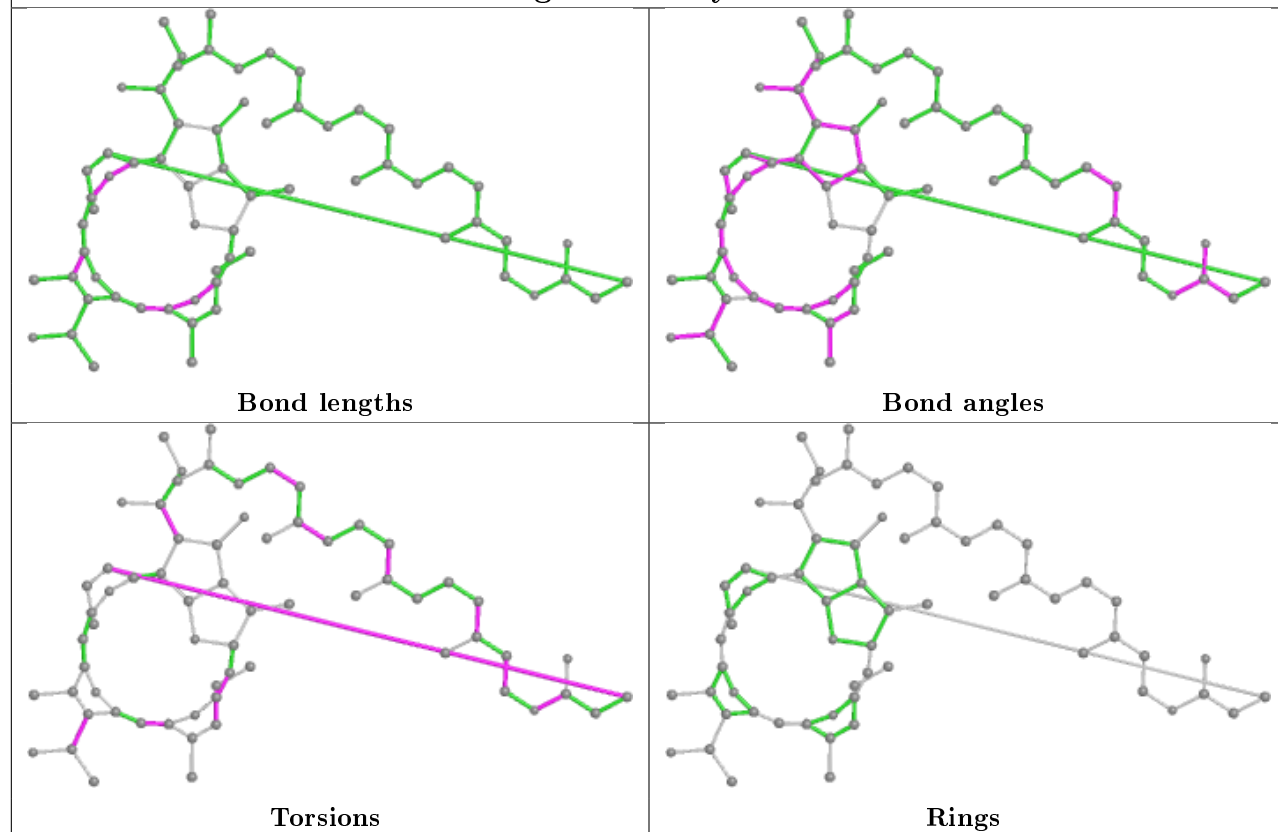
Ligand BCL i 102



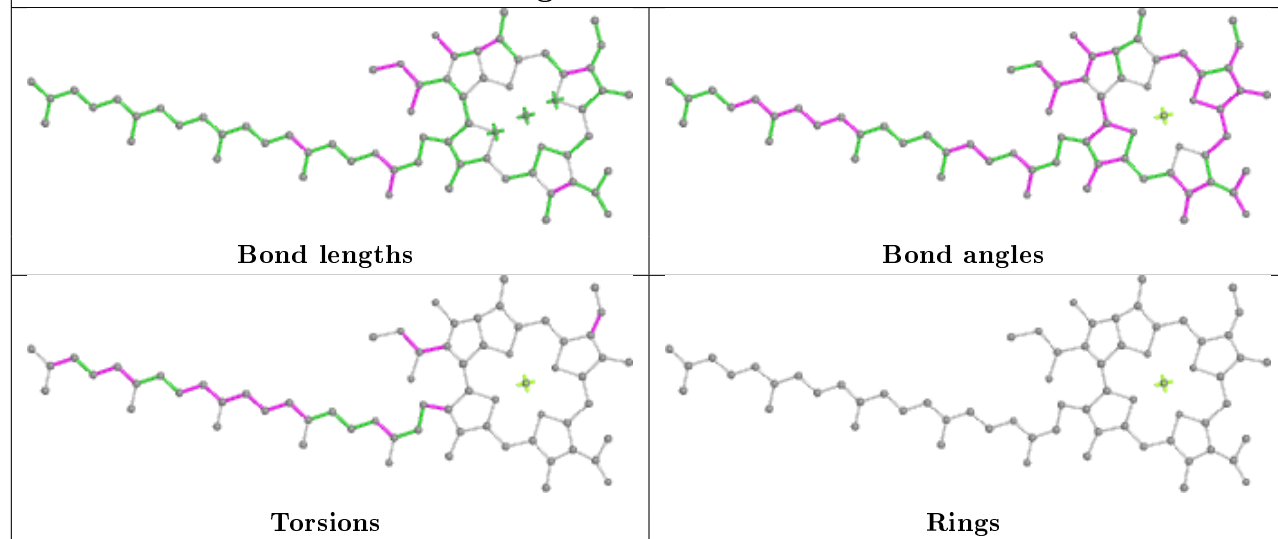
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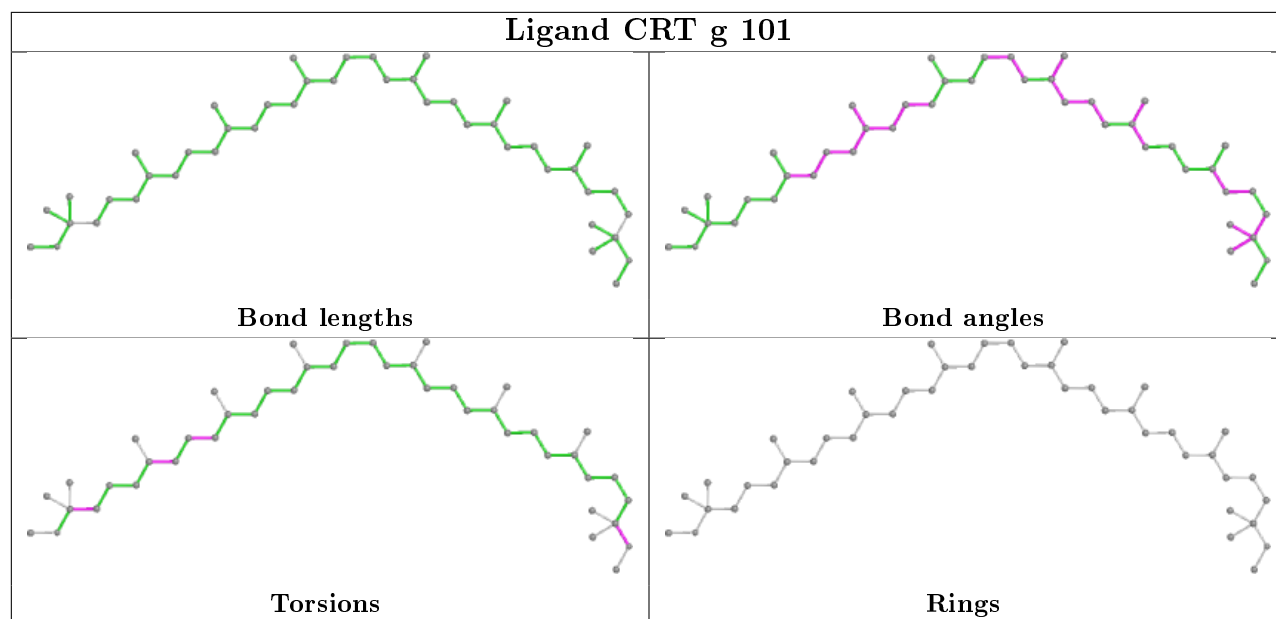
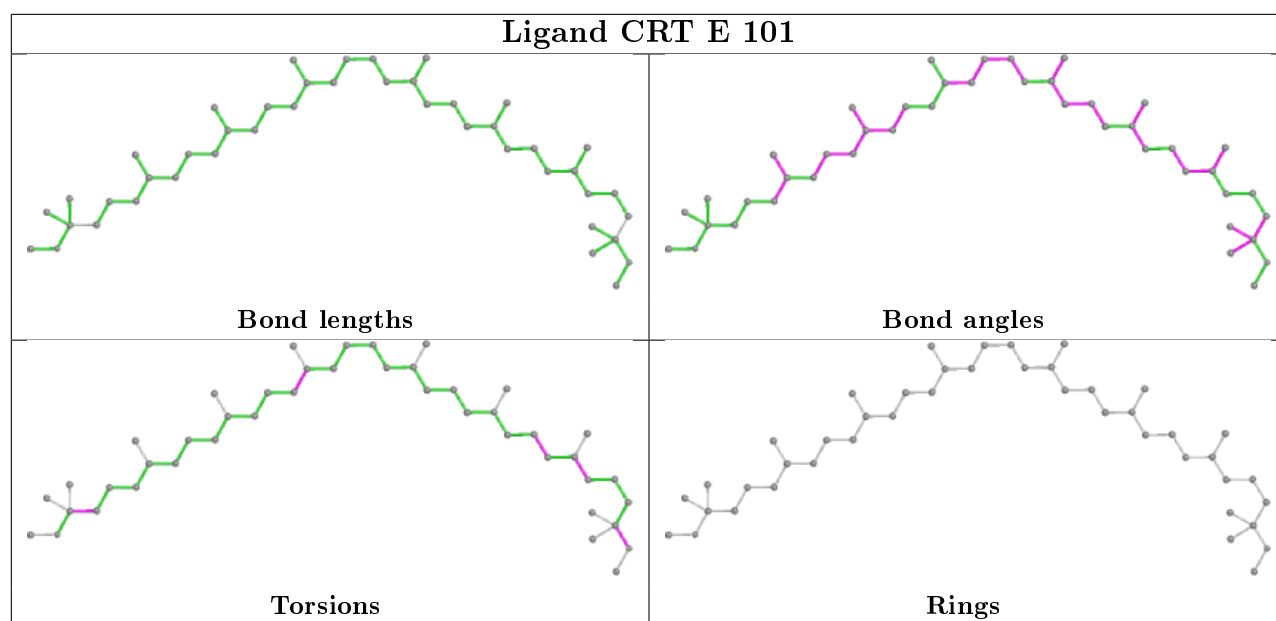


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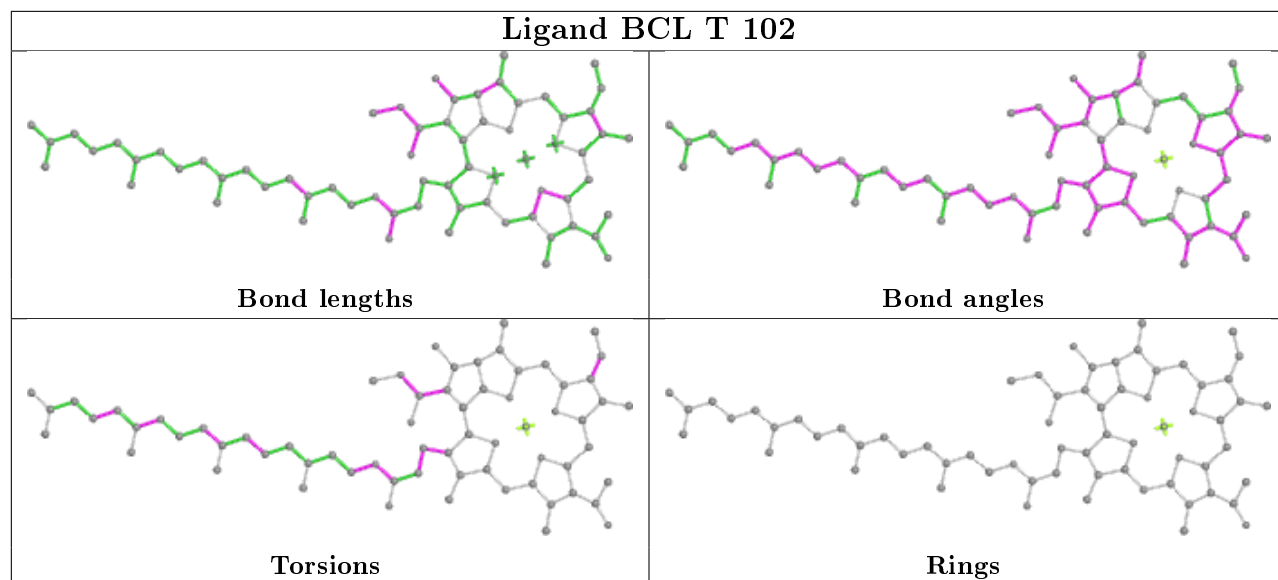


Ligand BCL u 101

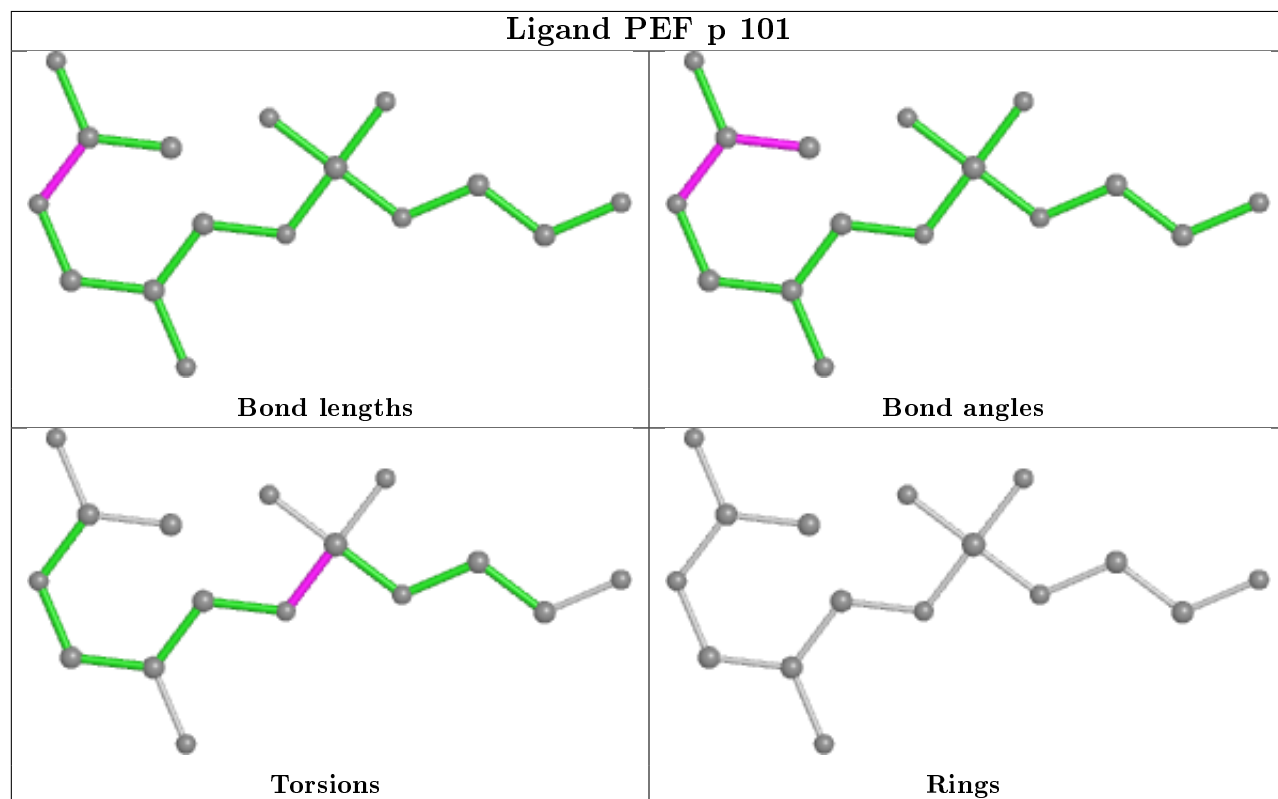


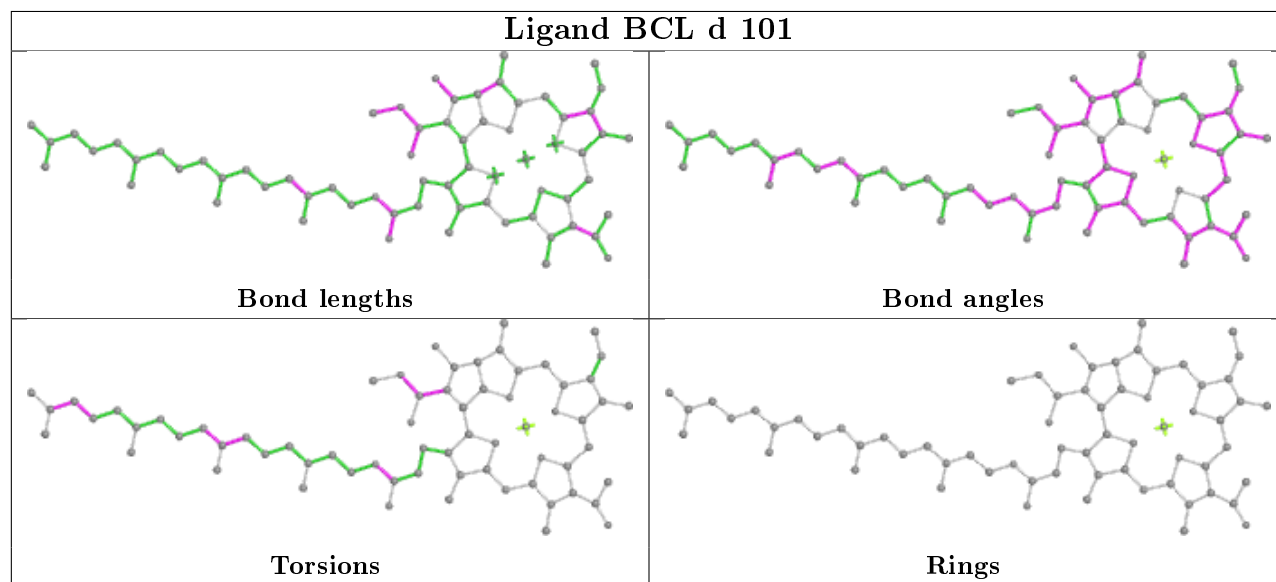
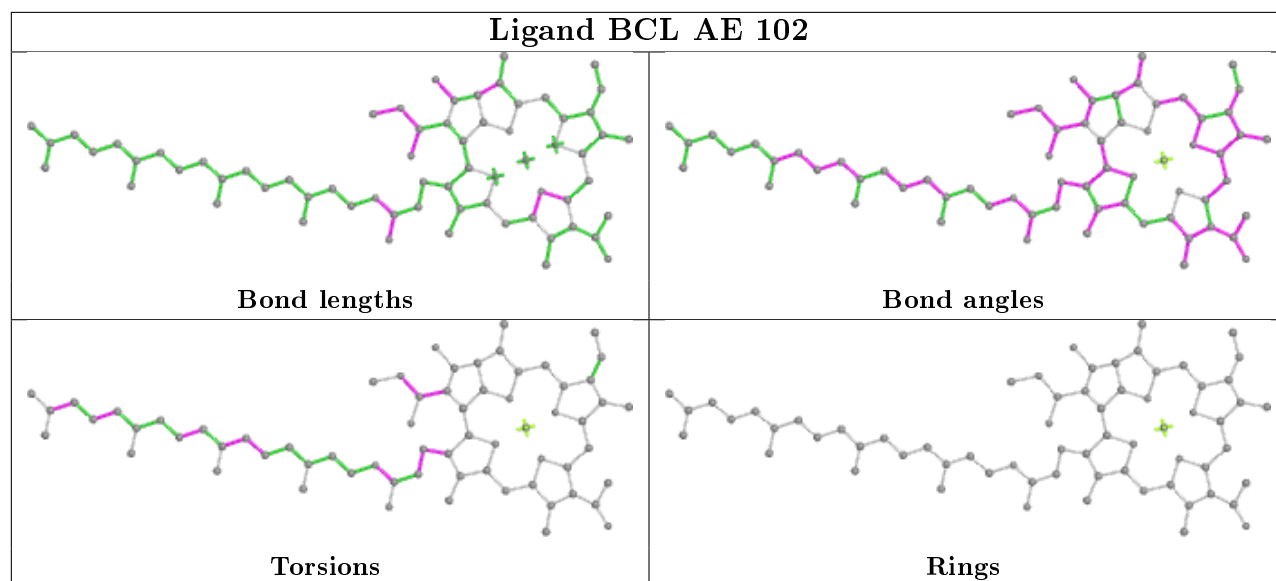
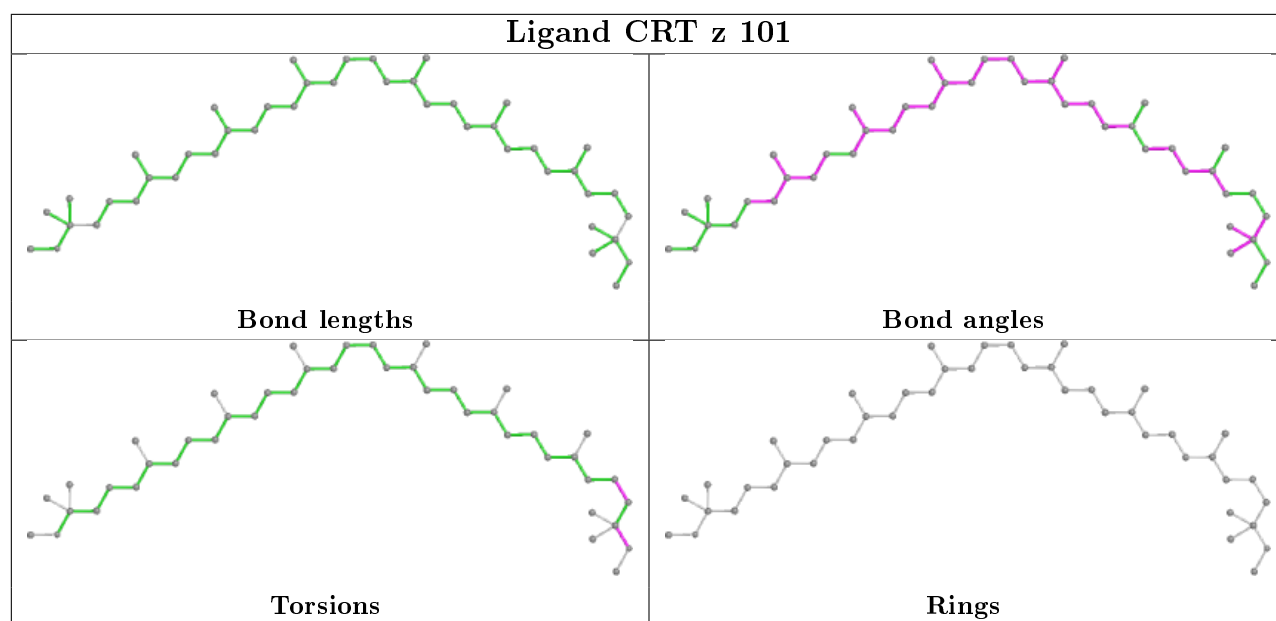


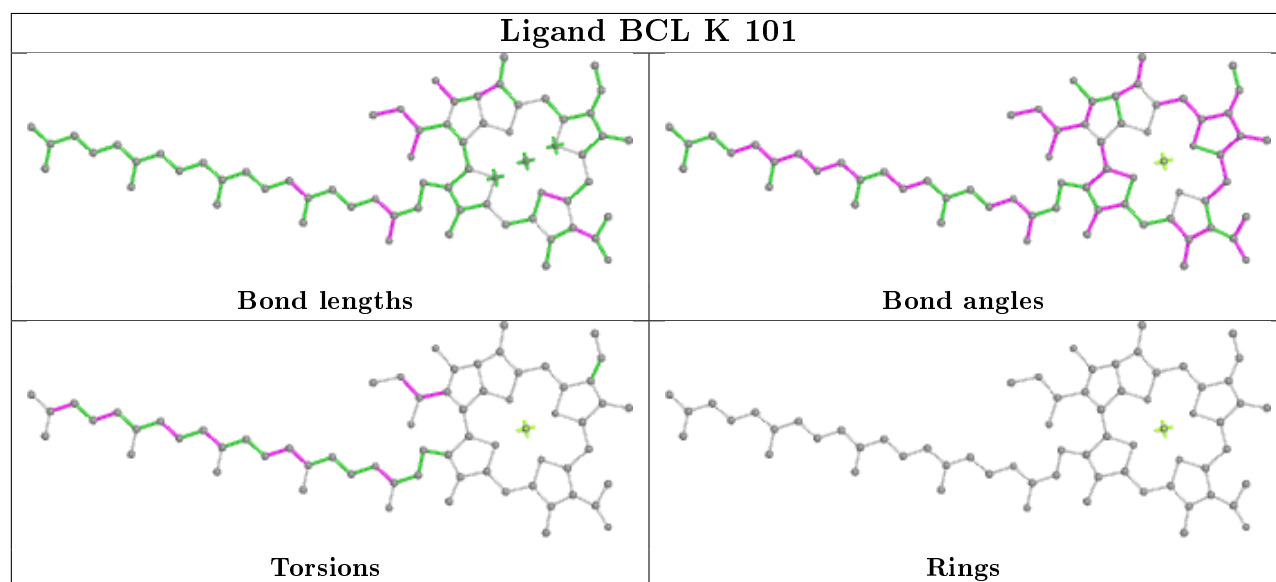
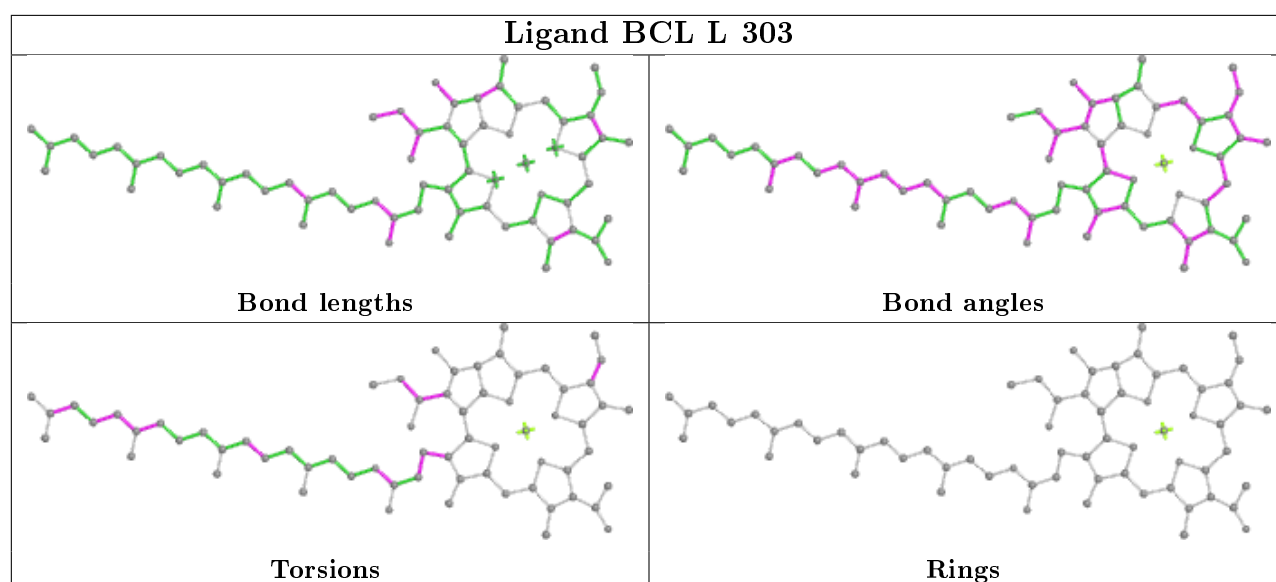
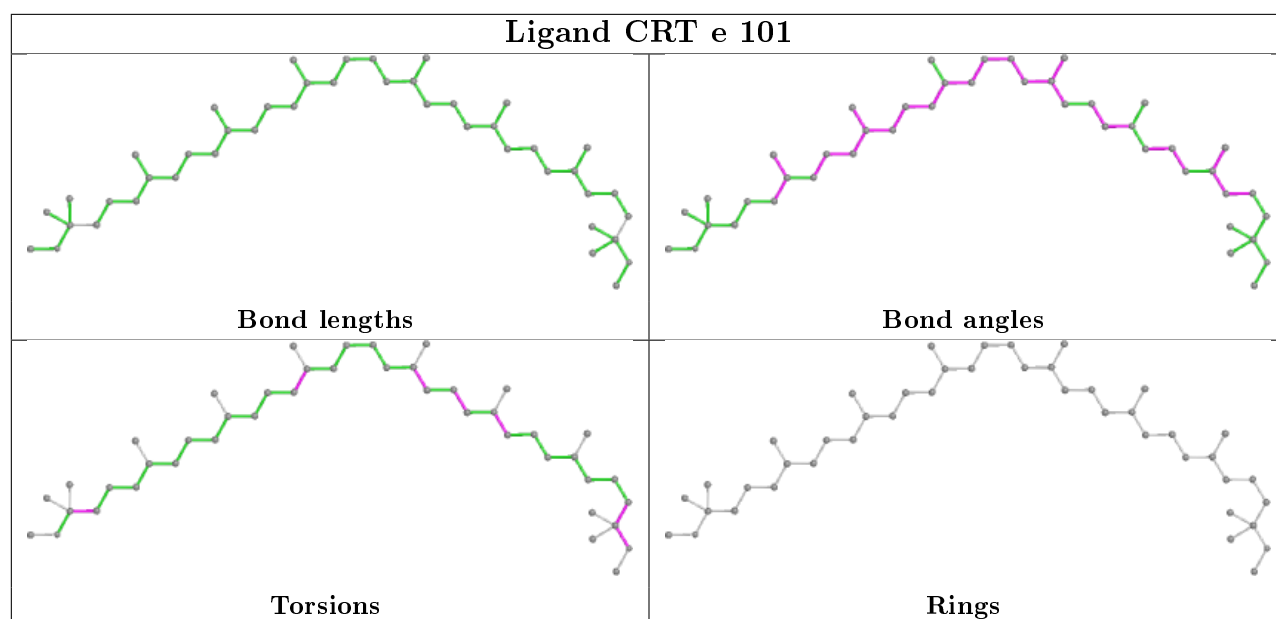
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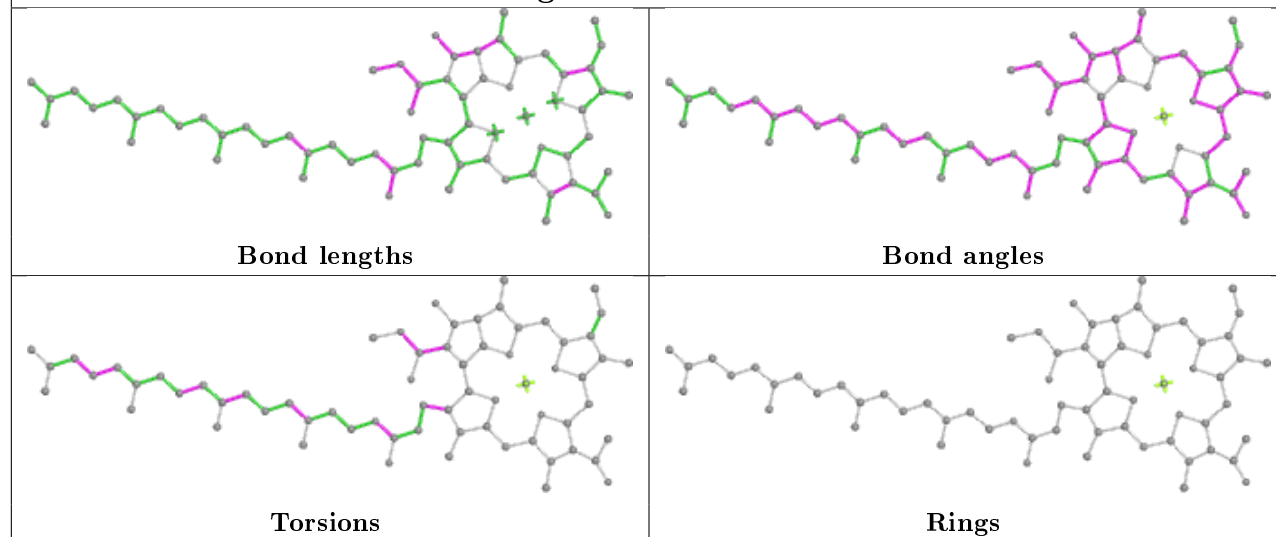
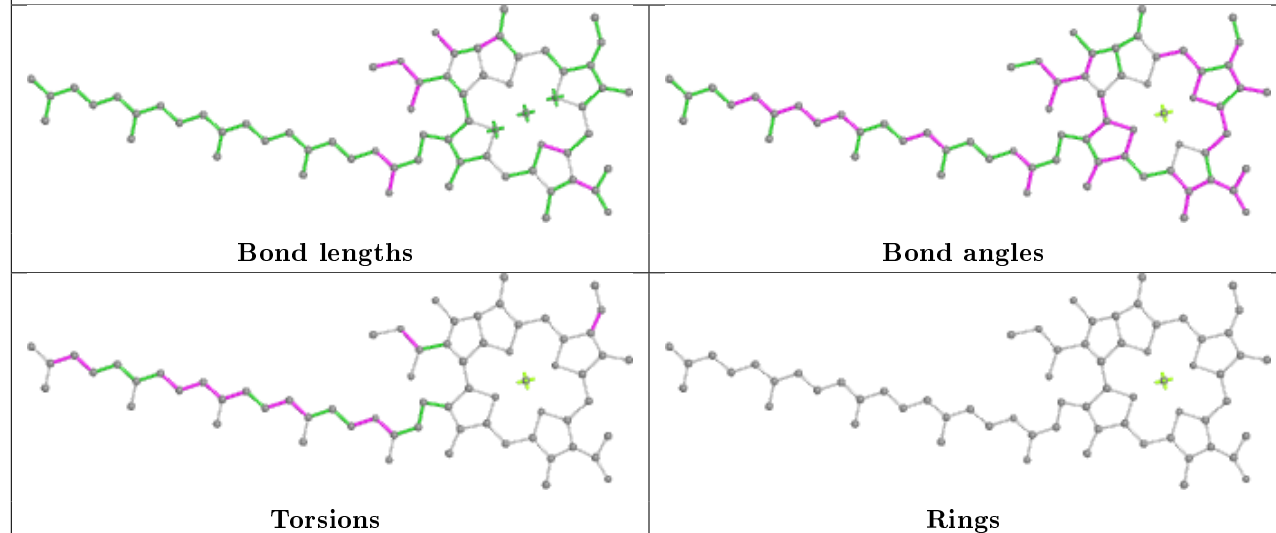
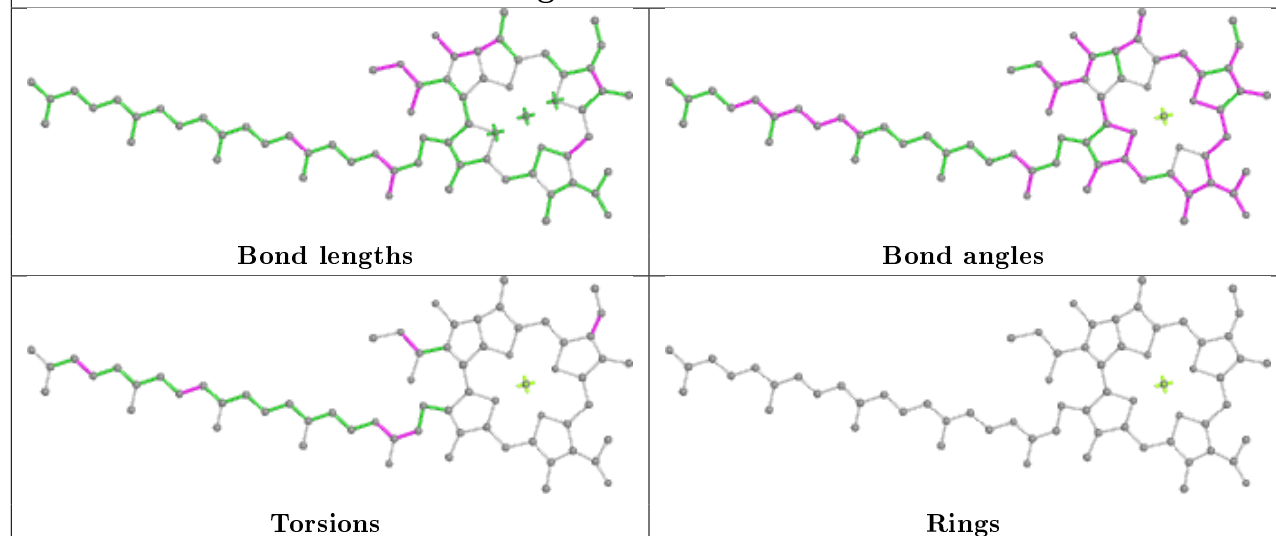


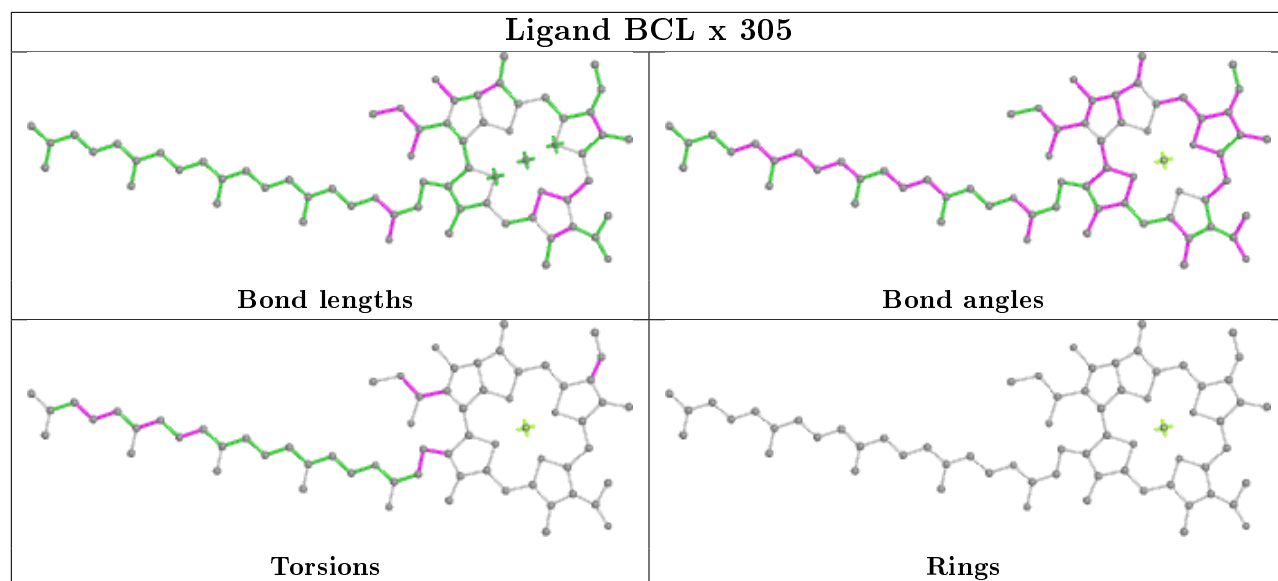
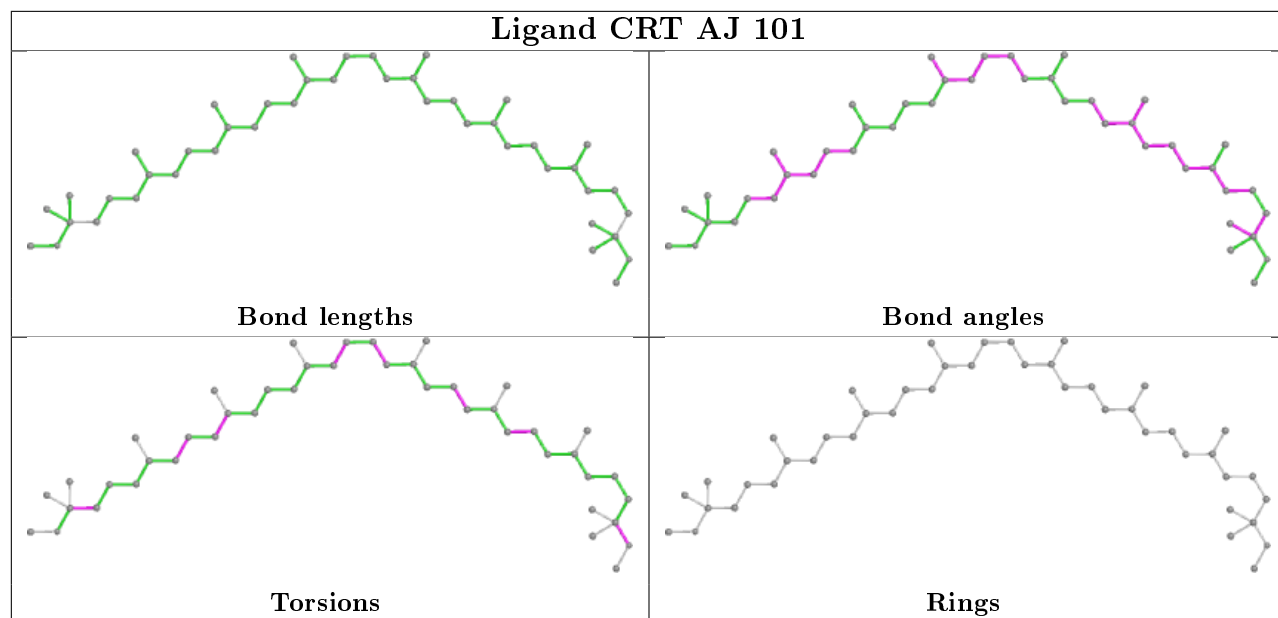
Ligand PEF p 101

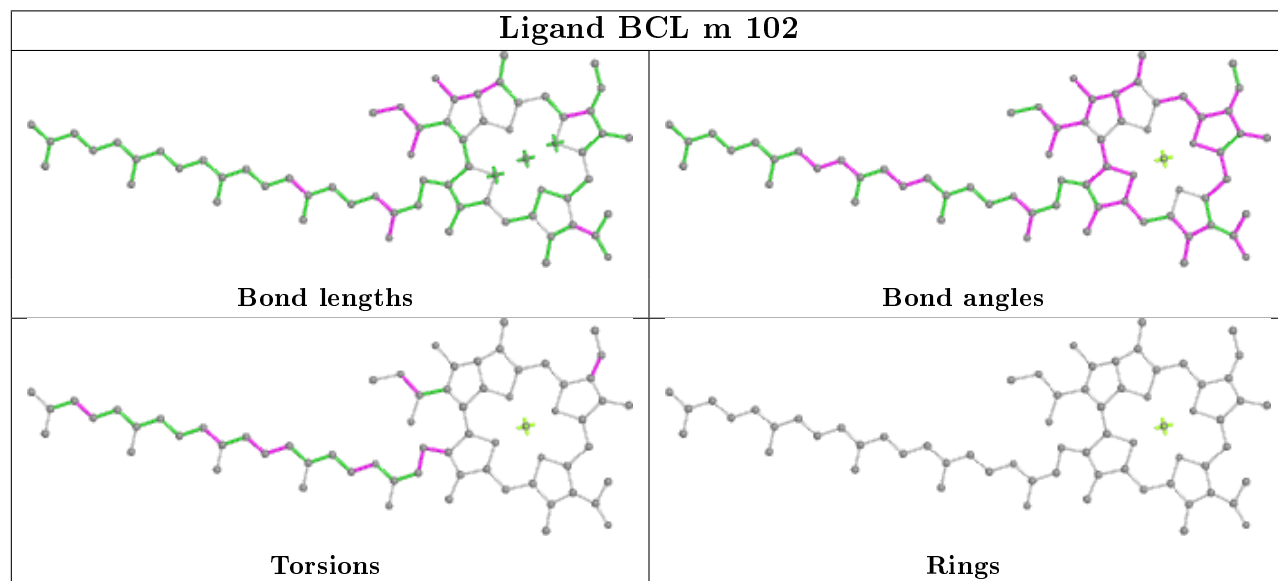
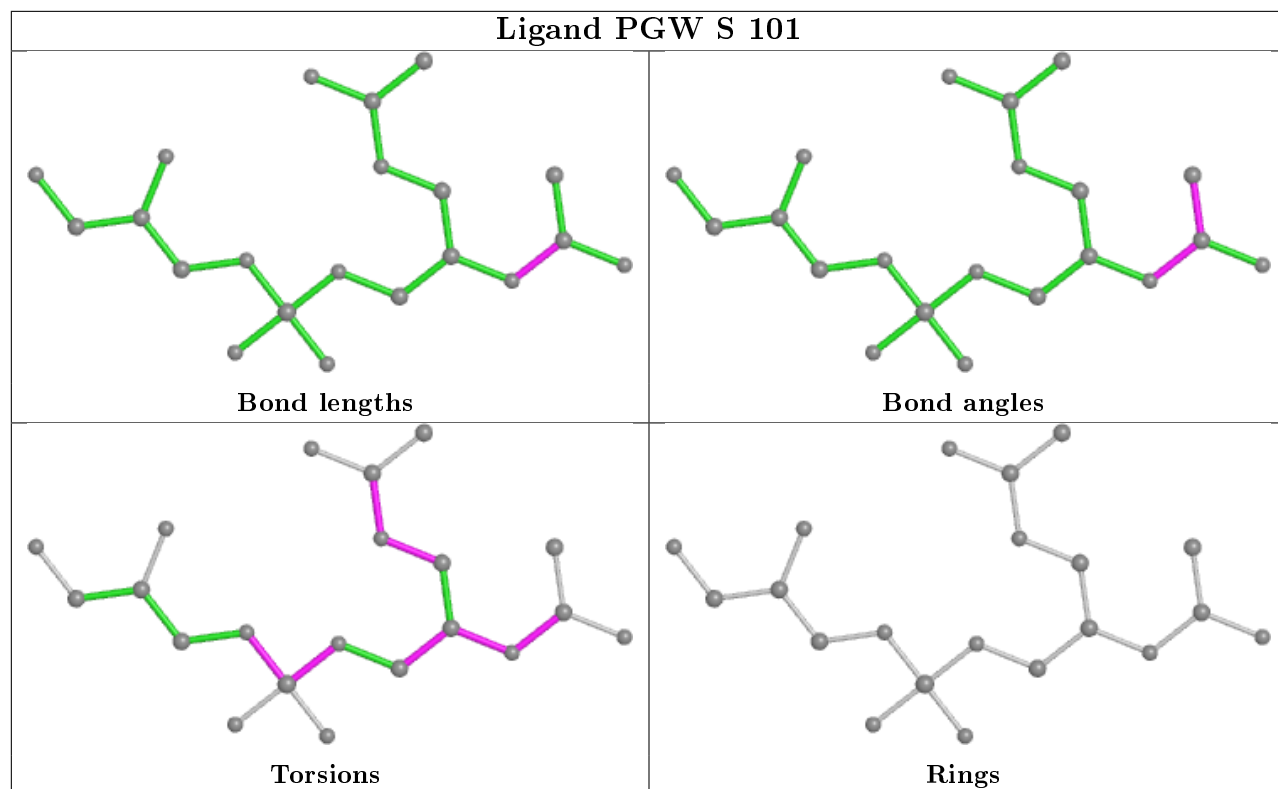


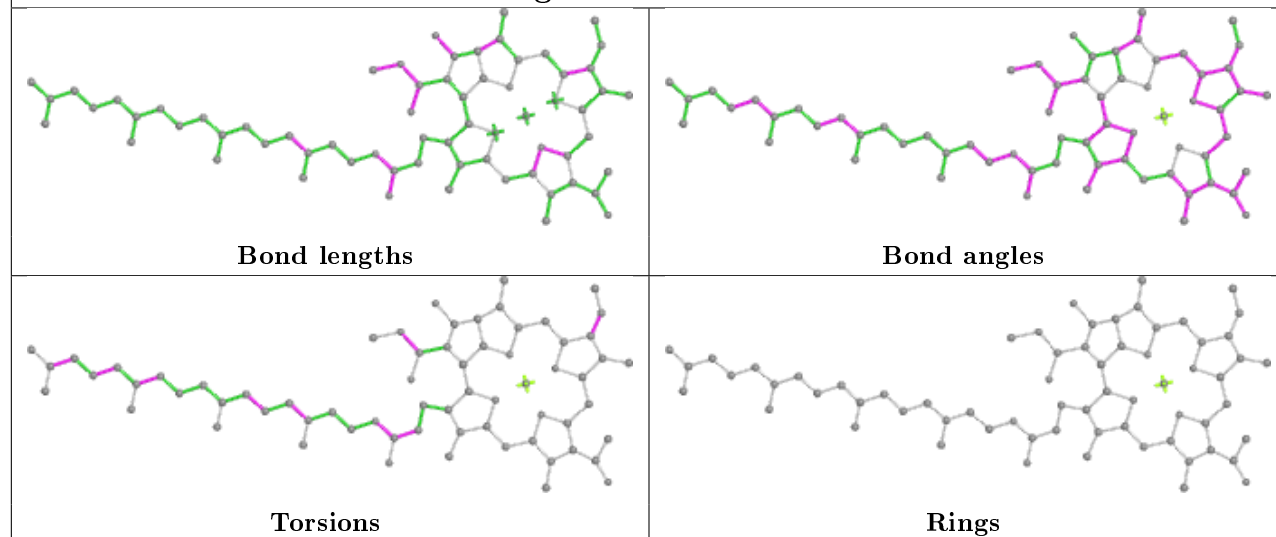
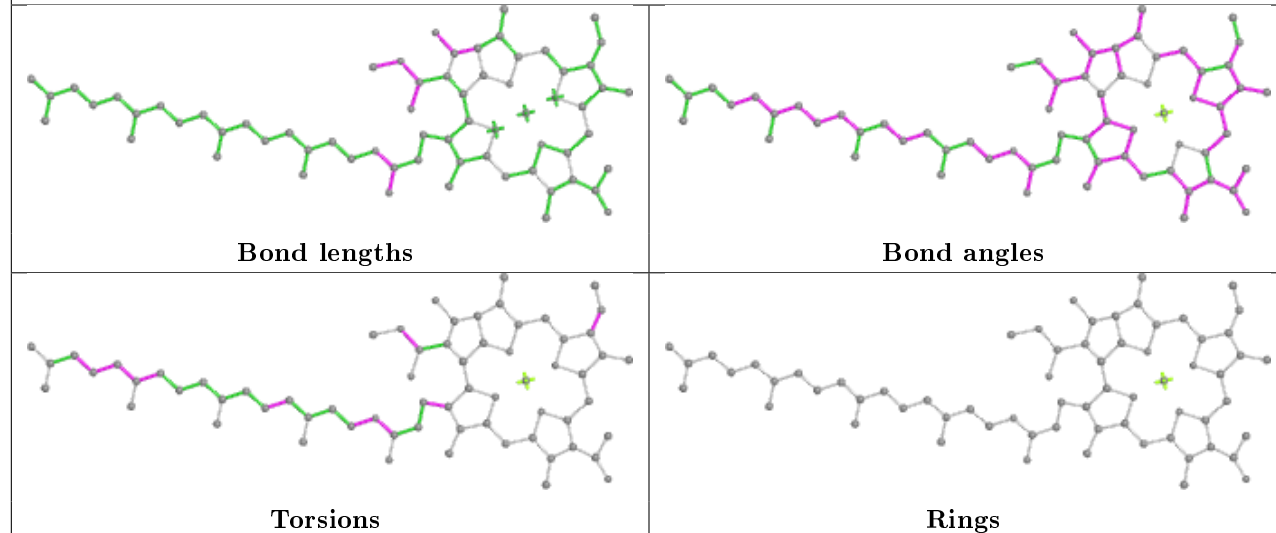
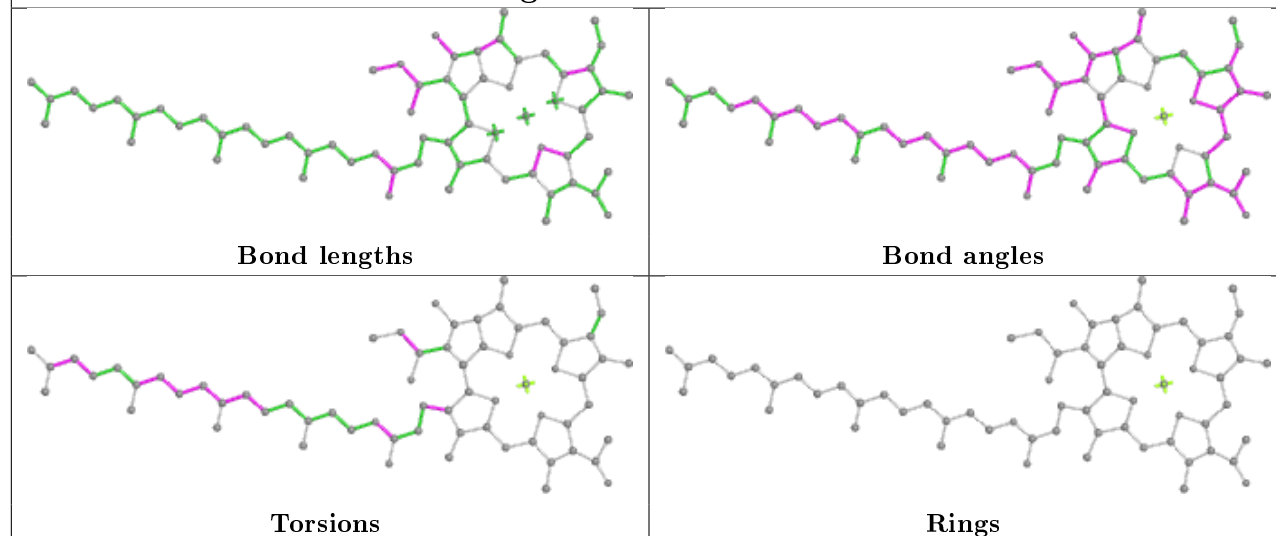


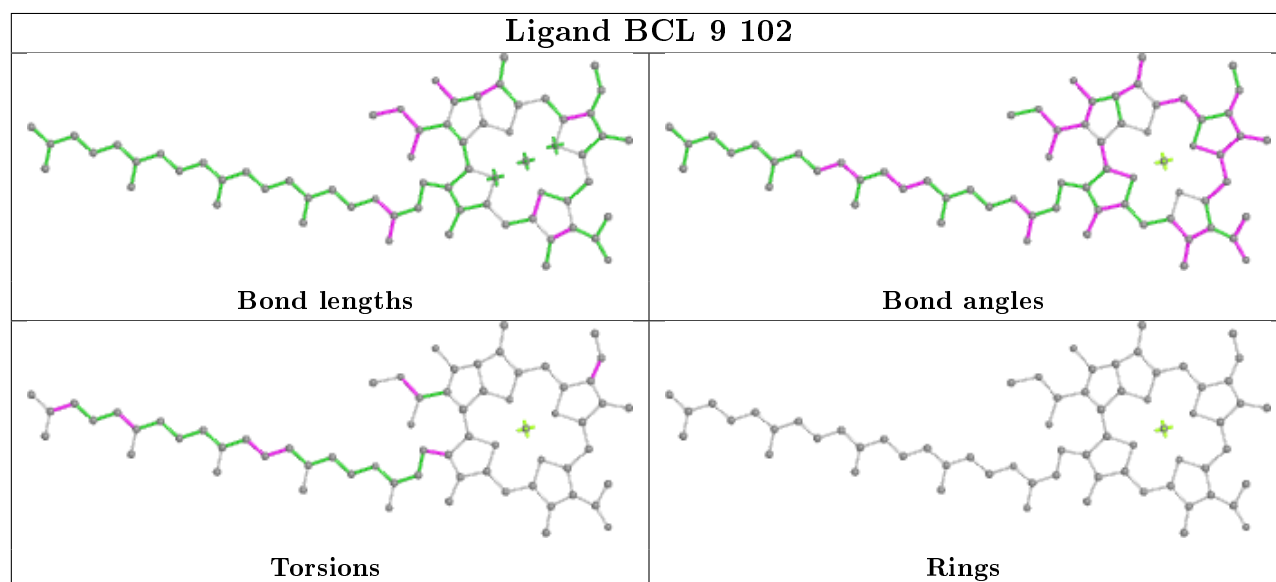
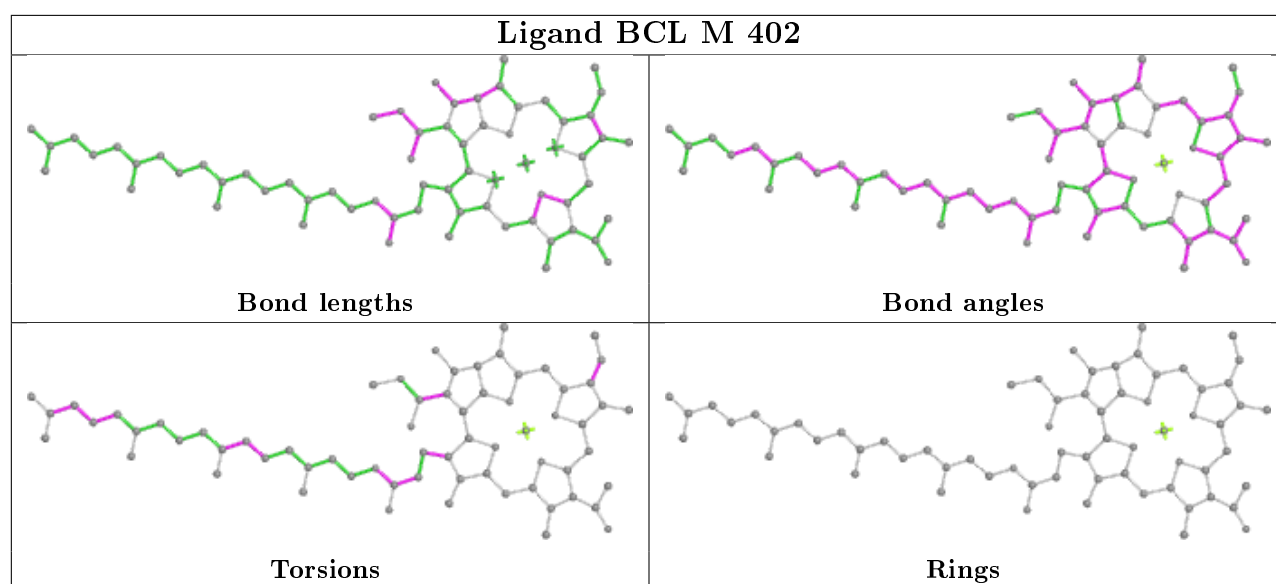
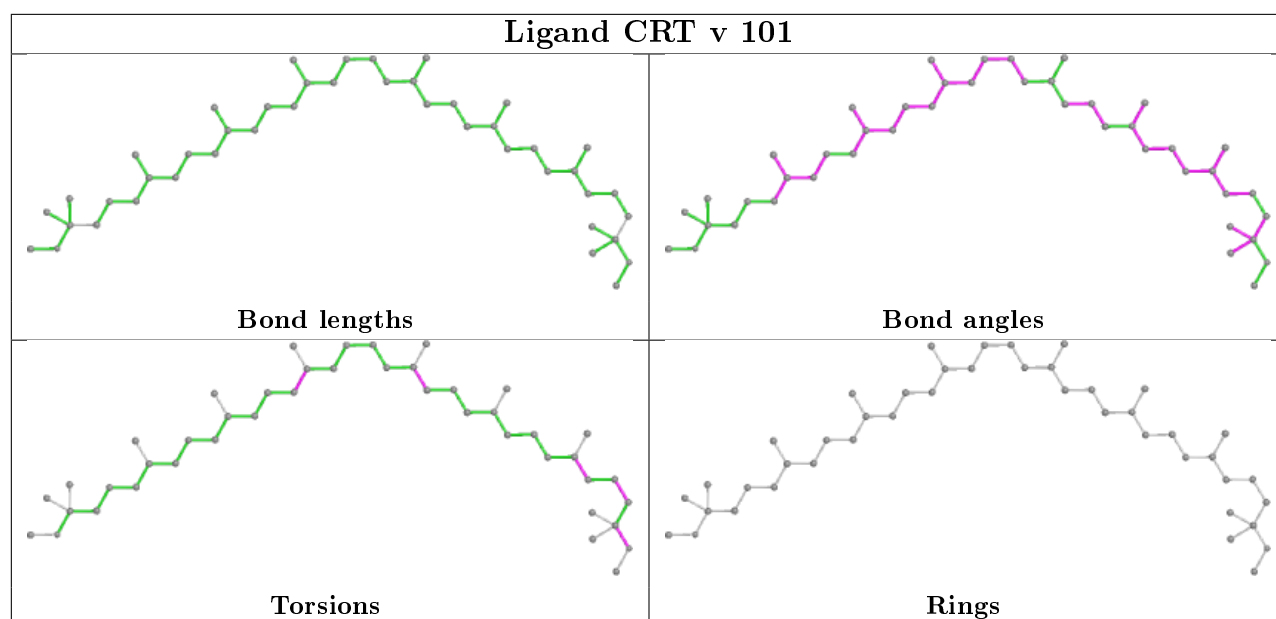


Ligand BCL 2 102**Ligand BCL 1 101****Ligand BCL 5 101**

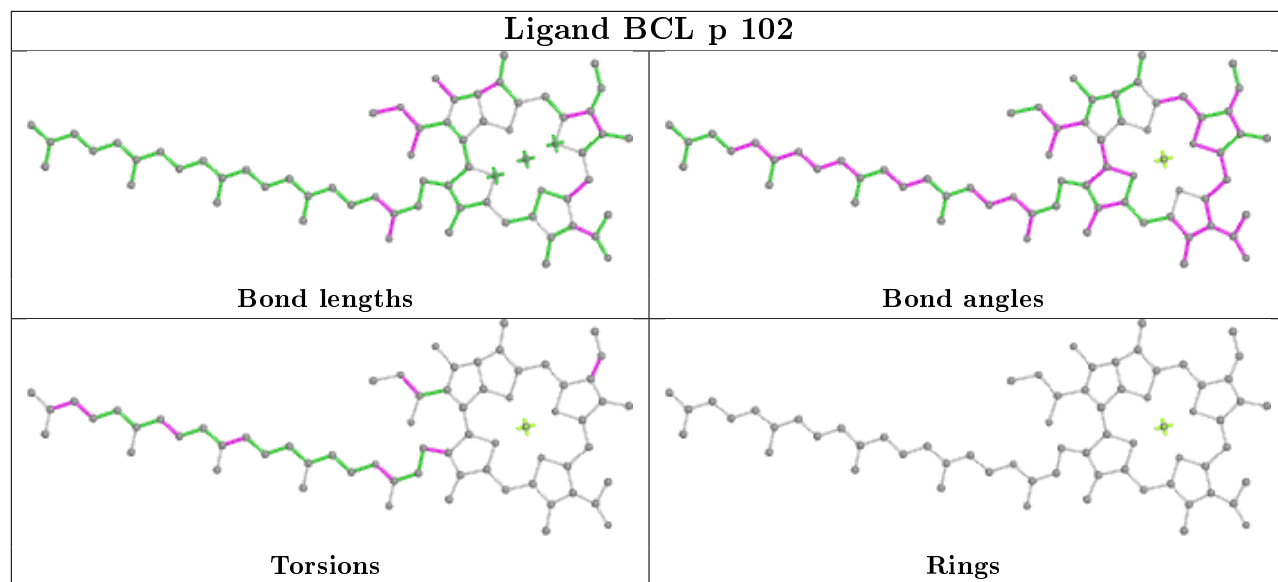




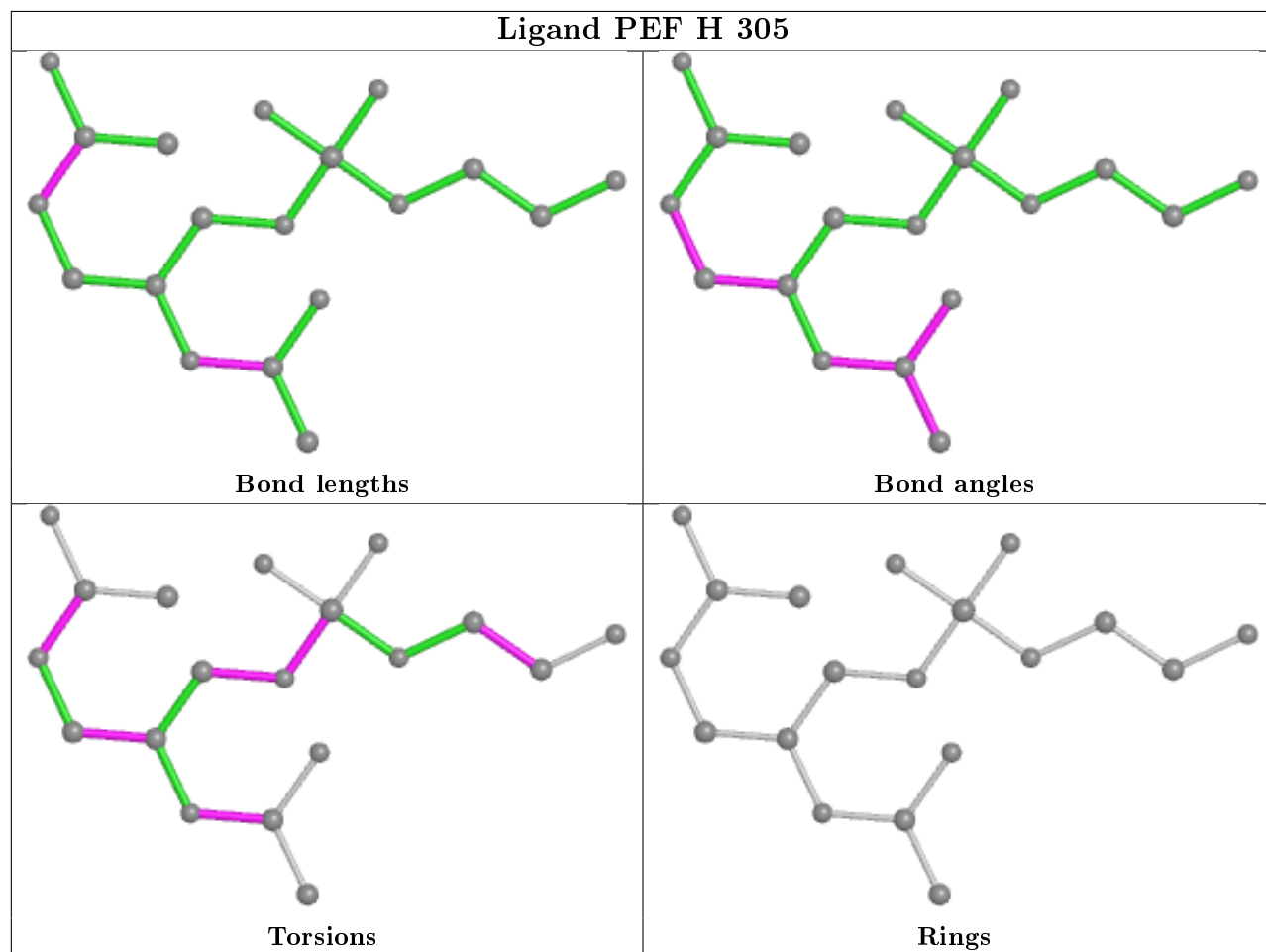
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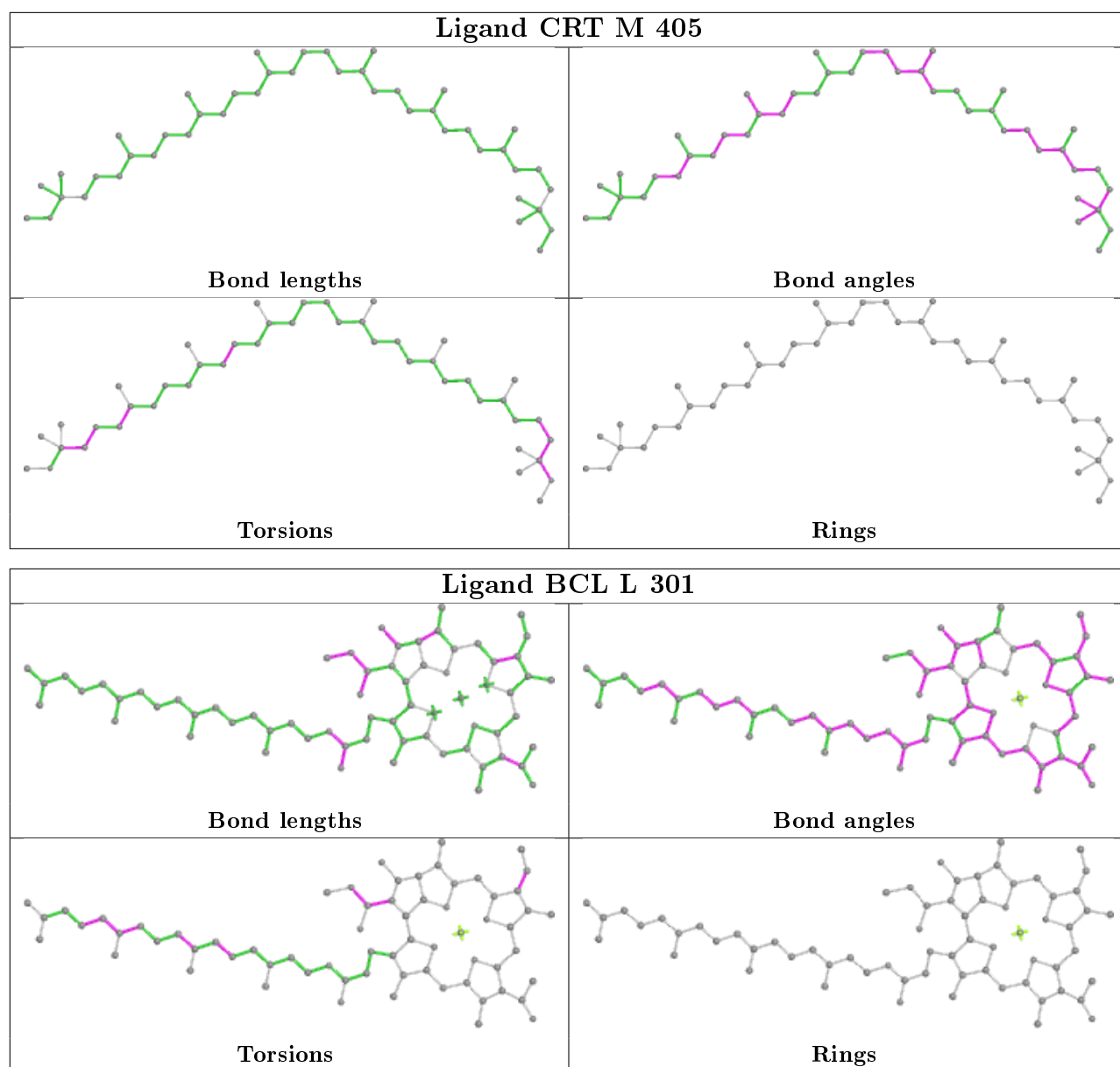


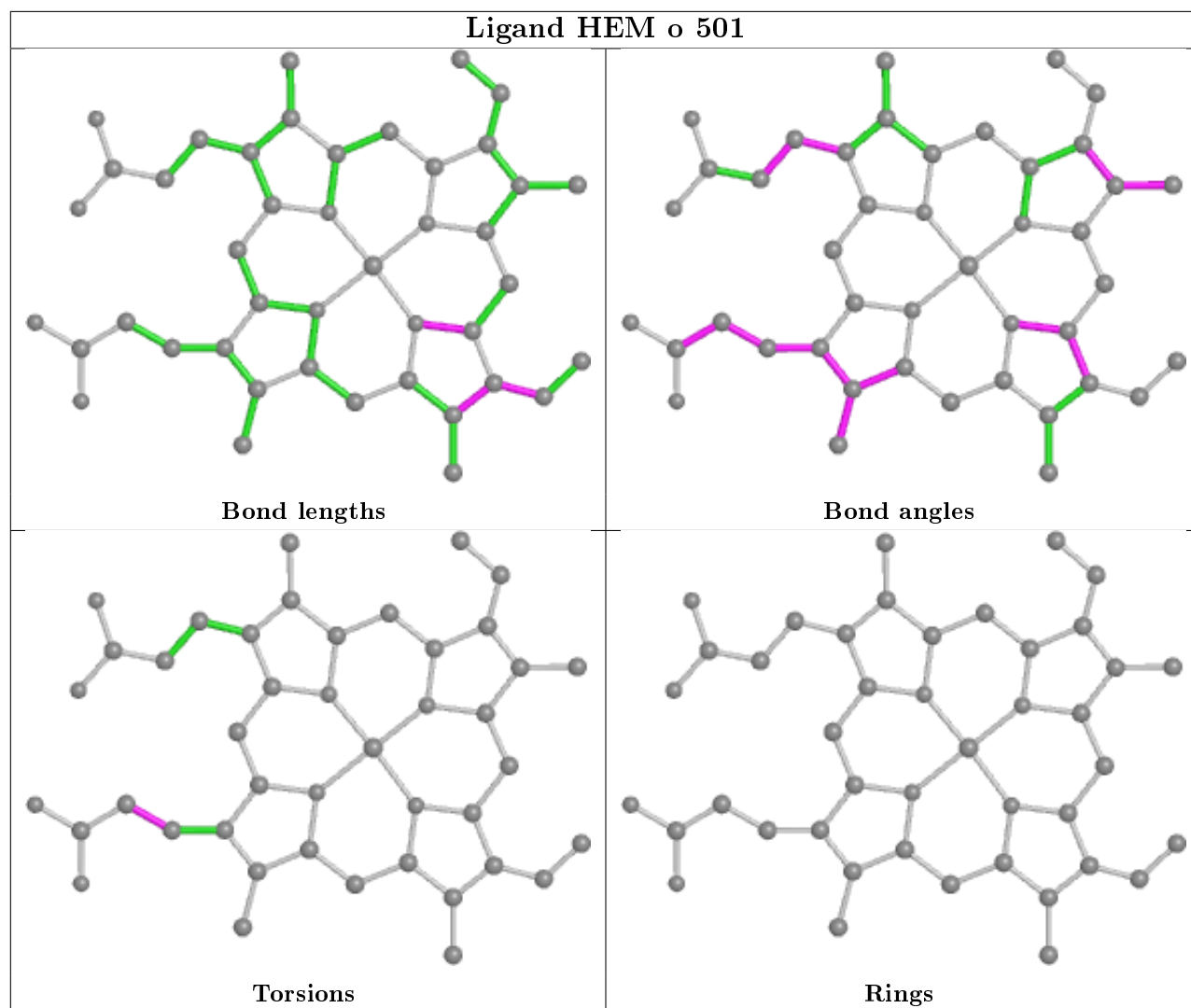
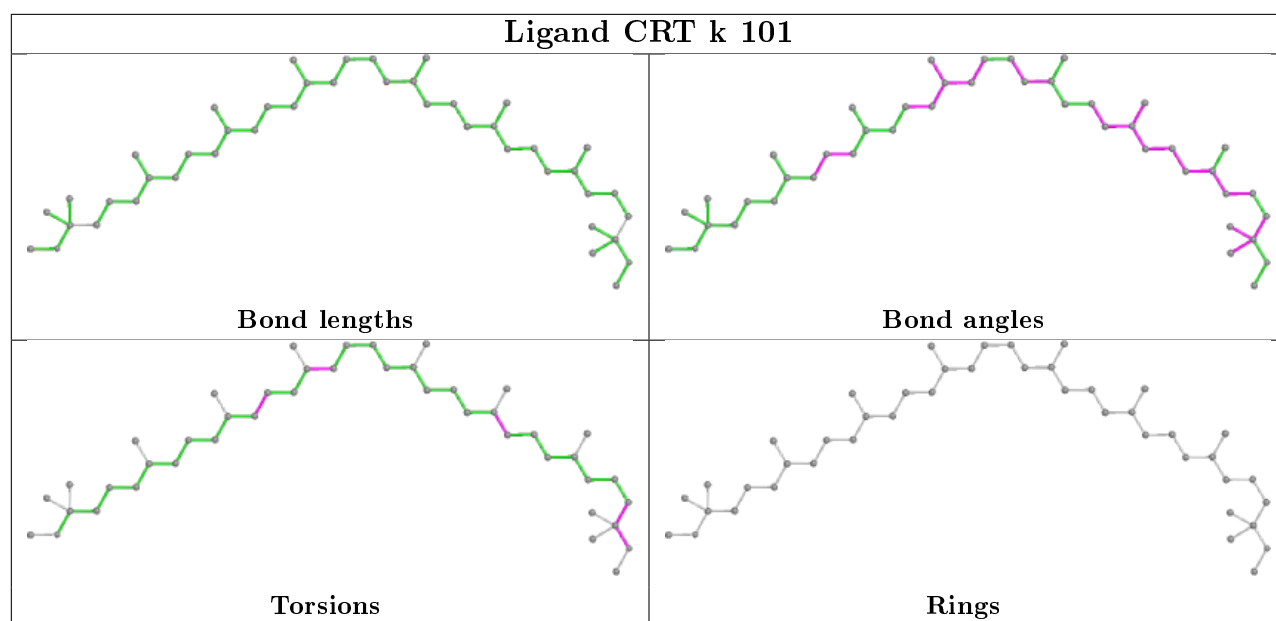
Ligand BCL p 102

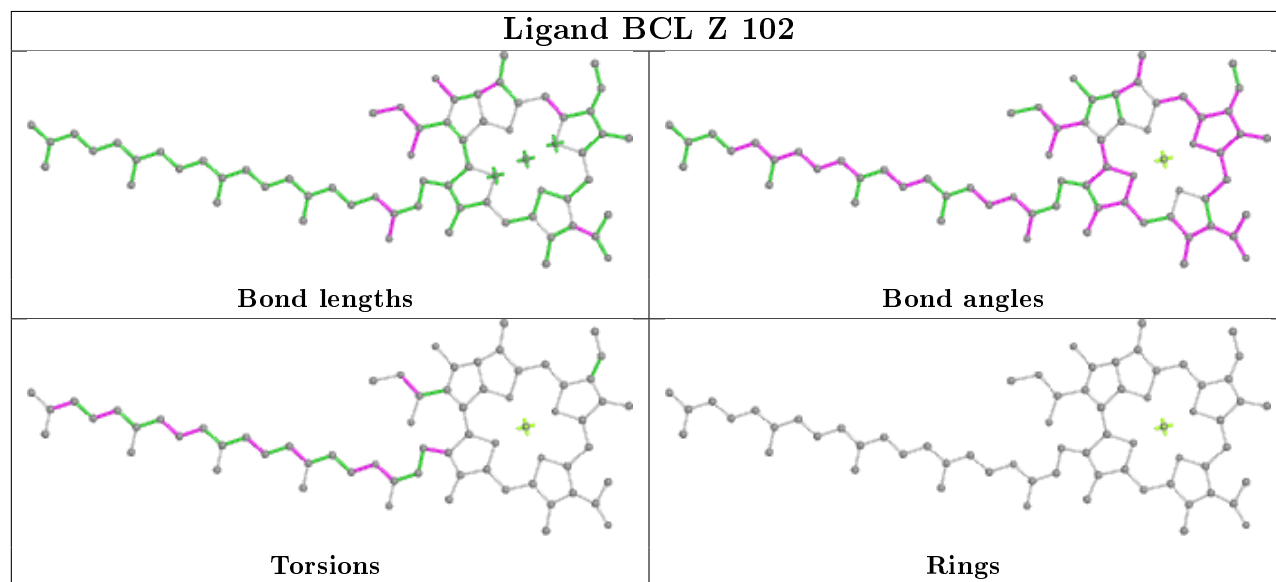
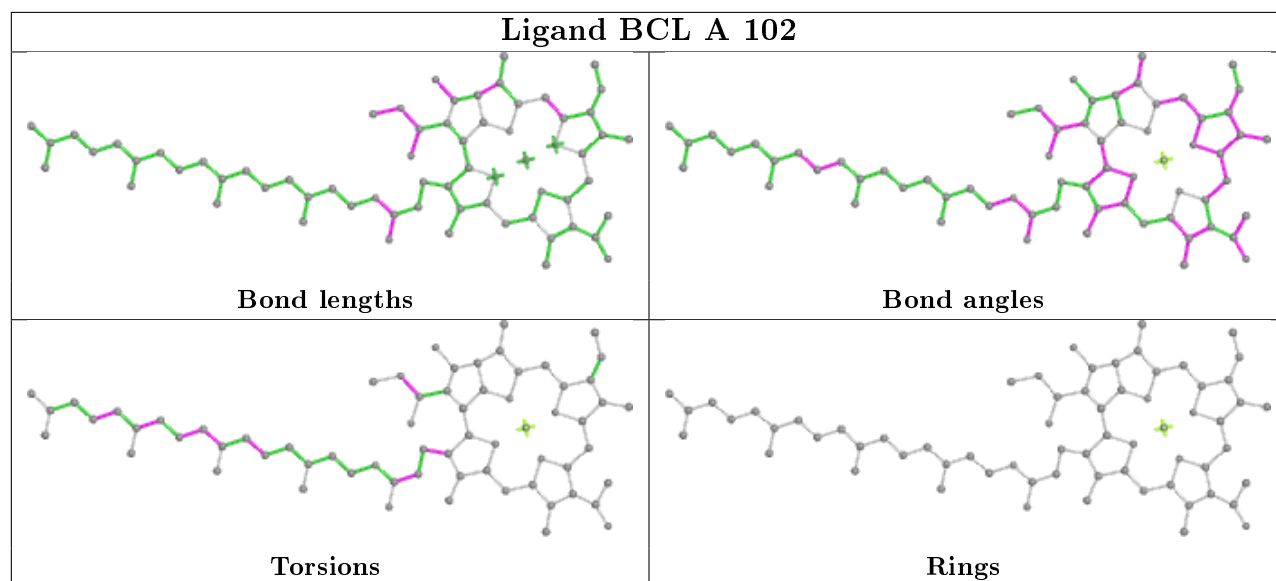
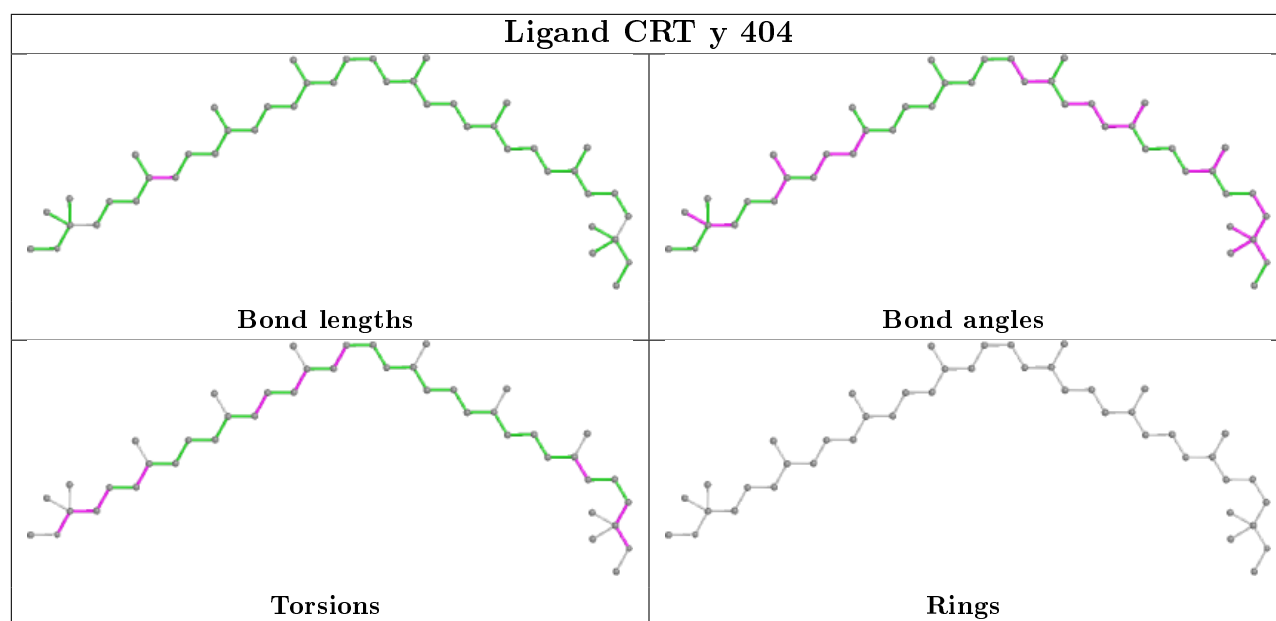


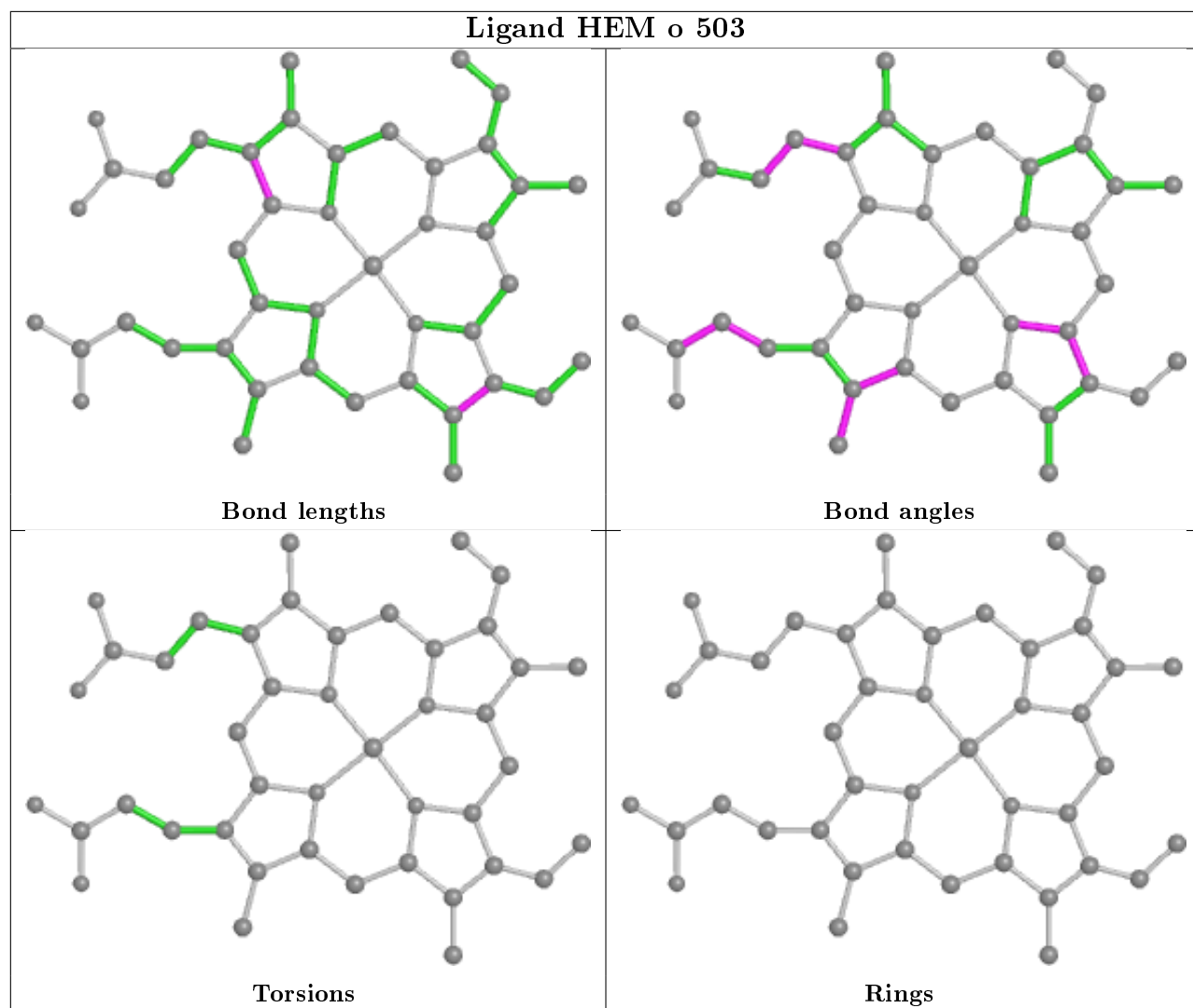
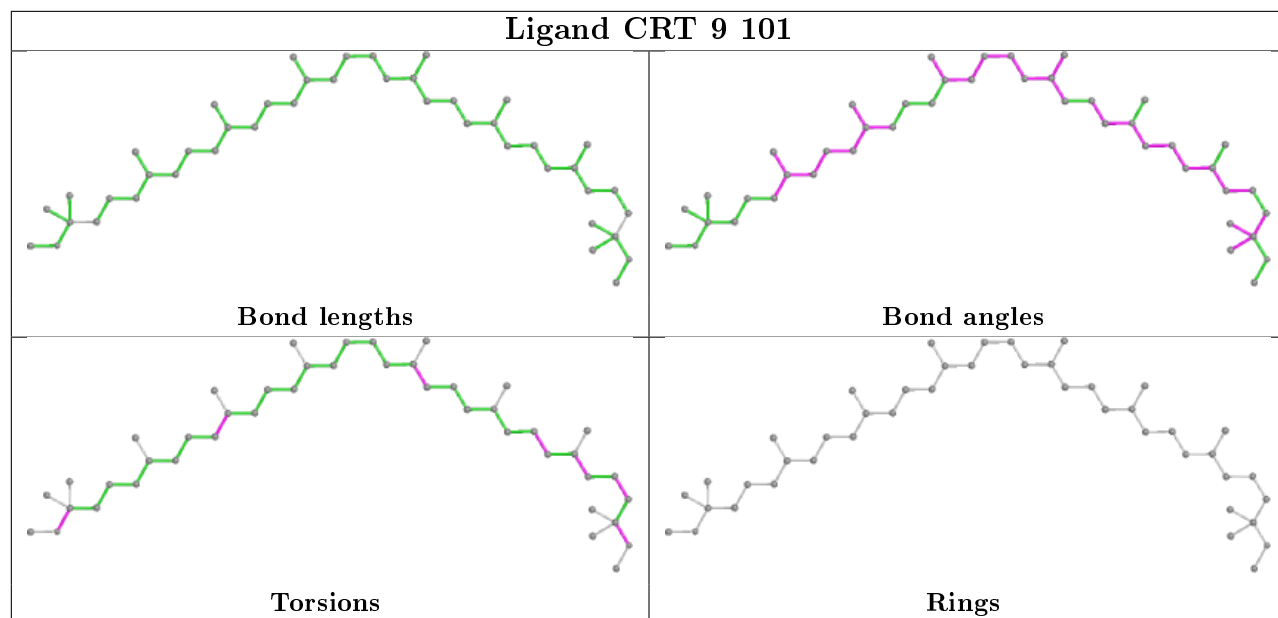
Ligand PEF H 305

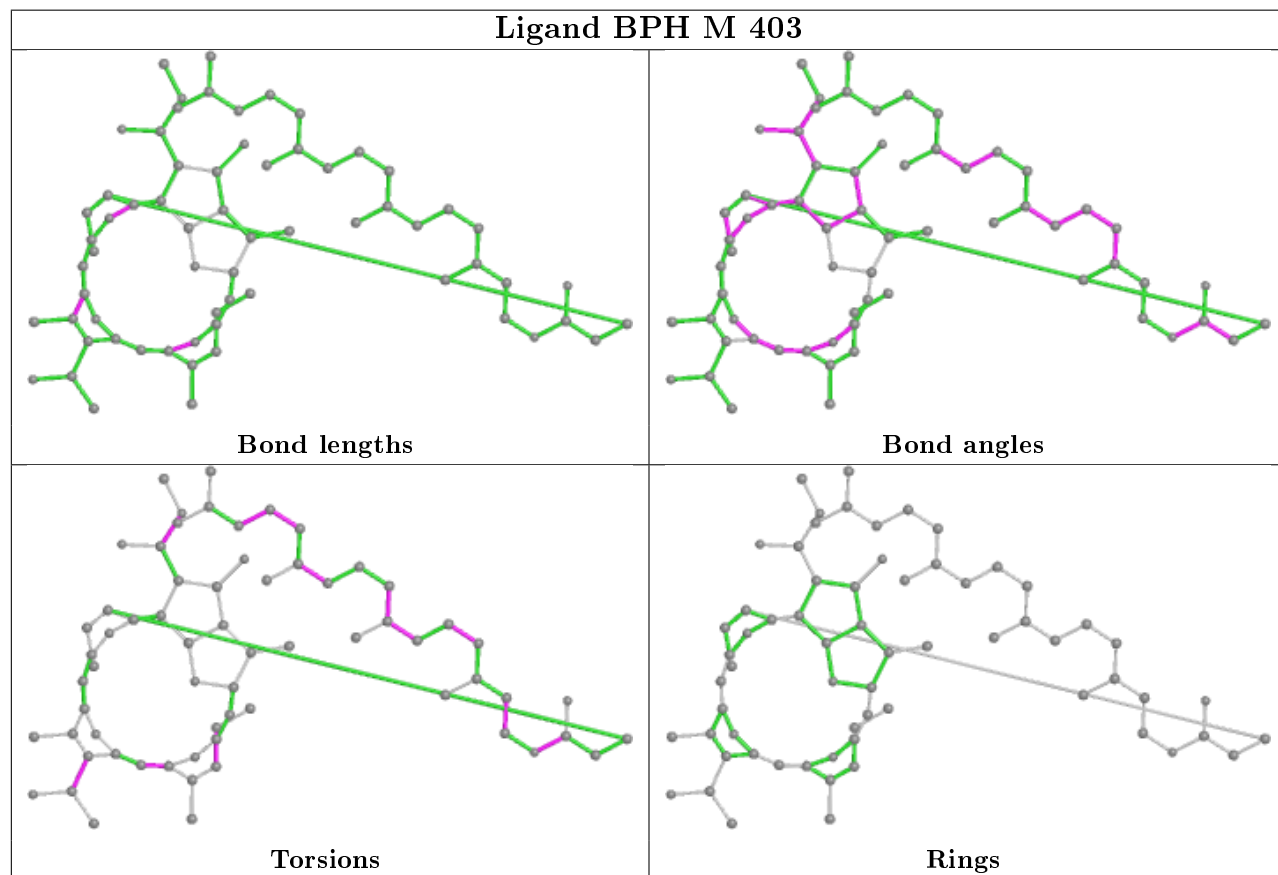
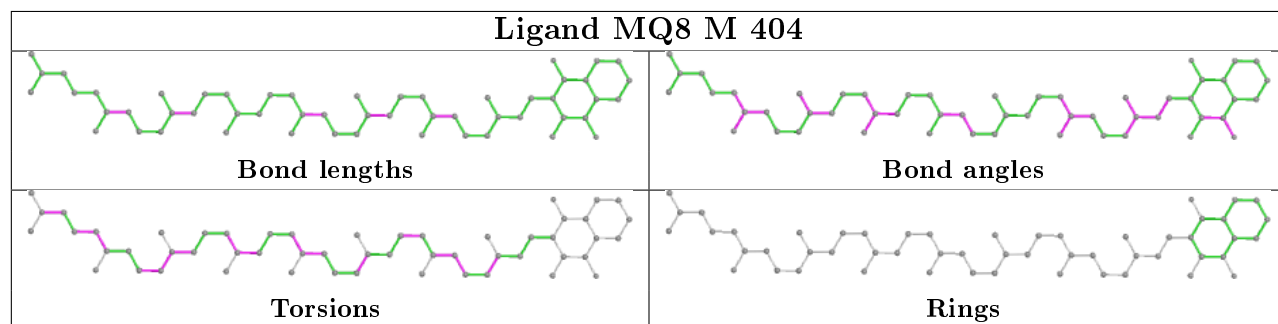
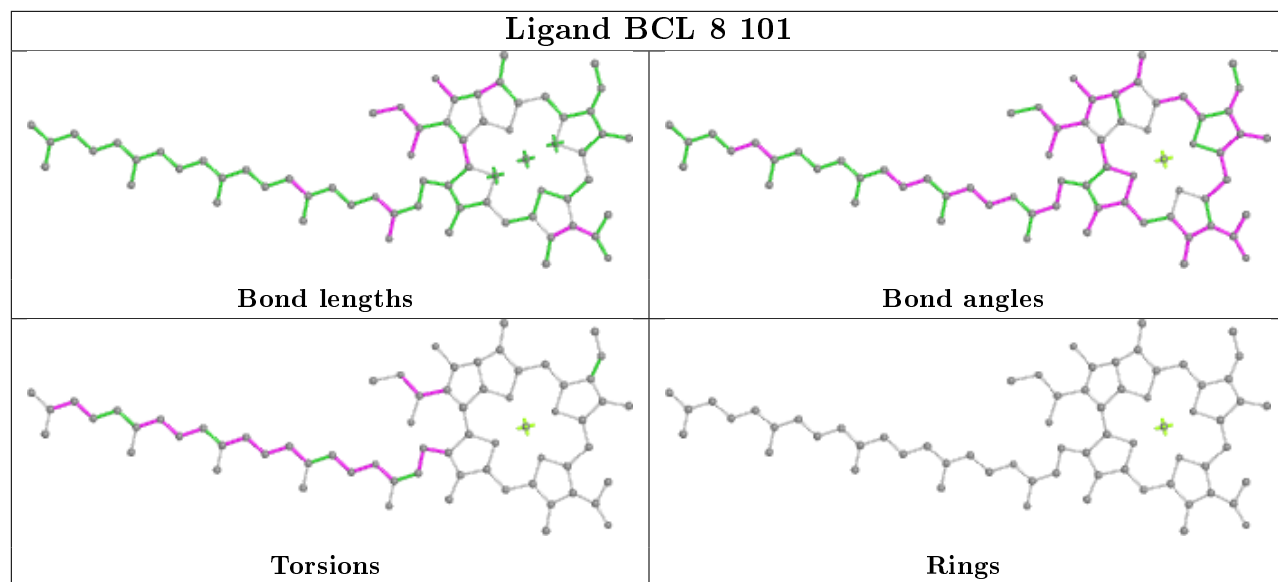


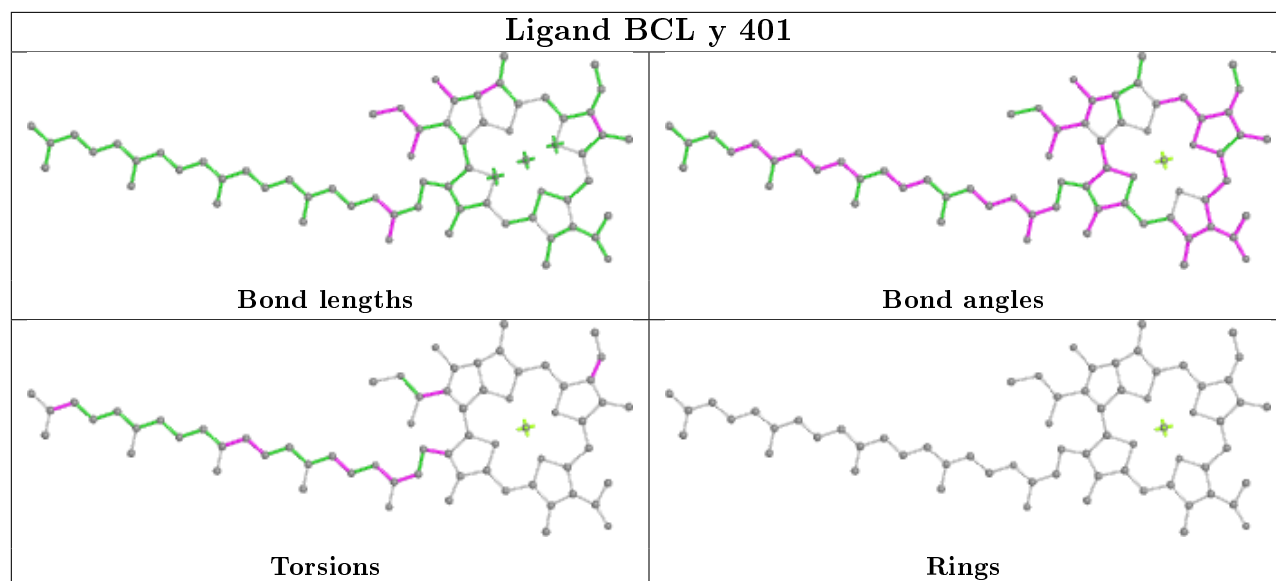
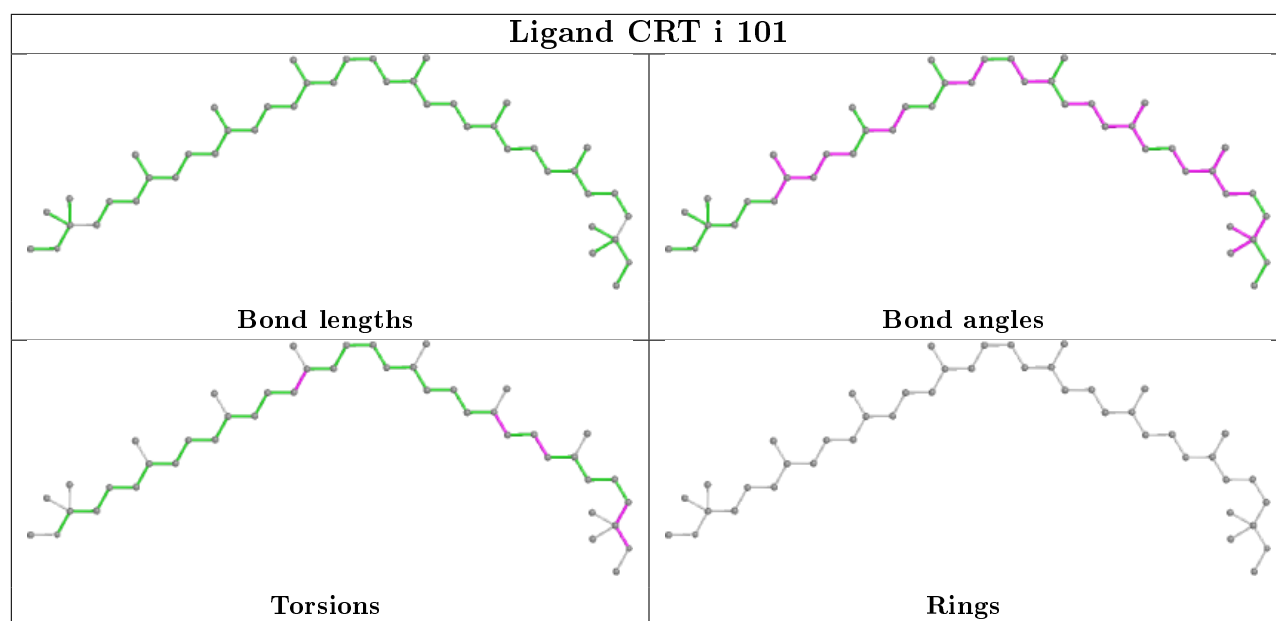


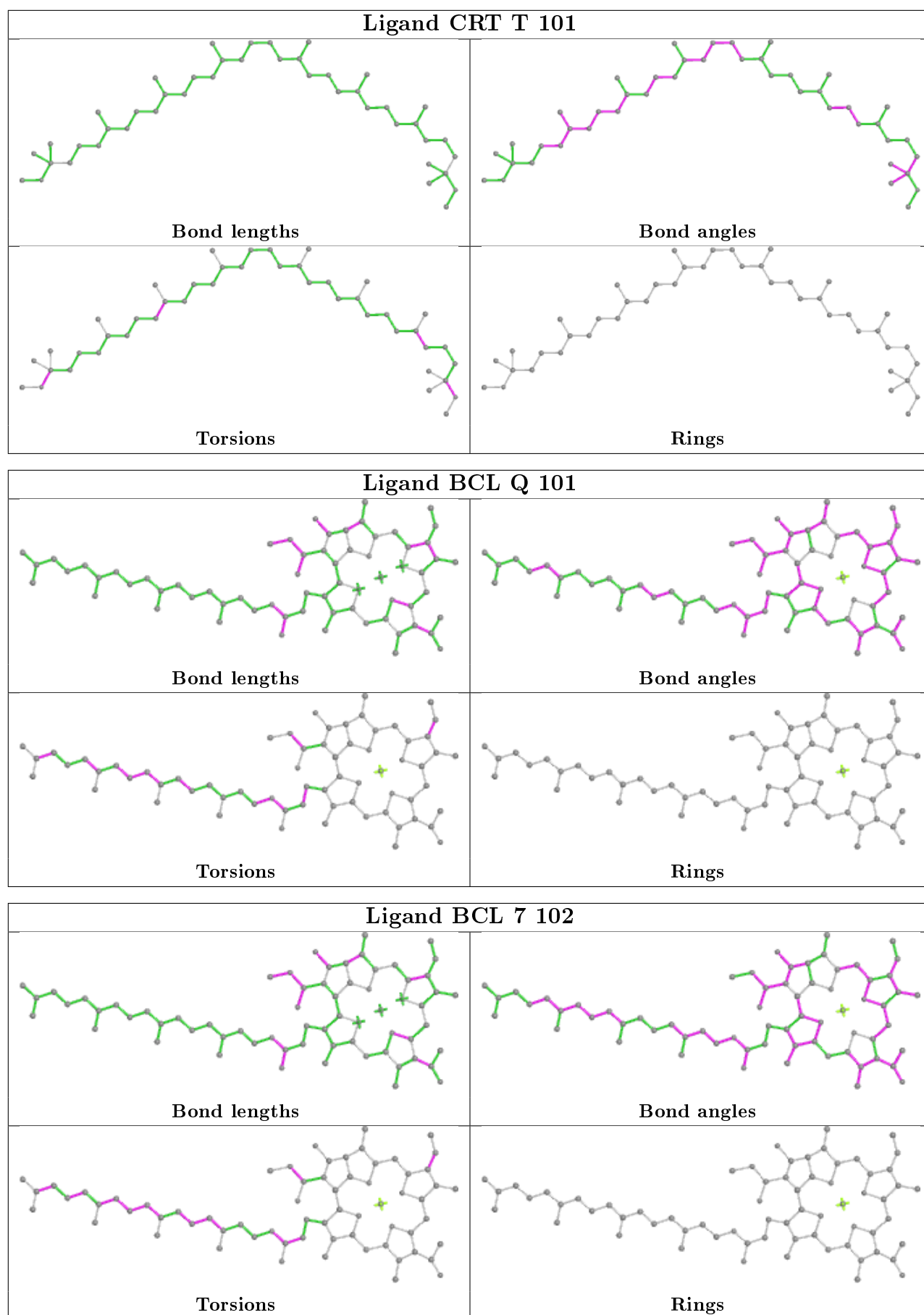


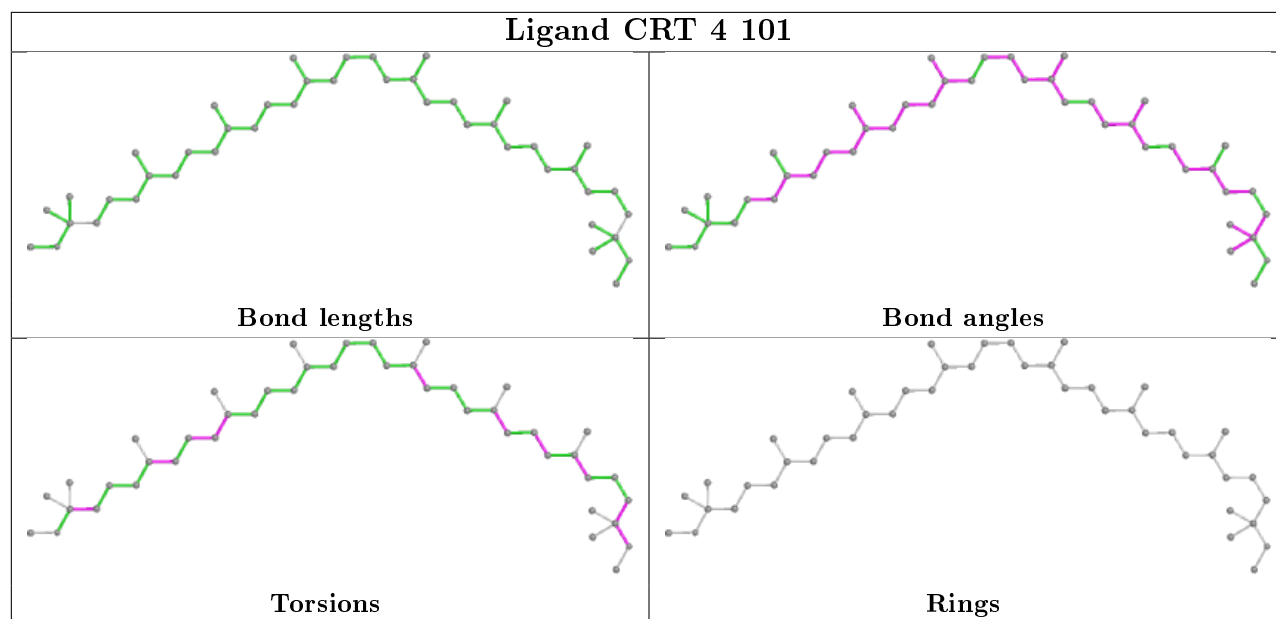
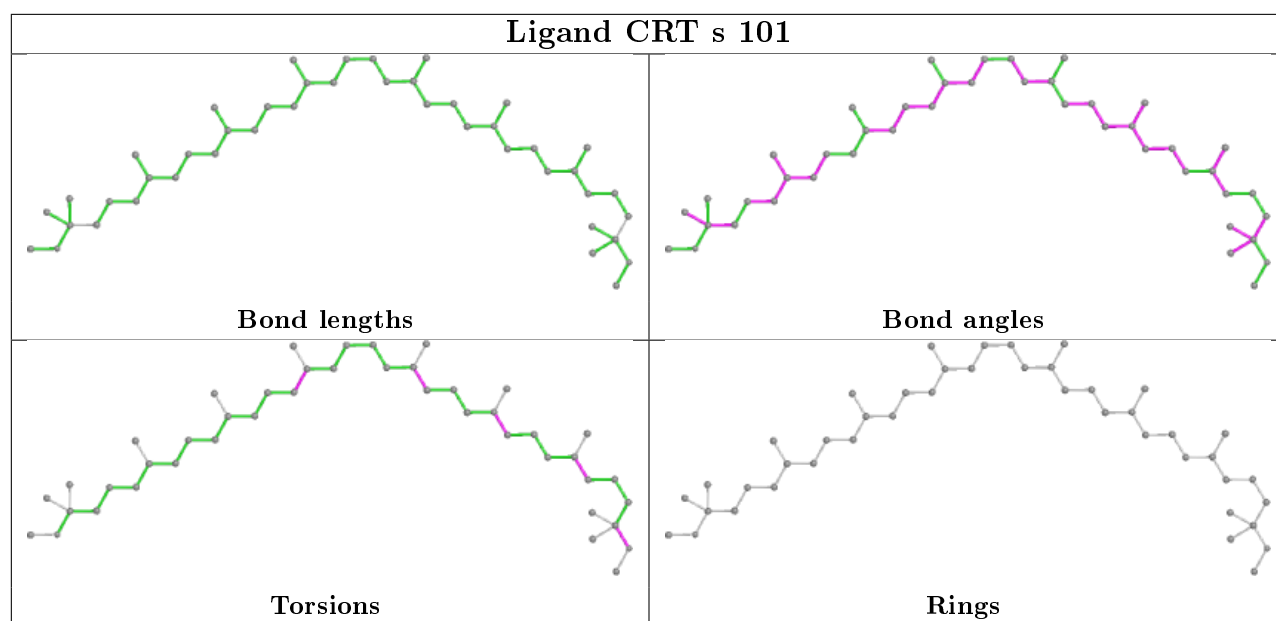


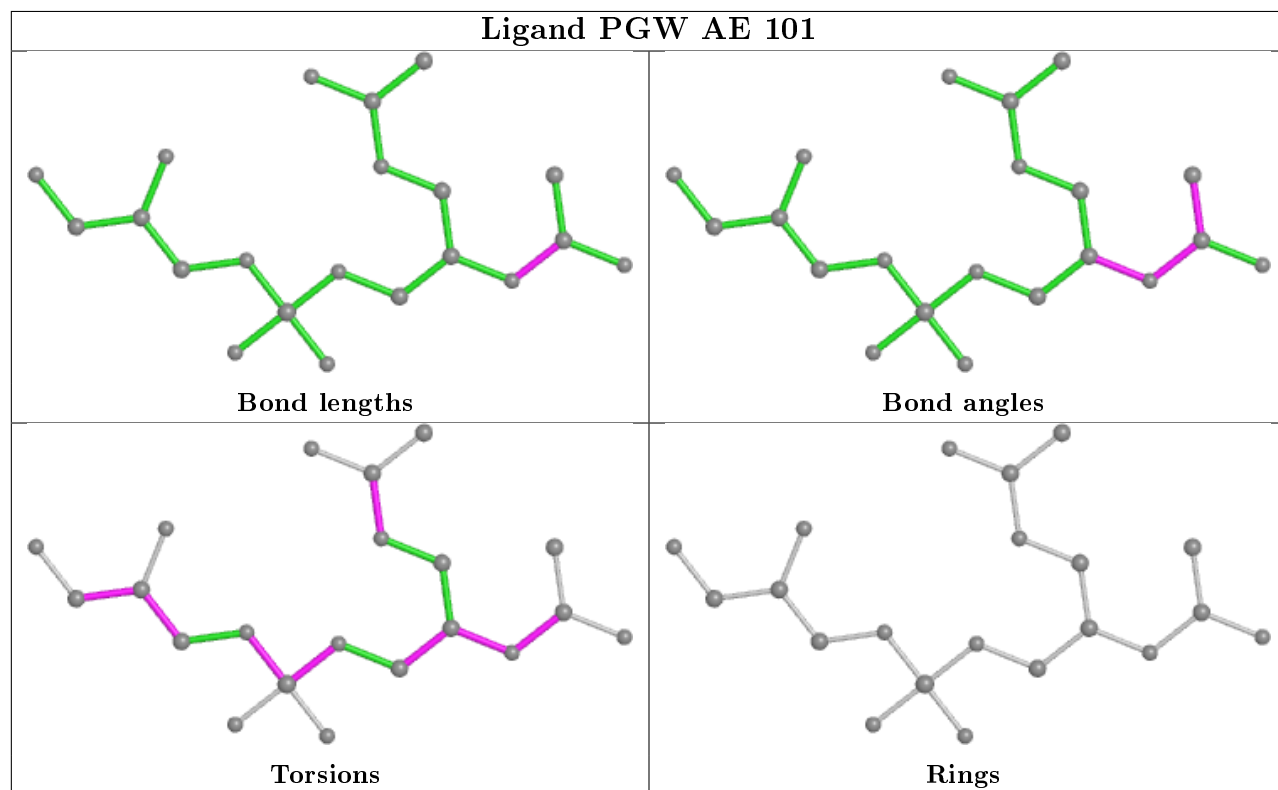
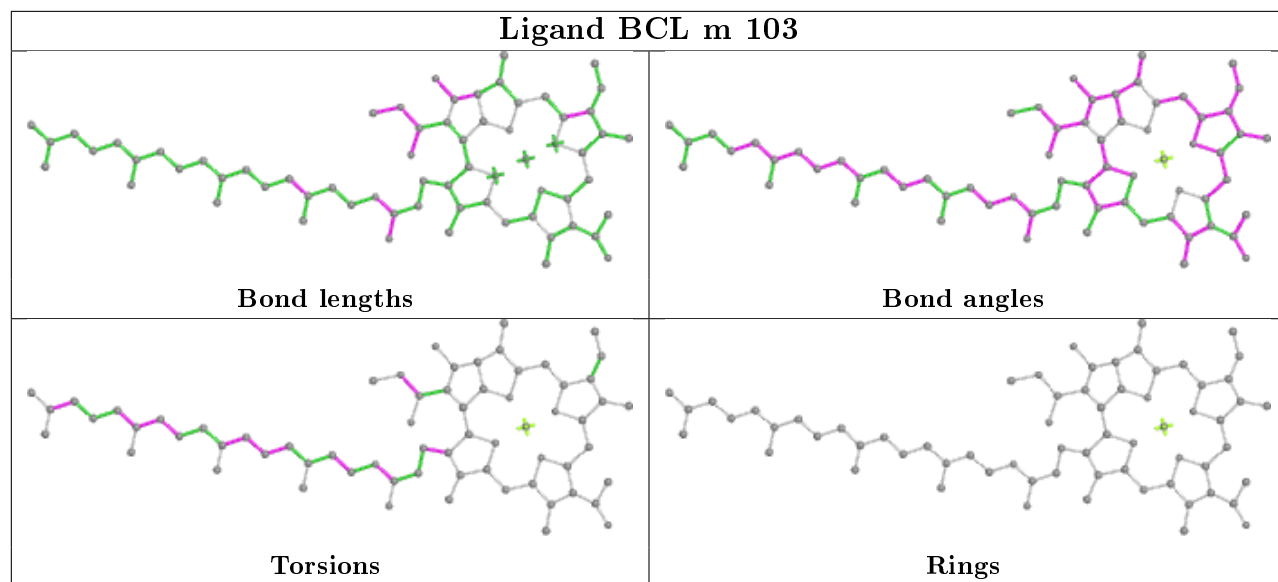


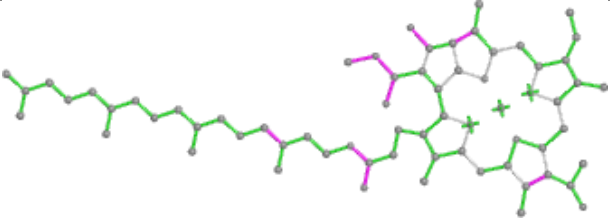
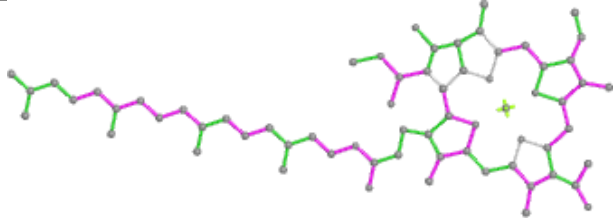
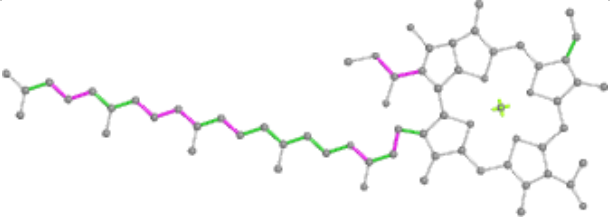
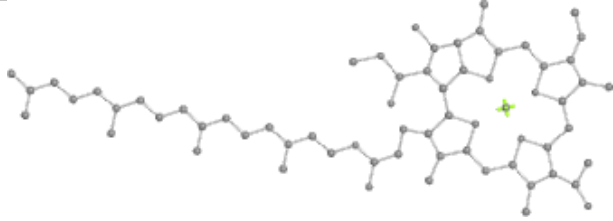
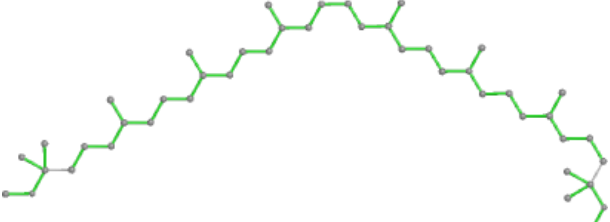
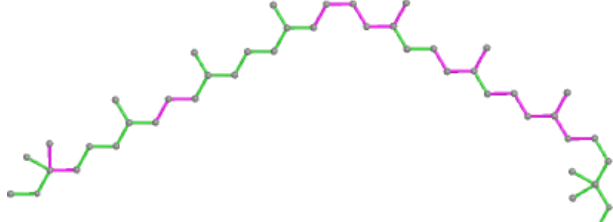
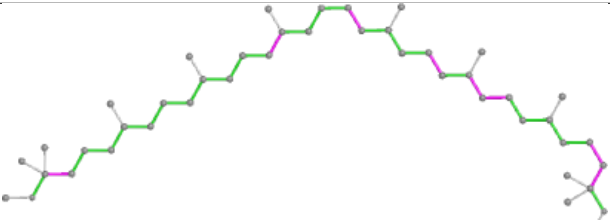
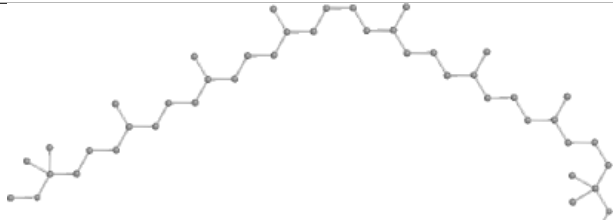
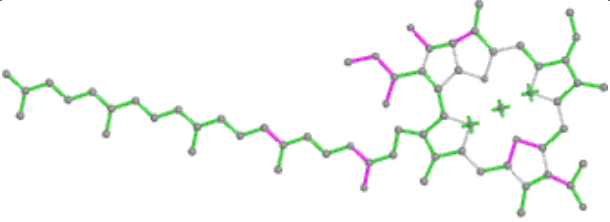
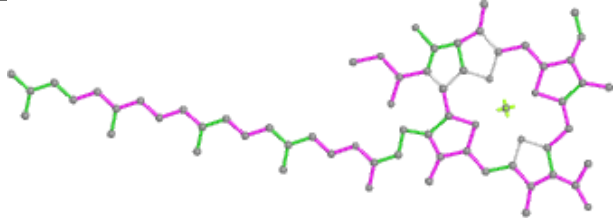
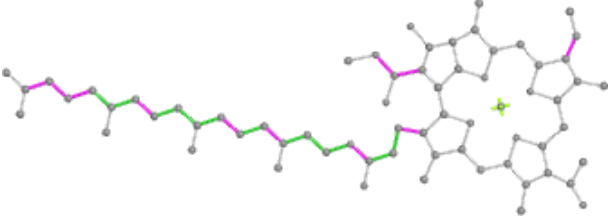
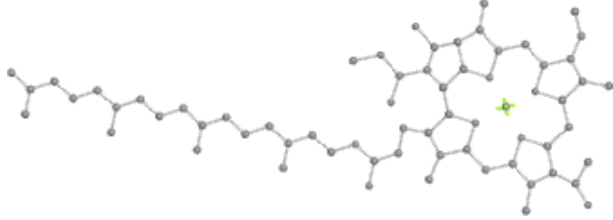


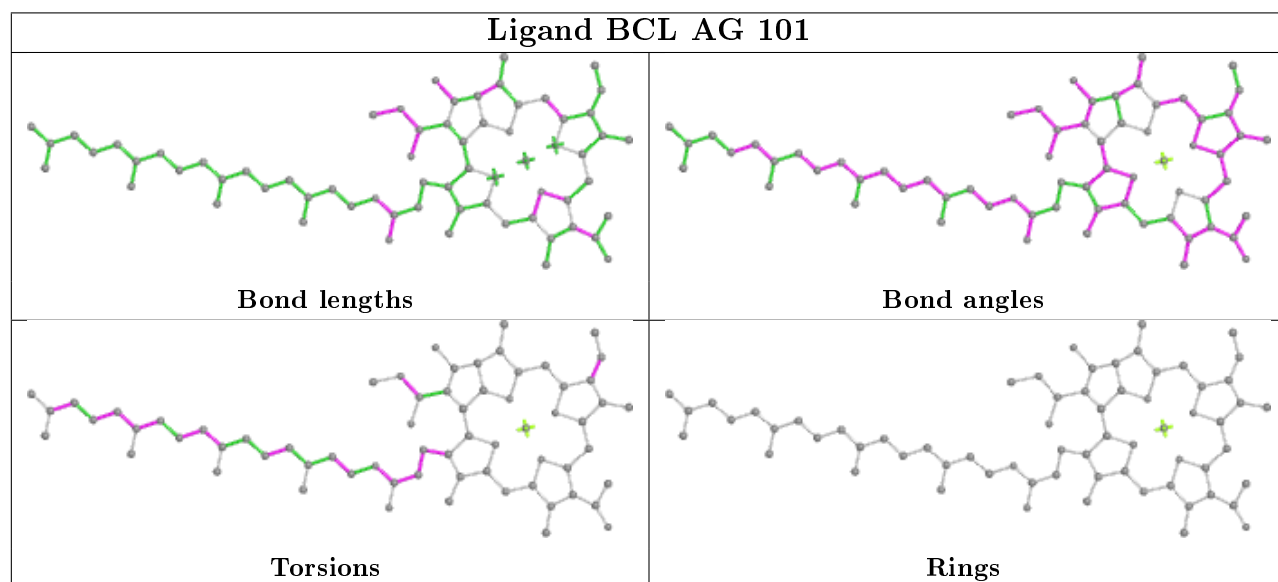
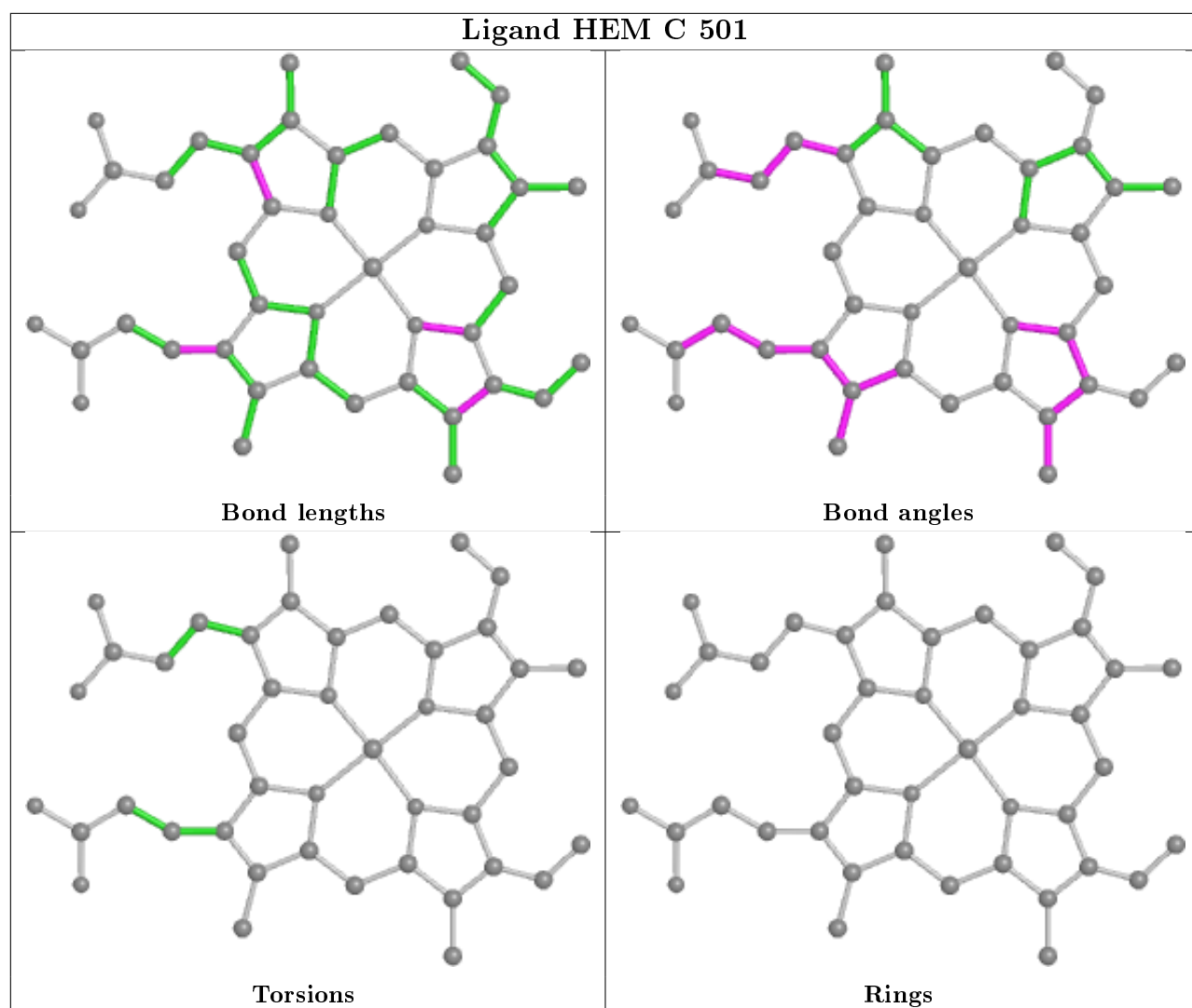




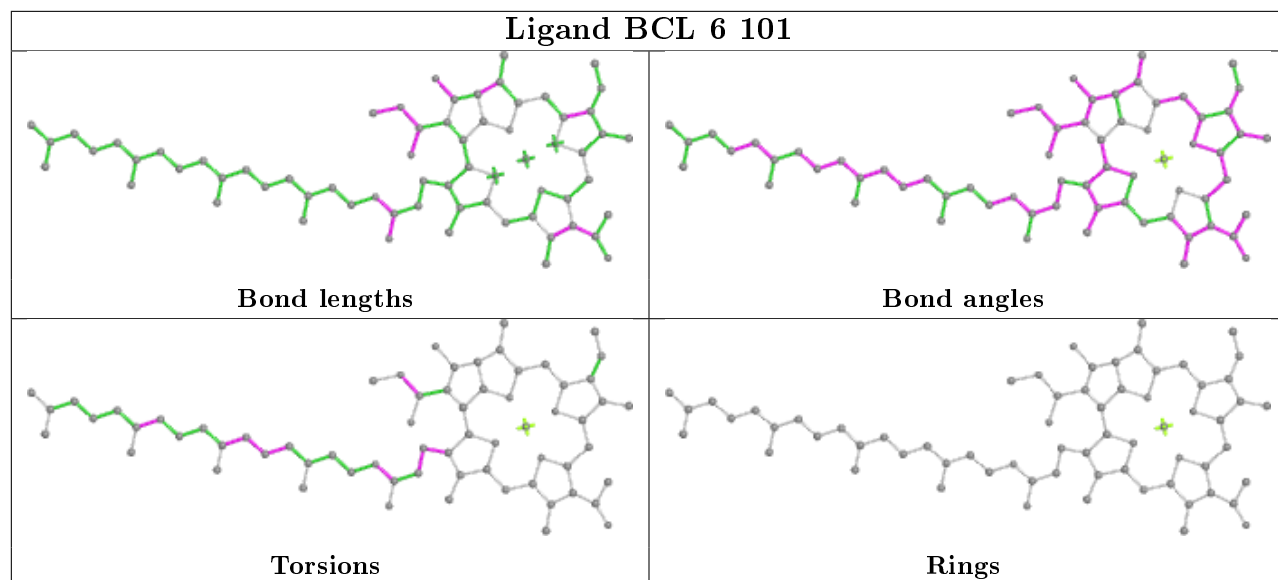




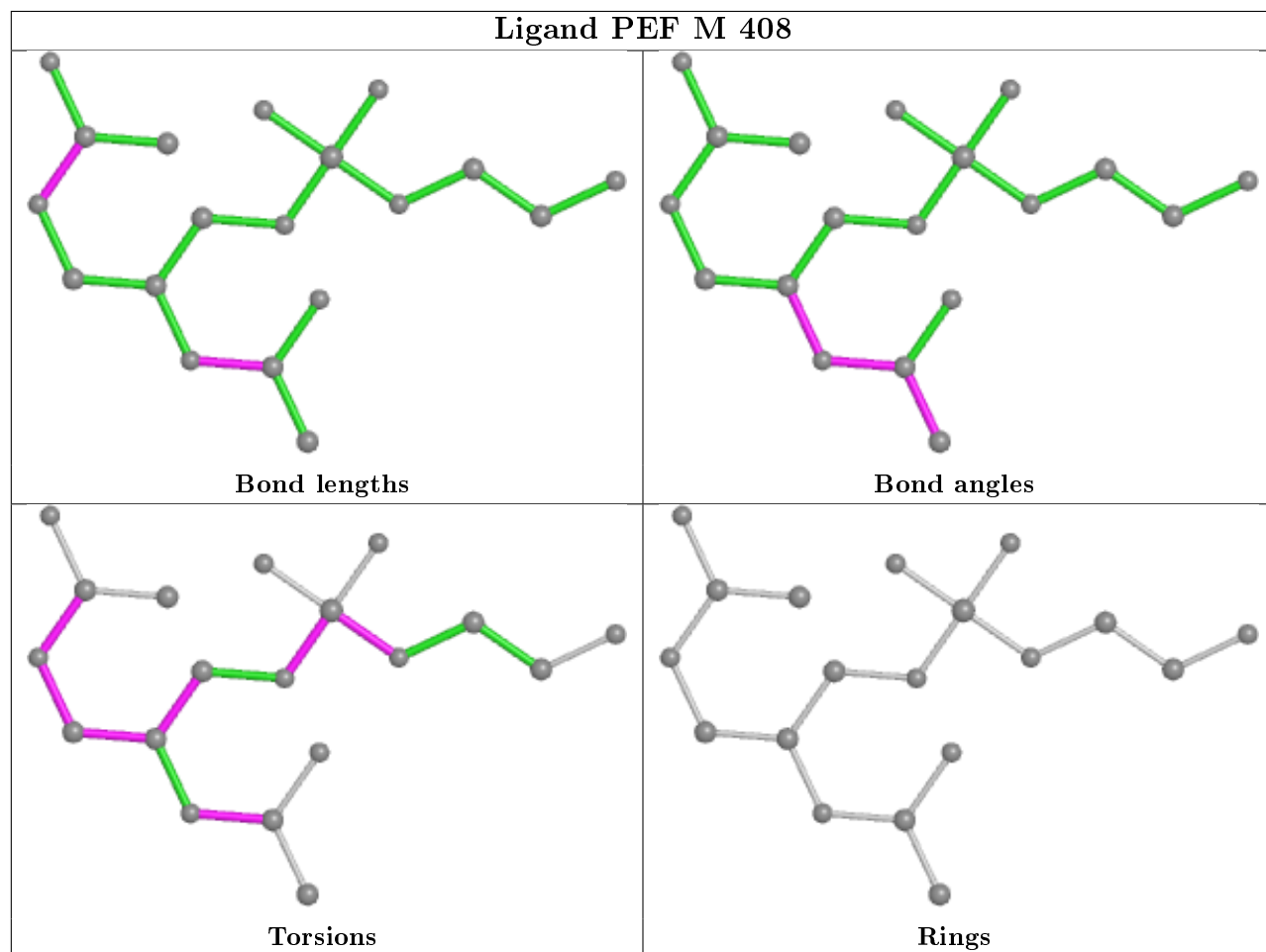
Ligand BCL 3 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CRT X 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL R 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

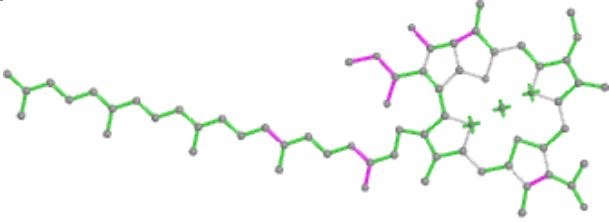
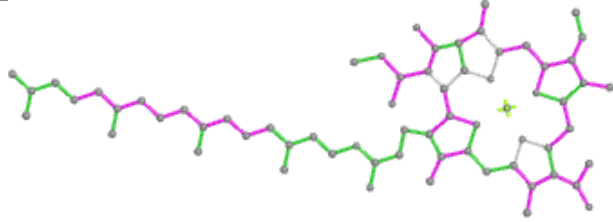
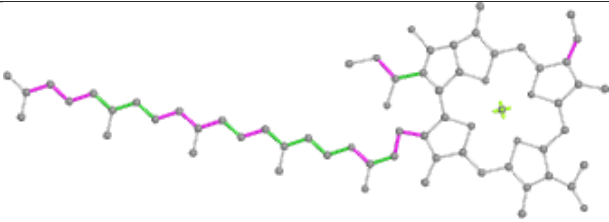
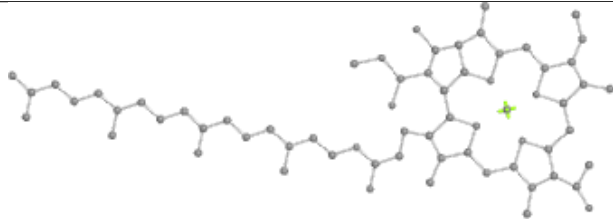
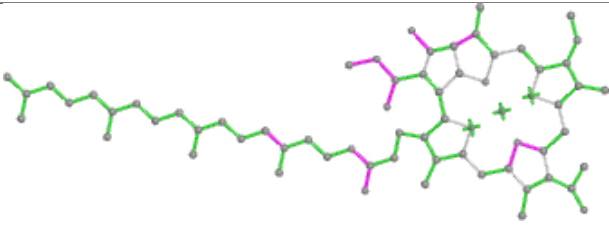
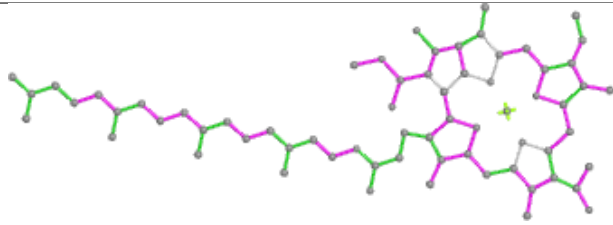
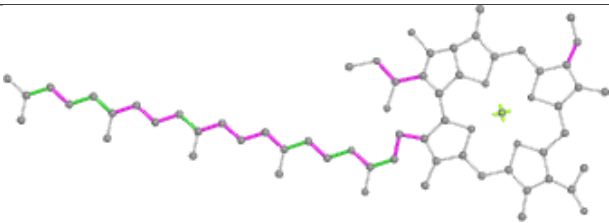
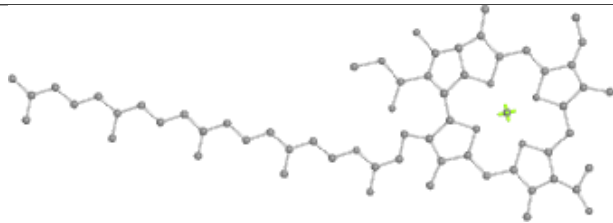
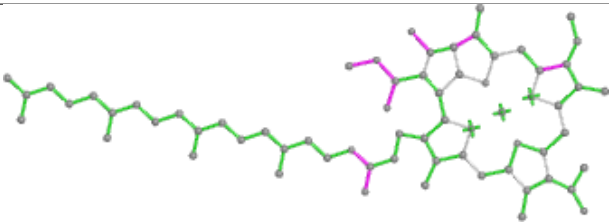
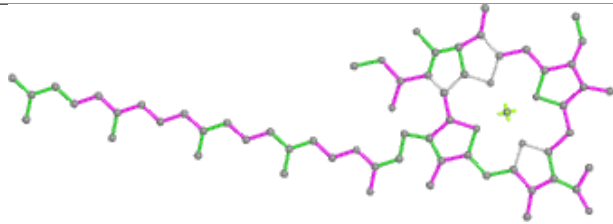
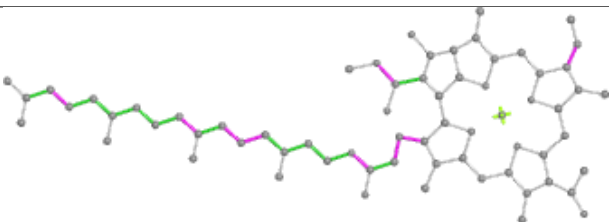
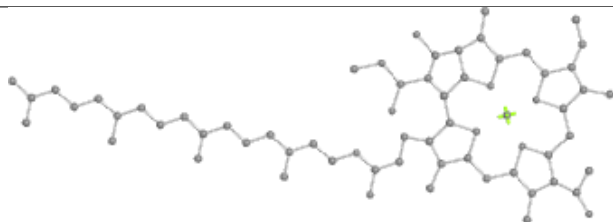


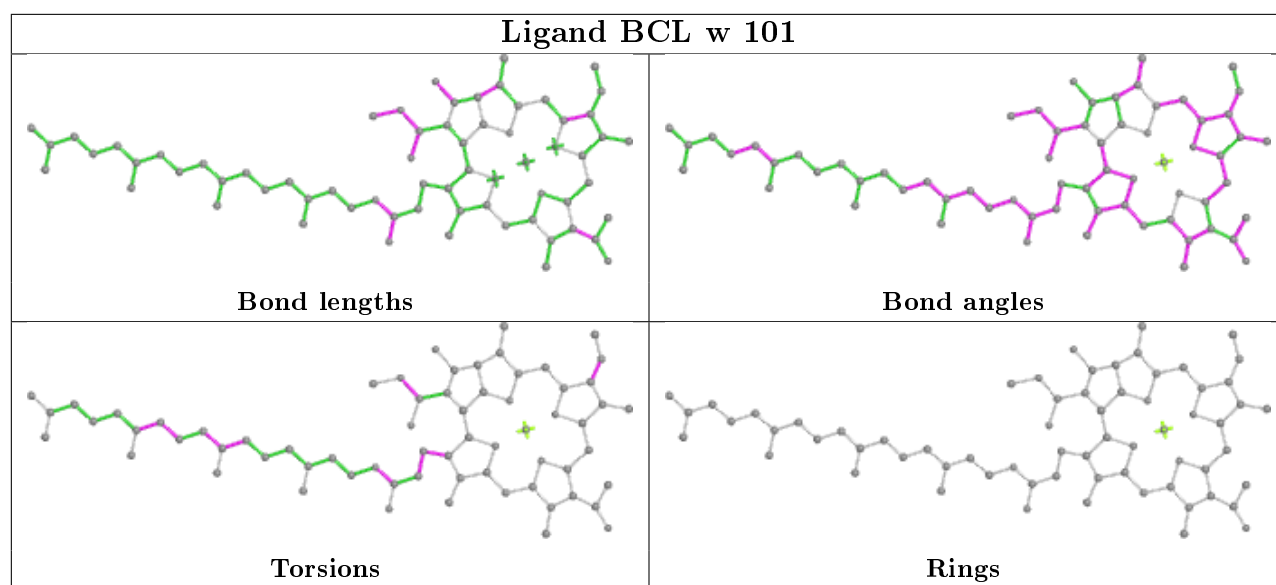
Ligand BCL 6 101



Ligand PEF M 408



Ligand BCL AI 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL k 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL I 103	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	0.55	37 (11%) 4 4	89, 118, 143, 160	0
1	o	317/333 (95%)	0.53	36 (11%) 5 4	97, 126, 153, 166	0
2	L	280/281 (99%)	0.25	19 (6%) 17 17	73, 99, 149, 173	0
2	x	280/281 (99%)	0.19	11 (3%) 39 37	75, 98, 145, 174	0
3	M	318/319 (99%)	0.18	12 (3%) 40 37	73, 105, 141, 160	0
3	y	318/319 (99%)	0.24	13 (4%) 37 35	73, 110, 148, 173	0
4	H	258/259 (99%)	0.50	23 (8%) 9 10	78, 105, 162, 245	0
4	t	258/259 (99%)	0.40	19 (7%) 14 14	84, 107, 140, 240	0
5	1	60/61 (98%)	0.79	11 (18%) 1 1	134, 157, 202, 223	0
5	3	60/61 (98%)	1.26	10 (16%) 1 1	137, 157, 204, 216	0
5	5	60/61 (98%)	1.14	13 (21%) 0 1	142, 169, 243, 251	0
5	7	60/61 (98%)	1.99	19 (31%) 0 0	155, 180, 257, 271	0
5	9	60/61 (98%)	1.02	8 (13%) 3 3	156, 191, 228, 241	0
5	A	60/61 (98%)	2.02	16 (26%) 0 0	165, 198, 248, 252	0
5	AA	60/61 (98%)	1.55	11 (18%) 1 1	157, 202, 261, 269	0
5	AC	60/61 (98%)	1.52	16 (26%) 0 0	161, 205, 258, 265	0
5	AE	60/61 (98%)	1.33	12 (20%) 1 1	169, 207, 255, 264	0
5	AG	60/61 (98%)	1.51	15 (25%) 0 0	161, 192, 245, 246	0
5	AI	60/61 (98%)	1.35	16 (26%) 0 0	145, 177, 226, 231	0
5	AK	60/61 (98%)	0.62	12 (20%) 1 1	139, 163, 219, 236	0
5	D	60/61 (98%)	1.86	22 (36%) 0 0	161, 206, 256, 265	0
5	F	60/61 (98%)	1.90	22 (36%) 0 0	169, 210, 255, 258	0
5	I	60/61 (98%)	1.45	14 (23%) 0 1	178, 209, 255, 264	0
5	K	60/61 (98%)	1.97	14 (23%) 0 1	162, 203, 269, 278	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
5	O	60/61 (98%)	1.35	14 (23%)	0	1	140, 193, 265, 272	0
5	Q	60/61 (98%)	1.81	19 (31%)	0	0	142, 180, 254, 258	0
5	S	60/61 (98%)	1.85	16 (26%)	0	0	154, 189, 247, 254	0
5	U	60/61 (98%)	1.47	13 (21%)	0	1	145, 178, 238, 244	0
5	W	60/61 (98%)	1.01	15 (25%)	0	0	131, 159, 215, 220	0
5	Y	60/61 (98%)	1.13	12 (20%)	1	1	128, 156, 221, 249	0
5	d	60/61 (98%)	0.86	11 (18%)	1	1	134, 165, 216, 223	0
5	f	60/61 (98%)	1.20	13 (21%)	0	1	143, 161, 217, 229	0
5	h	60/61 (98%)	0.76	11 (18%)	1	1	140, 170, 234, 249	0
5	j	60/61 (98%)	0.80	11 (18%)	1	1	149, 179, 230, 245	0
5	l	60/61 (98%)	0.97	12 (20%)	1	1	141, 174, 222, 231	0
5	m	60/61 (98%)	1.32	18 (30%)	0	0	142, 178, 239, 244	0
5	p	60/61 (98%)	1.80	16 (26%)	0	0	136, 182, 239, 240	0
5	r	60/61 (98%)	1.63	17 (28%)	0	0	143, 184, 248, 251	0
5	u	60/61 (98%)	1.40	18 (30%)	0	0	162, 195, 251, 260	0
5	w	60/61 (98%)	1.52	17 (28%)	0	0	165, 204, 259, 265	0
6	0	40/47 (85%)	0.82	8 (20%)	1	1	166, 222, 247, 250	0
6	2	40/47 (85%)	0.61	5 (12%)	3	3	164, 179, 206, 212	0
6	4	40/47 (85%)	0.11	5 (12%)	3	3	162, 176, 195, 200	0
6	6	40/47 (85%)	0.47	5 (12%)	3	3	174, 192, 206, 209	0
6	8	40/47 (85%)	0.63	5 (12%)	3	3	186, 217, 229, 232	0
6	AB	40/47 (85%)	0.53	3 (7%)	14	13	177, 217, 249, 252	0
6	AD	40/47 (85%)	0.89	10 (25%)	0	0	196, 226, 250, 256	0
6	AF	40/47 (85%)	0.57	5 (12%)	3	3	211, 233, 245, 251	0
6	AH	40/47 (85%)	0.71	10 (25%)	0	0	201, 219, 238, 243	0
6	AJ	40/47 (85%)	0.66	6 (15%)	2	2	180, 200, 220, 224	0
6	AL	40/47 (85%)	0.69	8 (20%)	1	1	169, 183, 204, 214	0
6	B	40/47 (85%)	1.32	10 (25%)	0	0	180, 225, 250, 252	0
6	E	40/47 (85%)	0.66	6 (15%)	2	2	186, 222, 253, 255	0
6	G	40/47 (85%)	1.19	13 (32%)	0	0	182, 227, 257, 259	0
6	J	40/47 (85%)	0.64	5 (12%)	3	3	187, 227, 259, 261	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	N	40/47 (85%)	0.53	5 (12%) 3 3	167, 212, 250, 252	0
6	P	40/47 (85%)	0.28	3 (7%) 14 13	166, 212, 248, 255	0
6	R	40/47 (85%)	1.20	11 (27%) 0 0	164, 208, 240, 243	0
6	T	40/47 (85%)	0.06	3 (7%) 14 13	178, 211, 230, 241	0
6	V	40/47 (85%)	0.03	1 (2%) 57 54	172, 198, 213, 222	0
6	X	40/47 (85%)	0.29	6 (15%) 2 2	162, 182, 195, 198	0
6	Z	40/47 (85%)	0.04	2 (5%) 28 27	161, 175, 196, 201	0
6	c	40/47 (85%)	1.68	13 (32%) 0 0	151, 202, 239, 250	0
6	e	40/47 (85%)	0.30	4 (10%) 7 7	172, 185, 215, 220	0
6	g	40/47 (85%)	0.20	4 (10%) 7 7	180, 190, 212, 218	0
6	i	40/47 (85%)	1.37	14 (35%) 0 0	182, 201, 214, 214	0
6	k	40/47 (85%)	0.54	3 (7%) 14 13	175, 212, 229, 243	0
6	n	40/47 (85%)	0.87	7 (17%) 1 1	146, 196, 239, 246	0
6	q	40/47 (85%)	0.60	5 (12%) 3 3	152, 190, 235, 243	0
6	s	40/47 (85%)	0.88	10 (25%) 0 0	156, 194, 238, 243	0
6	v	40/47 (85%)	0.31	7 (17%) 1 1	175, 201, 247, 250	0
6	z	40/47 (85%)	0.87	7 (17%) 1 1	176, 210, 255, 256	0
All	All	5546/5840 (94%)	0.78	843 (15%) 2 2	73, 162, 243, 278	0

The worst 5 of 843 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	p	54	SER	25.9
5	A	52	PRO	17.7
5	K	57	ALA	17.0
5	A	53	VAL	16.7
5	AE	54	SER	16.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
15	CRT	n	101	44/44	0.34	0.98	166,179,185,189	0
15	CRT	v	101	44/44	0.34	1.10	170,189,194,196	0
15	CRT	0	101	44/44	0.39	0.77	175,197,206,206	0
15	CRT	R	101	44/44	0.39	0.87	159,181,189,191	0
15	CRT	I	102	44/44	0.40	1.06	194,205,211,214	0
15	CRT	i	101	44/44	0.42	0.91	156,180,197,201	0
15	CRT	z	101	44/44	0.43	0.74	176,193,197,198	0
15	CRT	g	101	44/44	0.45	0.79	145,172,198,202	0
15	CRT	q	101	44/44	0.46	0.92	159,174,179,182	0
15	CRT	m	104	44/44	0.48	1.01	171,183,189,191	0
15	CRT	O	101	44/44	0.50	0.75	179,194,202,205	0
15	CRT	9	101	44/44	0.56	0.83	181,205,211,215	0
15	CRT	7	101	44/44	0.56	0.81	155,177,191,193	0
15	CRT	AC	101	44/44	0.58	0.94	180,197,200,202	0
15	CRT	P	102	44/44	0.59	0.75	170,186,189,190	0
15	CRT	7	103	44/44	0.60	0.63	171,193,205,208	0
12	PEF	p	101	16/47	0.62	0.30	131,142,148,151	0
15	CRT	AF	102	44/44	0.65	0.72	170,212,229,231	0
8	BA	w	102	1/1	0.67	0.09	271,271,271,271	0
14	MQ8	M	404	53/53	0.69	0.48	82,100,144,151	0
15	CRT	T	101	44/44	0.69	0.83	154,186,198,199	0
16	PO4	H	303	5/5	0.70	0.55	158,160,164,166	0
15	CRT	AD	101	44/44	0.70	0.49	175,204,211,213	0
15	CRT	E	101	44/44	0.70	0.58	179,205,211,213	0
16	PO4	t	302	5/5	0.71	0.33	142,142,144,149	0
12	PEF	A	101	19/47	0.73	0.46	142,147,157,161	0
9	BCL	AC	103	66/66	0.73	0.49	188,211,257,265	0
12	PEF	H	304	19/47	0.74	0.57	160,166,175,180	0
15	CRT	G	101	44/44	0.75	0.91	187,209,215,218	0
15	CRT	AH	102	44/44	0.76	0.60	155,198,229,231	0
15	CRT	M	405	44/44	0.76	0.41	90,108,139,148	0
15	CRT	AL	101	44/44	0.77	1.06	130,168,200,203	0
7	HEM	o	501	43/43	0.77	0.47	129,137,145,148	0
9	BCL	AB	102	66/66	0.78	0.53	187,214,258,267	0
15	CRT	4	101	44/44	0.78	0.52	141,166,185,190	0
15	CRT	V	101	44/44	0.78	0.69	140,179,197,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CRT	e	101	44/44	0.78	0.87	140,173,206,210	0
9	BCL	AG	101	66/66	0.78	0.34	179,190,215,226	0
15	CRT	k	101	44/44	0.79	0.60	166,186,199,202	0
15	CRT	AJ	101	44/44	0.79	0.88	139,182,214,217	0
15	CRT	y	404	44/44	0.79	0.38	99,115,146,154	0
8	BA	u	103	1/1	0.79	0.23	264,264,264,264	0
15	CRT	Z	101	44/44	0.80	1.06	127,160,186,189	0
15	CRT	2	101	44/44	0.80	1.04	136,165,190,194	0
9	BCL	AE	102	66/66	0.80	0.35	188,207,244,262	0
15	CRT	X	101	44/44	0.80	0.90	129,166,188,191	0
9	BCL	D	101	66/66	0.80	0.36	153,209,226,231	0
12	PEF	L	305	12/47	0.81	0.29	113,118,123,123	0
9	BCL	K	101	66/66	0.81	0.51	183,209,225,229	0
11	UQ8	L	304	53/53	0.81	0.60	81,86,88,89	0
12	PEF	y	406	19/47	0.81	0.24	116,122,128,131	0
8	BA	K	102	1/1	0.81	0.08	265,265,265,265	0
12	PEF	H	302	19/47	0.82	0.24	139,156,167,170	0
10	BPH	y	402	65/65	0.82	0.33	87,95,132,142	0
12	PEF	m	101	19/47	0.82	0.34	119,125,133,136	0
15	CRT	s	101	44/44	0.82	0.90	163,178,182,183	0
8	BA	AG	102	1/1	0.82	0.08	225,225,225,225	0
9	BCL	6	101	66/66	0.82	0.44	154,174,210,221	0
9	BCL	AC	102	66/66	0.83	0.38	181,205,218,228	0
17	PGW	S	101	21/51	0.83	0.23	122,133,142,147	0
9	BCL	m	102	66/66	0.83	0.43	157,190,207,214	0
9	BCL	z	102	66/66	0.83	0.39	183,211,253,269	0
14	MQ8	y	403	53/53	0.84	0.38	79,93,131,138	0
9	BCL	d	101	66/66	0.84	0.35	131,157,168,173	0
17	PGW	AE	101	21/51	0.84	0.37	141,155,167,171	0
12	PEF	y	407	19/47	0.84	0.23	97,101,106,108	0
8	BA	p	103	1/1	0.84	0.07	257,257,257,257	0
11	UQ8	x	304	53/53	0.84	0.55	80,87,90,91	0
12	PEF	M	408	19/47	0.84	0.28	95,99,103,105	0
9	BCL	I	103	66/66	0.85	0.37	200,223,264,273	0
9	BCL	0	102	66/66	0.86	0.40	183,208,254,257	0
9	BCL	g	102	66/66	0.86	0.38	153,171,206,215	0
9	BCL	N	101	66/66	0.86	0.37	189,213,255,262	0
9	BCL	j	101	66/66	0.86	0.33	166,183,198,203	0
9	BCL	f	101	66/66	0.86	0.49	144,163,174,180	0
9	BCL	D	102	66/66	0.86	0.48	194,218,258,259	0
9	BCL	p	102	66/66	0.87	0.34	128,189,203,208	0
9	BCL	y	401	66/66	0.87	0.40	86,93,102,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	BA	W	102	1/1	0.87	0.11	209,209,209,209	0
9	BCL	7	102	66/66	0.87	0.34	163,180,195,200	0
12	PEF	x	306	19/47	0.87	0.25	97,102,107,107	0
12	PEF	y	408	19/47	0.88	0.37	102,108,116,118	0
9	BCL	O	102	66/66	0.88	0.38	179,206,250,251	0
8	BA	AE	103	1/1	0.88	0.08	248,248,248,248	0
9	BCL	F	101	66/66	0.88	0.43	183,211,226,232	0
9	BCL	u	101	66/66	0.89	0.34	133,196,212,216	0
12	PEF	H	301	19/47	0.89	0.28	108,115,119,121	0
9	BCL	A	102	66/66	0.89	0.29	182,205,221,225	0
9	BCL	x	301	66/66	0.89	0.35	81,86,92,97	0
9	BCL	R	102	66/66	0.89	0.36	170,194,236,245	0
9	BCL	AF	101	66/66	0.89	0.34	161,205,215,225	0
10	BPH	M	403	65/65	0.89	0.28	84,88,117,126	0
9	BCL	i	102	66/66	0.89	0.33	161,181,218,232	0
9	BCL	k	102	66/66	0.89	0.33	171,195,223,234	0
9	BCL	AH	101	66/66	0.89	0.35	182,196,206,212	0
9	BCL	u	102	66/66	0.90	0.37	181,205,248,268	0
9	BCL	e	102	66/66	0.90	0.44	152,164,191,197	0
8	BA	F	102	1/1	0.90	0.09	271,271,271,271	0
9	BCL	m	103	66/66	0.90	0.29	173,198,219,230	0
9	BCL	P	101	66/66	0.90	0.35	173,201,216,221	0
9	BCL	3	101	66/66	0.90	0.42	138,153,165,168	0
9	BCL	G	102	66/66	0.90	0.34	197,220,264,265	0
12	PEF	t	303	19/47	0.90	0.19	94,97,104,104	0
9	BCL	I	101	66/66	0.90	0.36	149,216,231,234	0
10	BPH	L	302	65/65	0.90	0.24	79,88,109,114	0
9	BCL	8	101	66/66	0.90	0.32	173,196,221,230	0
9	BCL	AI	102	66/66	0.90	0.28	163,172,197,203	0
9	BCL	9	102	66/66	0.90	0.29	165,191,211,216	0
9	BCL	V	102	66/66	0.90	0.34	162,177,208,223	0
9	BCL	w	101	66/66	0.90	0.39	176,199,217,222	0
9	BCL	h	101	66/66	0.91	0.29	155,171,185,187	0
12	PEF	H	305	19/47	0.91	0.21	93,97,104,105	0
7	HEM	C	501	43/43	0.91	0.33	118,126,133,136	0
9	BCL	A	103	66/66	0.91	0.34	190,213,242,251	0
9	BCL	l	101	66/66	0.91	0.33	123,149,159,163	0
9	BCL	q	102	66/66	0.91	0.40	170,194,226,241	0
12	PEF	M	407	16/47	0.91	0.16	86,89,91,92	0
9	BCL	T	102	66/66	0.91	0.34	166,185,223,243	0
9	BCL	c	101	66/66	0.91	0.34	173,199,243,258	0
9	BCL	AB	101	66/66	0.91	0.29	176,202,220,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	PEF	t	301	19/47	0.92	0.24	100,104,107,108	0
8	BA	m	106	1/1	0.92	0.05	242,242,242,242	0
8	BA	L	306	1/1	0.92	0.22	185,185,185,185	0
10	BPH	x	302	65/65	0.92	0.27	78,84,104,106	0
8	BA	3	102	1/1	0.92	0.14	191,191,191,191	0
9	BCL	l	101	66/66	0.92	0.34	157,189,205,210	0
9	BCL	5	101	66/66	0.92	0.32	147,166,178,183	0
9	BCL	r	101	66/66	0.92	0.41	160,190,204,208	0
9	BCL	U	101	66/66	0.92	0.27	153,176,186,191	0
9	BCL	AI	101	66/66	0.92	0.35	167,179,190,196	0
9	BCL	Q	101	66/66	0.92	0.33	166,193,205,211	0
8	BA	x	308	1/1	0.92	0.16	175,175,175,175	0
9	BCL	x	303	66/66	0.92	0.33	82,89,97,98	0
9	BCL	2	102	66/66	0.93	0.34	145,156,185,195	0
9	BCL	W	101	66/66	0.93	0.33	152,165,171,179	0
9	BCL	M	401	66/66	0.93	0.29	86,94,107,114	0
7	HEM	o	503	43/43	0.93	0.38	98,109,122,124	0
7	HEM	C	502	43/43	0.93	0.36	108,114,120,121	0
7	HEM	C	504	43/43	0.93	0.35	105,106,110,111	0
9	BCL	S	102	66/66	0.93	0.34	136,186,197,205	0
9	BCL	4	102	66/66	0.93	0.29	144,159,189,198	0
9	BCL	L	301	66/66	0.93	0.29	79,84,98,103	0
8	BA	AK	102	1/1	0.93	0.03	186,186,186,186	0
9	BCL	AL	102	66/66	0.93	0.34	152,161,183,190	0
9	BCL	L	303	66/66	0.93	0.32	79,86,91,96	0
8	BA	D	103	1/1	0.93	0.17	252,252,252,252	0
9	BCL	s	102	66/66	0.93	0.47	174,198,247,260	0
8	BA	d	102	1/1	0.94	0.05	174,174,174,174	0
7	HEM	o	504	43/43	0.94	0.32	111,114,119,122	0
9	BCL	X	102	66/66	0.94	0.36	148,159,180,192	0
9	BCL	AK	101	66/66	0.94	0.34	152,162,177,193	0
8	BA	O	103	1/1	0.94	0.10	244,244,244,244	0
7	HEM	o	502	43/43	0.94	0.42	119,124,128,129	0
8	BA	f	102	1/1	0.94	0.05	205,205,205,205	0
9	BCL	M	402	66/66	0.94	0.36	83,90,96,99	0
9	BCL	Z	102	66/66	0.94	0.32	143,151,174,182	0
9	BCL	x	305	66/66	0.94	0.29	83,90,98,105	0
8	BA	j	102	1/1	0.94	0.03	228,228,228,228	0
9	BCL	Y	101	66/66	0.94	0.35	142,152,162,174	0
8	BA	Q	102	1/1	0.95	0.03	245,245,245,245	0
7	HEM	C	503	43/43	0.95	0.37	96,107,121,123	0
8	BA	AA	101	1/1	0.95	0.02	260,260,260,260	0

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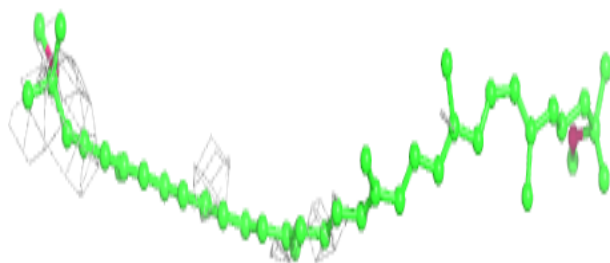
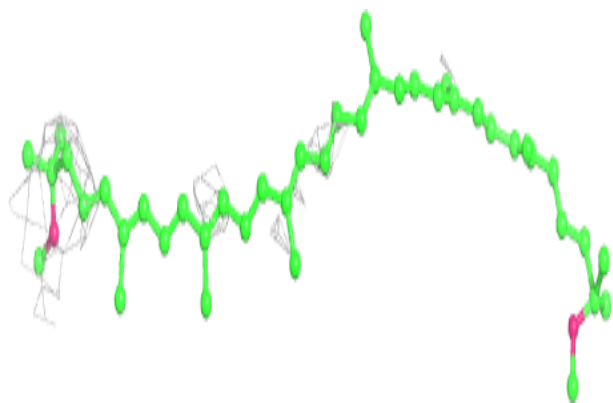
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	BA	7	104	1/1	0.95	0.19	215,215,215,215	0
8	BA	AI	103	1/1	0.95	0.11	210,210,210,210	0
16	PO4	M	406	5/5	0.95	0.11	121,126,127,128	0
8	BA	5	102	1/1	0.95	0.09	212,212,212,212	0
8	BA	L	307	1/1	0.95	0.24	160,160,160,160	0
8	BA	I	104	1/1	0.95	0.09	276,276,276,276	0
8	BA	1	102	1/1	0.96	0.02	177,177,177,177	0
8	BA	h	102	1/1	0.96	0.04	210,210,210,210	0
8	BA	AC	104	1/1	0.96	0.11	257,257,257,257	0
8	BA	A	105	1/1	0.96	0.15	243,243,243,243	0
8	BA	A	104	1/1	0.96	0.08	247,247,247,247	0
16	PO4	y	405	5/5	0.96	0.18	134,136,141,141	0
8	BA	S	103	1/1	0.97	0.02	227,227,227,227	0
8	BA	x	307	1/1	0.97	0.21	186,186,186,186	0
8	BA	m	105	1/1	0.97	0.03	226,226,226,226	0
8	BA	r	102	1/1	0.97	0.06	250,250,250,250	0
8	BA	U	102	1/1	0.97	0.18	224,224,224,224	0
8	BA	Y	102	1/1	0.97	0.05	181,181,181,181	0
13	FE	x	309	1/1	0.98	0.17	76,76,76,76	0
13	FE	L	308	1/1	0.98	0.15	76,76,76,76	0
8	BA	C	505	1/1	0.99	0.24	93,93,93,93	0
8	BA	o	505	1/1	1.00	0.25	100,100,100,100	0

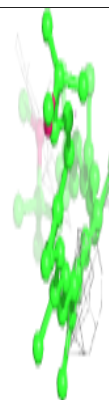
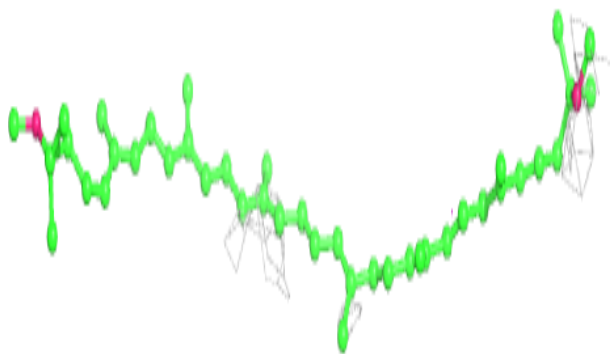
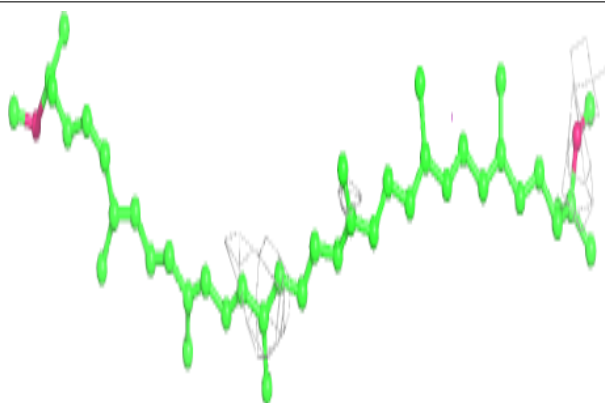
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

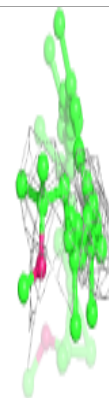
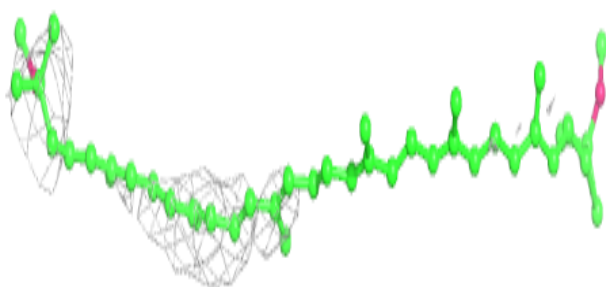
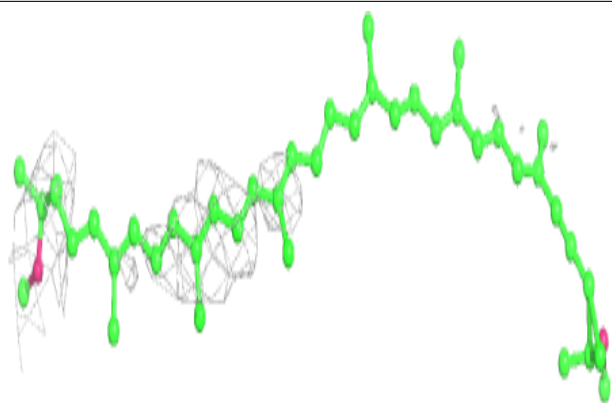
**Electron density around CRT v 101:**

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

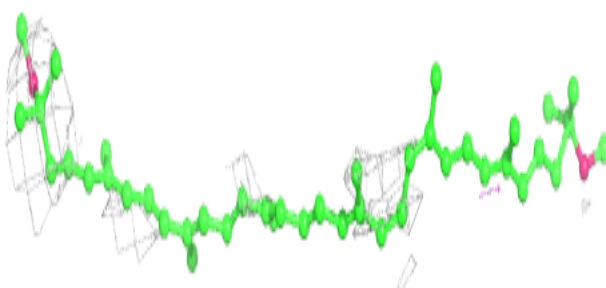
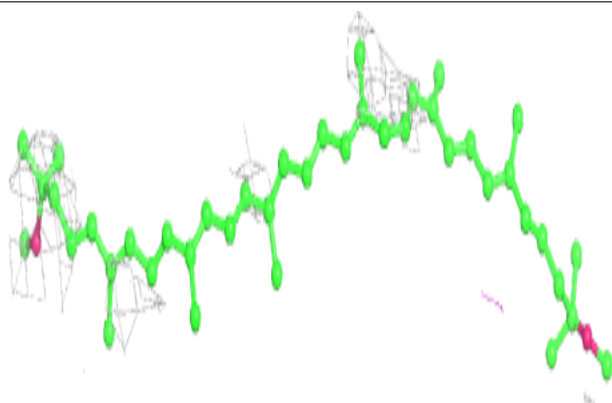


Electron density around CRT 0 101:

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

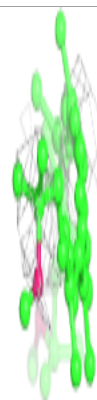
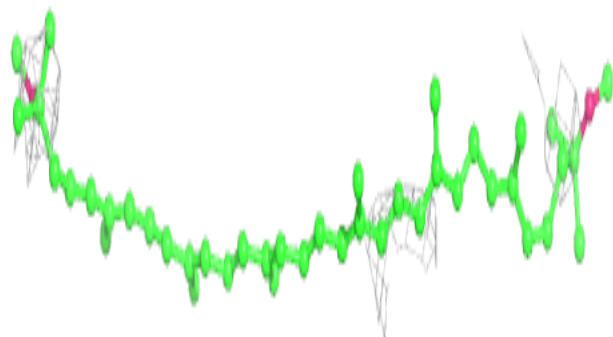
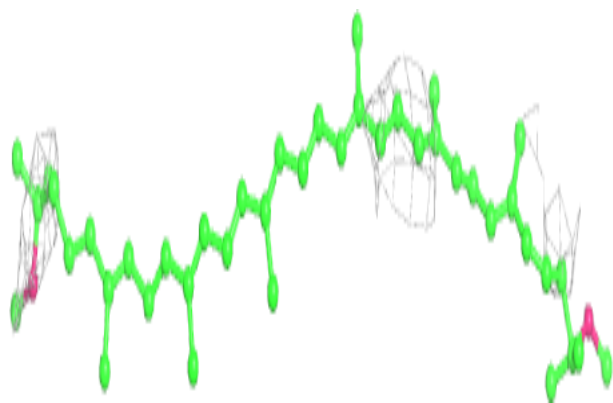
**Electron density around CRT R 101:**

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

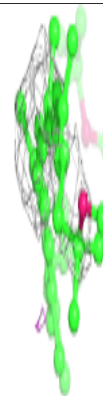
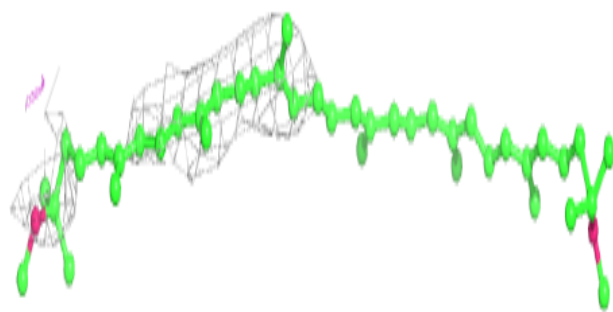
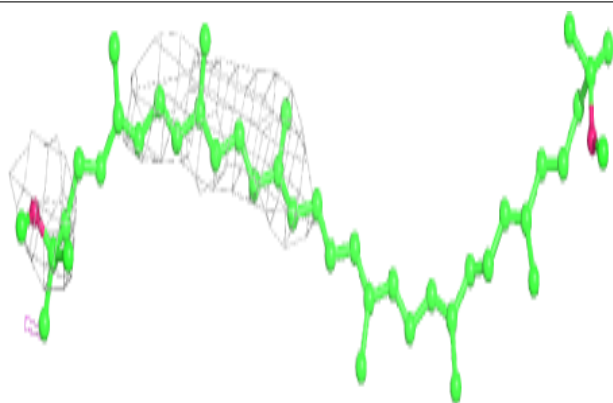


Electron density around CRT I 102:

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

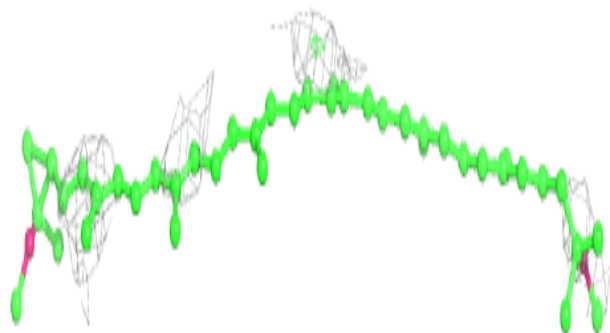
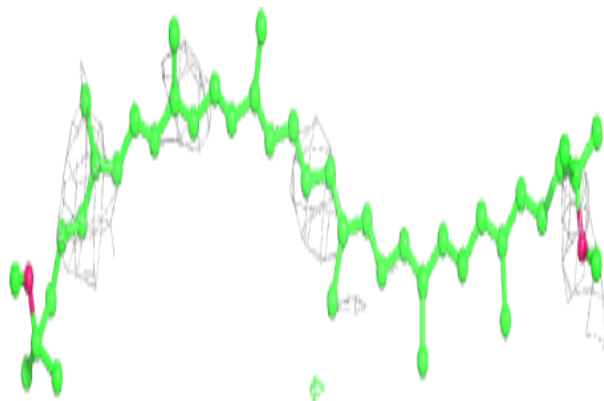
**Electron density around CRT i 101:**

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

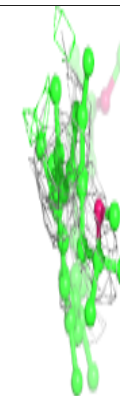
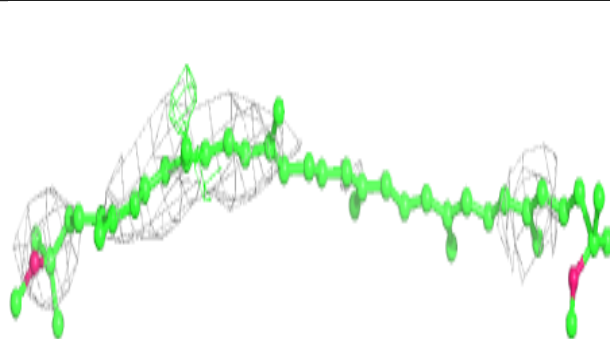
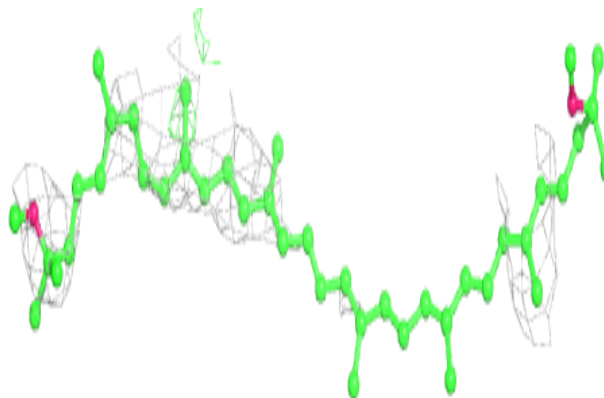


Electron density around CRT z 101:

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

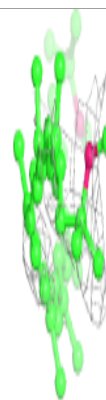
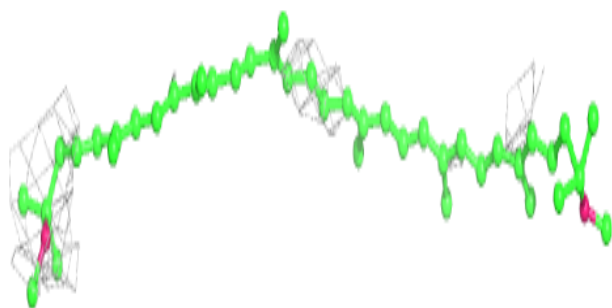
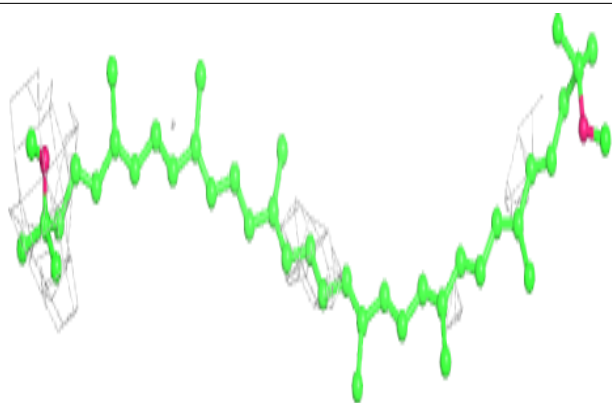
**Electron density around CRT g 101:**

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

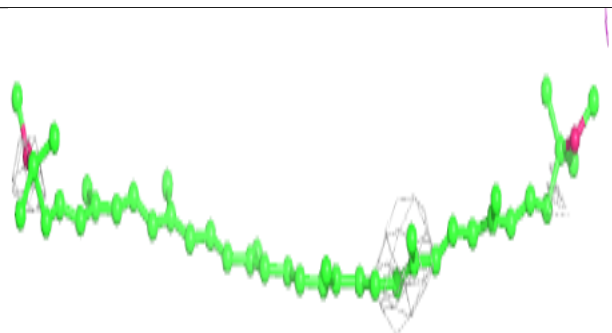
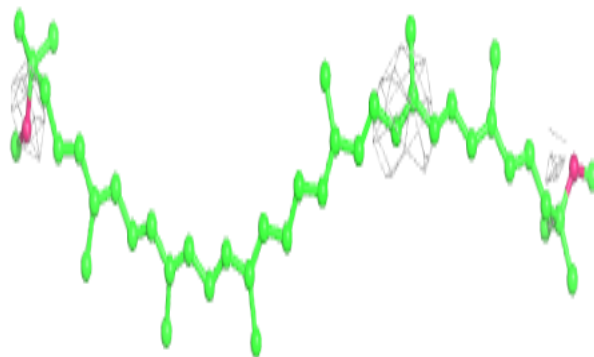


Electron density around CRT q 101:

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

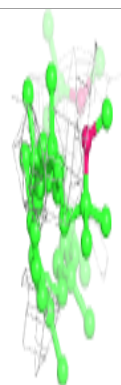
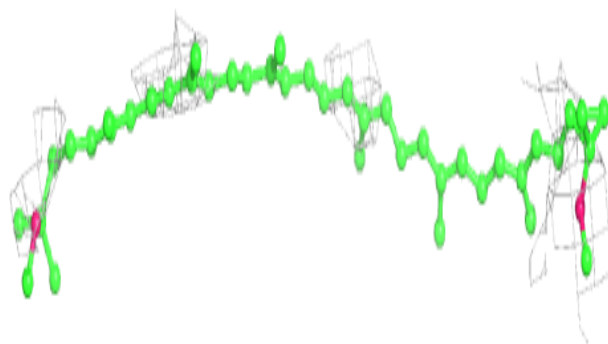
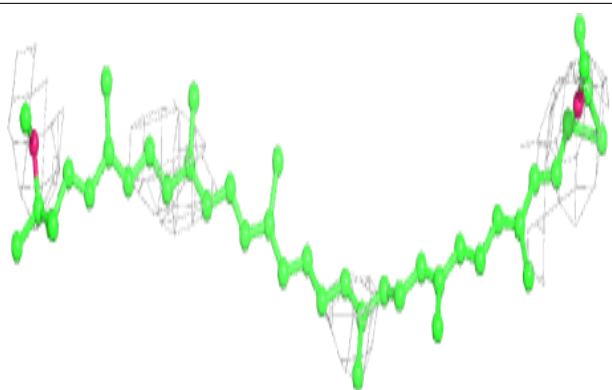
**Electron density around CRT m 104:**

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

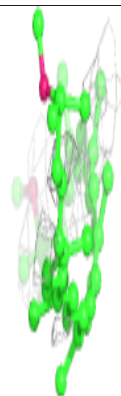
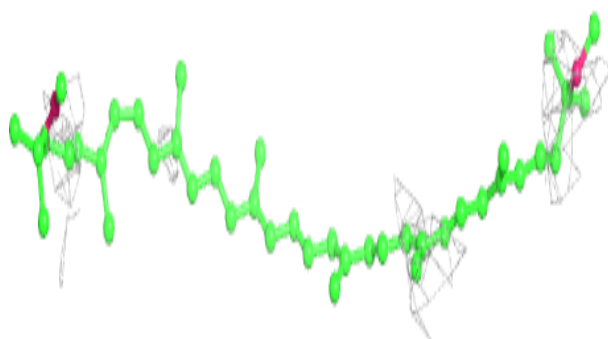
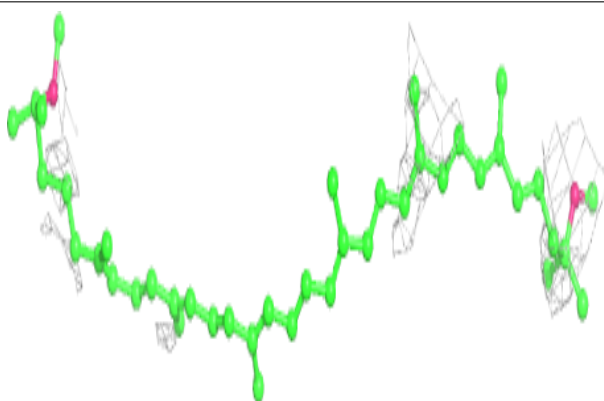


Electron density around CRT O 101:

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

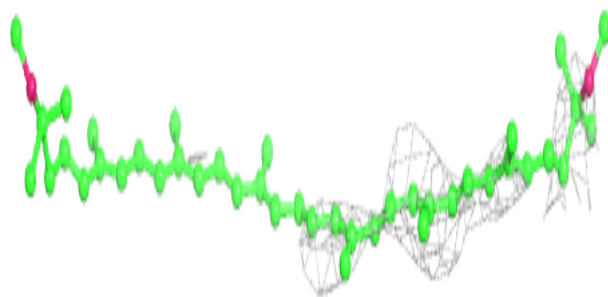
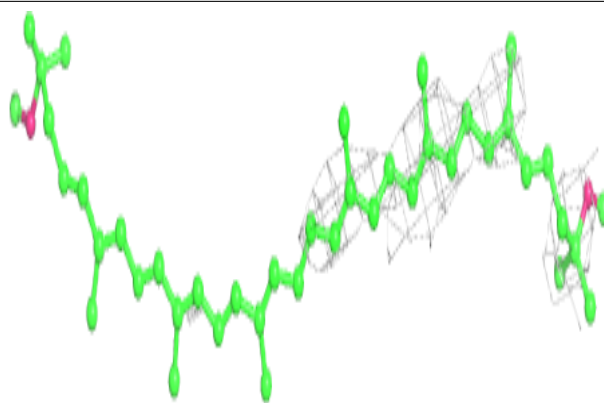
**Electron density around CRT 9 101:**

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

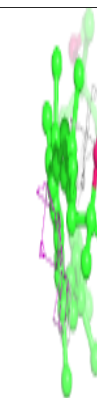
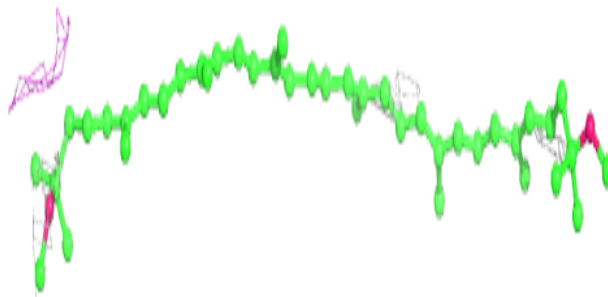
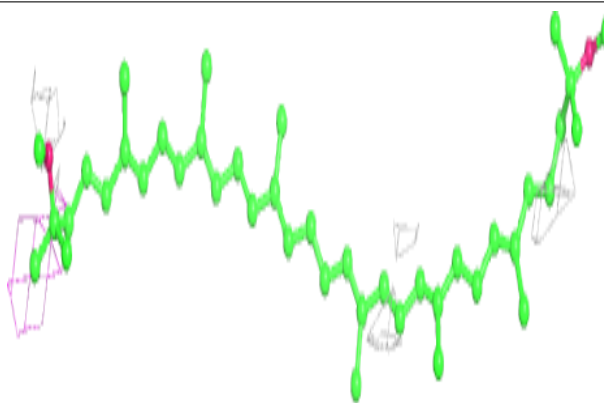


Electron density around CRT 7 101:

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

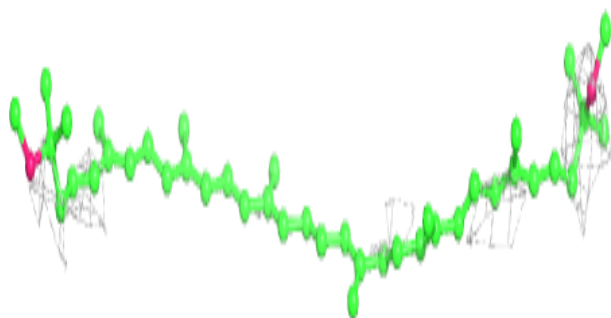
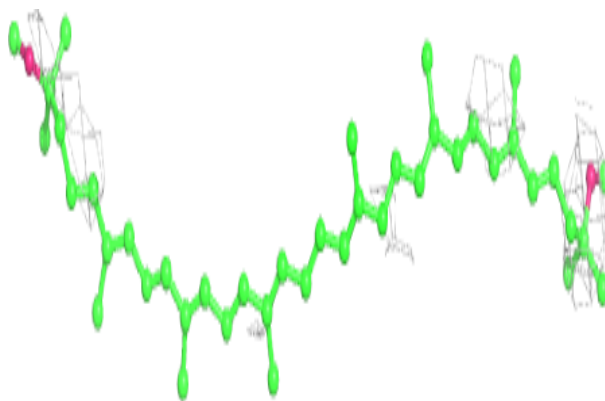
**Electron density around CRT AC 101:**

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

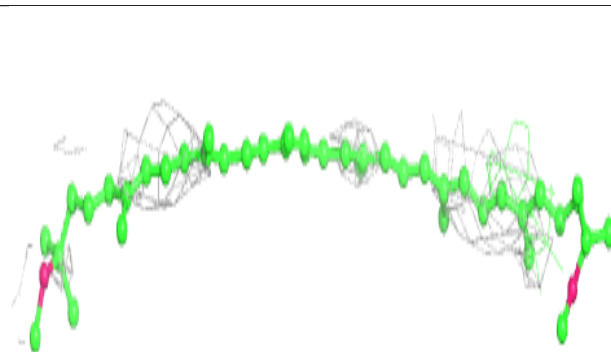
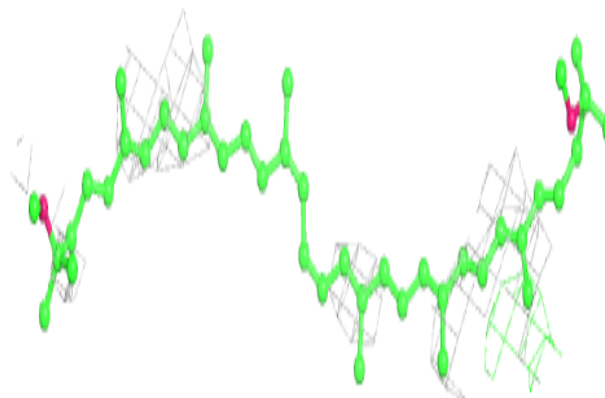


Electron density around CRT P 102:

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

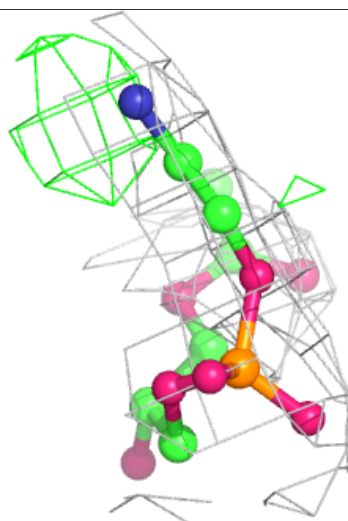
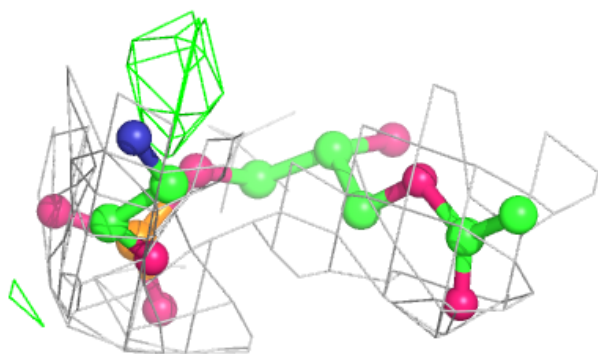
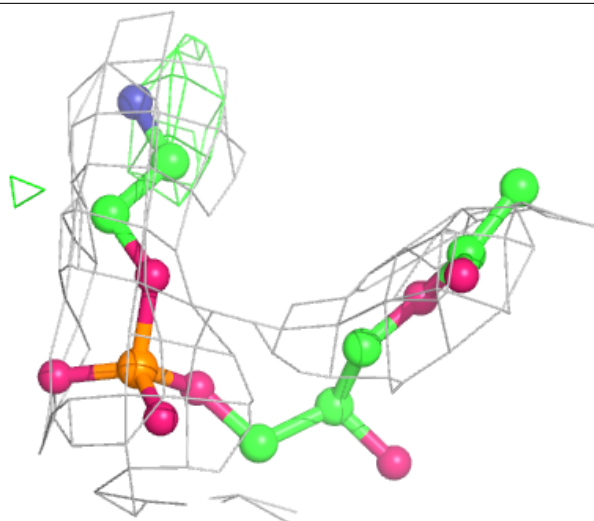
**Electron density around CRT 7 103:**

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



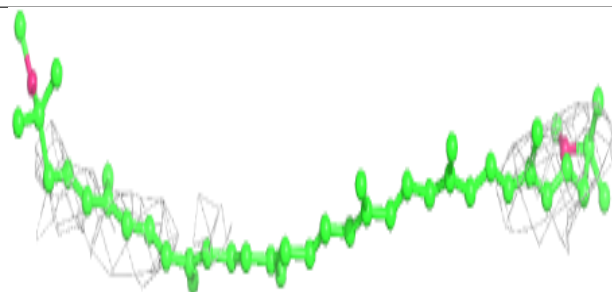
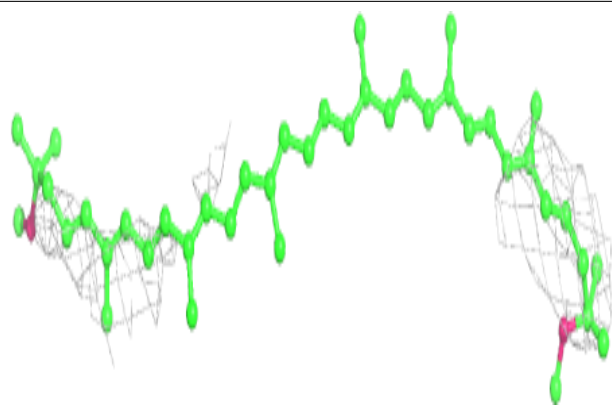
Electron density around PEF p 101:

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

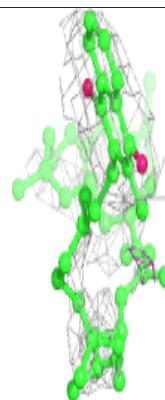
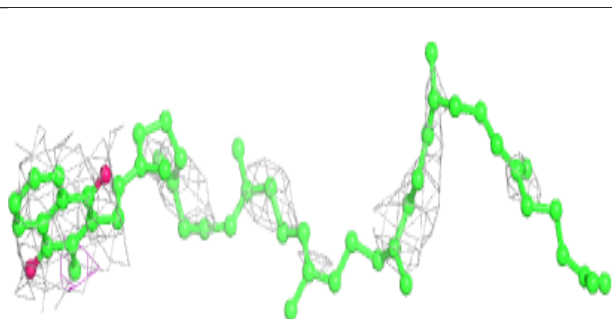
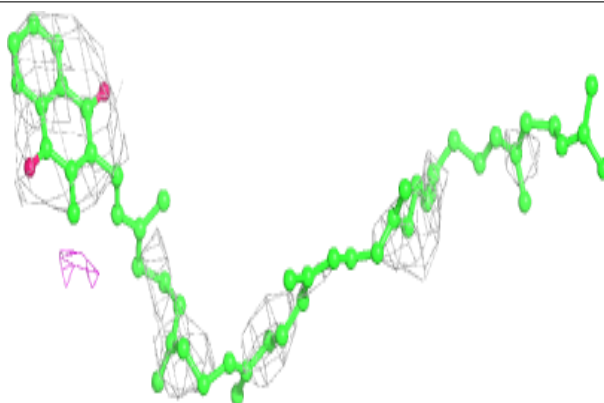


Electron density around CRT AF 102:

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

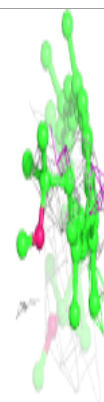
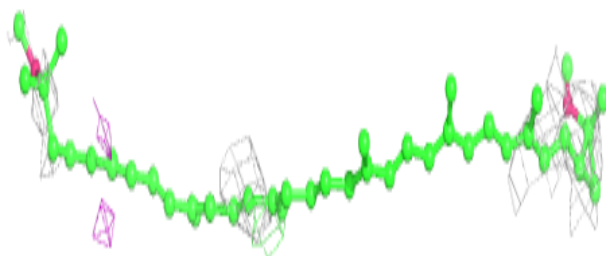
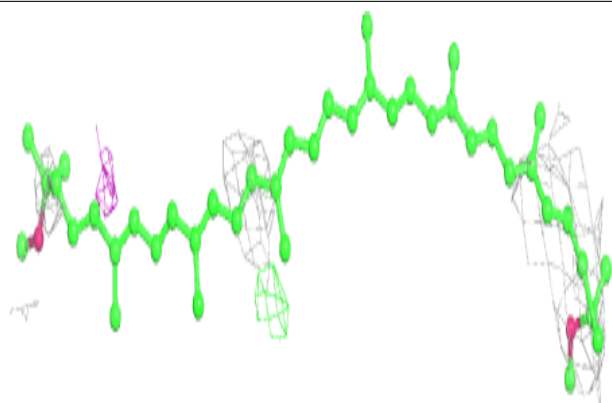
**Electron density around MQ8 M 404:**

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

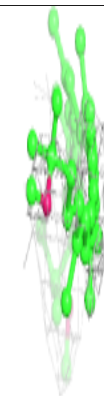
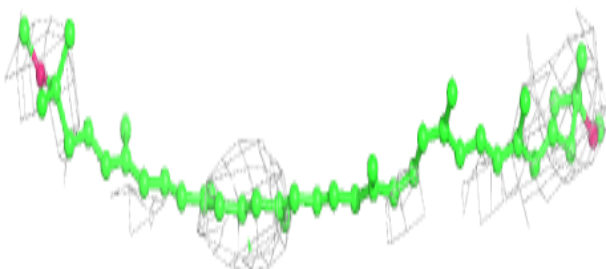
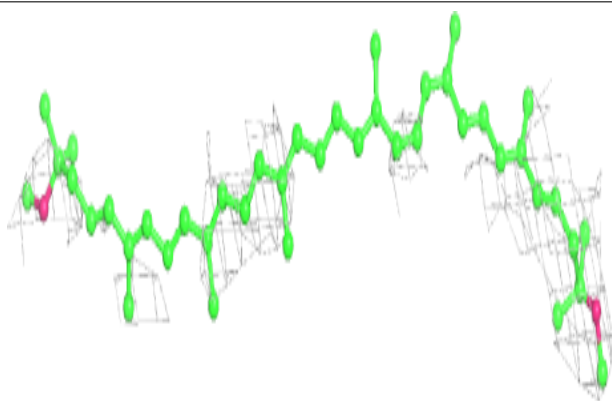


Electron density around CRT T 101:

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

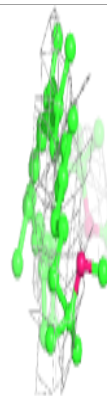
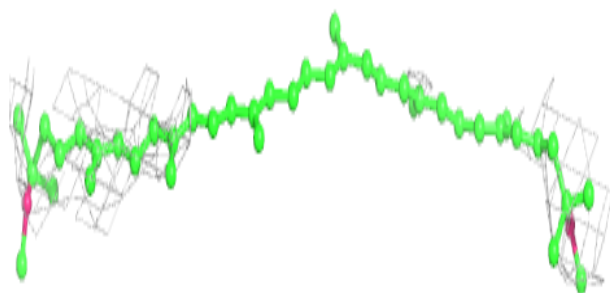
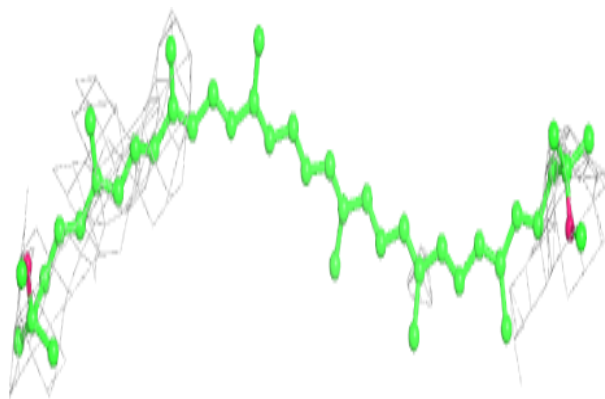
**Electron density around CRT AD 101:**

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

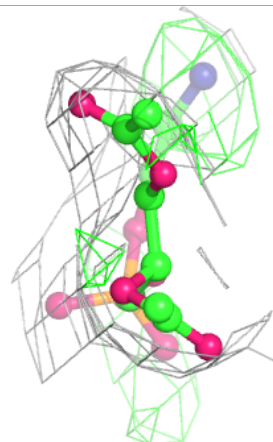
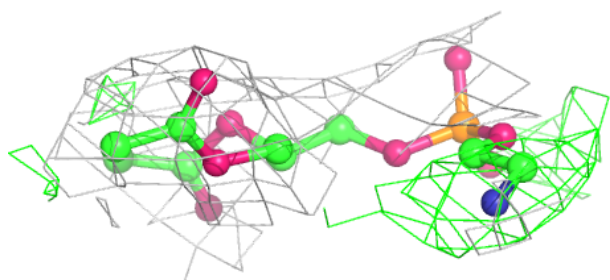
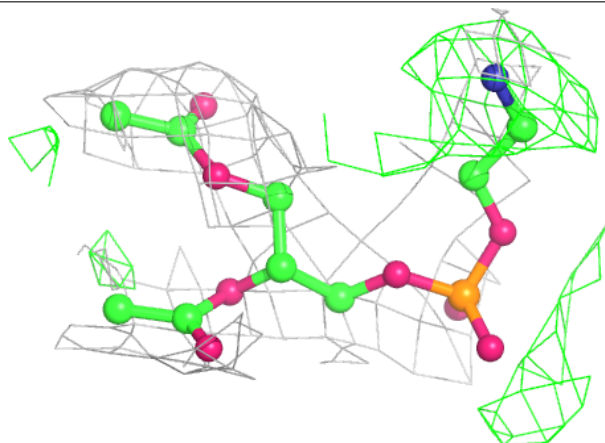


Electron density around CRT E 101:

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

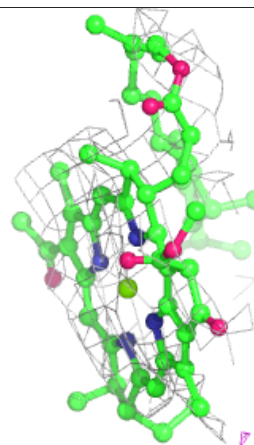
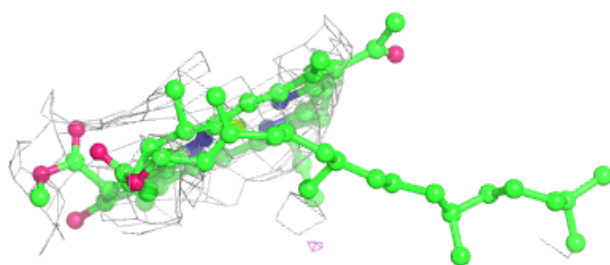
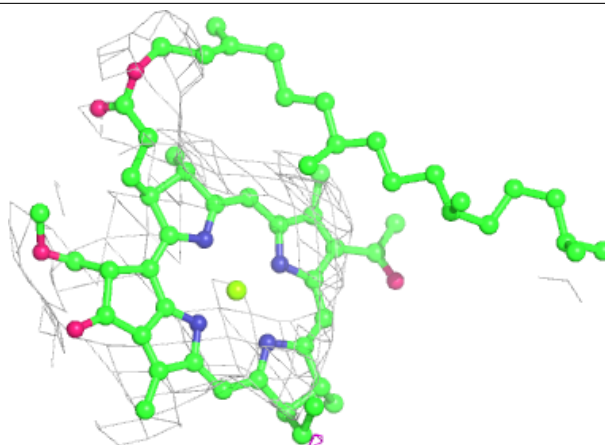
**Electron density around PEF A 101:**

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



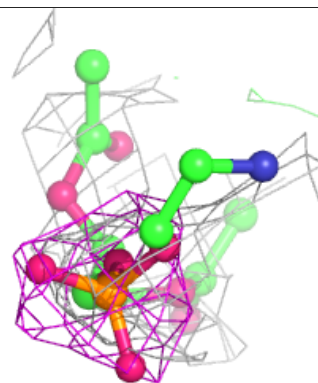
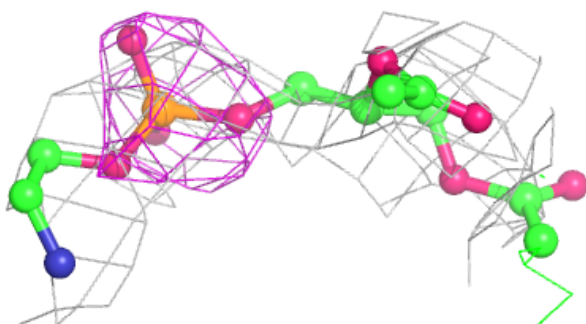
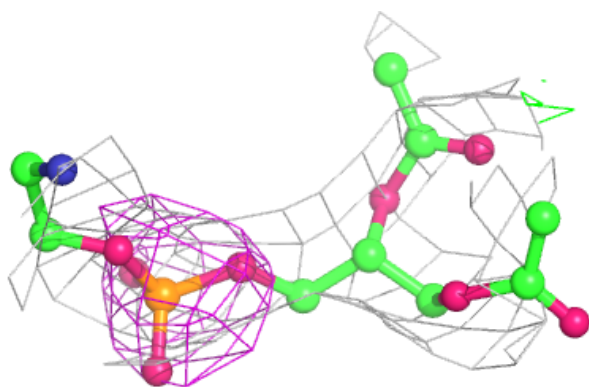
Electron density around BCL AC 103:

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

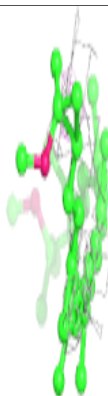
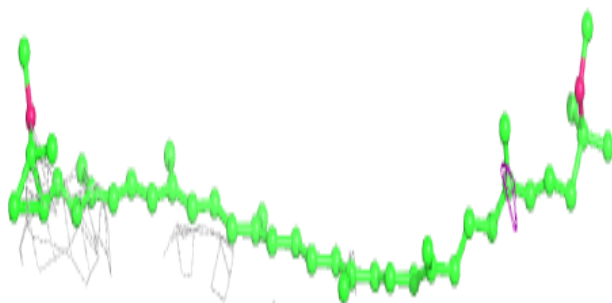
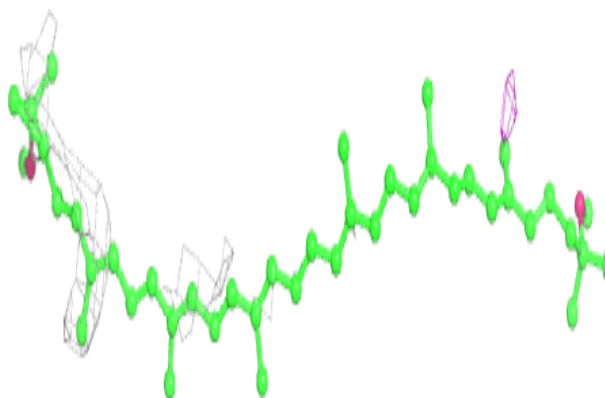


Electron density around PEF H 304:

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

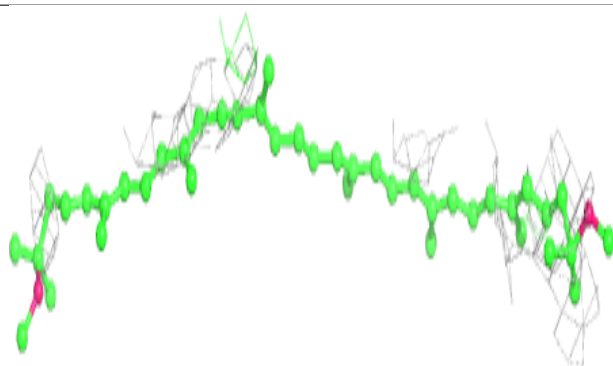
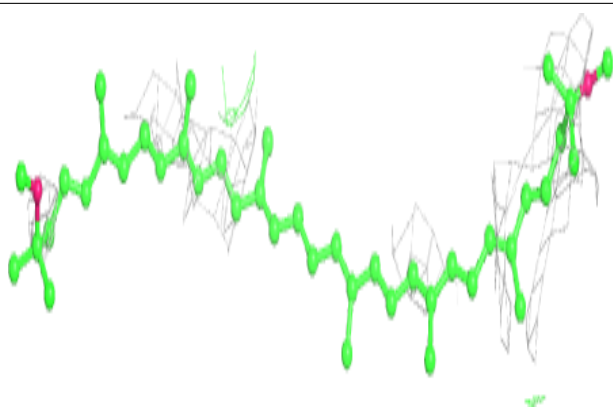
**Electron density around CRT G 101:**

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

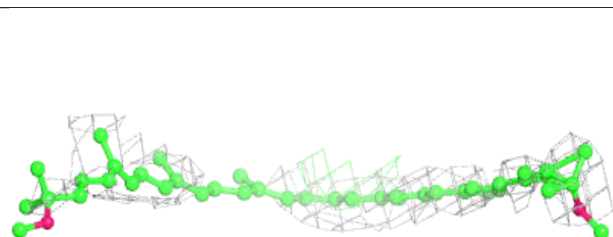
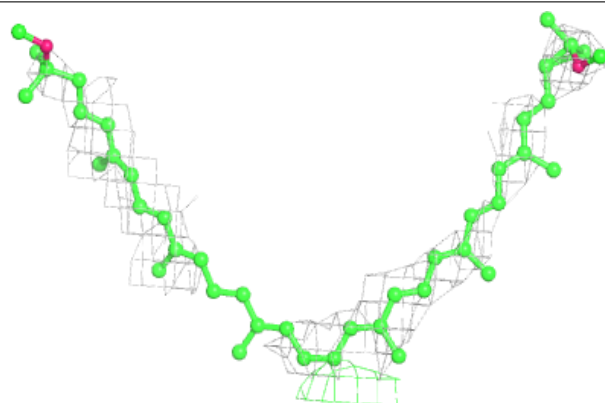


Electron density around CRT AH 102:

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

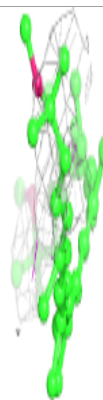
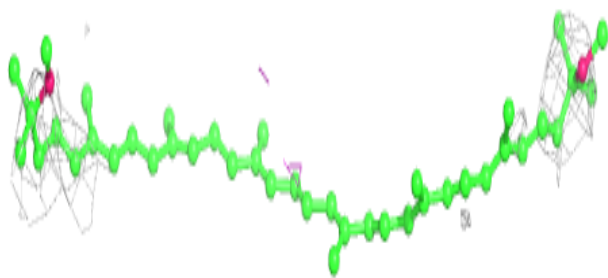
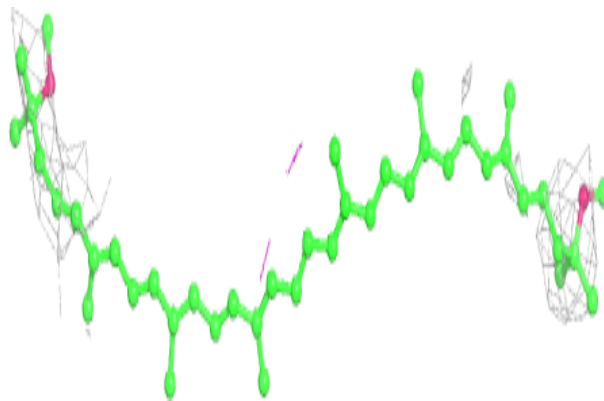
**Electron density around CRT M 405:**

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



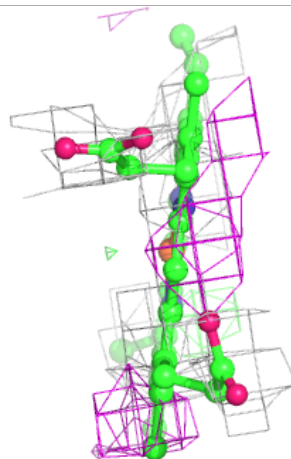
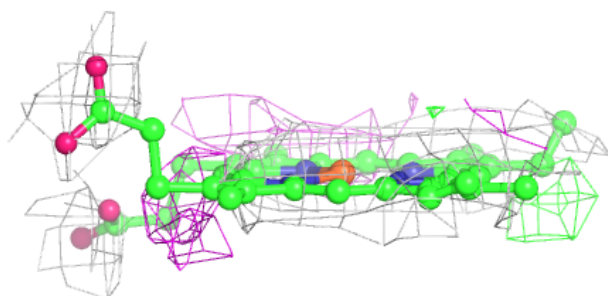
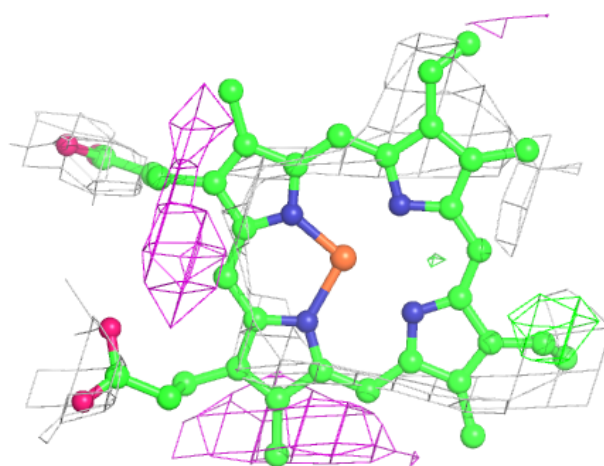
Electron density around CRT AL 101:

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



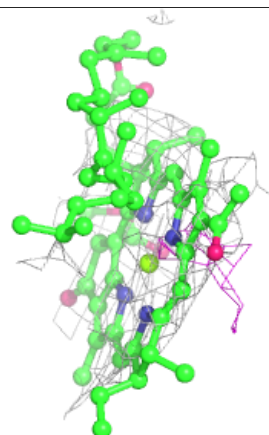
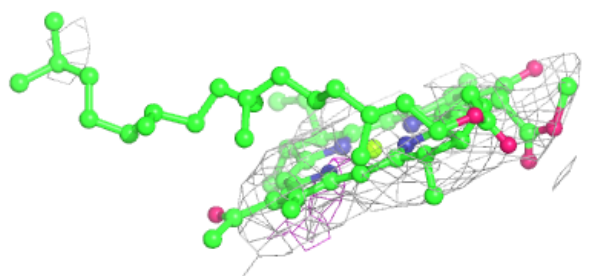
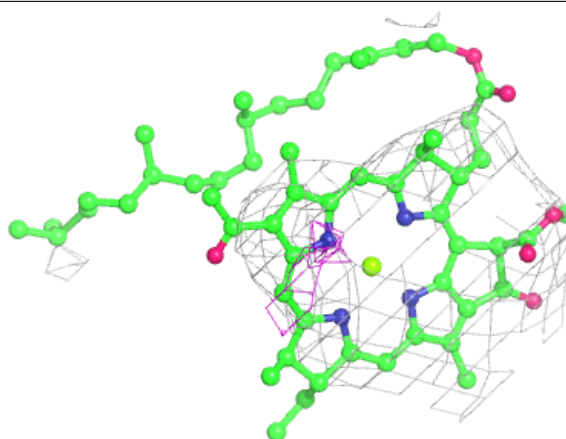
Electron density around HEM o 501:

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

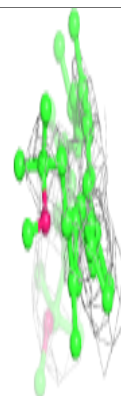
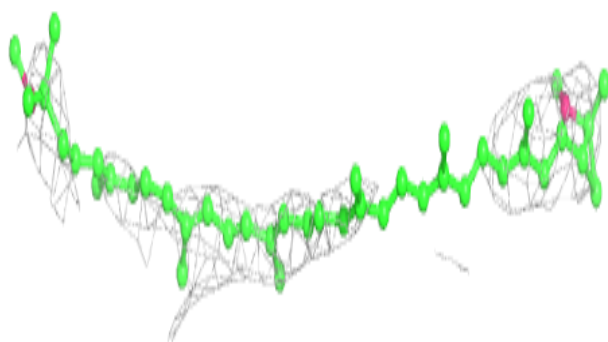
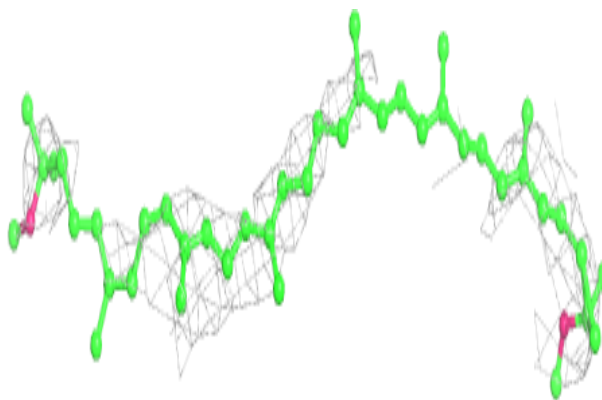


Electron density around BCL AB 102:

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

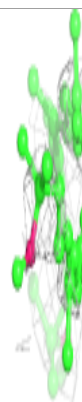
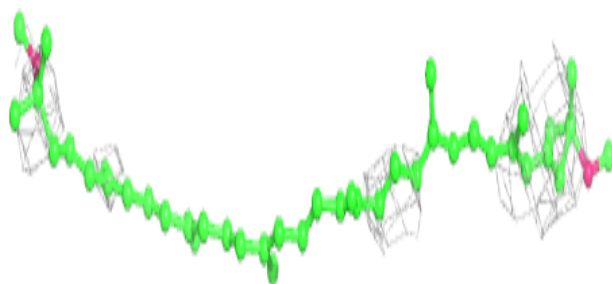
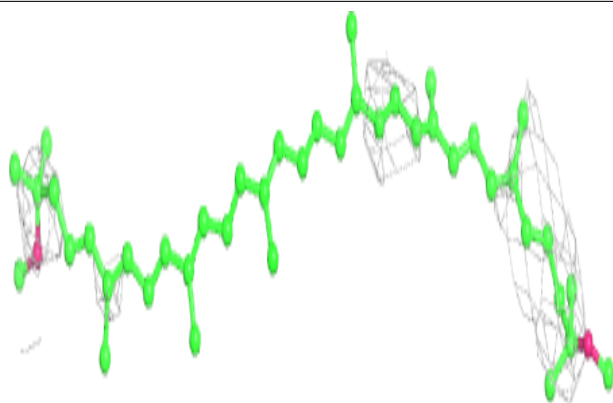
**Electron density around CRT 4 101:**

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

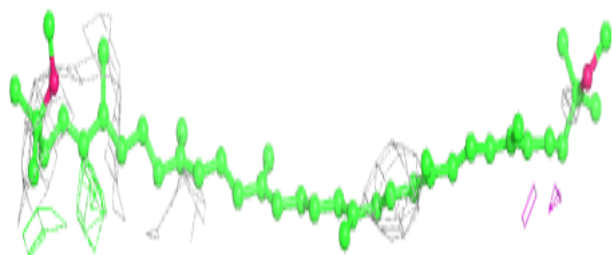
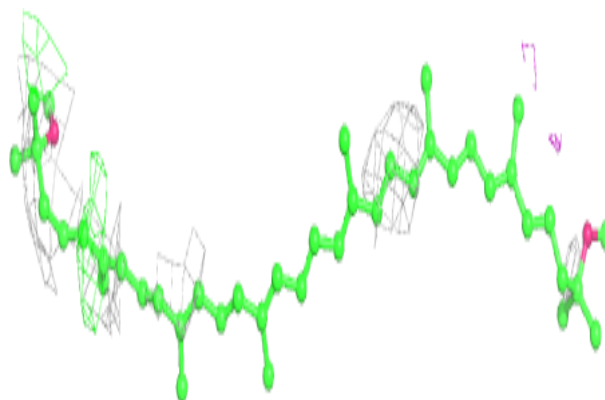


Electron density around CRT V 101:

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

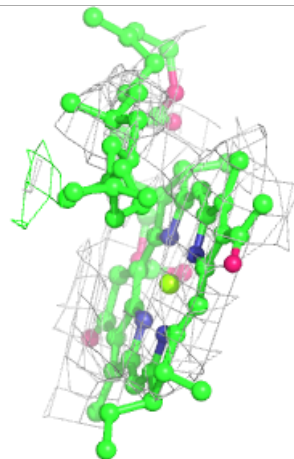
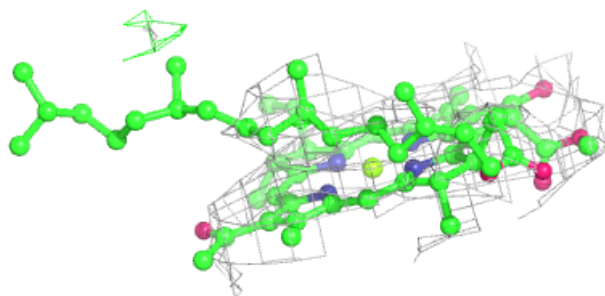
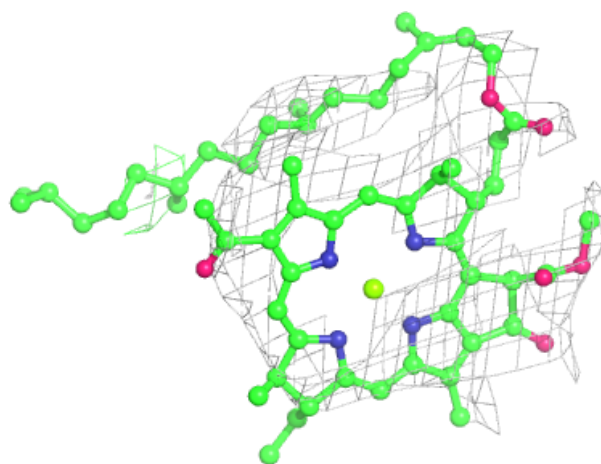
**Electron density around CRT e 101:**

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



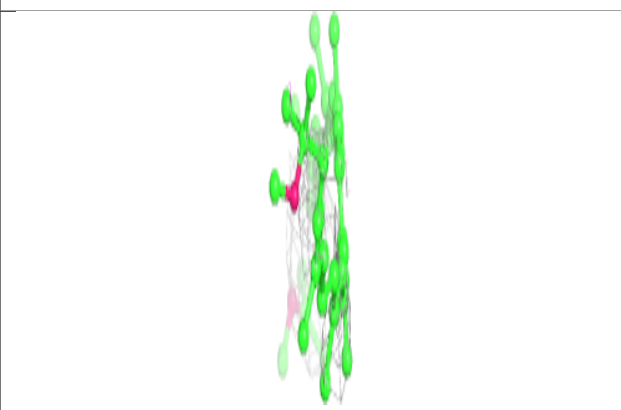
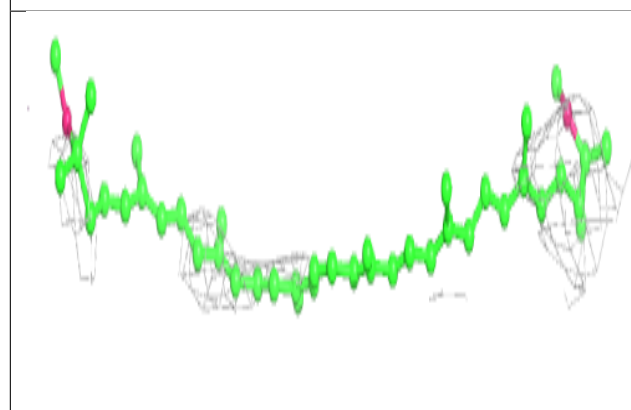
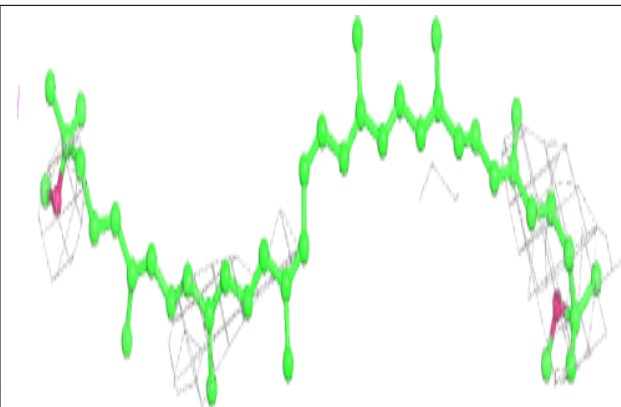
Electron density around BCL AG 101:

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

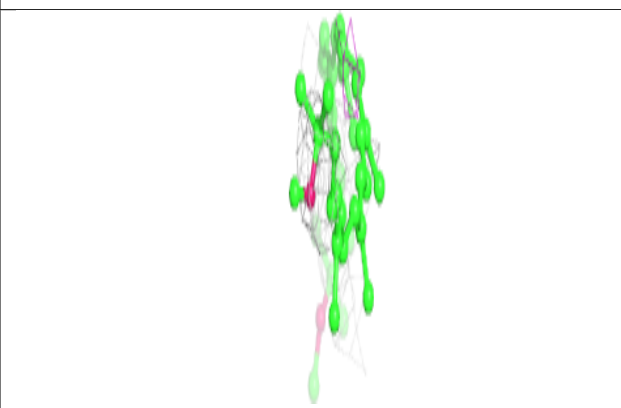
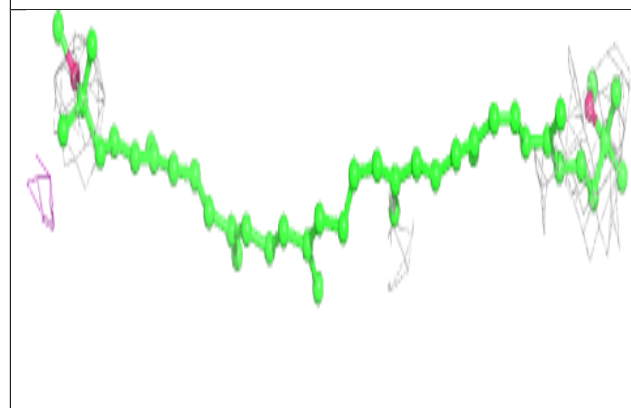
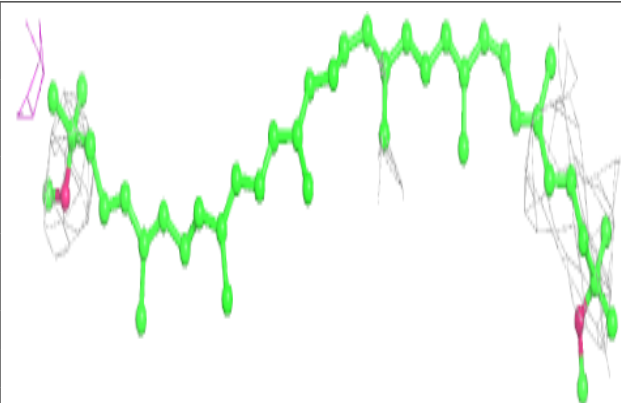


Electron density around CRT k 101:

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

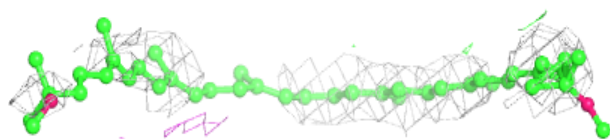
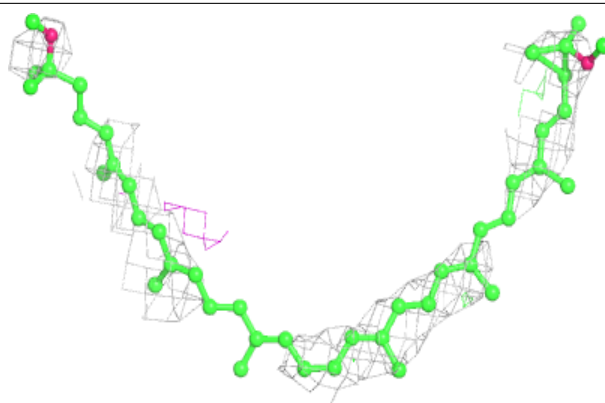
**Electron density around CRT AJ 101:**

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

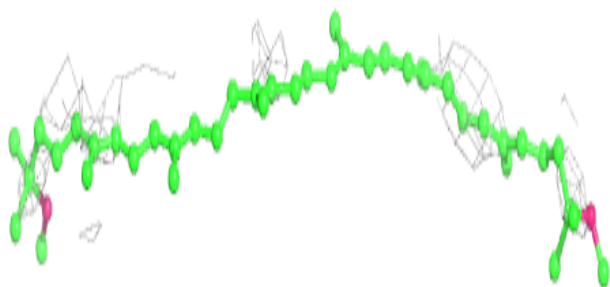
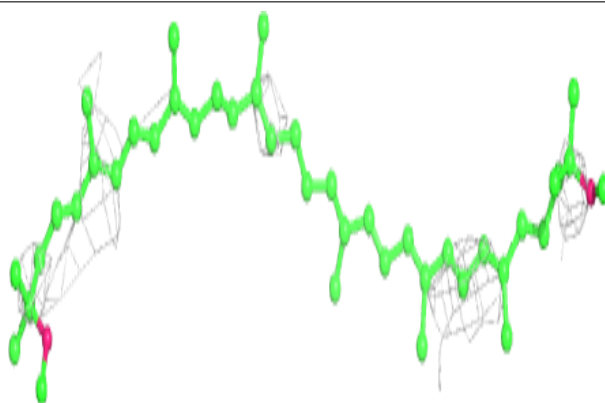


Electron density around CRT y 404:

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

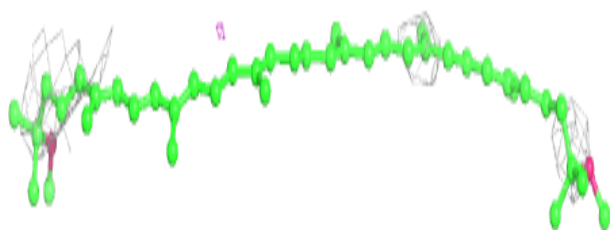
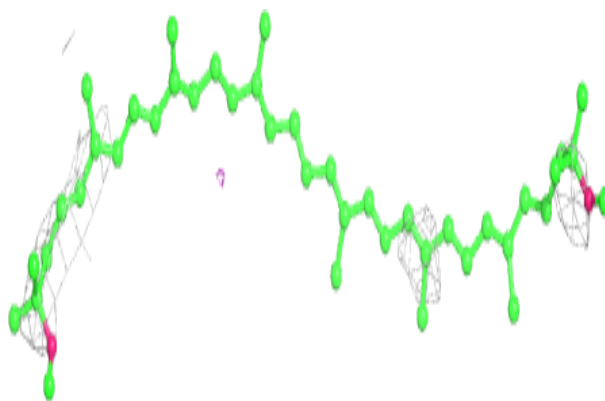
**Electron density around CRT Z 101:**

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

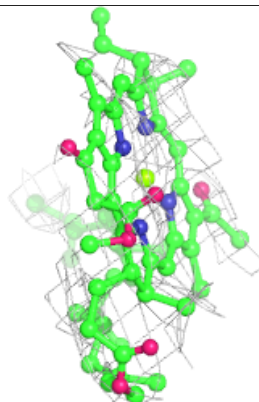
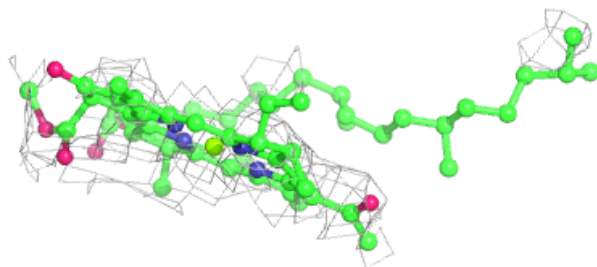
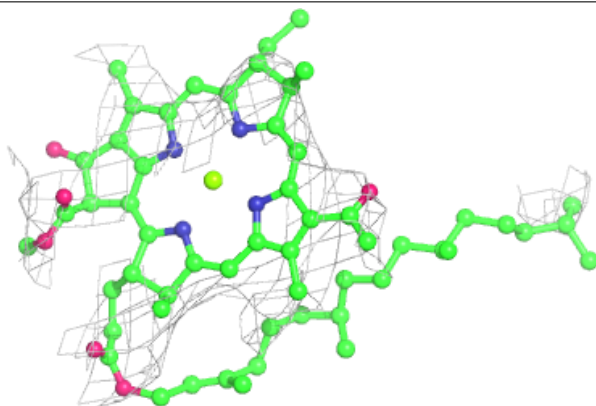


Electron density around CRT 2 101:

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

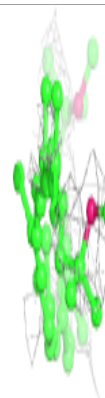
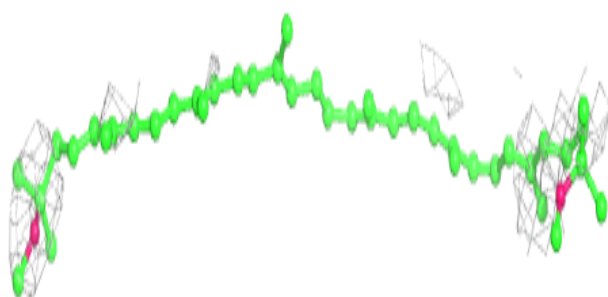
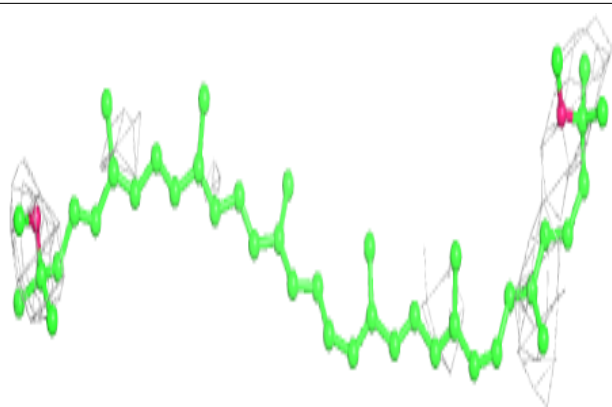
**Electron density around BCL AE 102:**

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

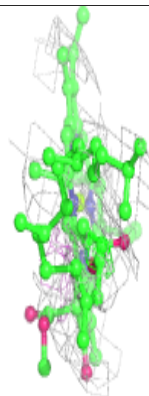
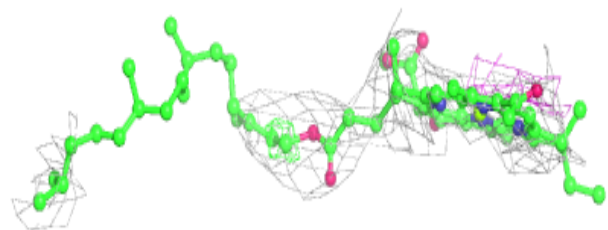
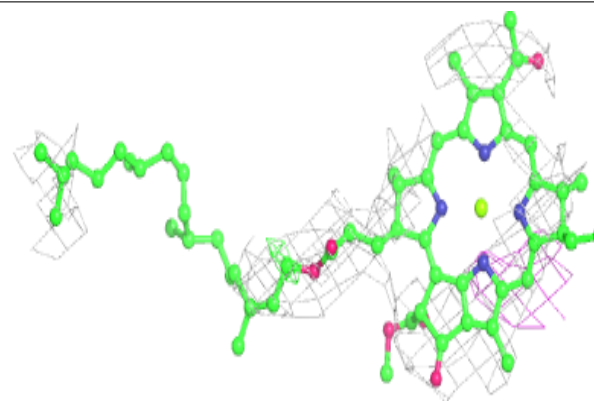


Electron density around CRT X 101:

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

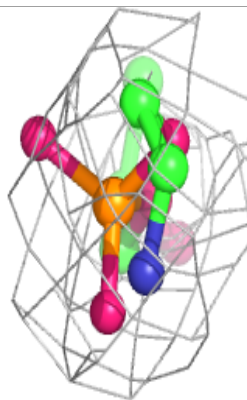
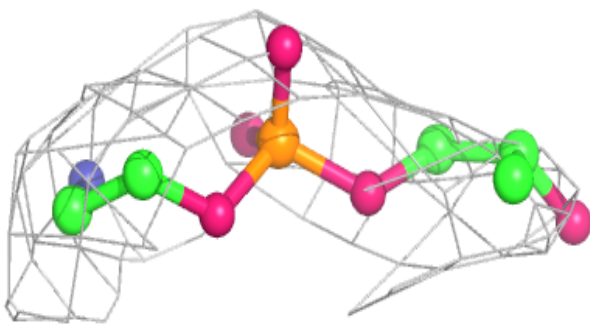
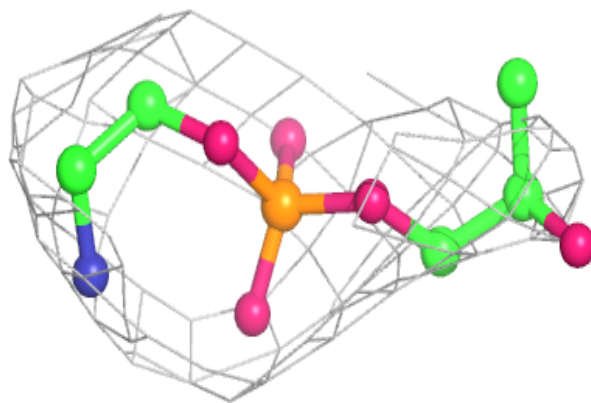
**Electron density around BCL D 101:**

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

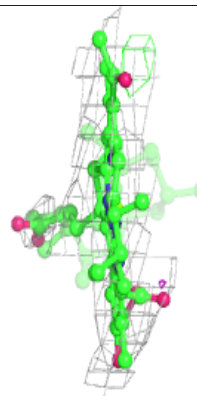
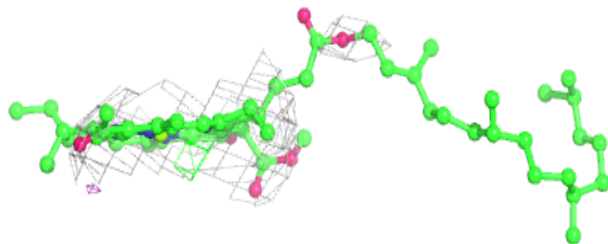
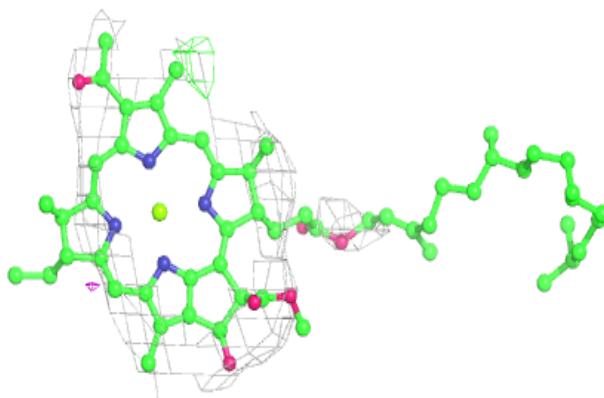


Electron density around PEF L 305:

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

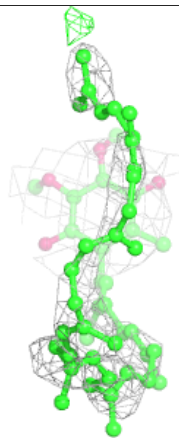
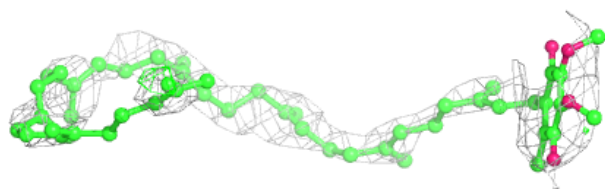
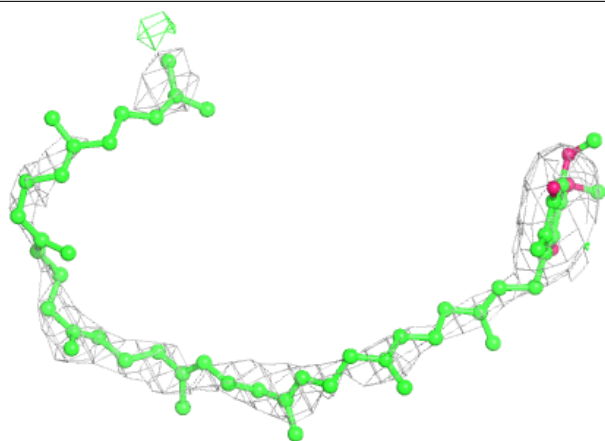
**Electron density around BCL K 101:**

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



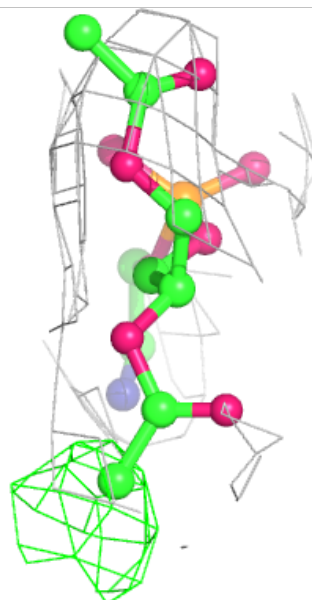
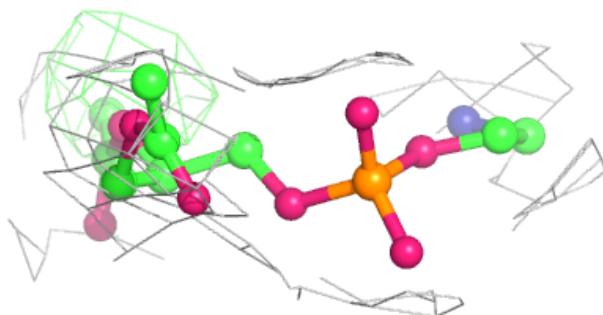
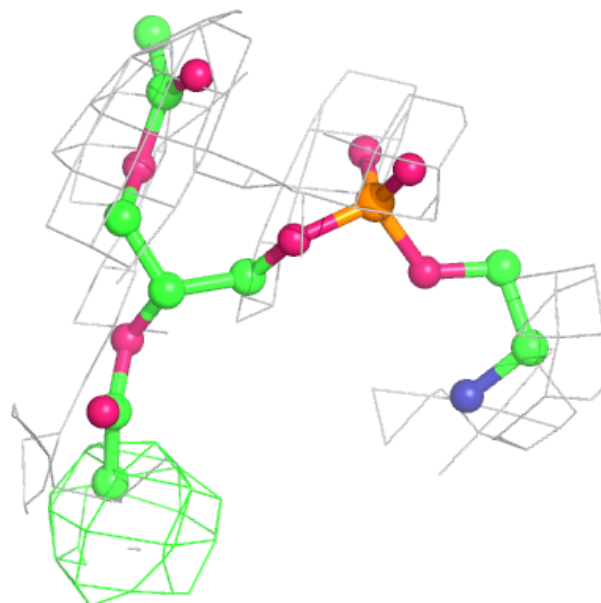
Electron density around UQ8 L 304:

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



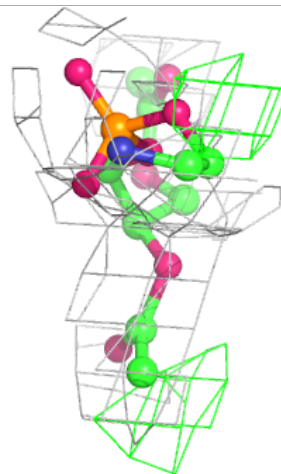
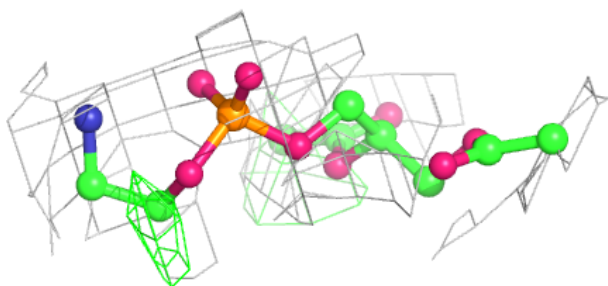
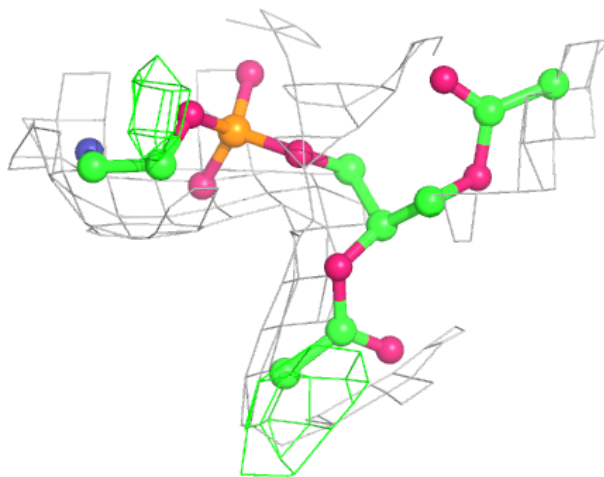
Electron density around PEF y 406:

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



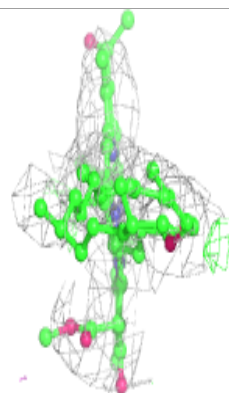
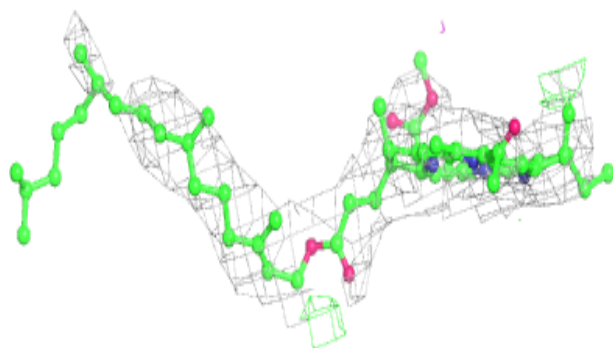
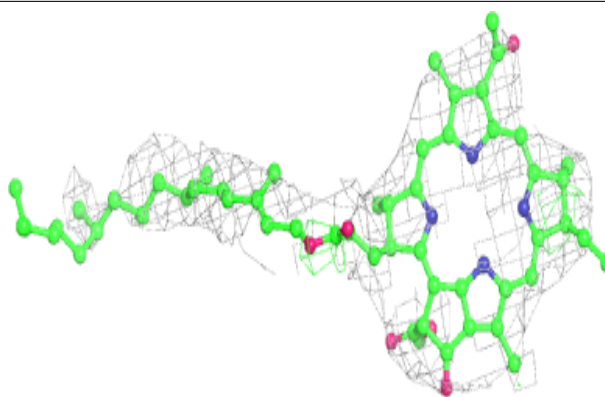
Electron density around PEF H 302:

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



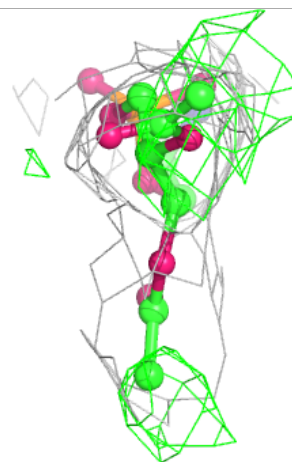
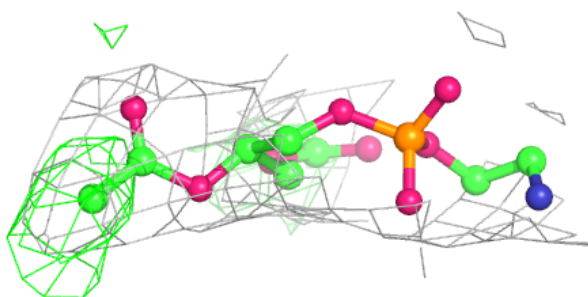
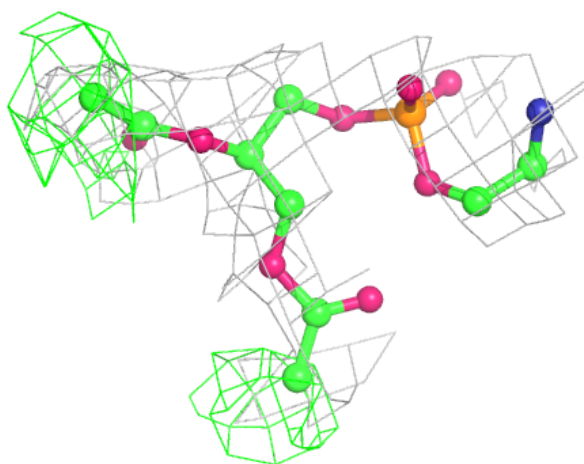
Electron density around BPH y 402:

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



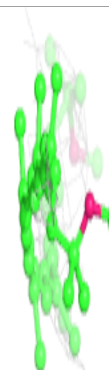
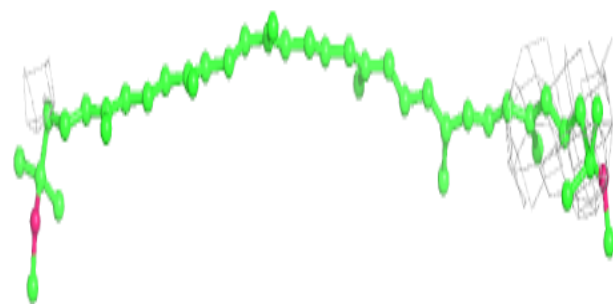
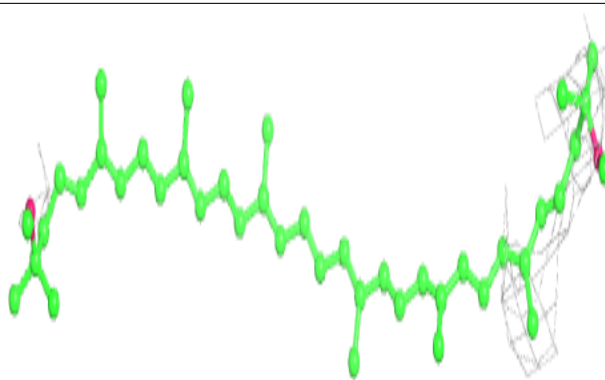
Electron density around PEF m 101:

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



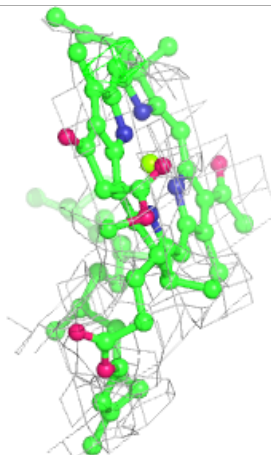
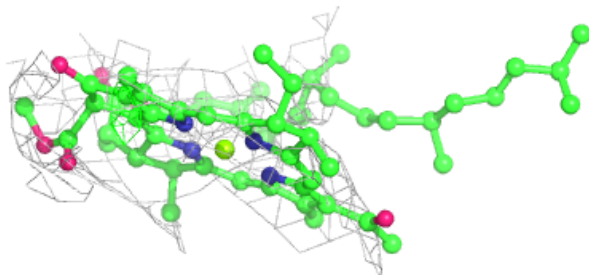
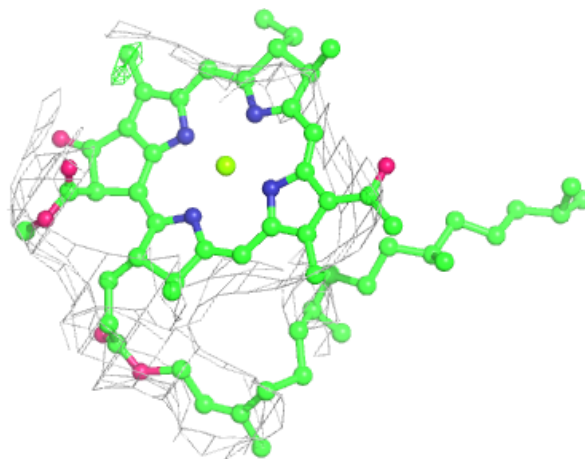
Electron density around CRT s 101:

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



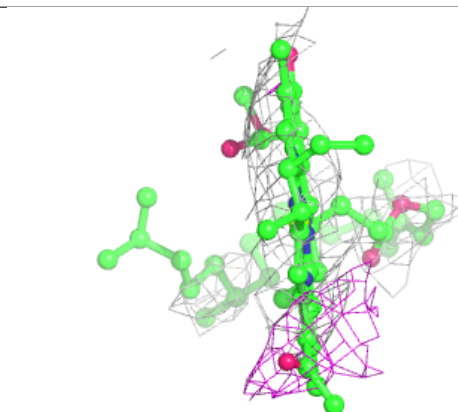
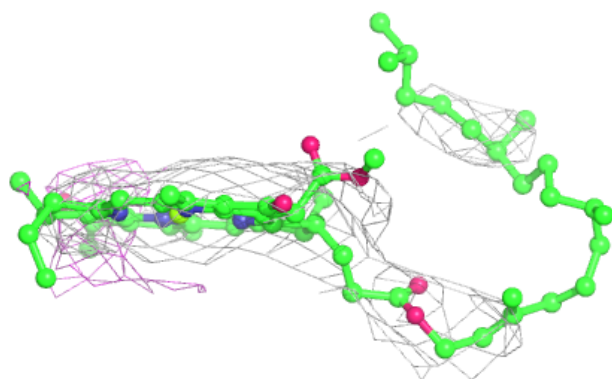
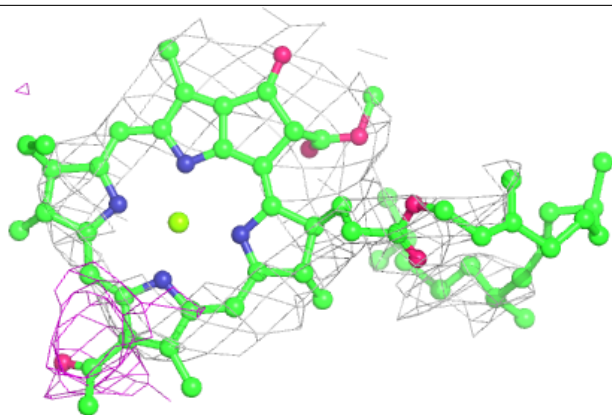
Electron density around BCL 6 101:

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

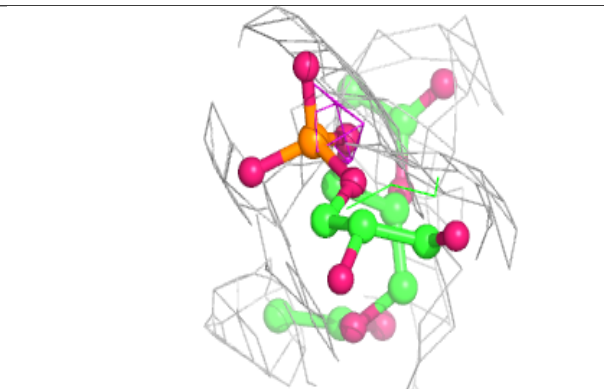
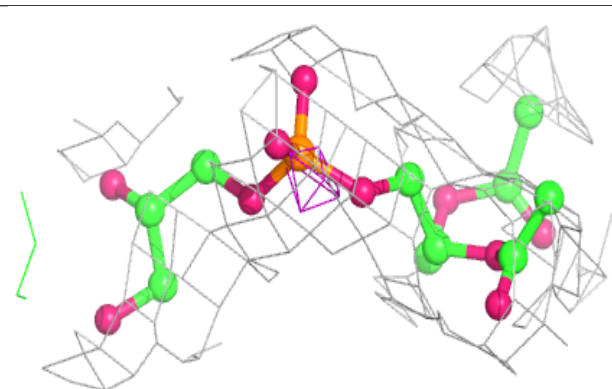
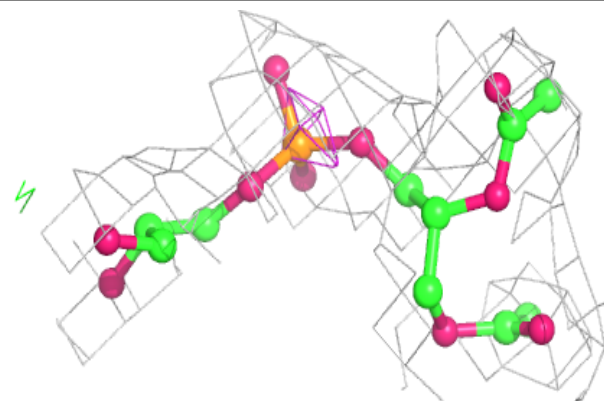


Electron density around BCL AC 102:

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

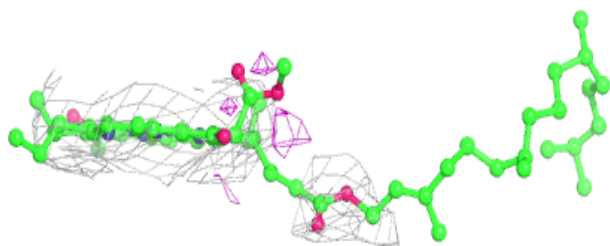
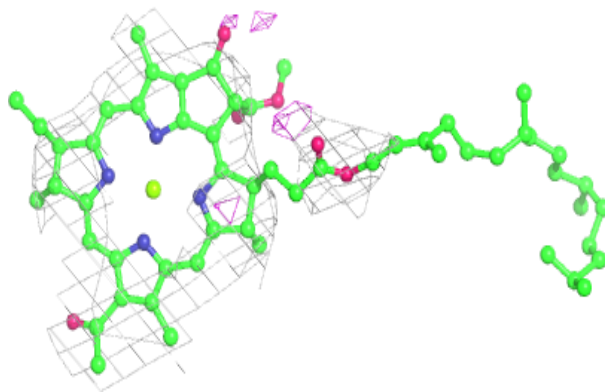
**Electron density around PGW S 101:**

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



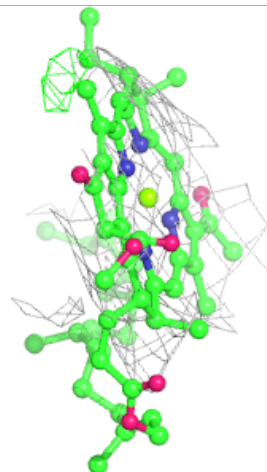
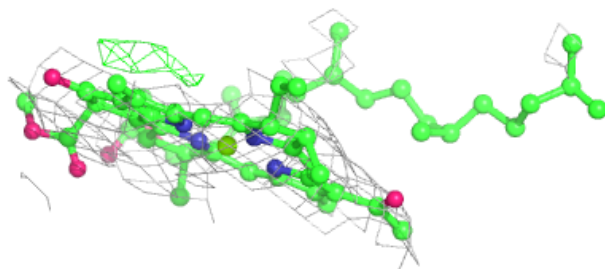
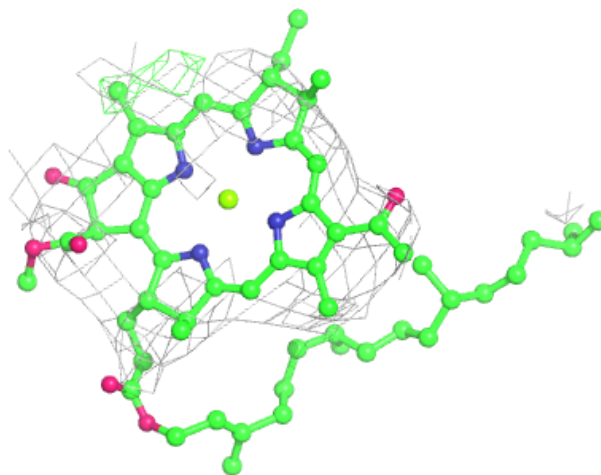
Electron density around BCL m 102:

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



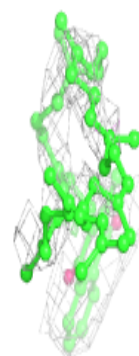
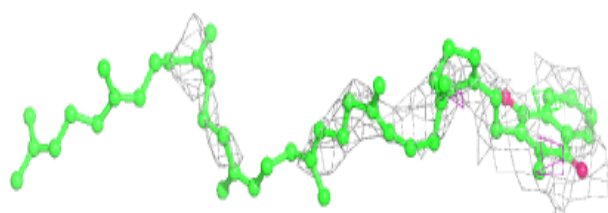
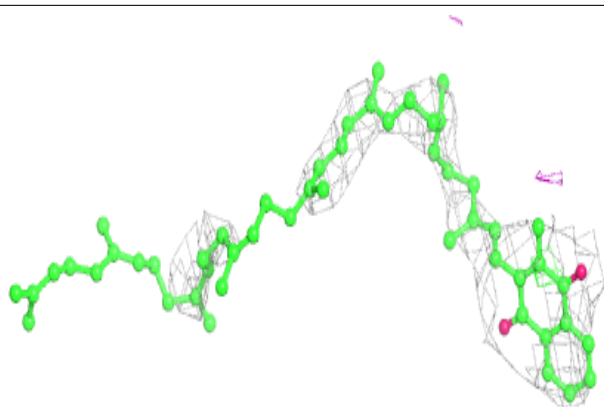
Electron density around BCL z 102:

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

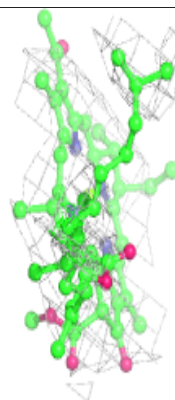
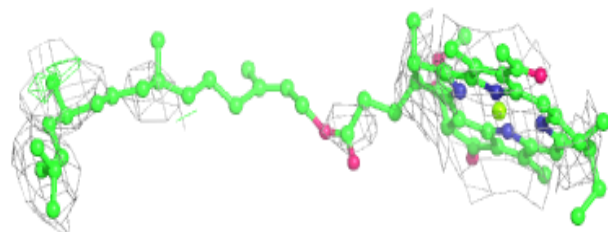
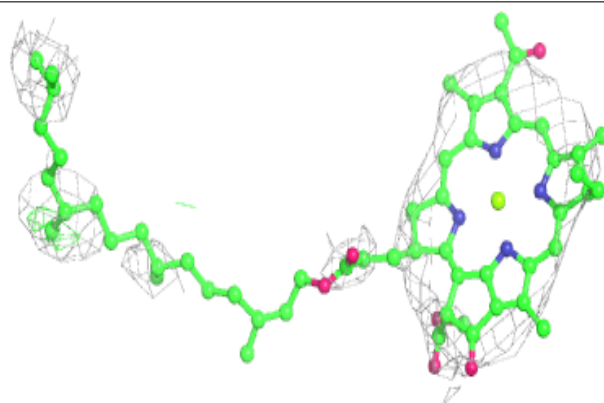


Electron density around MQ8 y 403:

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

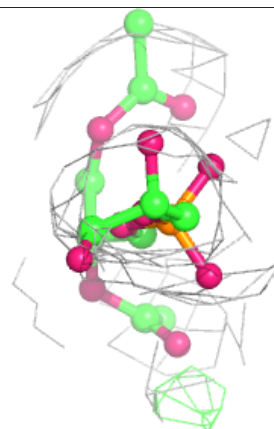
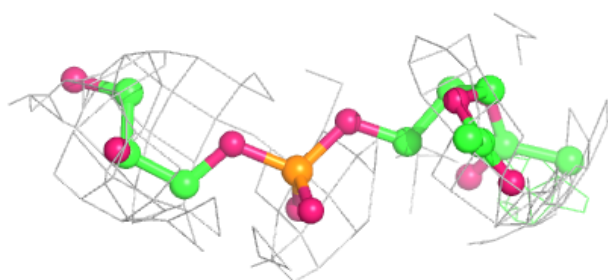
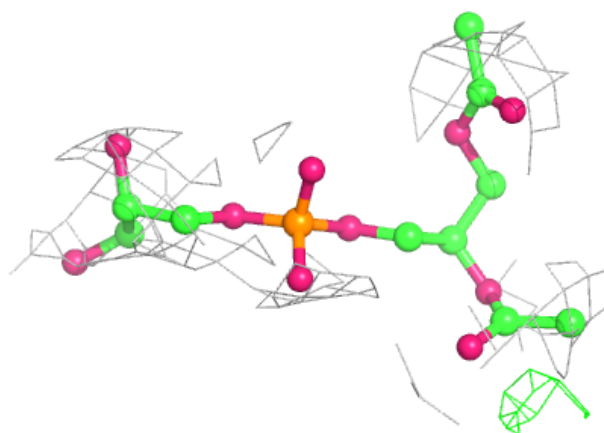
**Electron density around BCL d 101:**

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

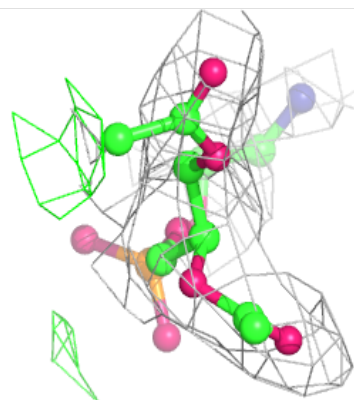
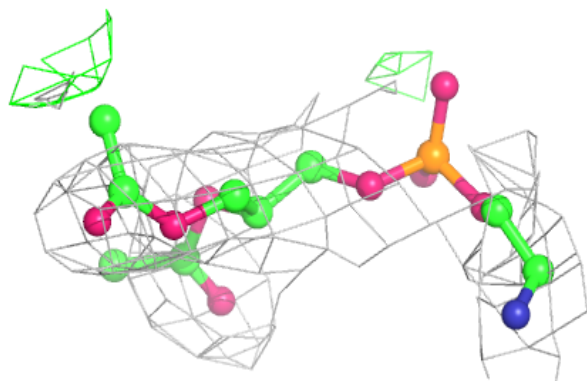
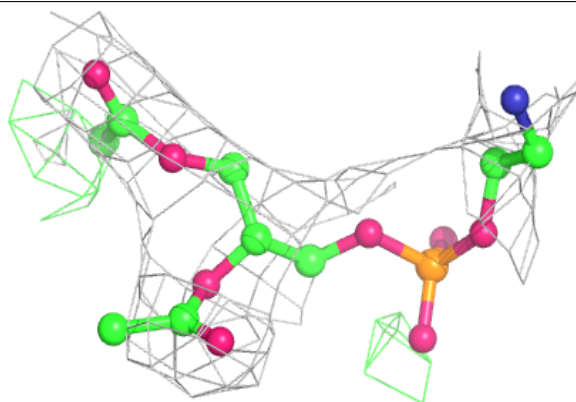


Electron density around PGW AE 101:

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

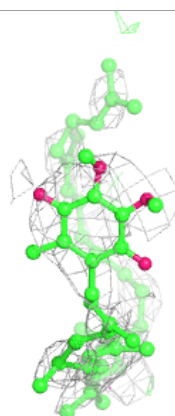
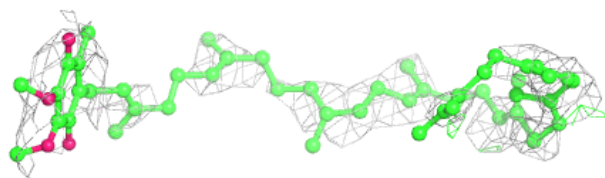
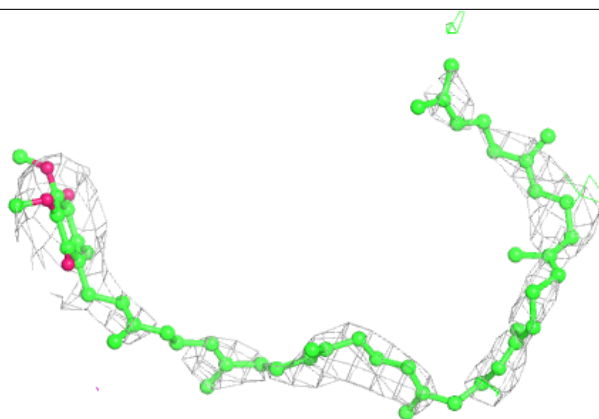
**Electron density around PEF y 407:**

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



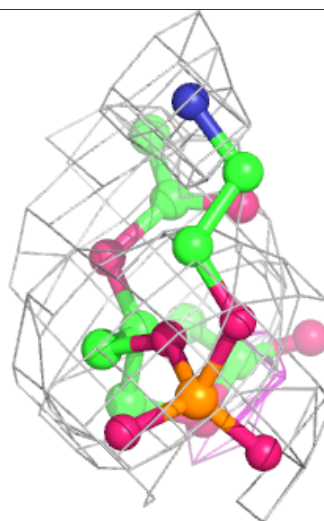
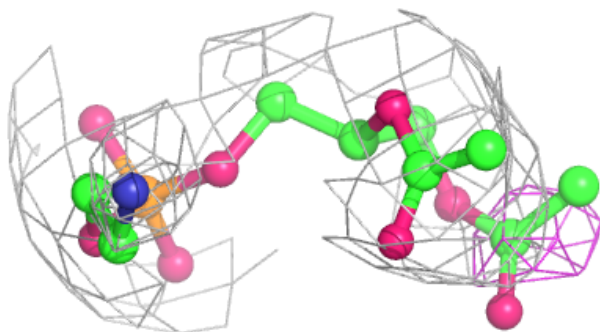
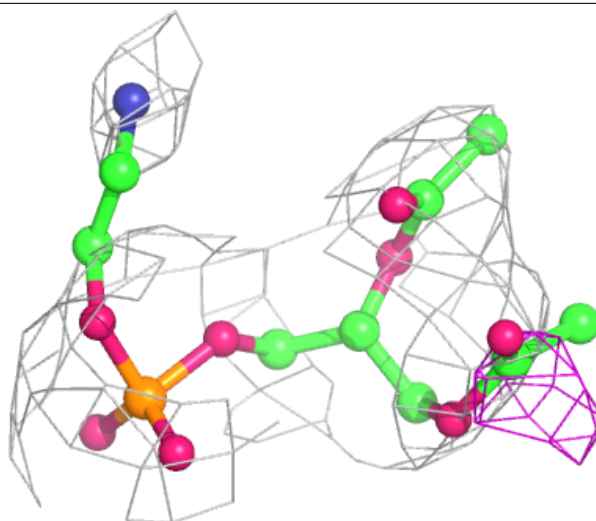
Electron density around UQ8 x 304:

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



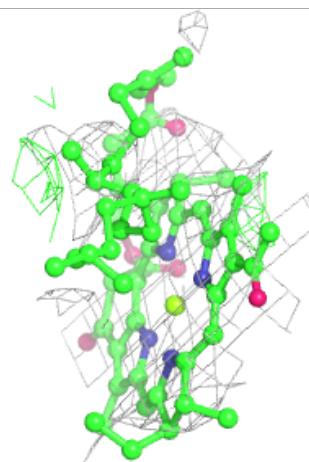
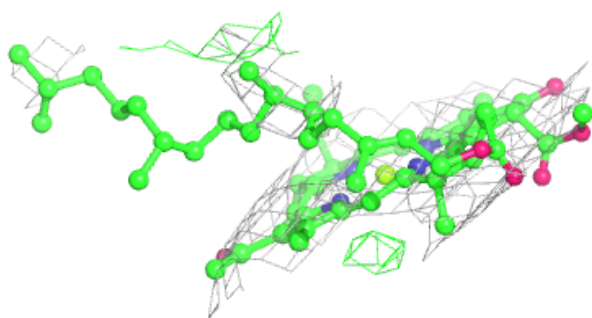
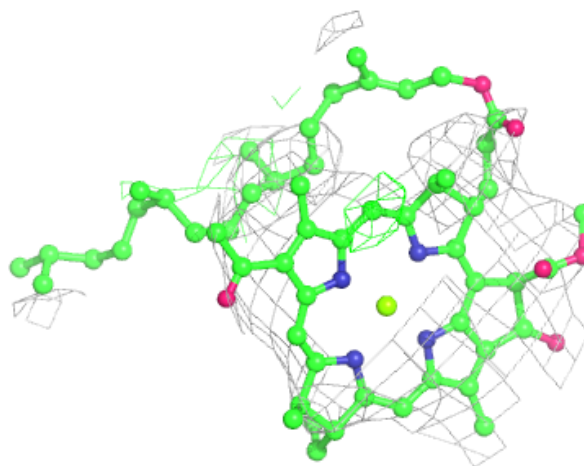
Electron density around PEF M 408:

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



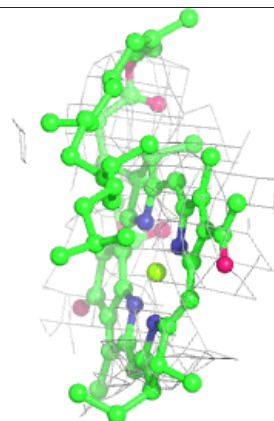
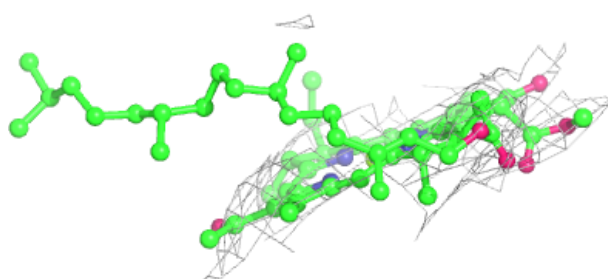
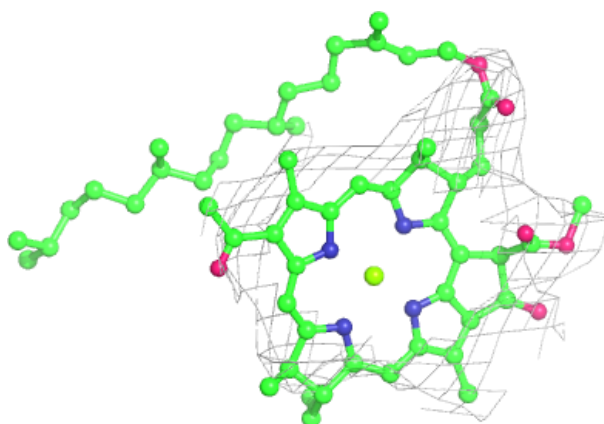
Electron density around BCL I 103:

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

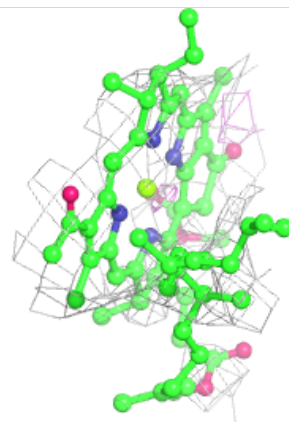
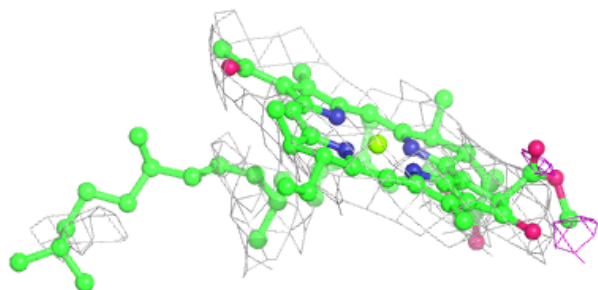
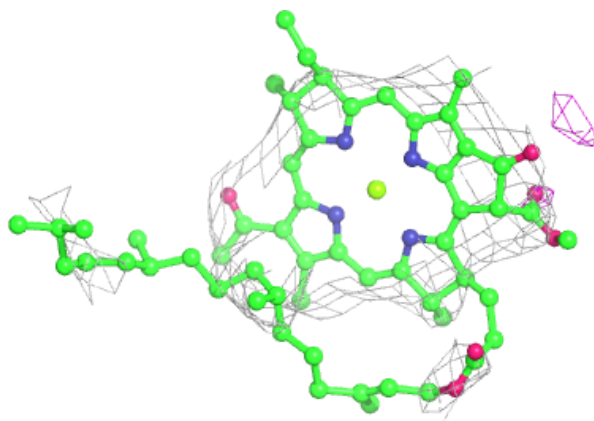


Electron density around BCL 0 102:

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

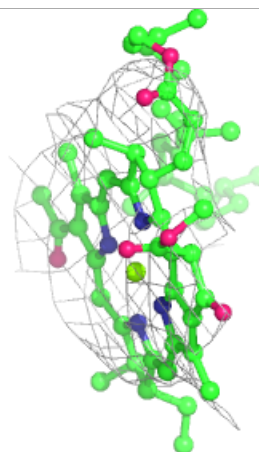
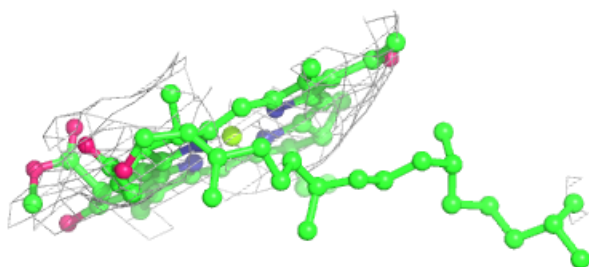
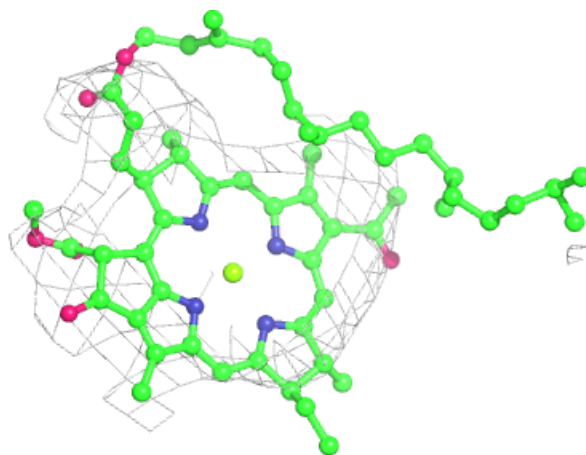
**Electron density around BCL g 102:**

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



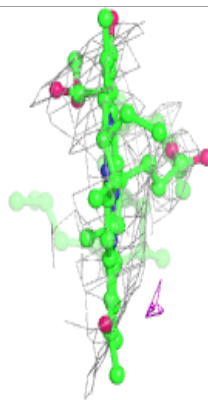
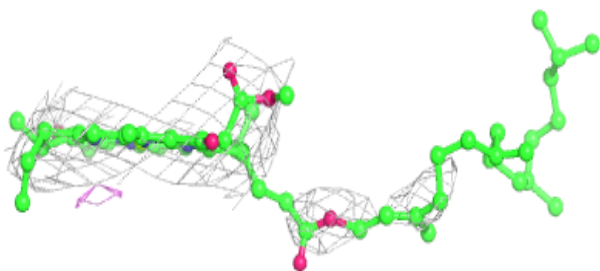
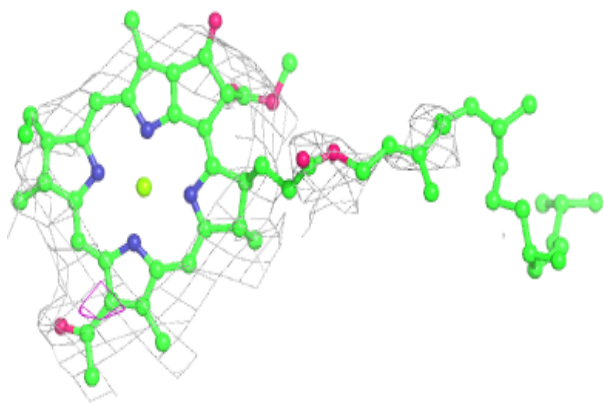
Electron density around BCL N 101:

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

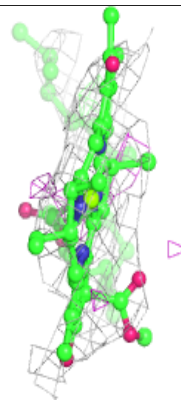
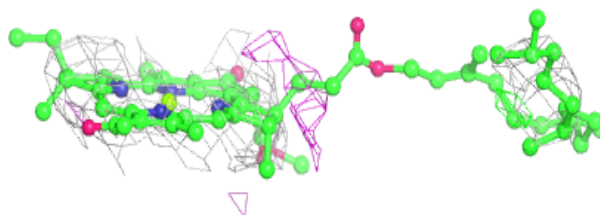
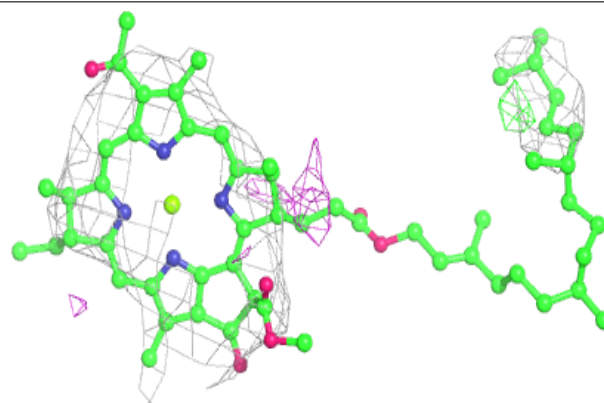


Electron density around BCL j 101:

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

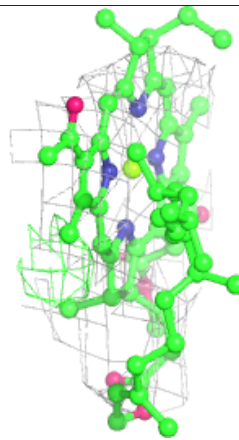
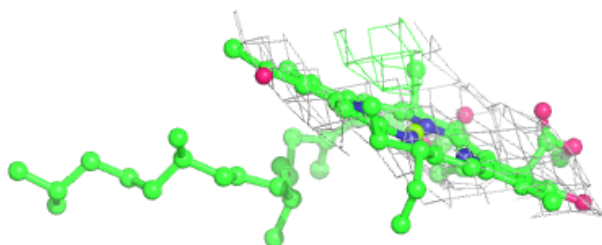
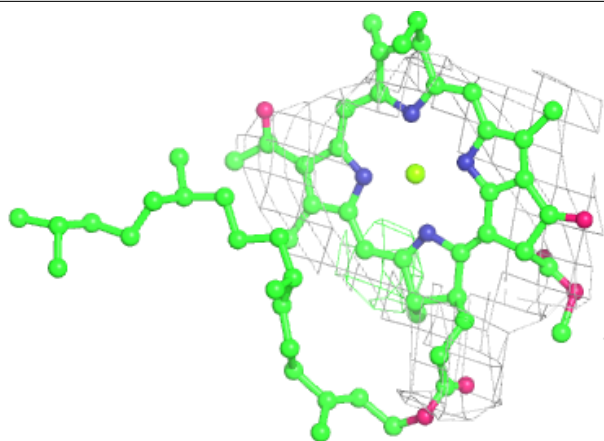
**Electron density around BCL f 101:**

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

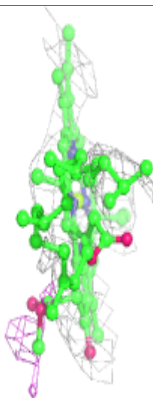
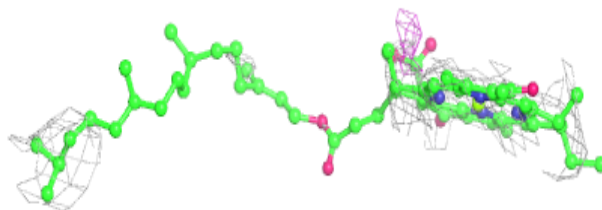
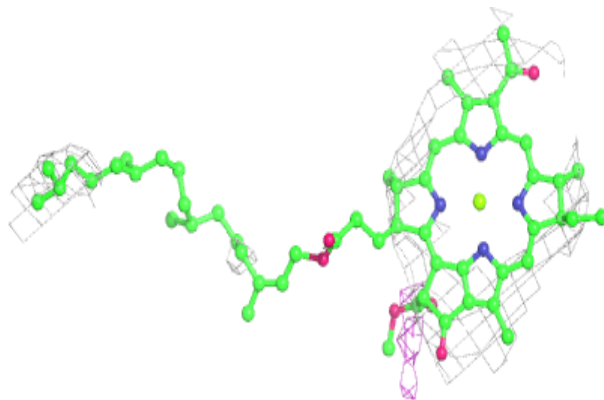


Electron density around BCL D 102:

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

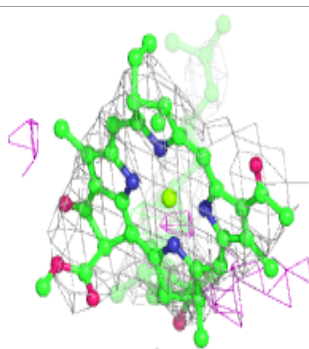
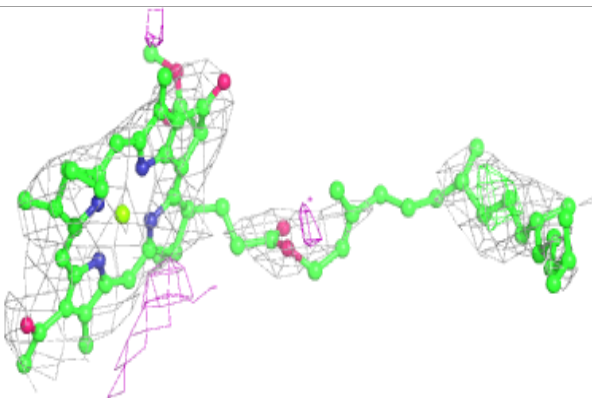
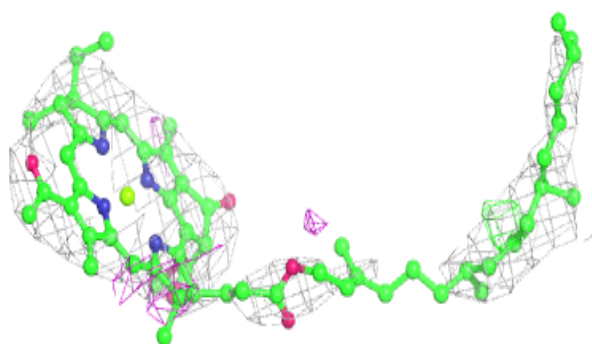
**Electron density around BCL p 102:**

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

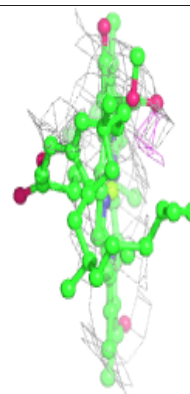
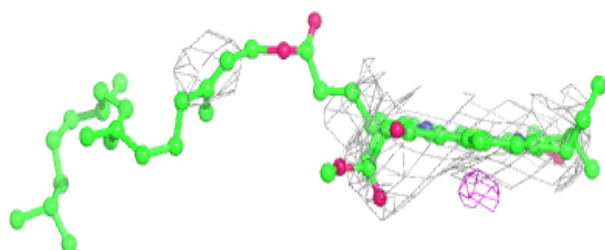
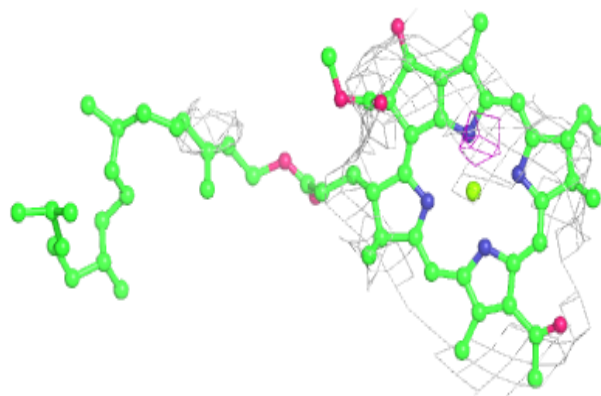


Electron density around BCL y 401:

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

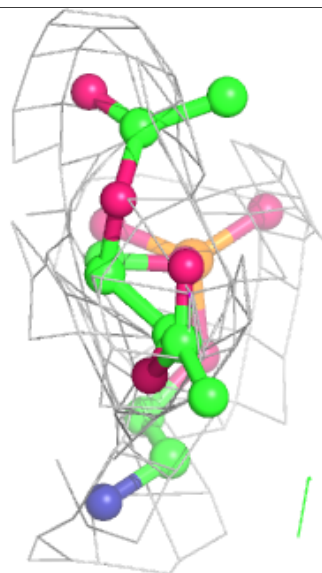
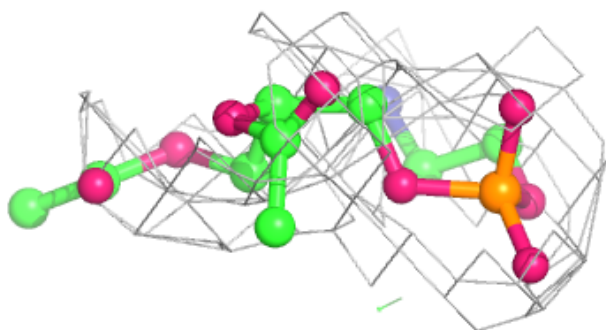
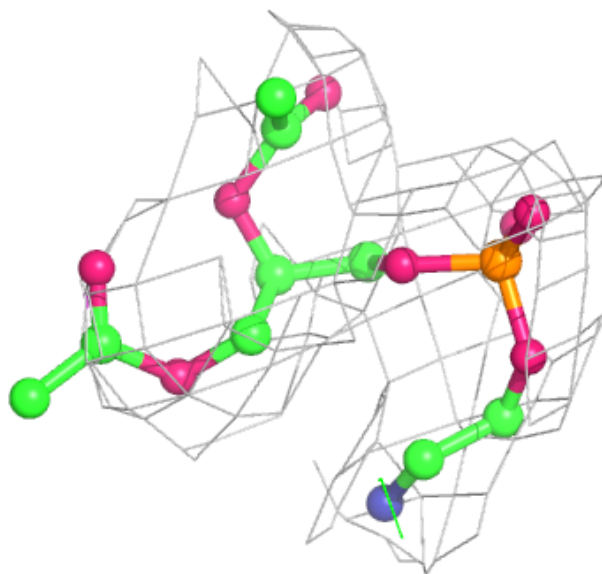
**Electron density around BCL 7 102:**

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



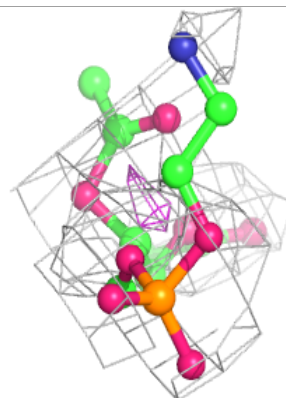
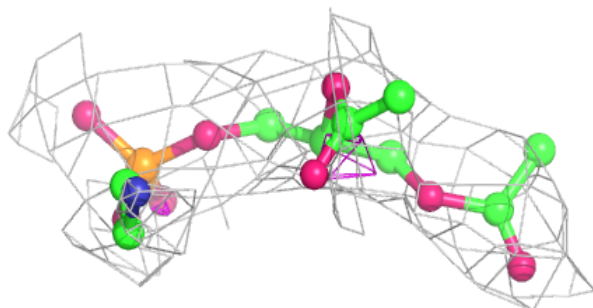
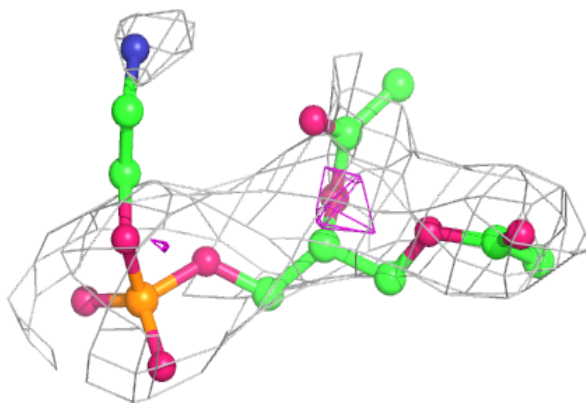
Electron density around PEF x 306:

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

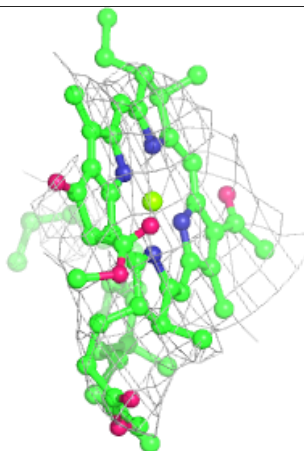
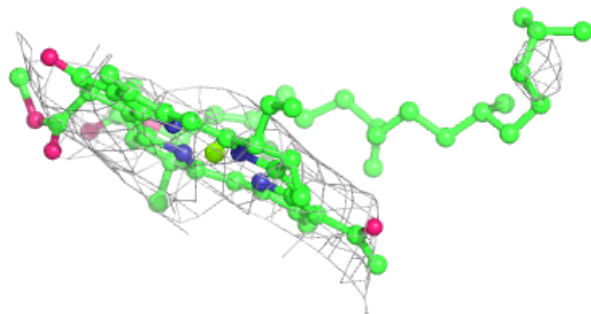
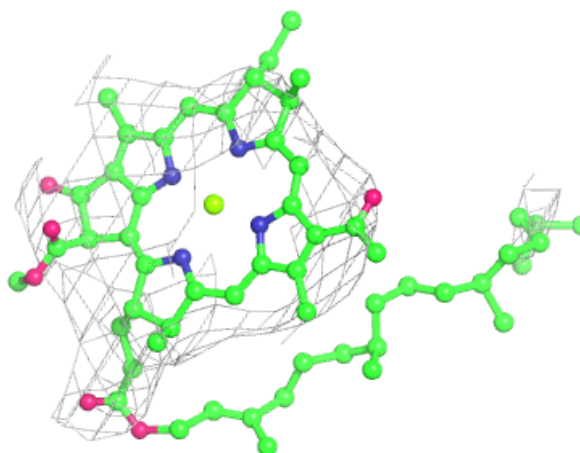


Electron density around PEF y 408:

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

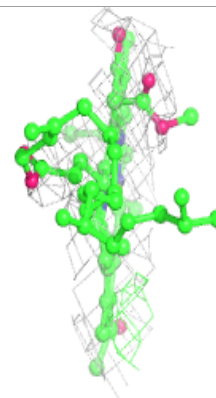
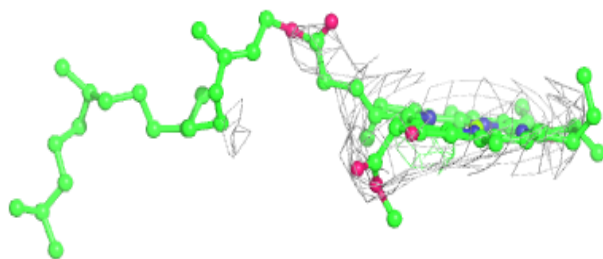
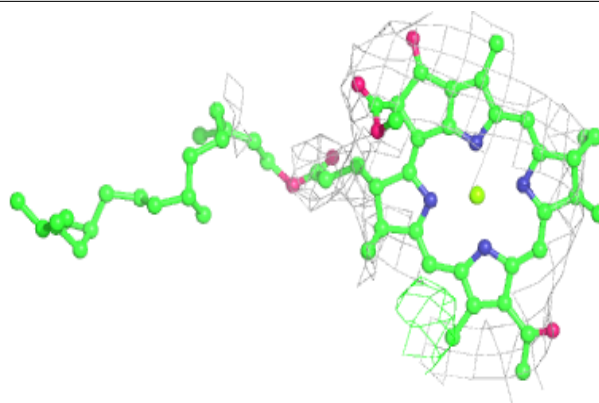
**Electron density around BCL O 102:**

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

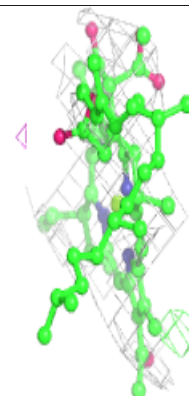
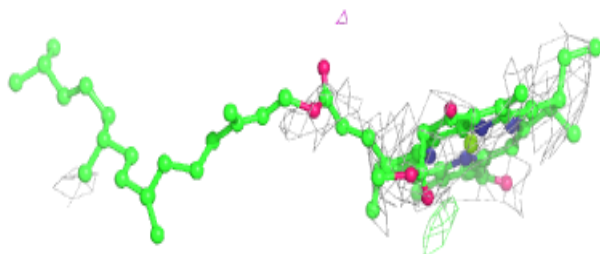
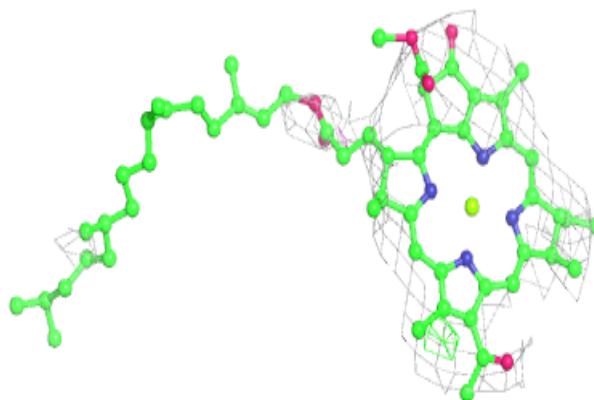


Electron density around BCL F 101:

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

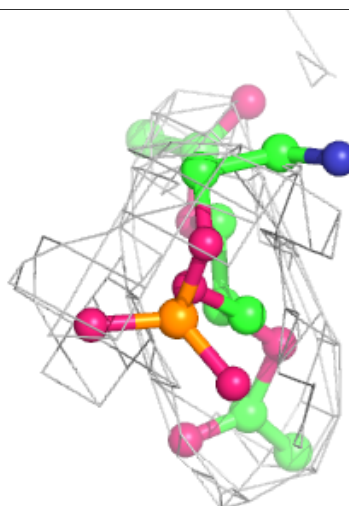
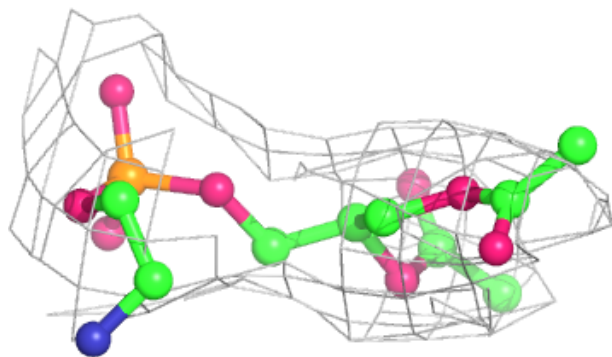
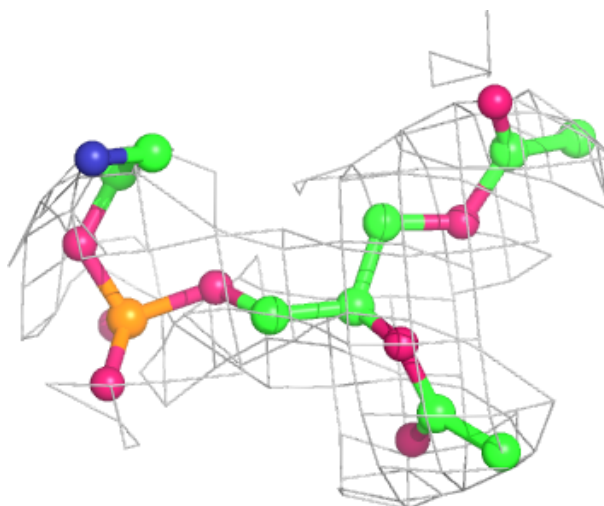
**Electron density around BCL u 101:**

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



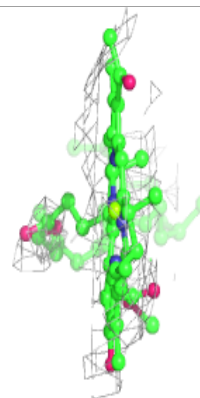
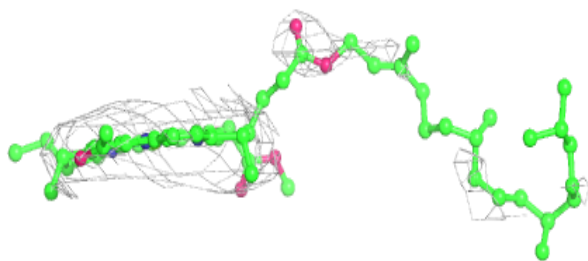
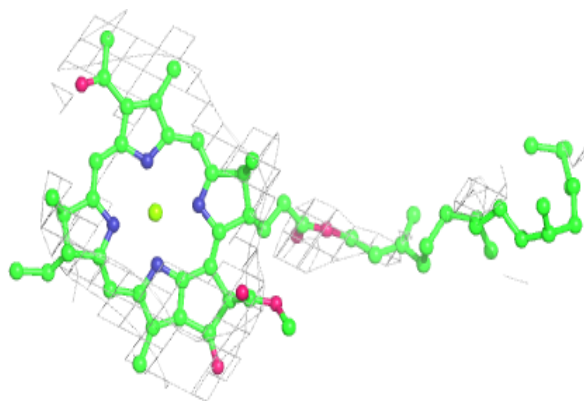
Electron density around PEF H 301:

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

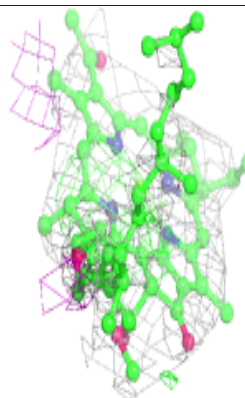
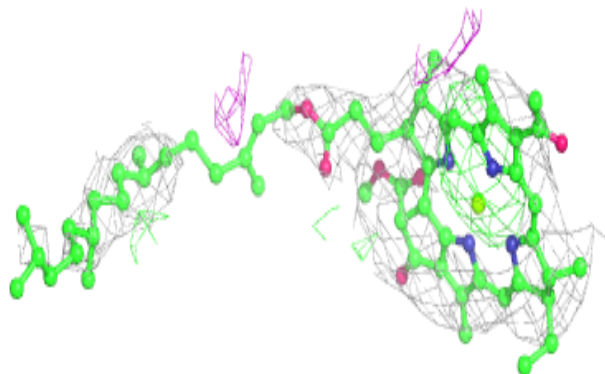
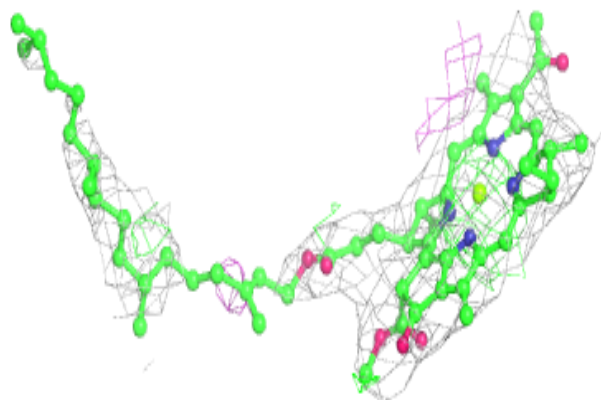


Electron density around BCL A 102:

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

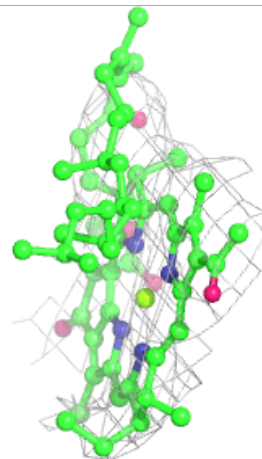
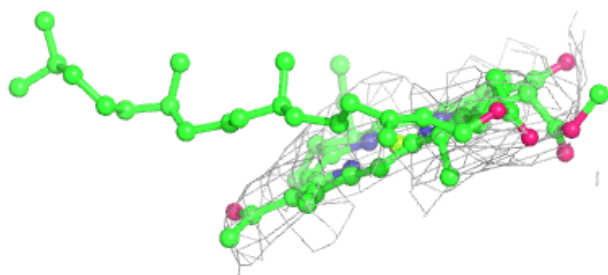
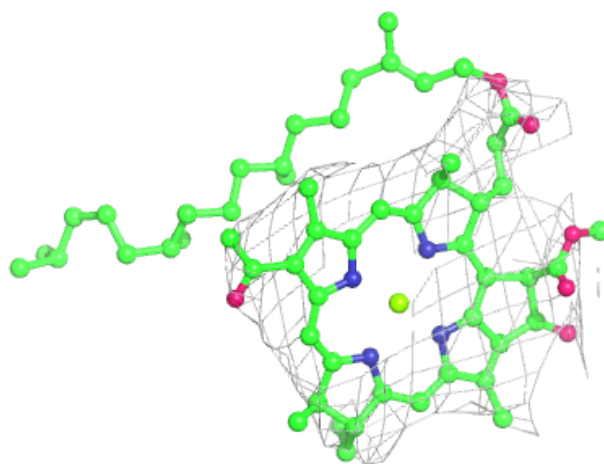
**Electron density around BCL x 301:**

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



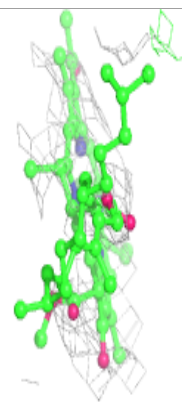
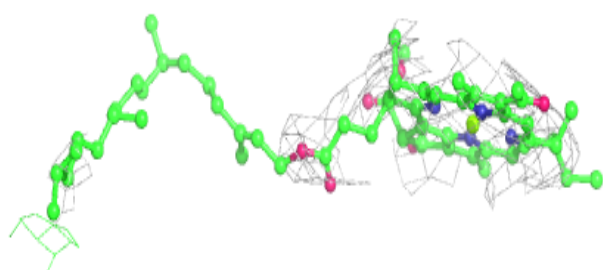
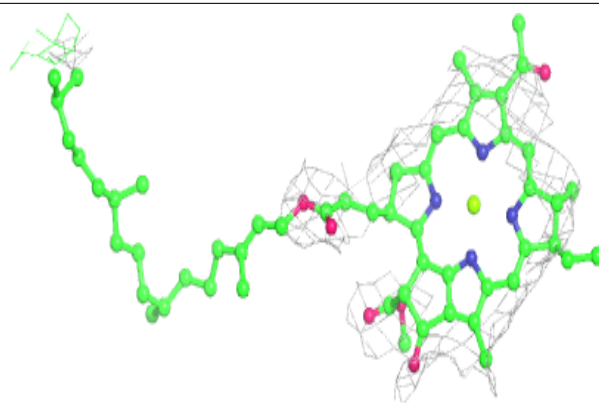
Electron density around BCL R 102:

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

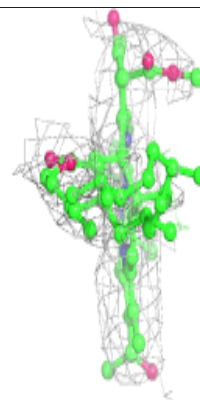
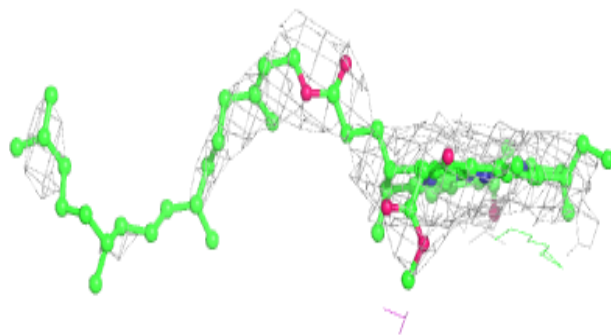
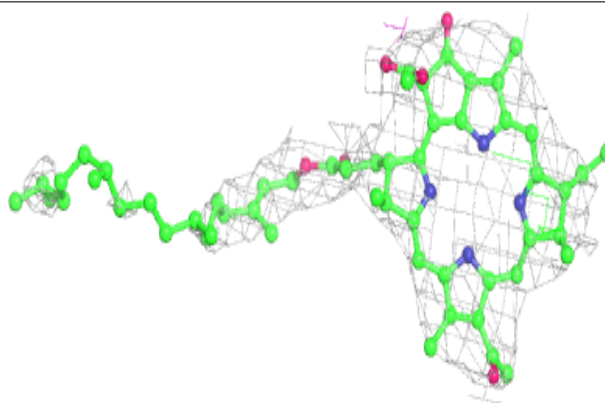


Electron density around BCL AF 101:

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

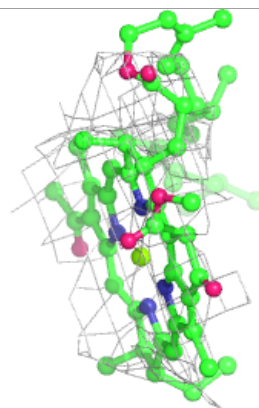
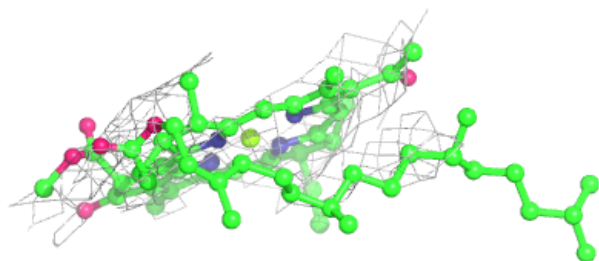
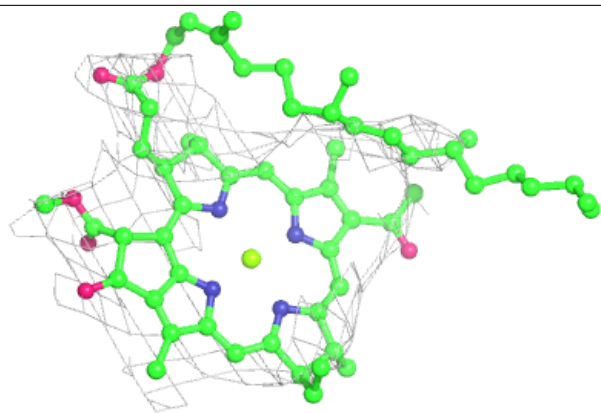
**Electron density around BPH M 403:**

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



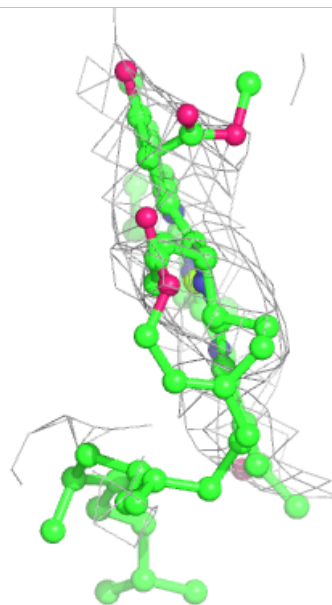
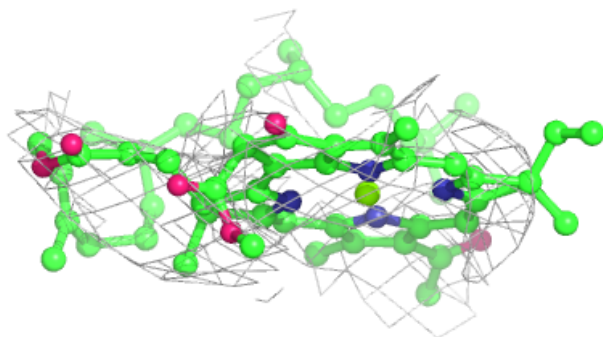
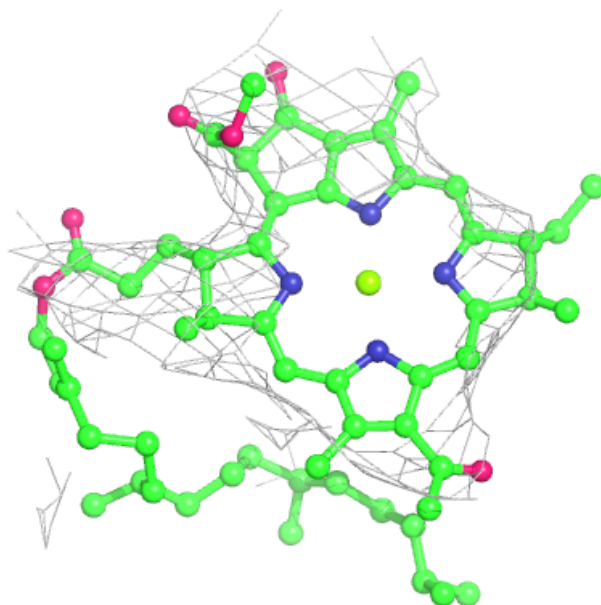
Electron density around BCL i 102:

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



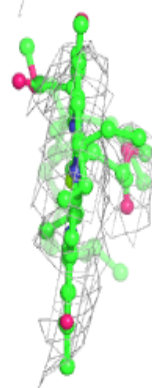
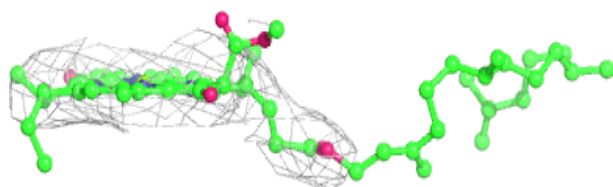
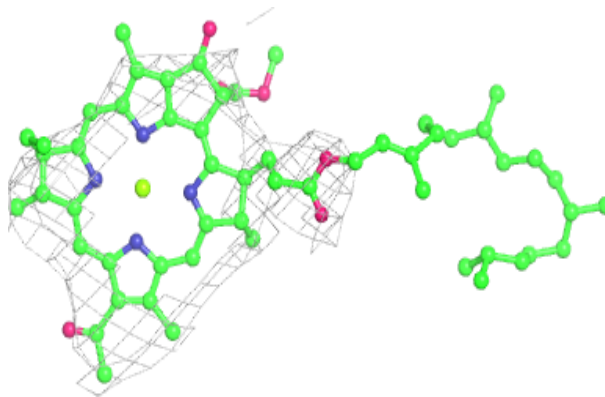
Electron density around BCL k 102:

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

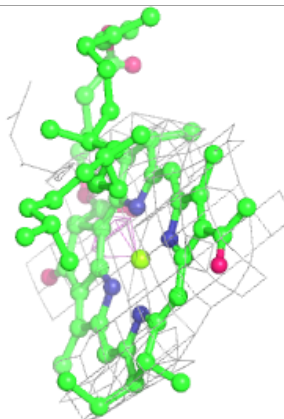
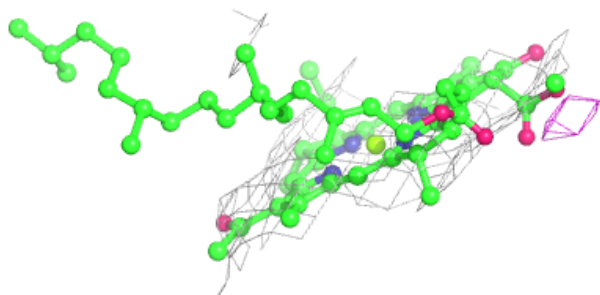
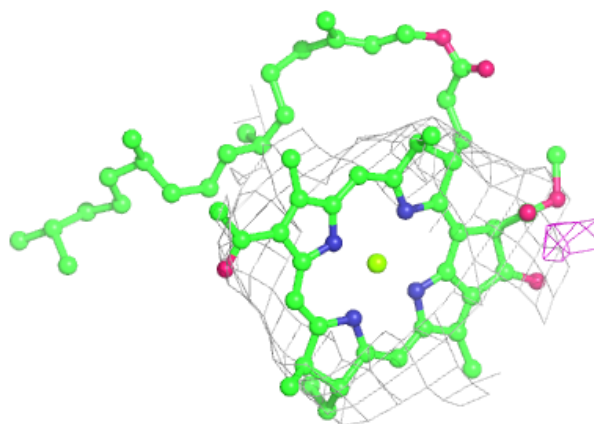


Electron density around BCL AH 101:

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

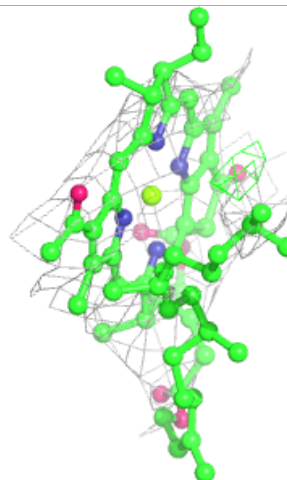
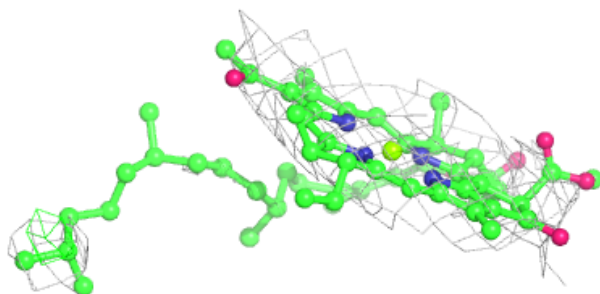
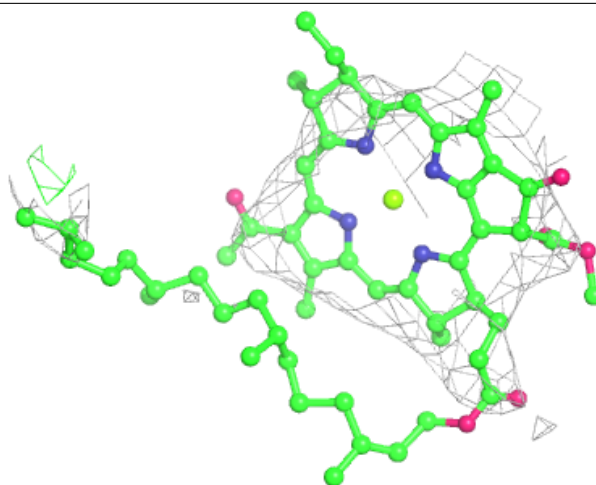
**Electron density around BCL u 102:**

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



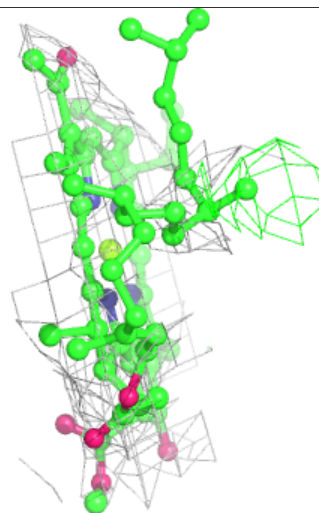
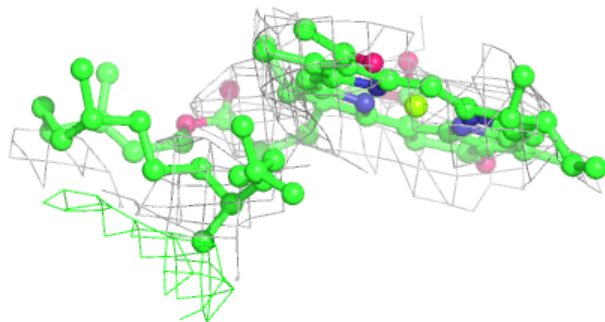
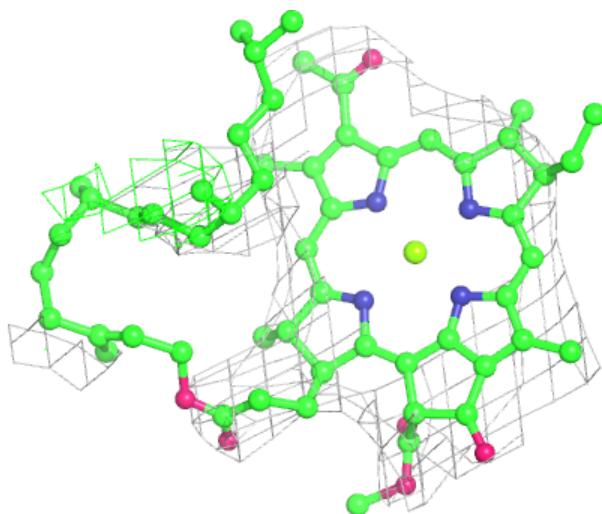
Electron density around BCL e 102:

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



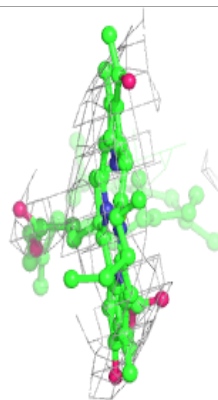
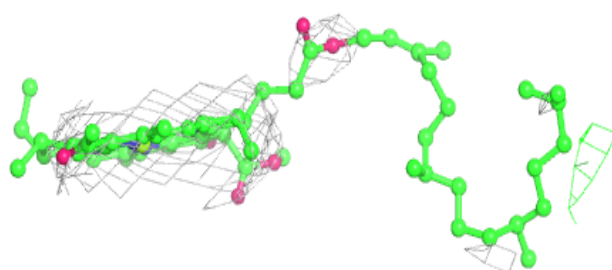
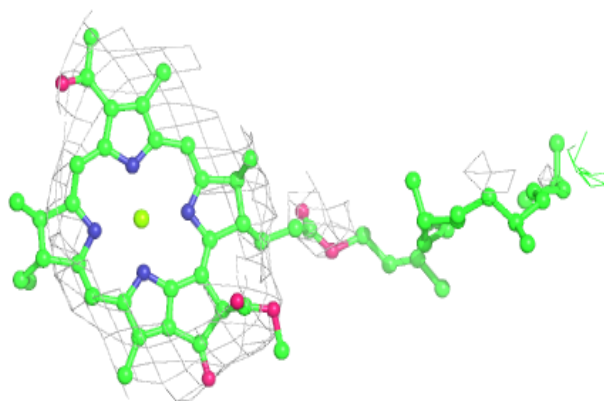
Electron density around BCL m 103:

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

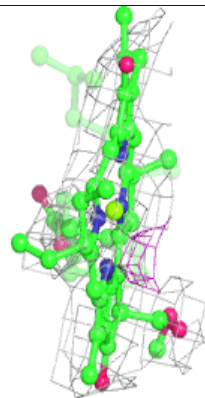
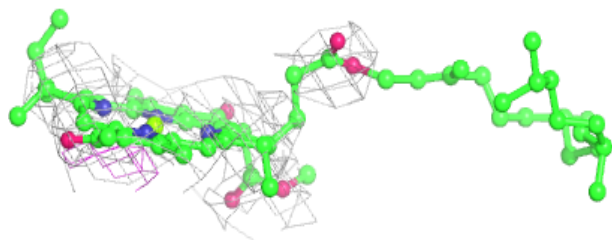
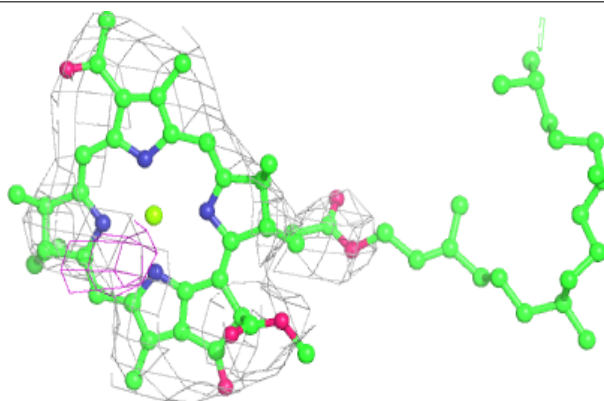


Electron density around BCL P 101:

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

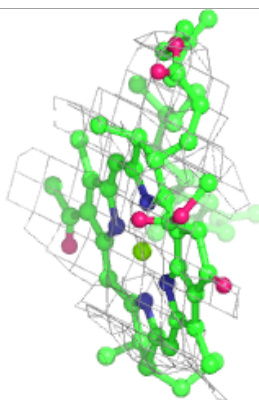
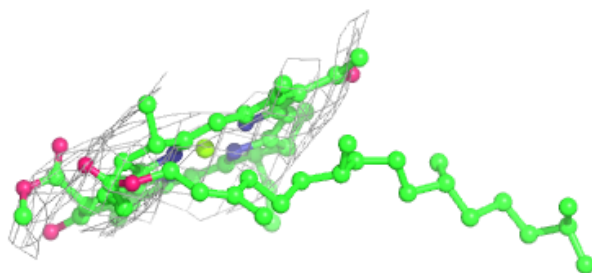
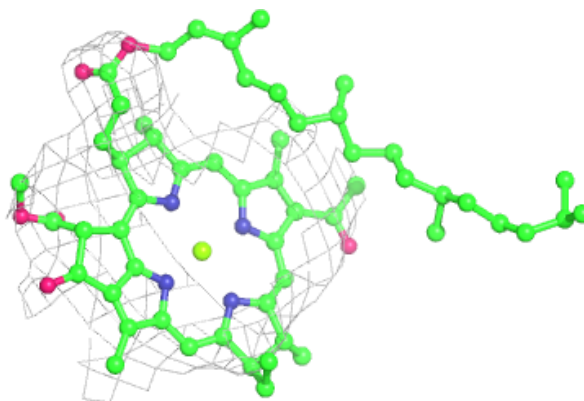
**Electron density around BCL 3 101:**

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

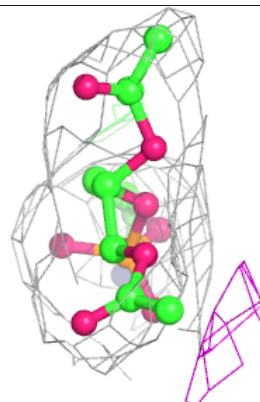
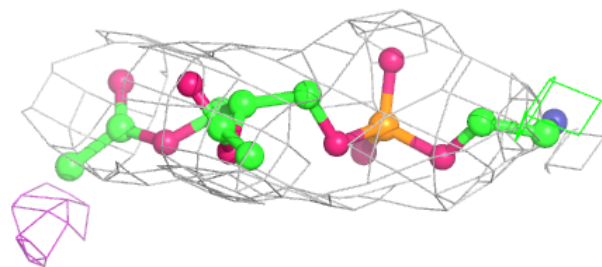
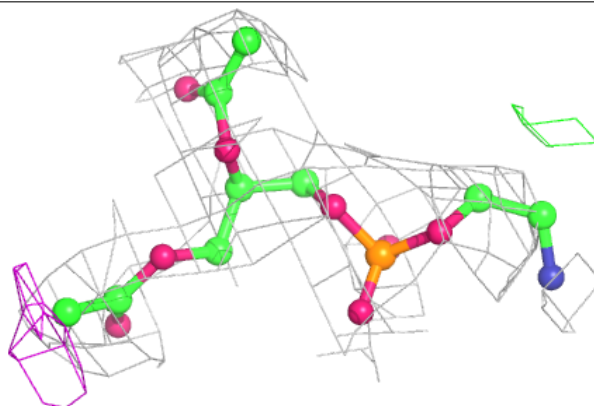


Electron density around BCL G 102:

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

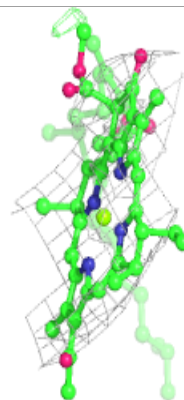
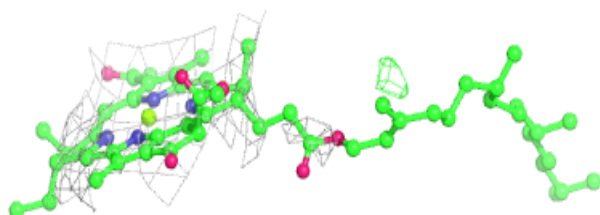
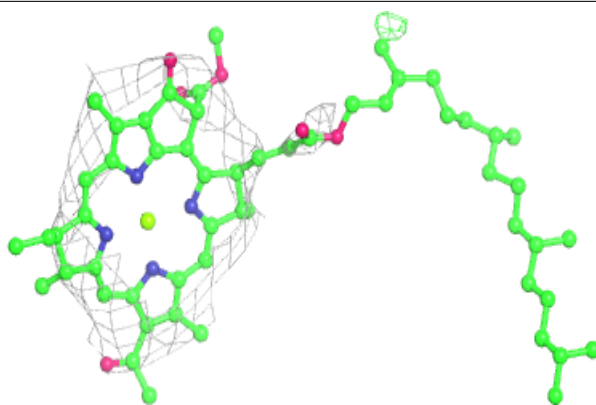
**Electron density around PEF t 303:**

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



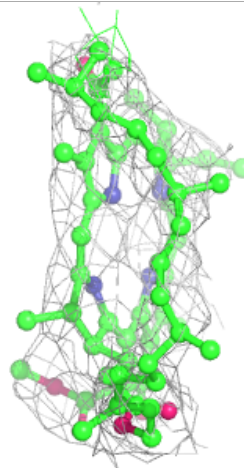
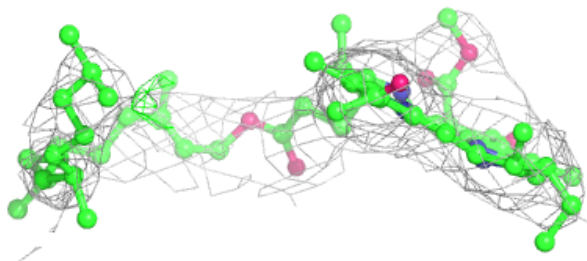
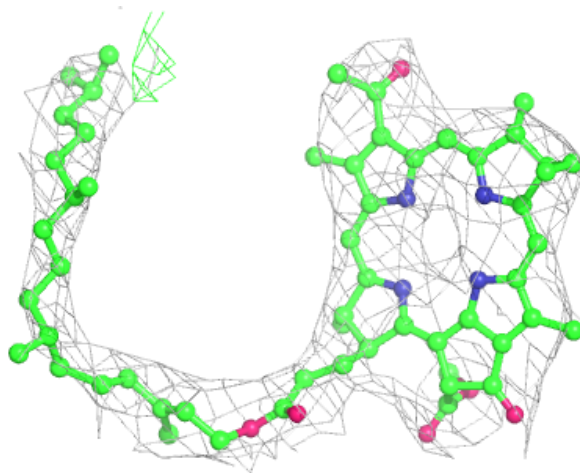
Electron density around BCL I 101:

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



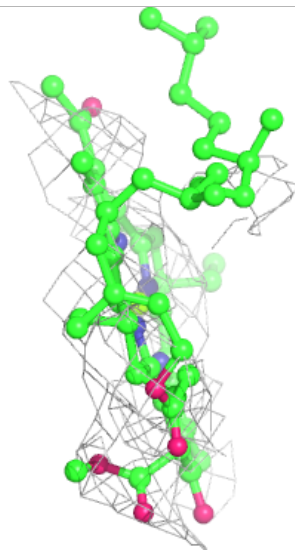
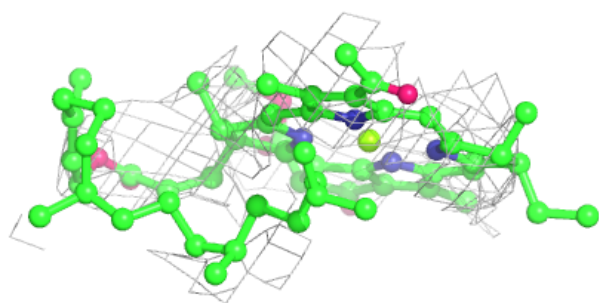
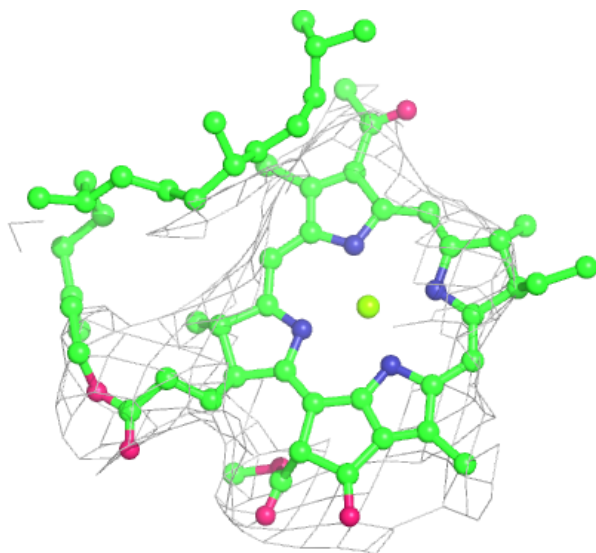
Electron density around BPH L 302:

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



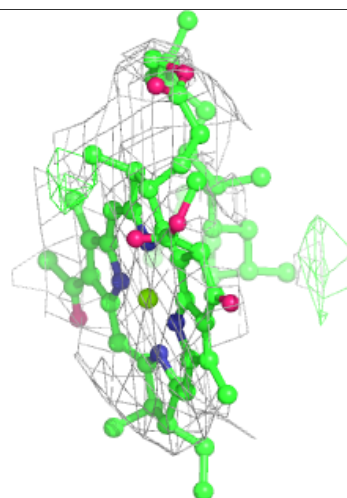
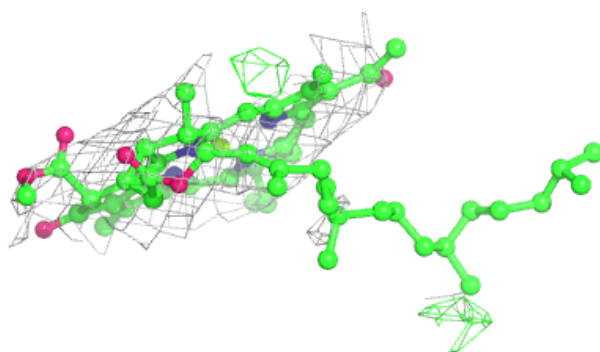
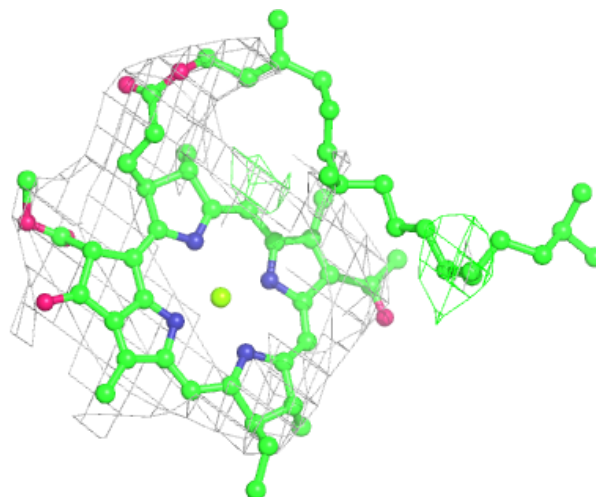
Electron density around BCL 8 101:

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



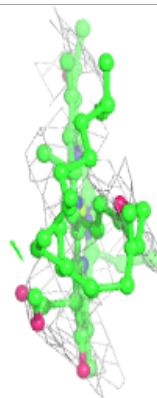
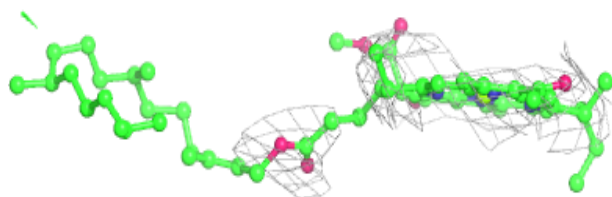
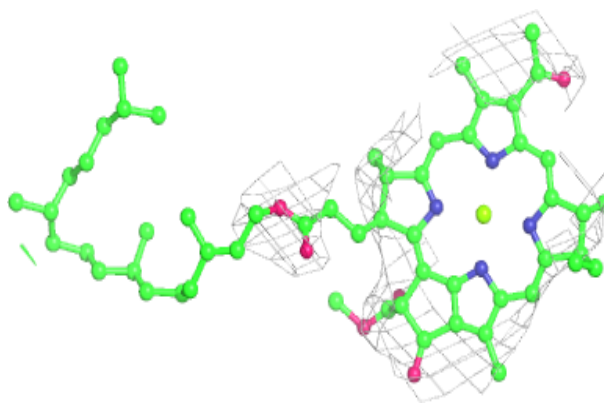
Electron density around BCL AI 102:

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



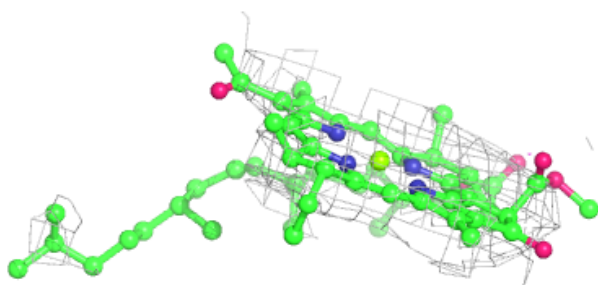
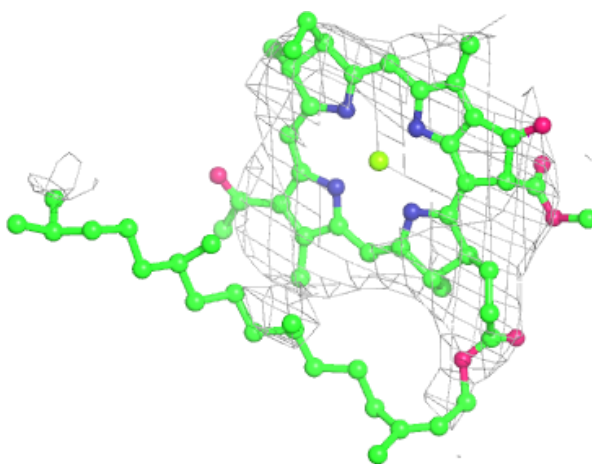
Electron density around BCL 9 102:

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



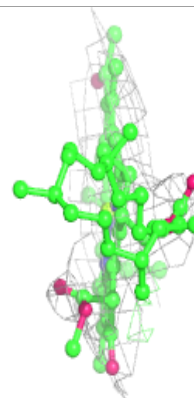
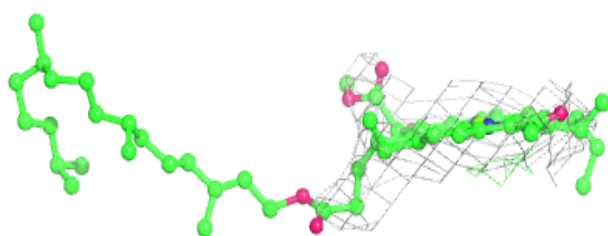
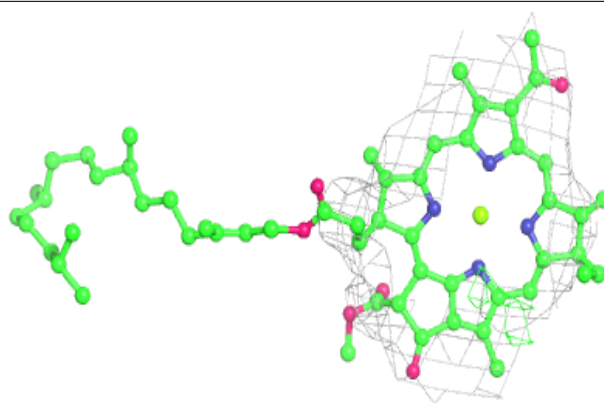
Electron density around BCL V 102:

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

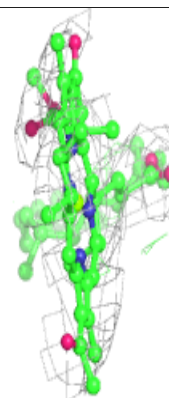
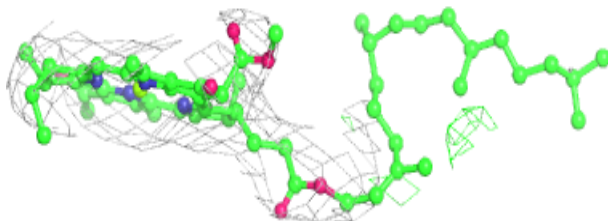
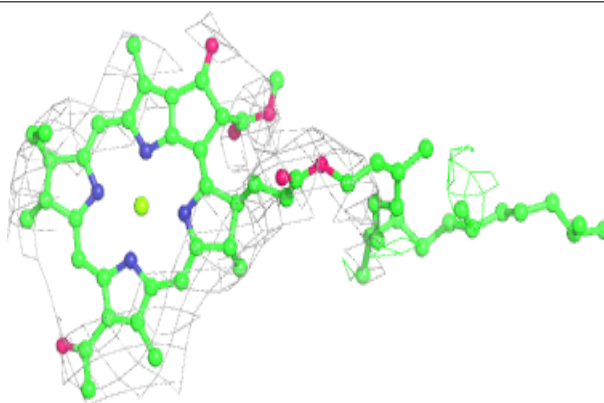


Electron density around BCL w 101:

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

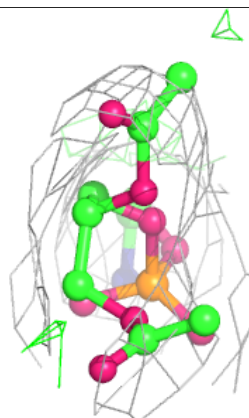
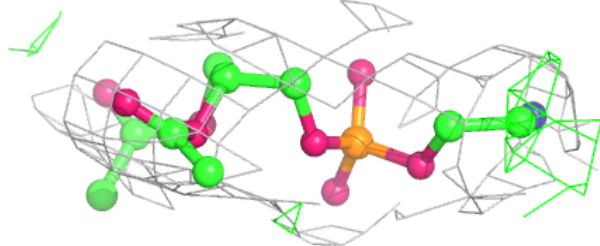
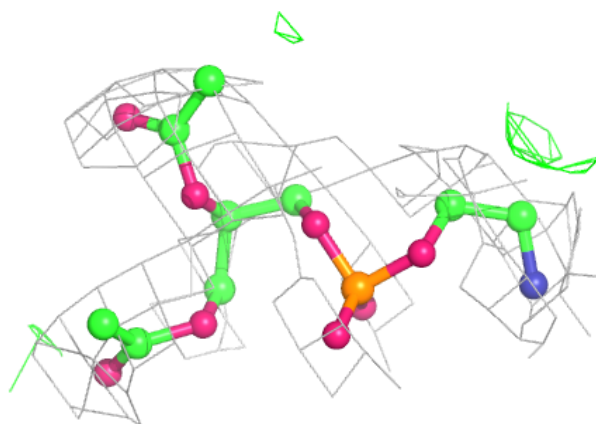
**Electron density around BCL h 101:**

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



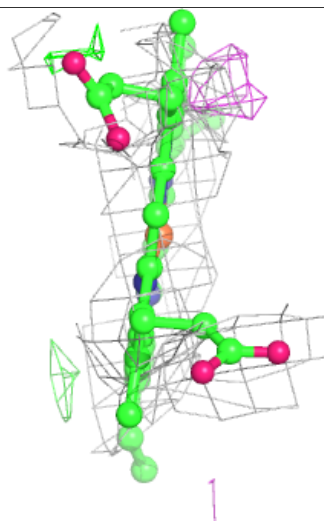
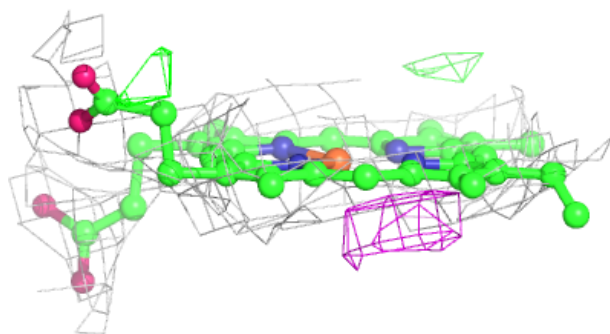
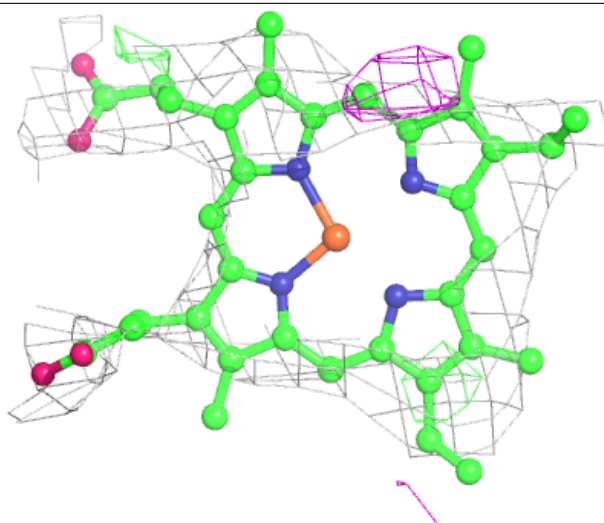
Electron density around PEF H 305:

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



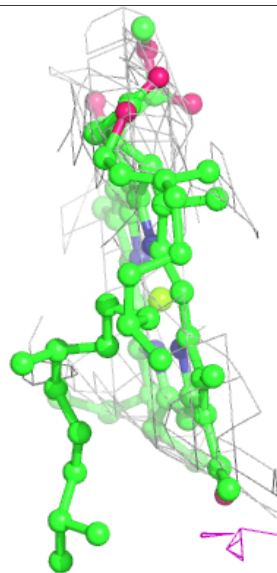
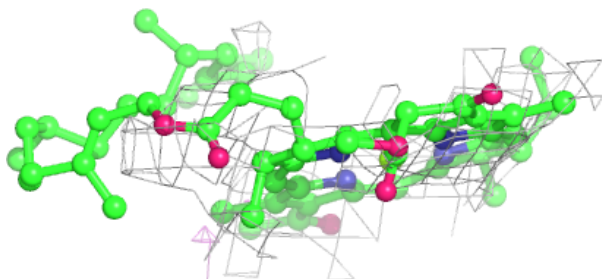
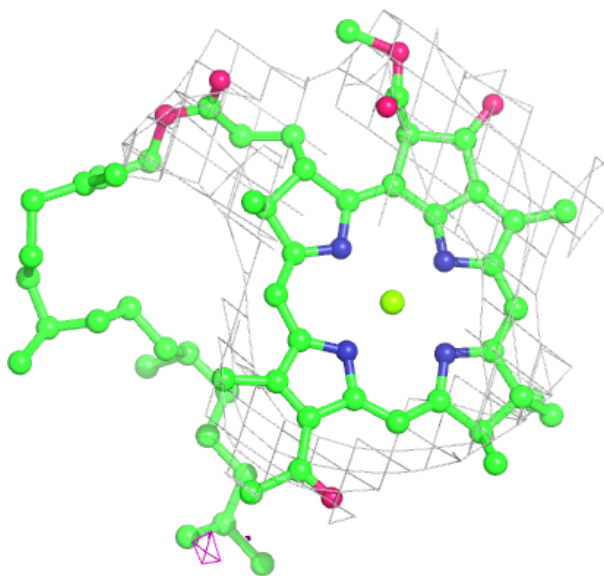
Electron density around HEM C 501:

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



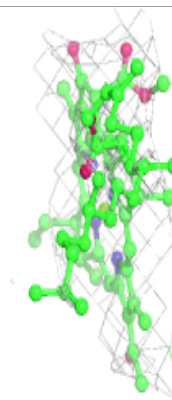
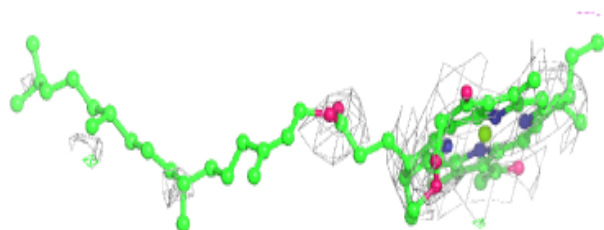
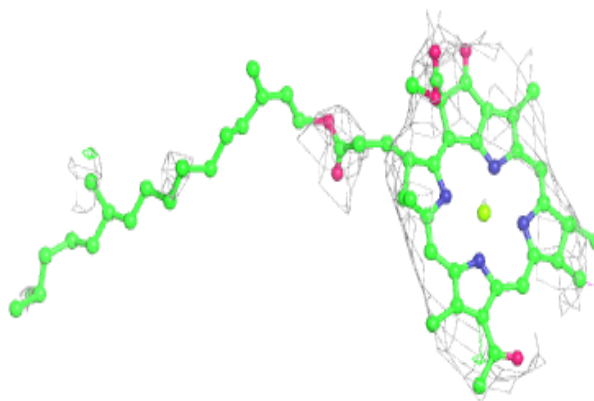
Electron density around BCL A 103:

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



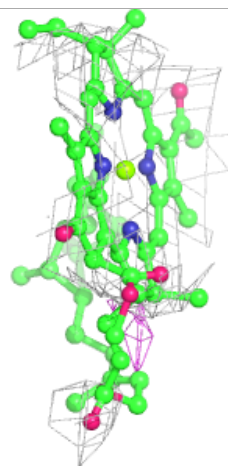
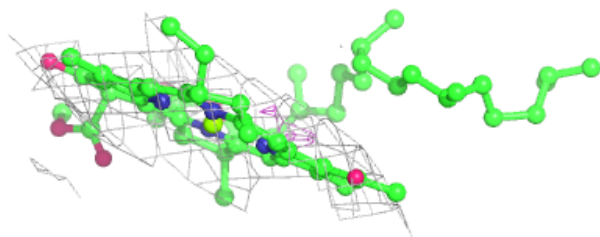
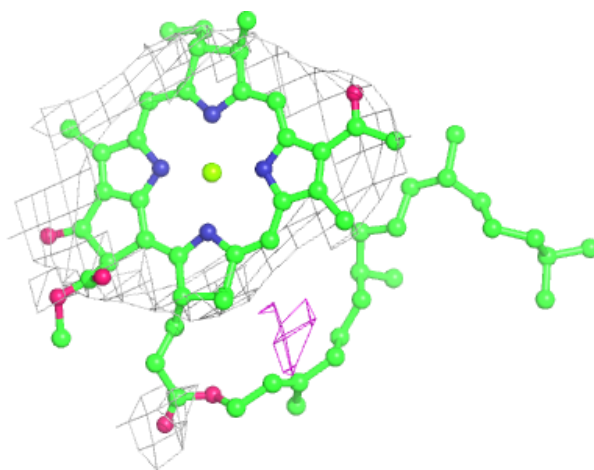
Electron density around BCL 1 101:

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



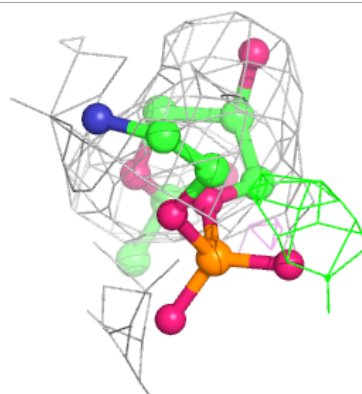
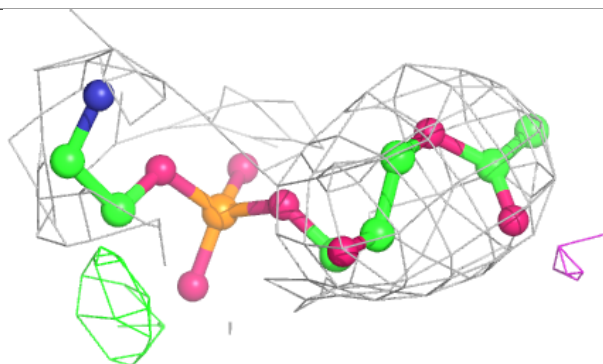
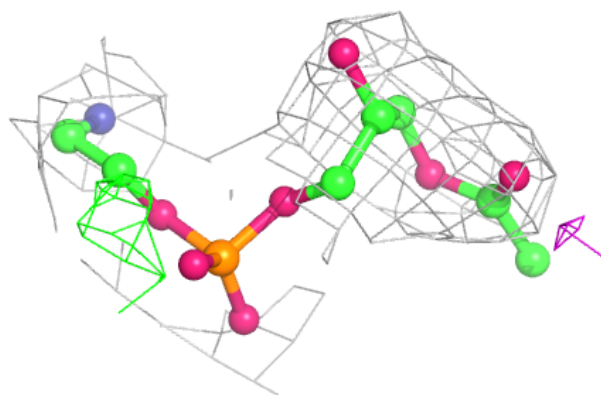
Electron density around BCL q 102:

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

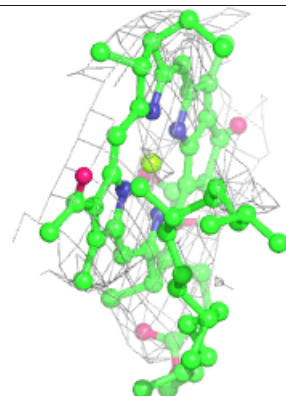
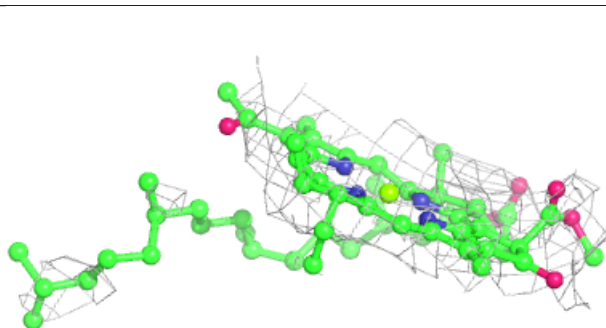
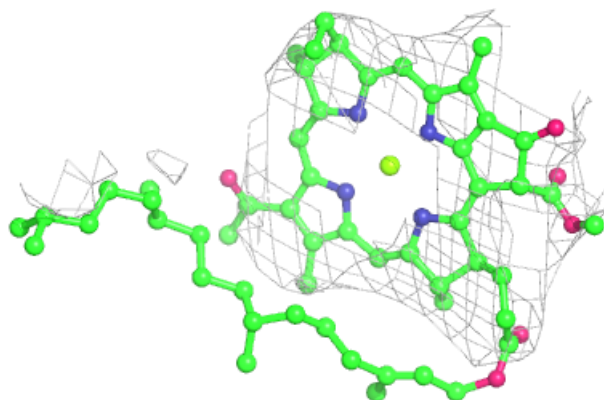


Electron density around PEF M 407:

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

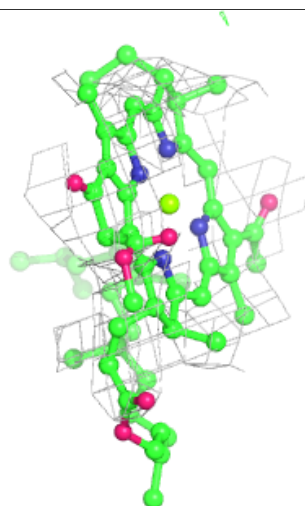
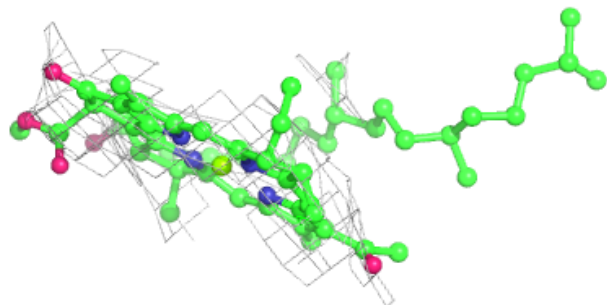
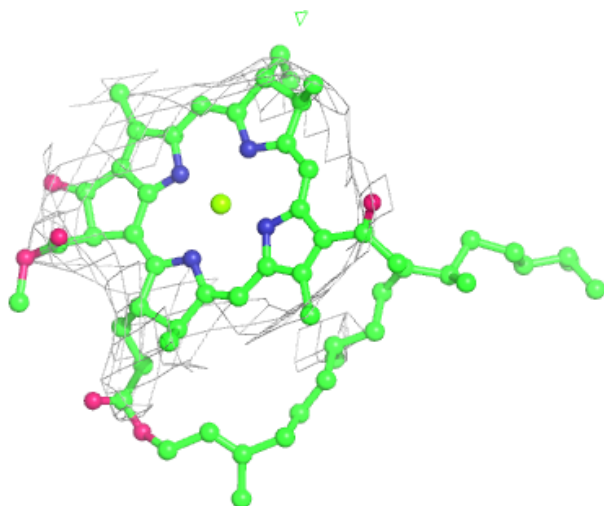
**Electron density around BCL T 102:**

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



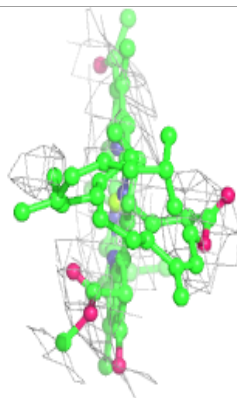
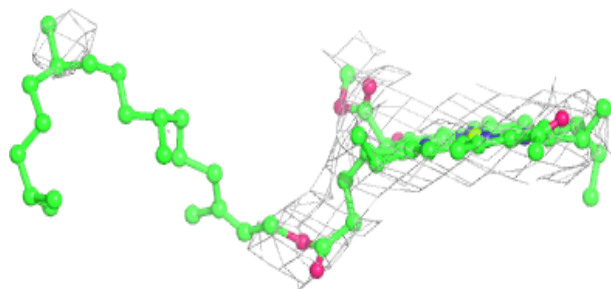
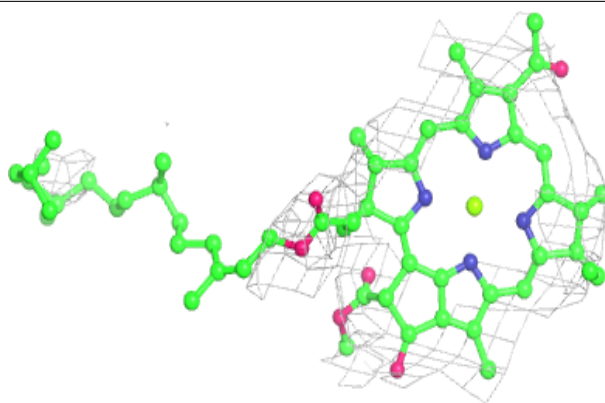
Electron density around BCL c 101:

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



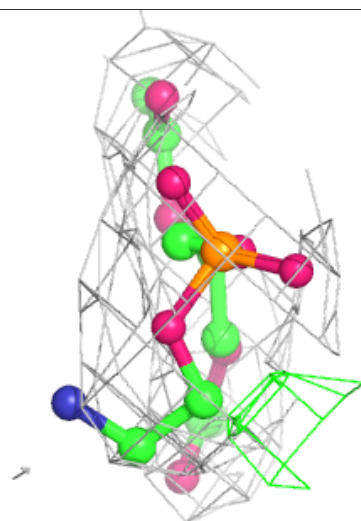
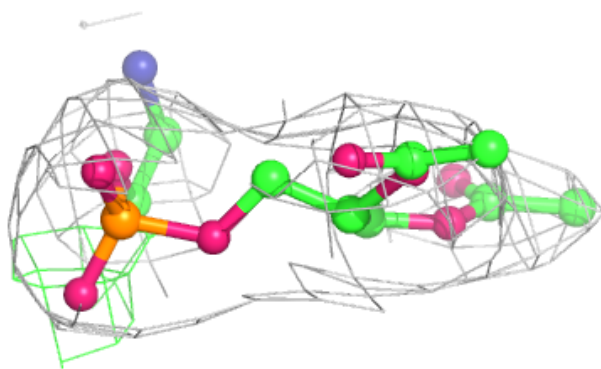
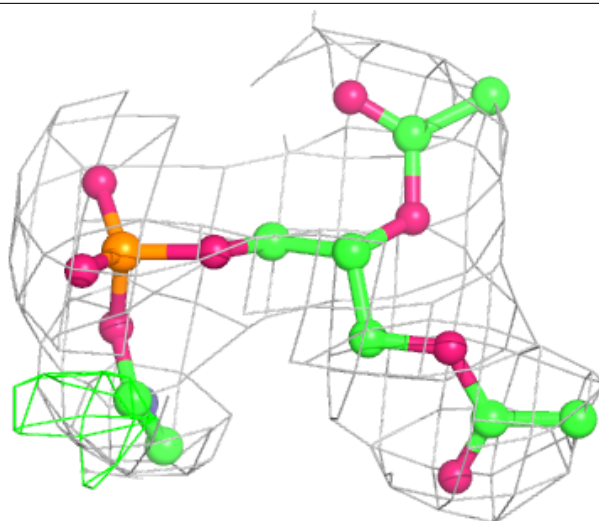
Electron density around BCL AB 101:

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



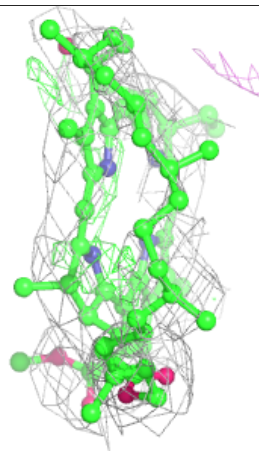
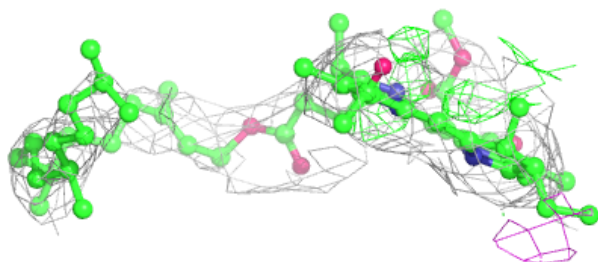
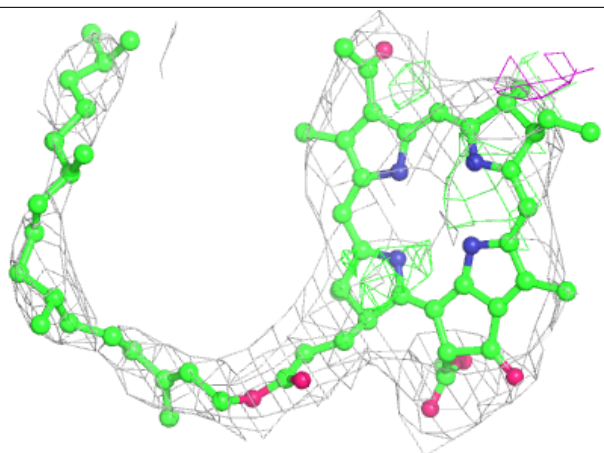
Electron density around PEF t 301:

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

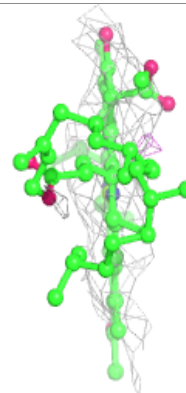
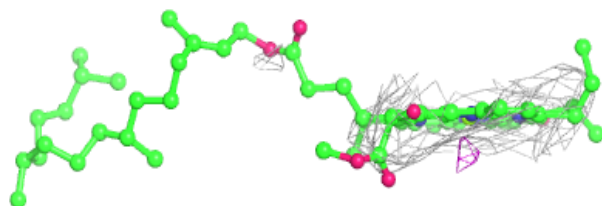
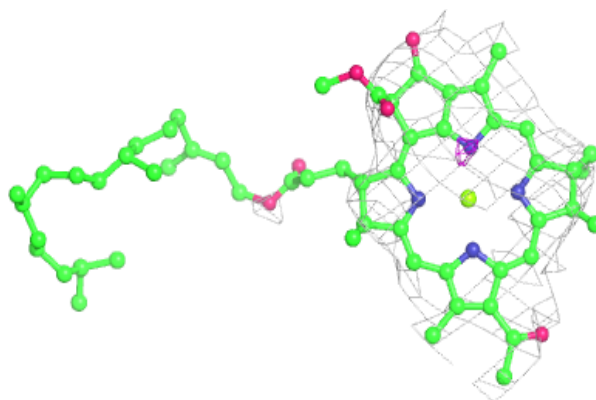


Electron density around BPH x 302:

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

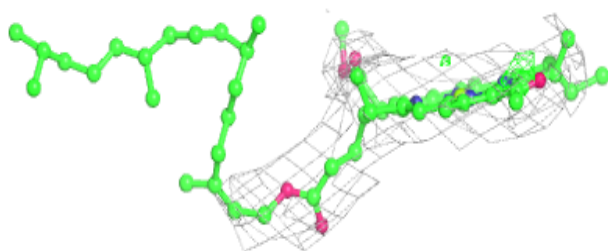
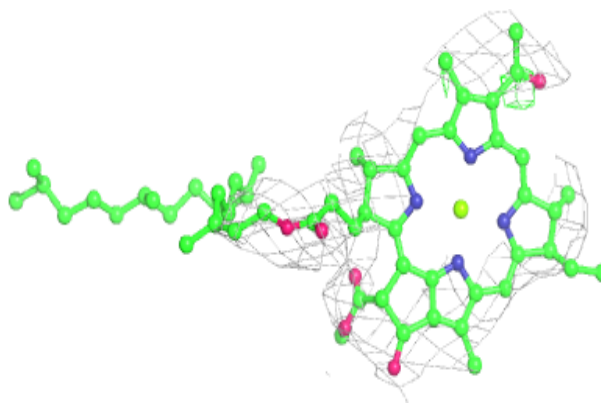
**Electron density around BCL 1 101:**

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

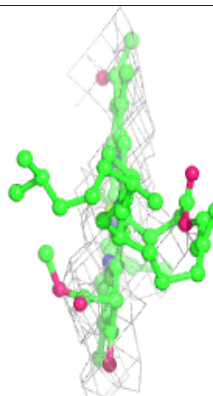
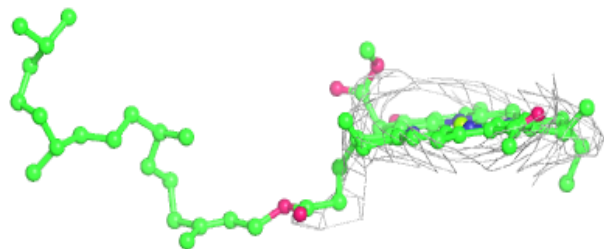
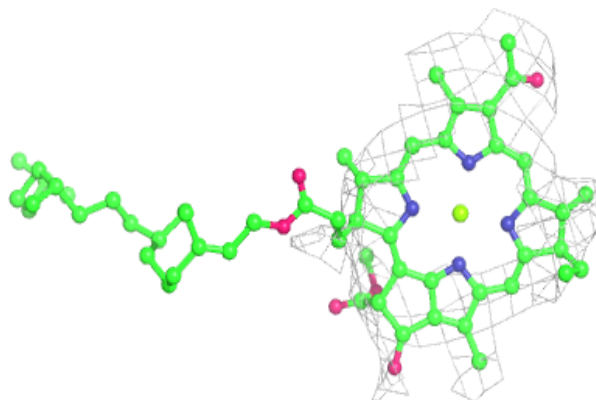


Electron density around BCL 5 101:

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

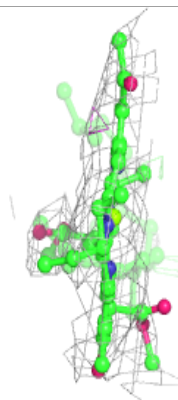
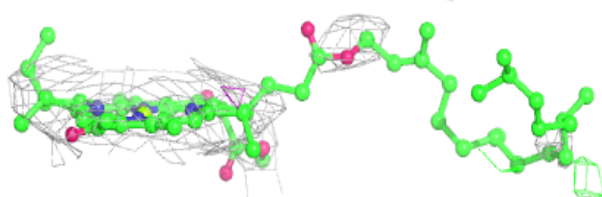
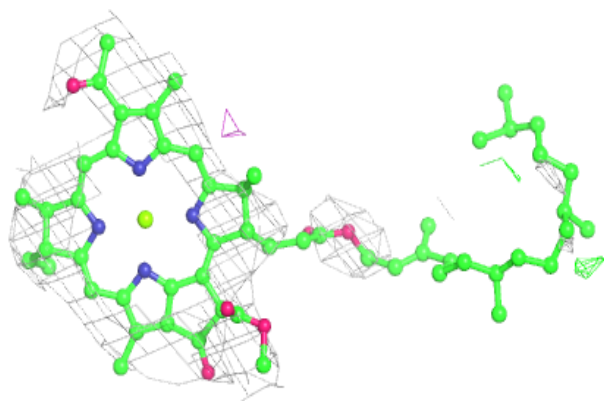
**Electron density around BCL r 101:**

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

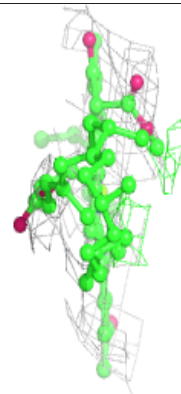
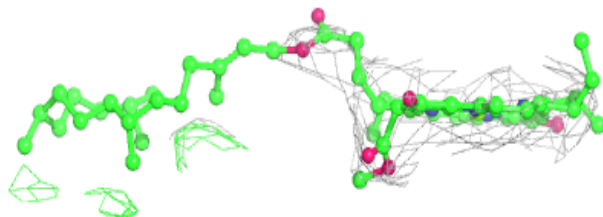
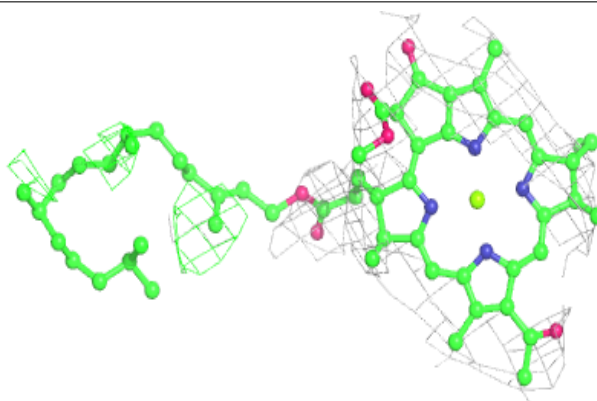


Electron density around BCL U 101:

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

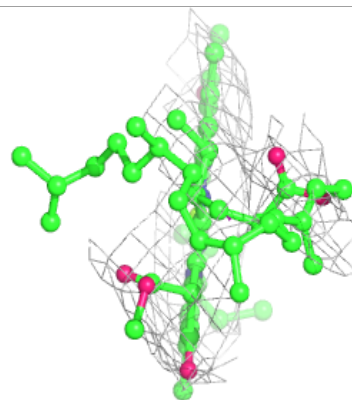
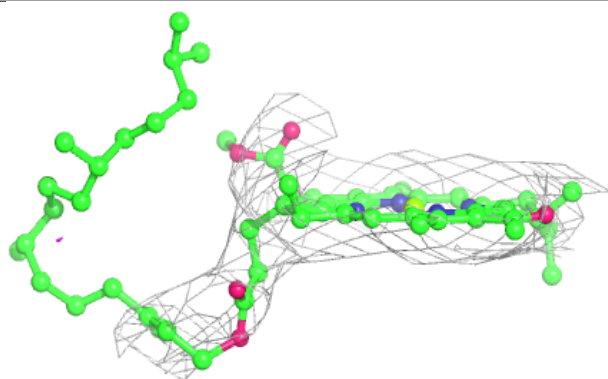
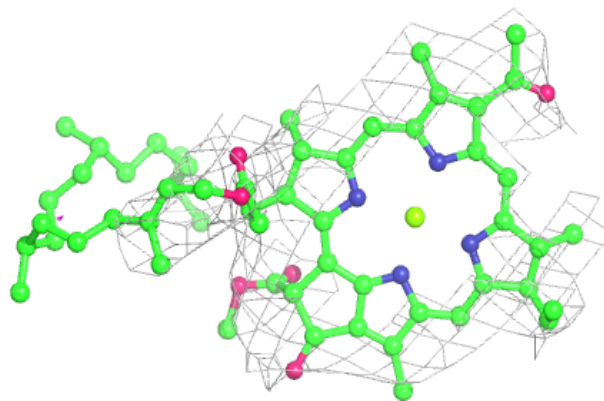
**Electron density around BCL AI 101:**

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

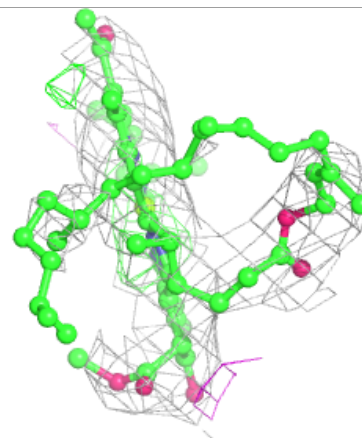
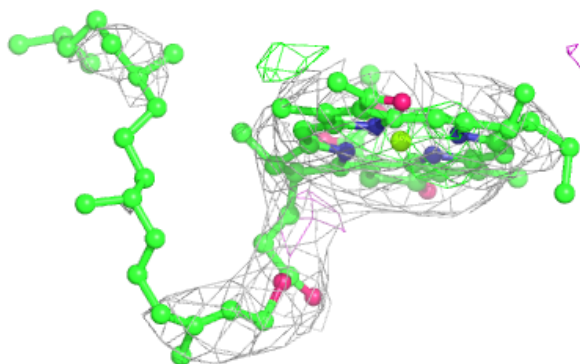
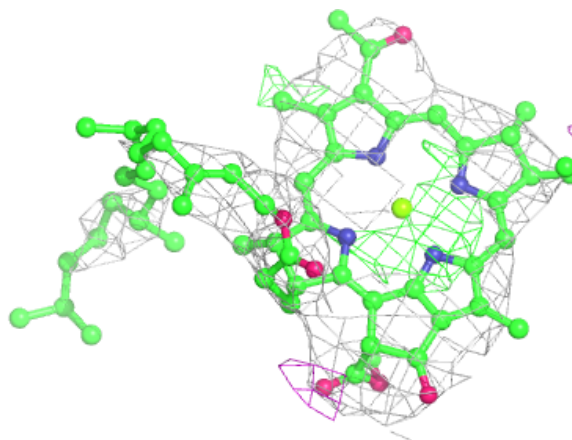


Electron density around BCL Q 101:

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

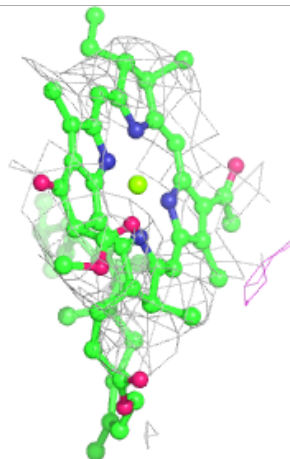
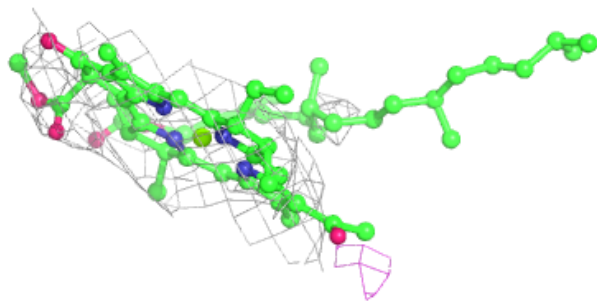
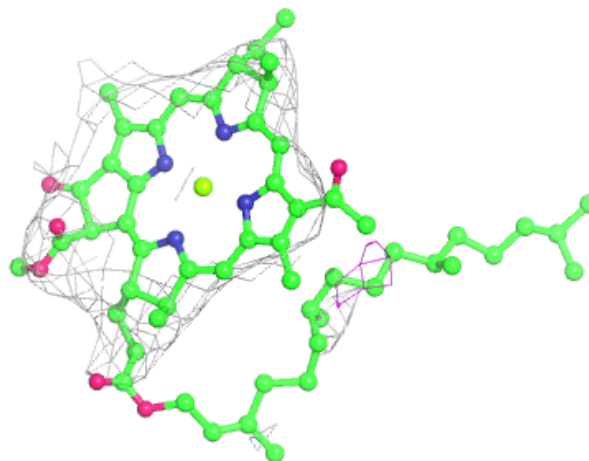
**Electron density around BCL x 303:**

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



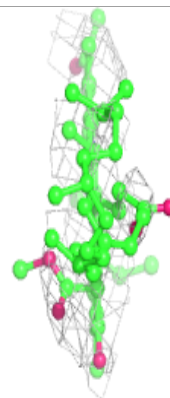
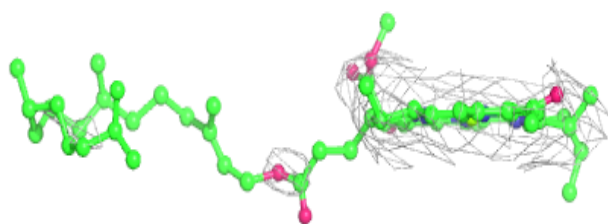
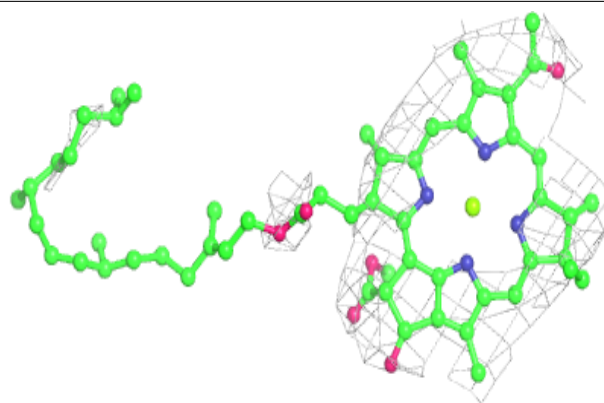
Electron density around BCL 2 102:

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



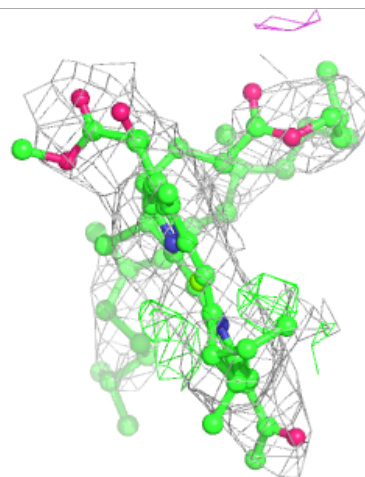
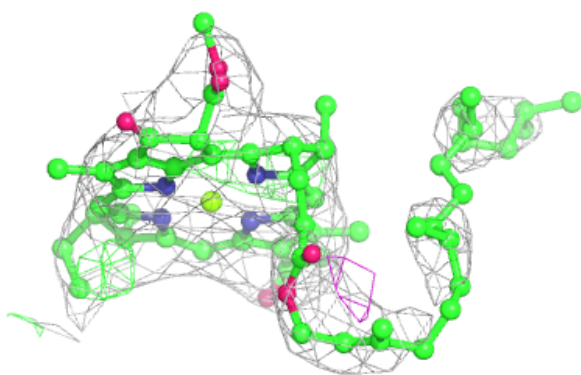
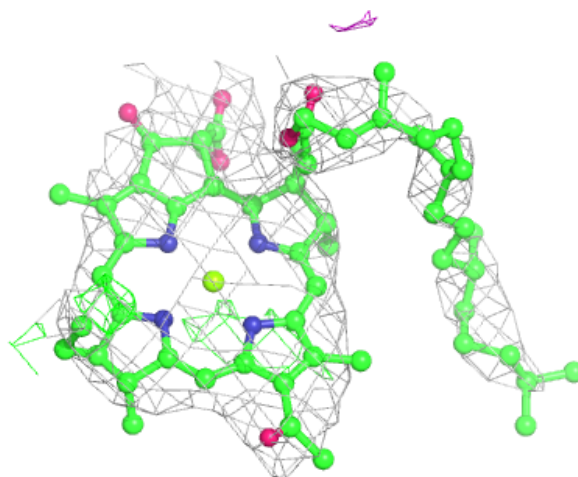
Electron density around BCL W 101:

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



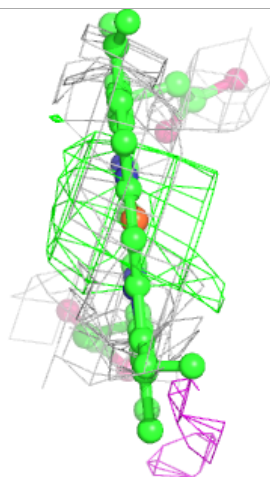
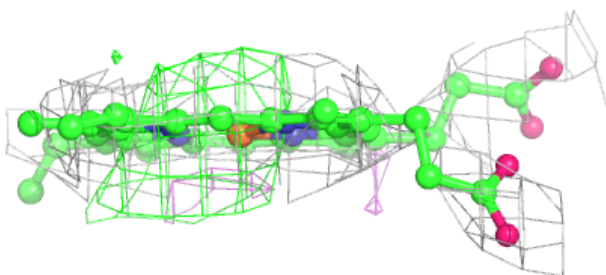
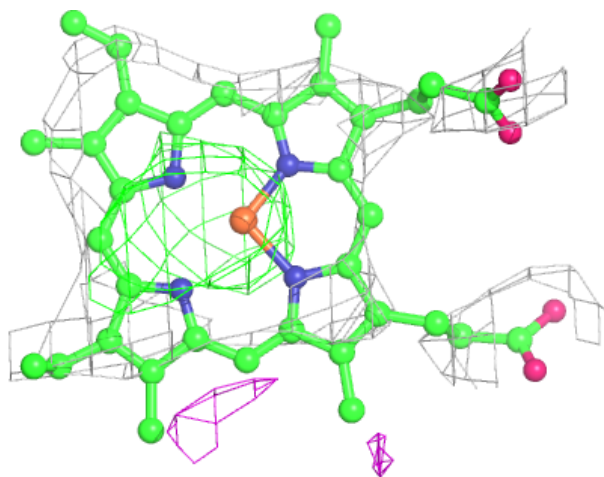
Electron density around BCL M 401:

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



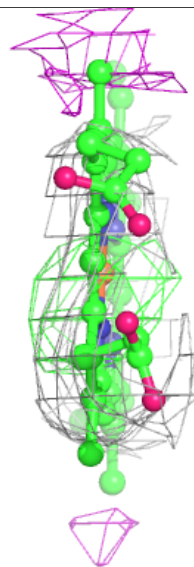
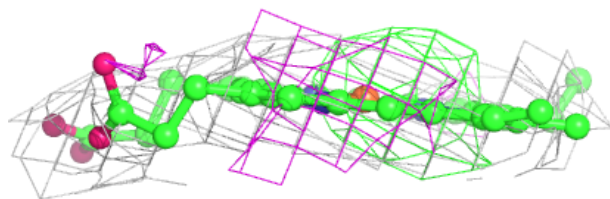
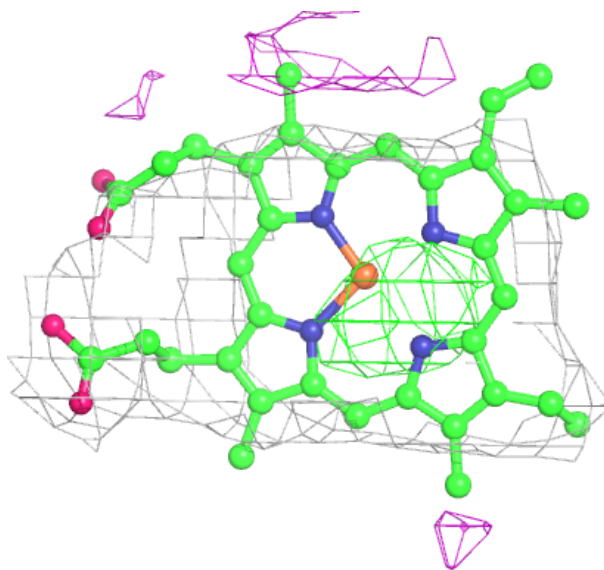
Electron density around HEM o 503:

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



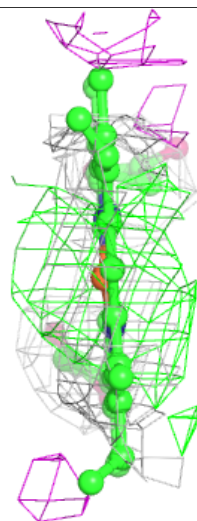
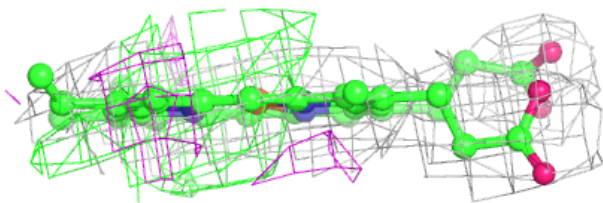
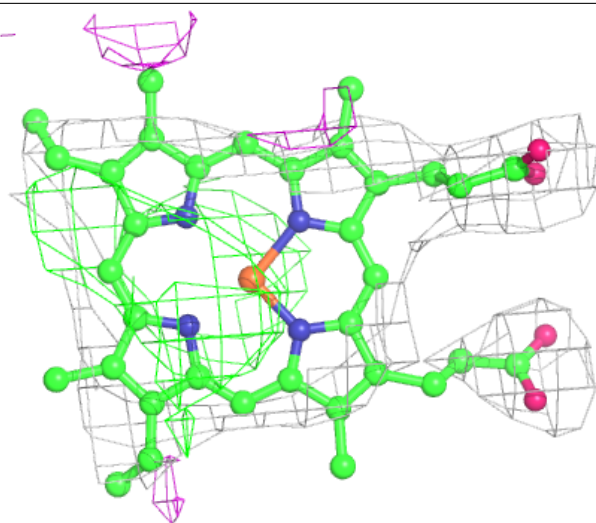
Electron density around HEM C 502:

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



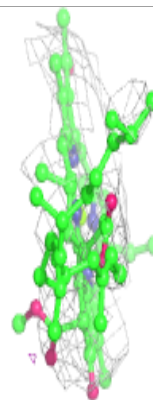
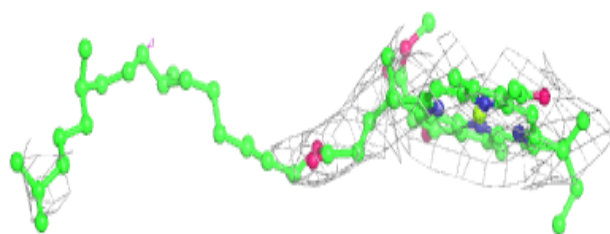
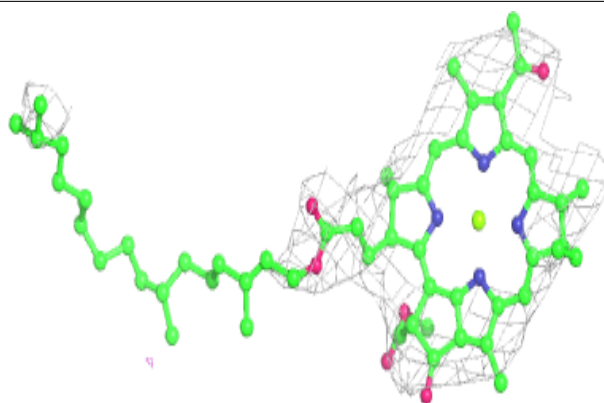
Electron density around HEM C 504:

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



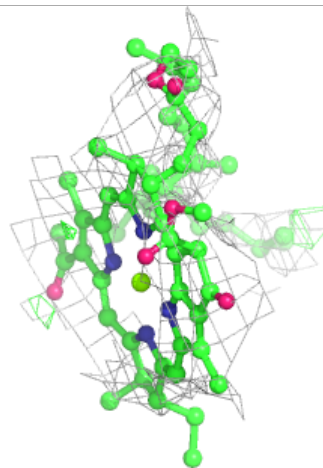
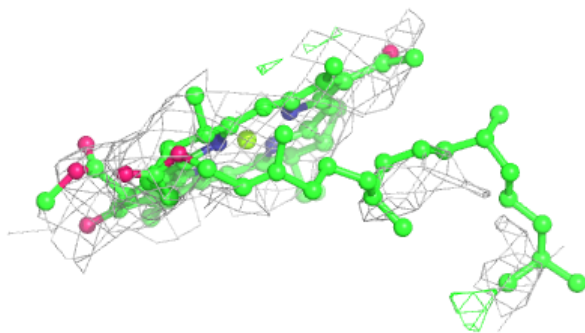
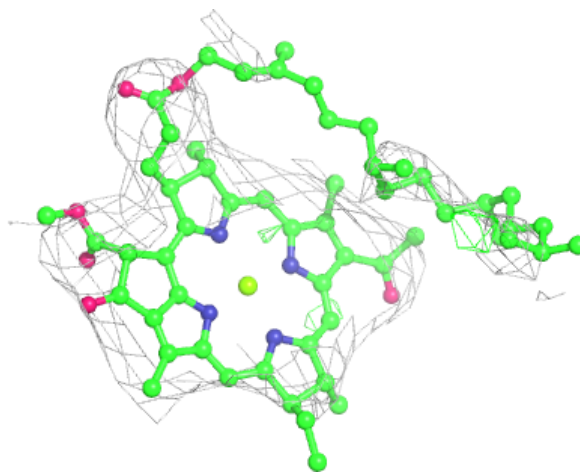
Electron density around BCL S 102:

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



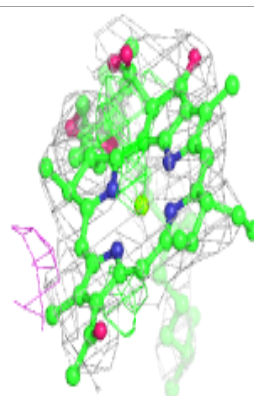
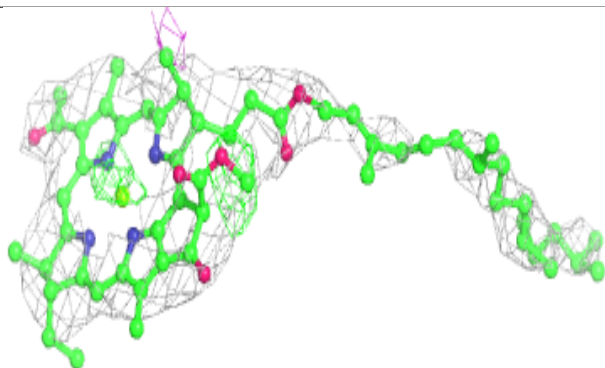
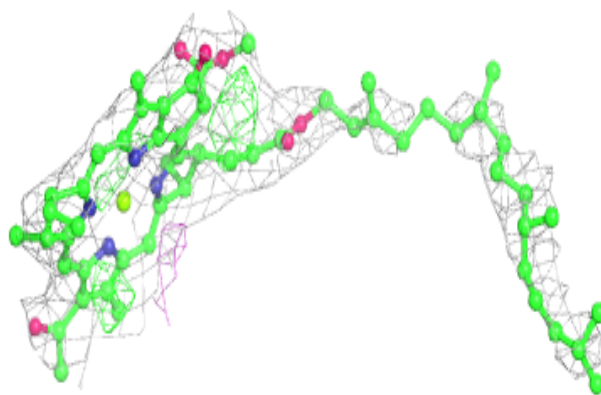
Electron density around BCL 4 102:

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

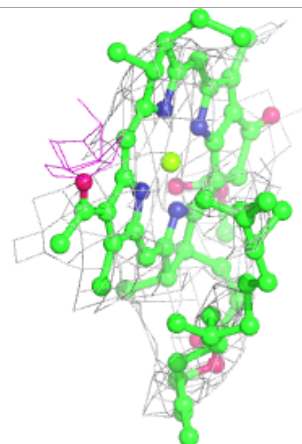
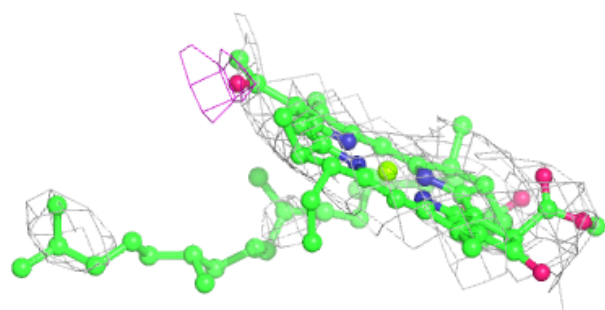
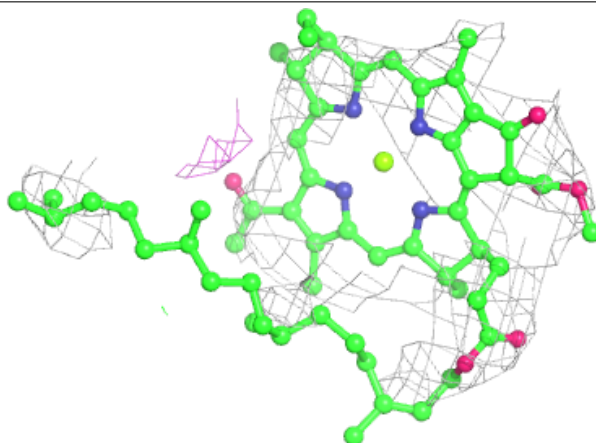


Electron density around BCL L 301:

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

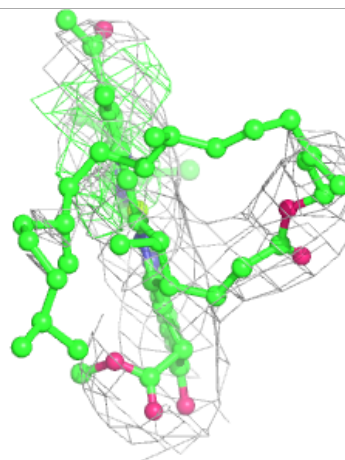
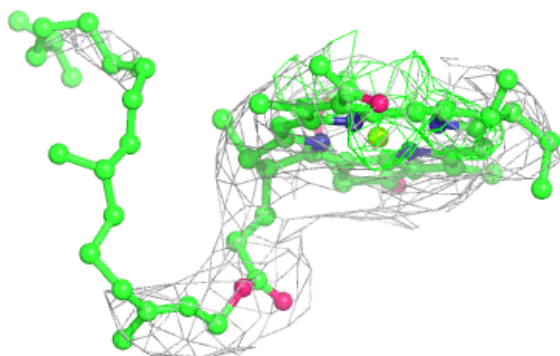
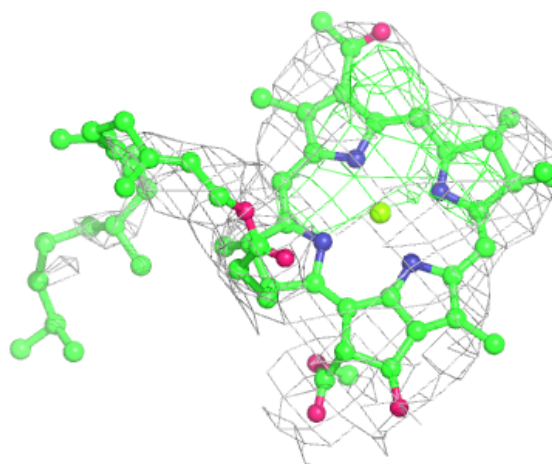
**Electron density around BCL AL 102:**

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



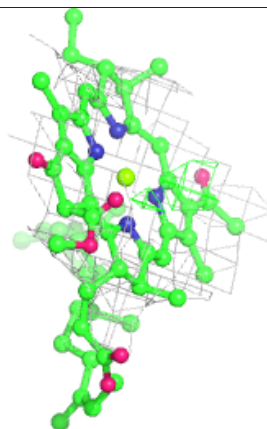
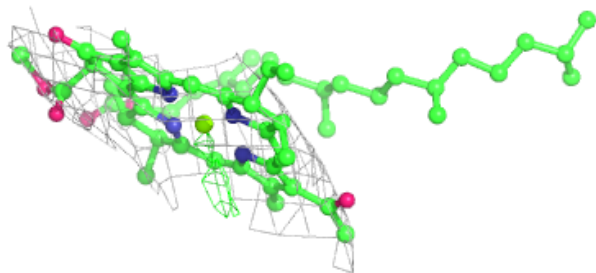
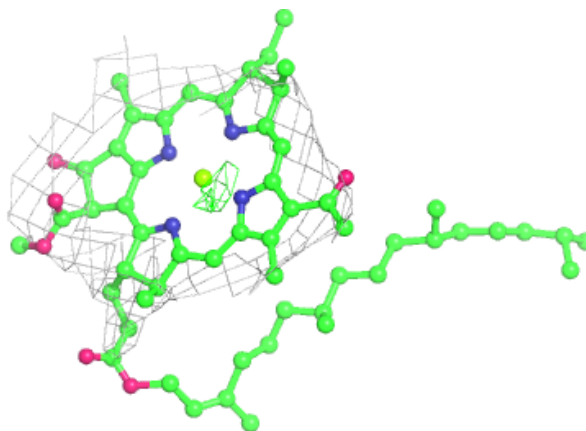
Electron density around BCL L 303:

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



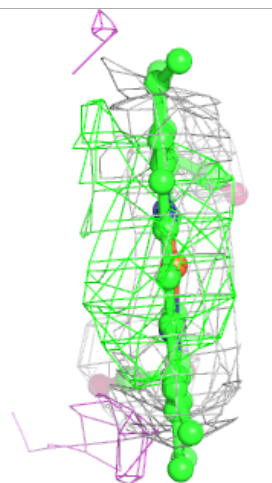
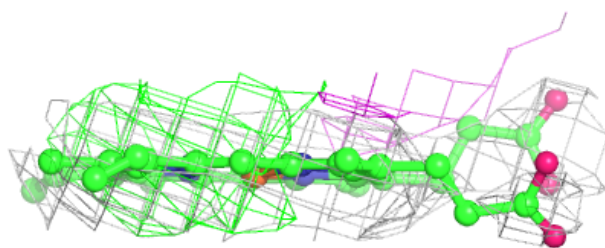
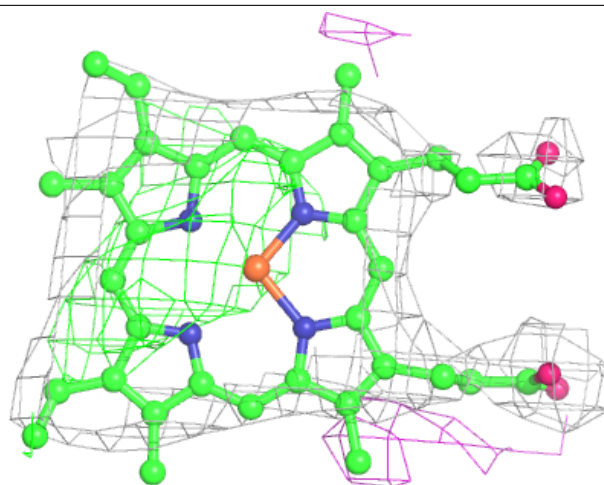
Electron density around BCL s 102:

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



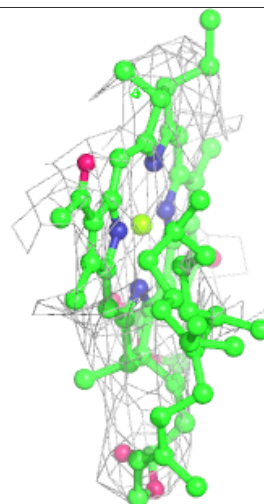
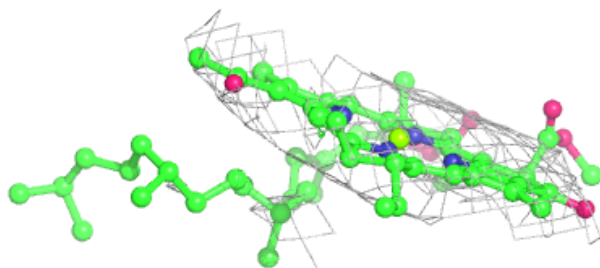
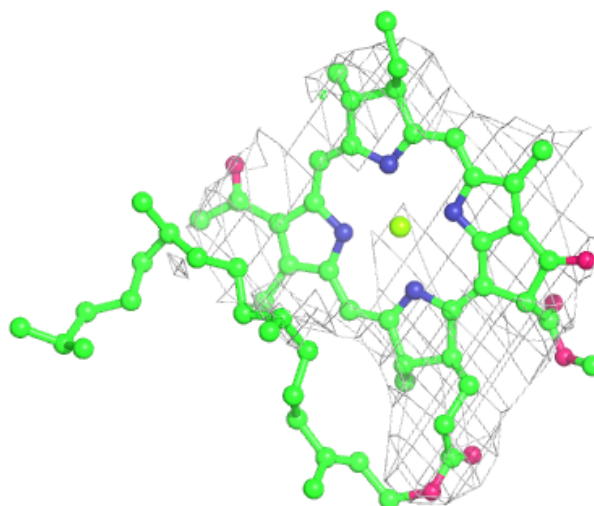
Electron density around HEM o 504:

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



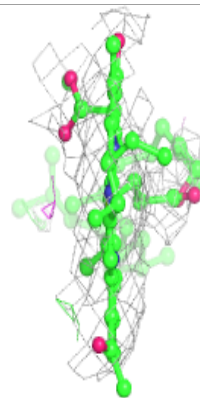
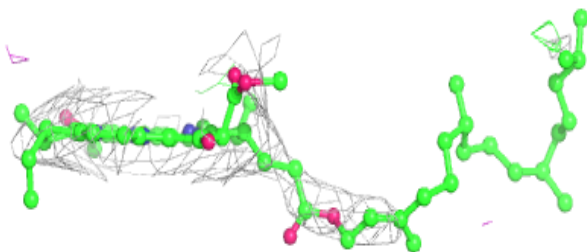
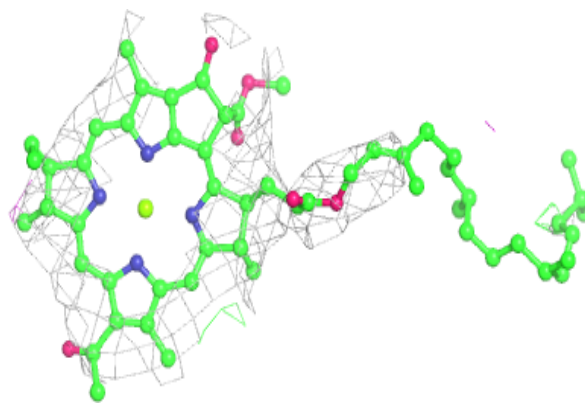
Electron density around BCL X 102:

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



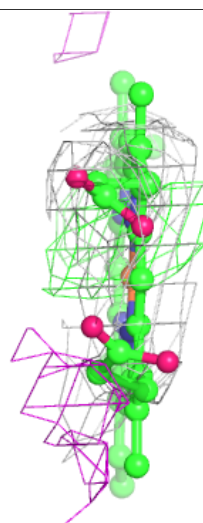
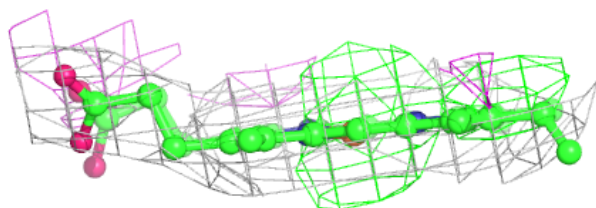
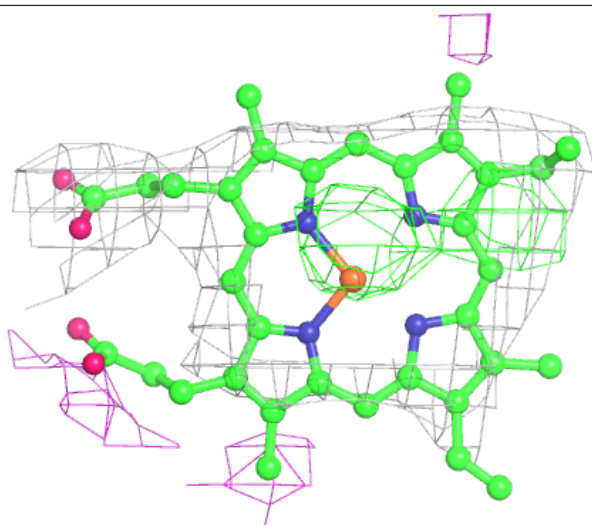
Electron density around BCL AK 101:

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



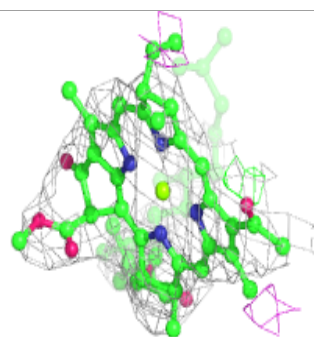
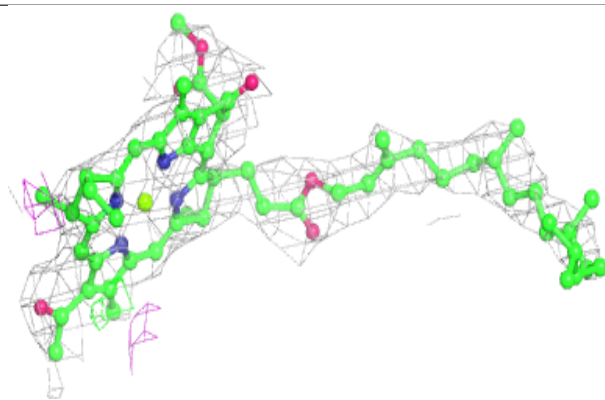
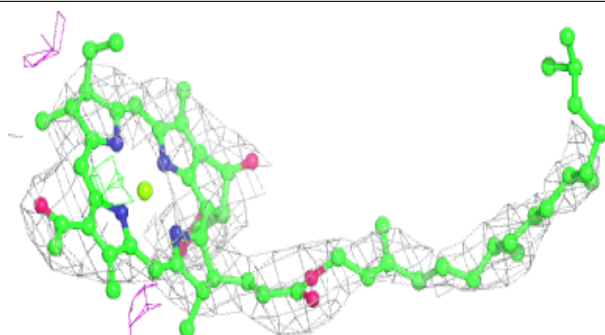
Electron density around HEM o 502:

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



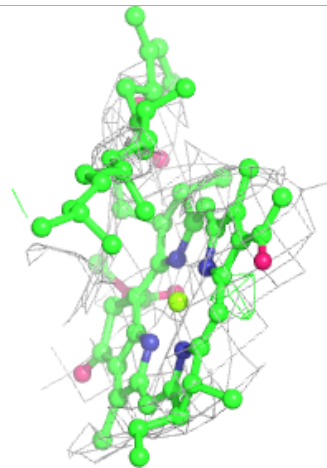
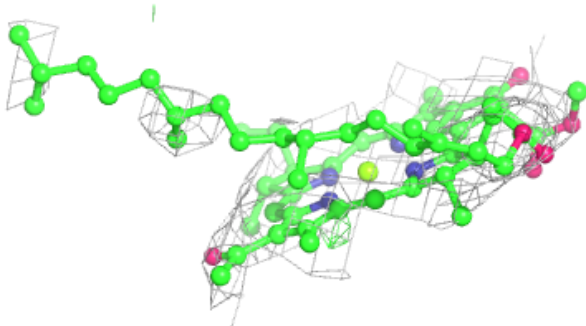
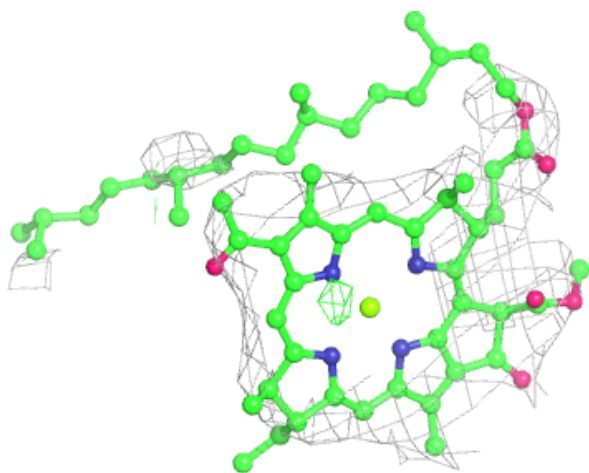
Electron density around BCL M 402:

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



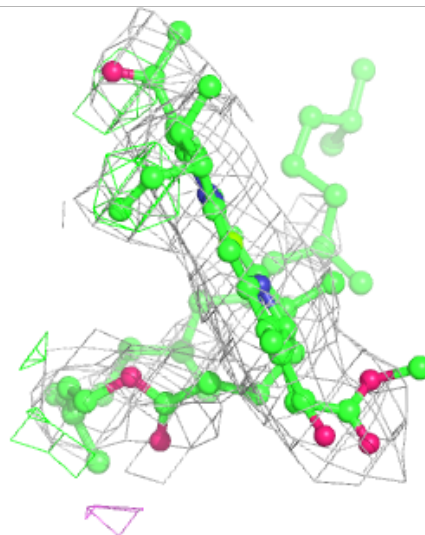
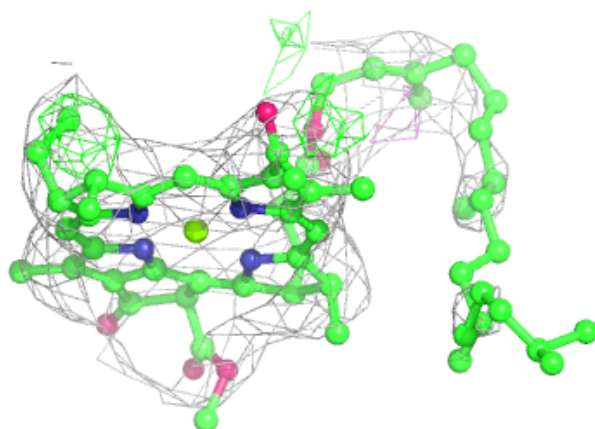
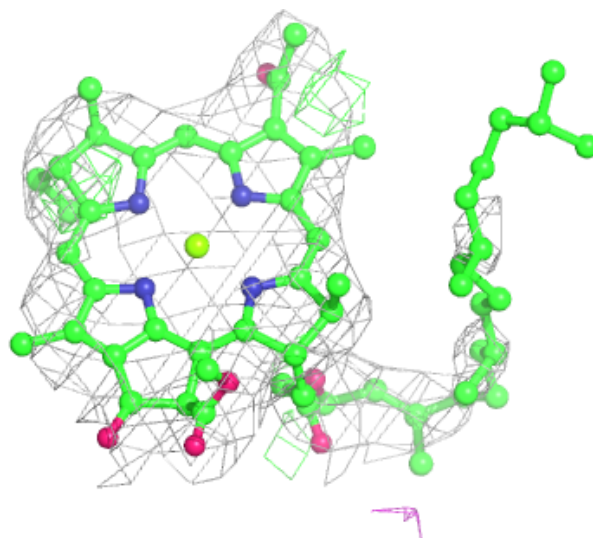
Electron density around BCL Z 102:

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



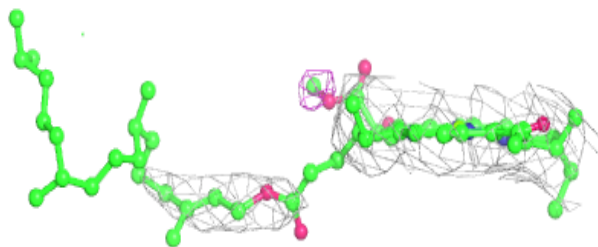
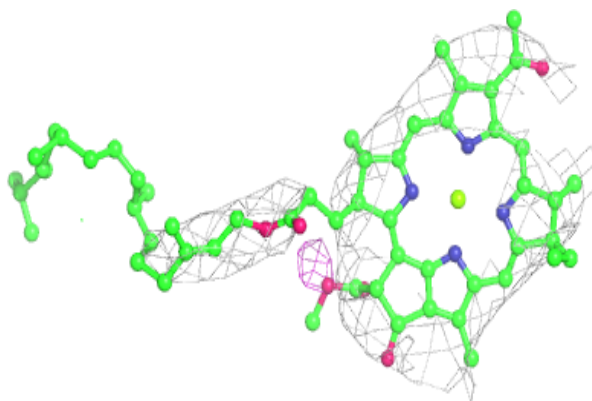
Electron density around BCL x 305:

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



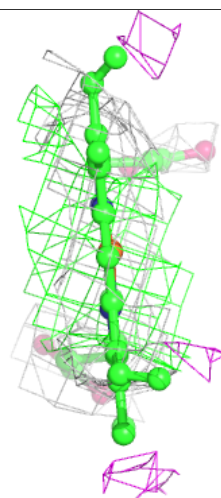
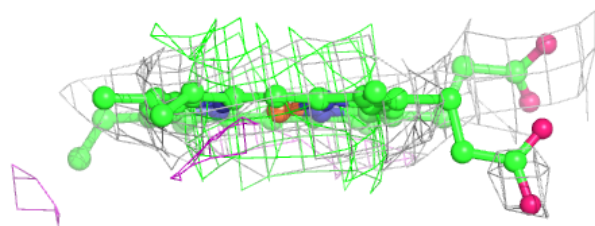
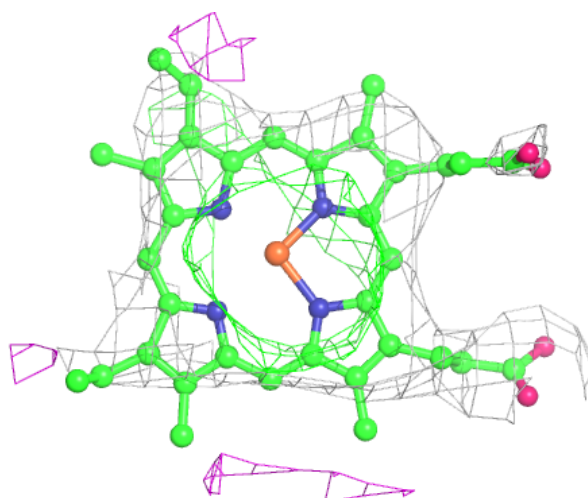
Electron density around BCL Y 101:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.