wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2023 – 03:24 PM JST

PDB ID	:	5B5M
Title	:	Crystal structure of the Sr-substituted LH1-RC complex from Tch. tepidum
Authors	:	Wang-Otomo, Z.-Y.; Yu, L.-J.
Deposited on	:	2016-05-12
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

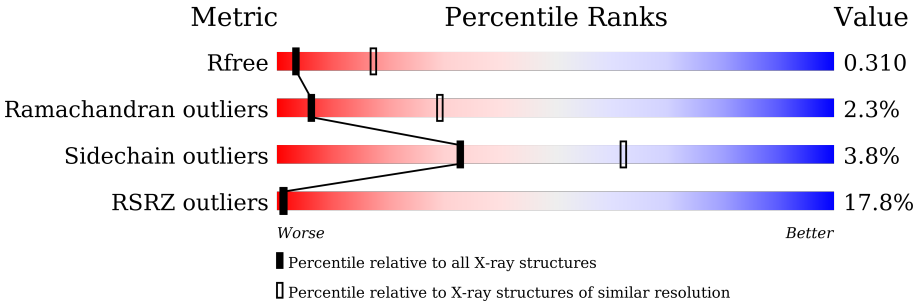
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	12% 84% 11% • 5%
1	o	333	13% 85% 9% • 5%
2	L	281	6% 91% 8% •
2	x	281	6% 90% 10%
3	M	319	4% 90% 10%
3	y	319	5% 89% 11%
4	H	259	11% 88% 9% •

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Mol	Chain	Length	Quality of chain
4	t	259	12% 86% 11%
5	1	61	21% 92%
5	3	61	25% 89% 10%
5	5	61	16% 93% 5%
5	7	61	34% 93% 5%
5	9	61	26% 90% 8%
5	A	61	43% 95%
5	AA	61	38% 90% 8%
5	AC	61	34% 92% 7%
5	AE	61	39% 92% 7%
5	AG	61	23% 93% 5%
5	AI	61	28% 95%
5	AK	61	20% 95%
5	D	61	44% 93% 5%
5	F	61	36% 93% 5%
5	I	61	31% 90% 8%
5	K	61	31% 97%
5	O	61	28% 93% 5%
5	Q	61	23% 84% 15%
5	S	61	28% 89% 10%
5	U	61	16% 93% 5%
5	W	61	23% 92% 7%
5	Y	61	33% 93% 5%
5	d	61	21% 93% 5%
5	f	61	23% 93% 5%

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Mol	Chain	Length	Quality of chain
5	h	61	26% 92% 5%
5	j	61	21% 93% 5%
5	l	61	34% 92% 7%
5	m	61	36% 95%
5	p	61	30% 89% 10%
5	r	61	25% 90% 8%
5	u	61	28% 95%
5	w	61	39% 95%
6	0	47	19% 83% 15%
6	2	47	13% 85% 15%
6	4	47	2% 85% 15%
6	6	47	13% 85% 15%
6	8	47	23% 85% 15%
6	AB	47	13% 85% 15%
6	AD	47	9% 85% 15%
6	AF	47	19% 85% 15%
6	AH	47	17% 85% 15%
6	AJ	47	17% 81% 15%
6	AL	47	19% 85% 15%
6	B	47	23% 79% 6% 15%
6	E	47	13% 85% 15%
6	G	47	11% 85% 15%
6	J	47	26% 83% 15%
6	N	47	17% 83% 15%
6	P	47	17% 81% 15%

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Mol	Chain	Length	Quality of chain
6	R	47	15% 85% 15%
6	T	47	13% 79% 6% 15%
6	V	47	9% 85% 15%
6	X	47	2% 79% 6% 15%
6	Z	47	2% 85% 15%
6	c	47	19% 85% 15%
6	e	47	9% 85% 15%
6	g	47	13% 83% 15%
6	i	47	17% 85% 15%
6	k	47	26% 83% 15%
6	n	47	21% 85% 15%
6	q	47	9% 83% 15%
6	s	47	11% 85% 15%
6	v	47	17% 85% 15%
6	z	47	19% 85% 15%

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
11	UQ8	L	304	-	-	-	X
11	UQ8	x	304	-	-	-	X
12	PEF	A	101	-	-	-	X
14	MQ8	M	403	-	-	-	X
14	MQ8	y	403	-	-	-	X
15	CRT	2	101	-	-	-	X
15	CRT	4	101	-	-	-	X
15	CRT	6	101	-	-	-	X
15	CRT	8	101	-	-	-	X
15	CRT	9	102	-	-	-	X
15	CRT	A	103	-	-	-	X
15	CRT	AC	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CRT	AD	102	-	-	-	X
15	CRT	AE	103	-	-	-	X
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	J	101	-	-	-	X
15	CRT	M	404	-	-	-	X
15	CRT	N	101	-	-	-	X
15	CRT	P	102	-	-	-	X
15	CRT	R	101	-	-	-	X
15	CRT	T	101	-	-	-	X
15	CRT	U	102	-	-	-	X
15	CRT	X	101	-	-	-	X
15	CRT	c	101	-	-	-	X
15	CRT	e	101	-	-	-	X
15	CRT	f	102	-	-	-	X
15	CRT	i	101	-	-	-	X
15	CRT	k	101	-	-	-	X
15	CRT	n	101	-	-	-	X
15	CRT	p	103	-	-	-	X
15	CRT	s	101	-	-	-	X
15	CRT	v	101	-	-	-	X
15	CRT	y	404	-	-	-	X
15	CRT	z	101	-	-	-	X
16	PO4	H	302	-	-	-	X
9	BCL	AC	102	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	C	317	2458	1551	430	460	17	0	0	0
1	o	317	2458	1551	430	460	17	0	0	0

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

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

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

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

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

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

- Molecule 5 is a protein called LH1 alpha polypeptide.

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

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

- Molecule 6 is a protein called LH1 beta polypeptide.

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

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

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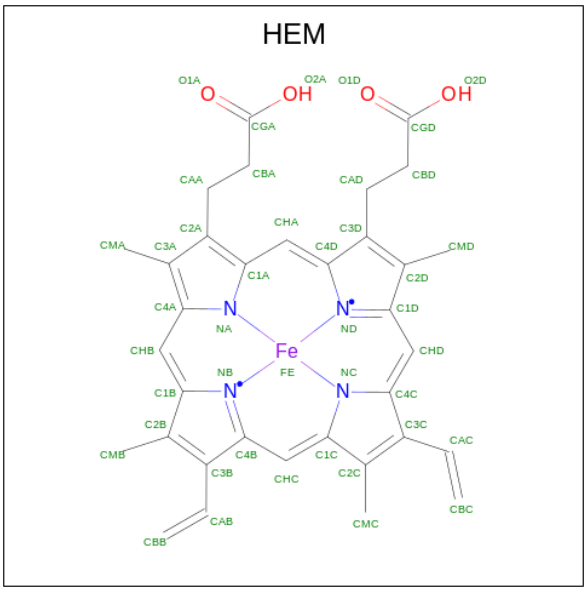
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	k	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	c	40	337	228	52	55	2	0	0	0

- 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
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	o	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	o	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	o	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
7	o	1	43	34	1	4	4	0	0

- Molecule 8 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

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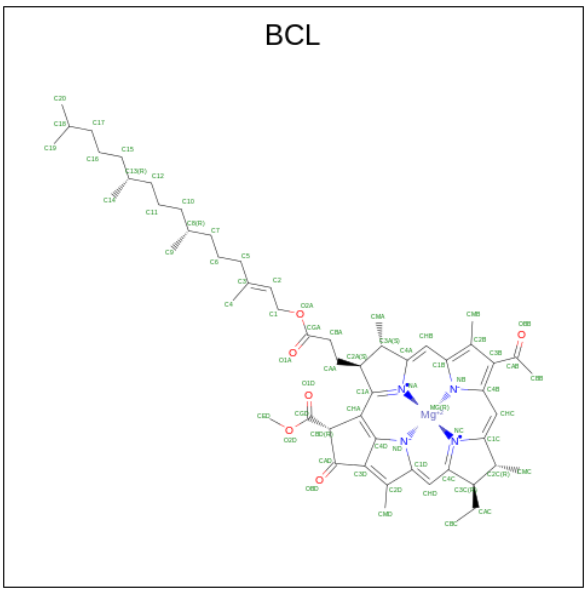
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	w	2	Total Sr 2 2	0	0
8	AA	1	Total Sr 1 1	0	0
8	AC	1	Total Sr 1 1	0	0
8	AE	1	Total Sr 1 1	0	0
8	AI	2	Total Sr 2 2	0	0
8	AK	1	Total Sr 1 1	0	0
8	d	1	Total Sr 1 1	0	0
8	f	1	Total Sr 1 1	0	0
8	h	1	Total Sr 1 1	0	0
8	j	1	Total Sr 1 1	0	0
8	l	1	Total Sr 1 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

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

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

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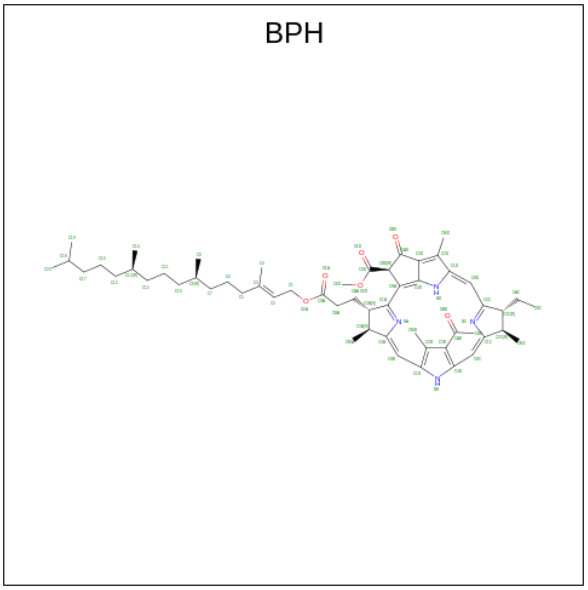
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
9	f	1	66	55	1	4	6	0	0
9	g	1	66	55	1	4	6	0	0
9	h	1	66	55	1	4	6	0	0
9	i	1	66	55	1	4	6	0	0
9	j	1	66	55	1	4	6	0	0
9	k	1	66	55	1	4	6	0	0
9	l	1	66	55	1	4	6	0	0
9	c	1	66	55	1	4	6	0	0

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



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

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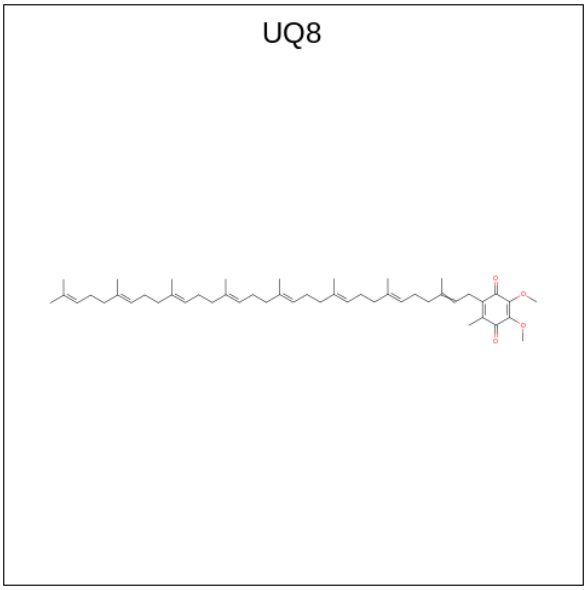
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	y	1	65	55	4	6	0	0

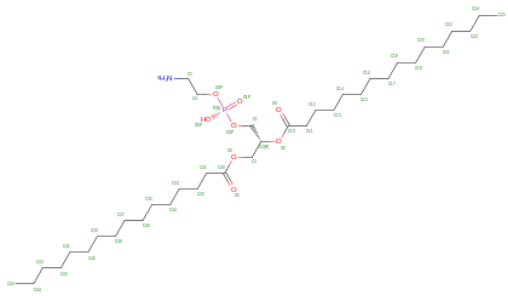
- Molecule 11 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



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

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

PEF



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

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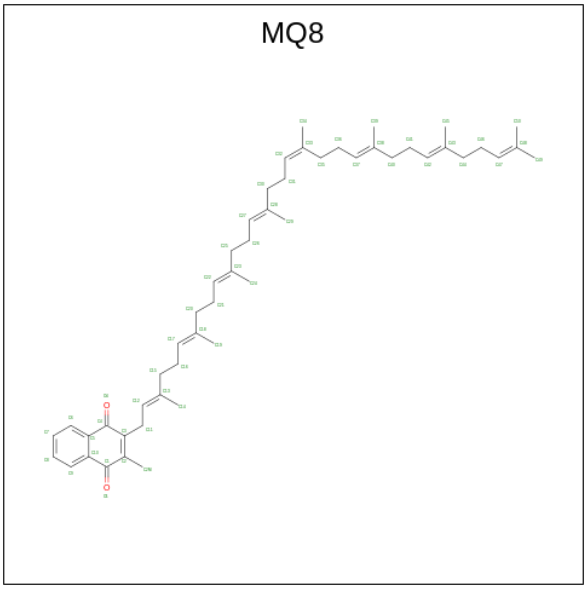
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	m	1	19	9	1	8	1	0	0
12	p	1	16	7	1	7	1	0	0

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

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

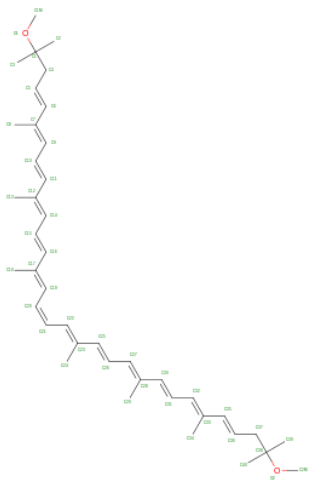
- Molecule 14 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



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

- Molecule 15 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).

CRT



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	M	1	44	42	2	0	0
15	A	1	44	42	2	0	0
15	E	1	44	42	2	0	0
15	G	1	44	42	2	0	0
15	J	1	44	42	2	0	0
15	N	1	44	42	2	0	0
15	P	1	44	42	2	0	0
15	R	1	44	42	2	0	0
15	T	1	44	42	2	0	0
15	U	1	44	42	2	0	0
15	X	1	44	42	2	0	0
15	Z	1	44	42	2	0	0
15	2	1	44	42	2	0	0
15	4	1	44	42	2	0	0

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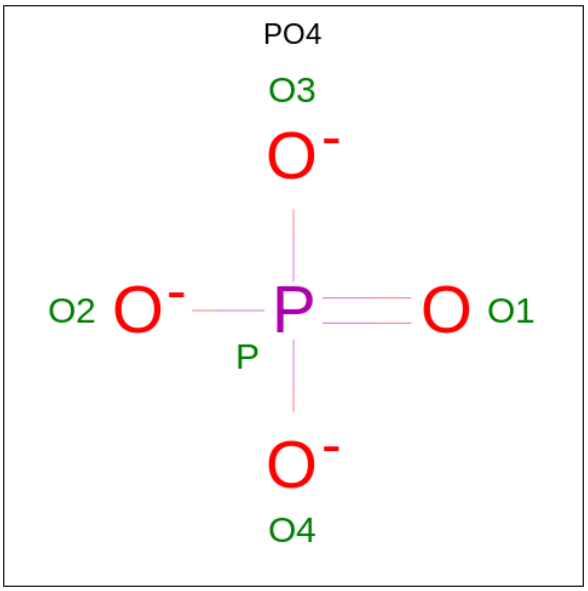
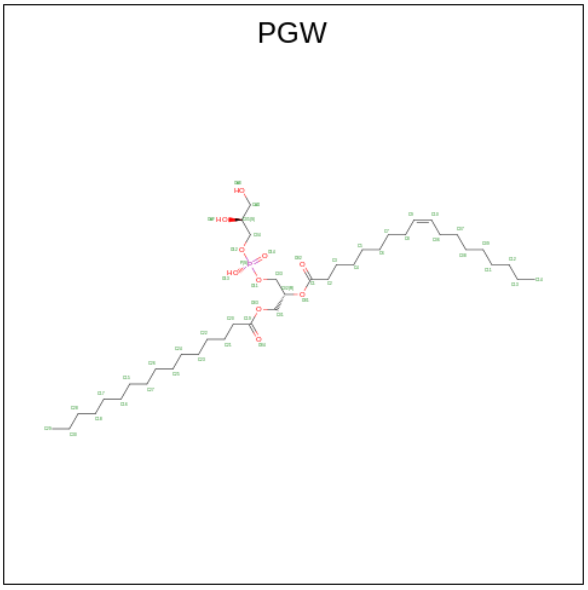
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	6	1	44	42	2	0	0
			Total	C	O		
15	8	1	44	42	2	0	0
			Total	C	O		
15	9	1	44	42	2	0	0
			Total	C	O		
15	y	1	44	42	2	0	0
			Total	C	O		
15	n	1	44	42	2	0	0
			Total	C	O		
15	p	1	44	42	2	0	0
			Total	C	O		
15	s	1	44	42	2	0	0
			Total	C	O		
15	v	1	44	42	2	0	0
			Total	C	O		
15	z	1	44	42	2	0	0
			Total	C	O		
15	AC	1	44	42	2	0	0
			Total	C	O		
15	AD	1	44	42	2	0	0
			Total	C	O		
15	AE	1	44	42	2	0	0
			Total	C	O		
15	AH	1	44	42	2	0	0
			Total	C	O		
15	AJ	1	44	42	2	0	0
			Total	C	O		
15	AL	1	44	42	2	0	0
			Total	C	O		
15	e	1	44	42	2	0	0
			Total	C	O		
15	f	1	44	42	2	0	0
			Total	C	O		
15	i	1	44	42	2	0	0
			Total	C	O		
15	k	1	44	42	2	0	0
			Total	C	O		
15	c	1	44	42	2	0	0

- Molecule 16 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- 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: $C_{40}H_{77}O_{10}P$).



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

- Molecule 18 is water.

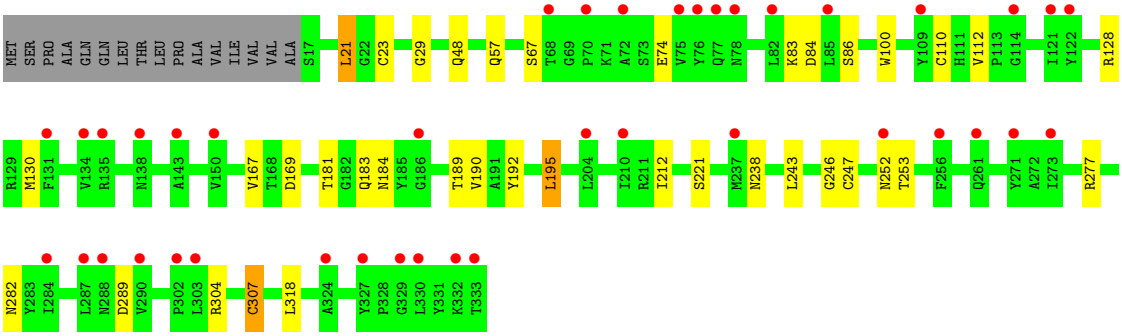
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	C	1	1	1	0	0
18	L	1	1	1	0	0
18	W	1	1	1	0	0
18	o	1	1	1	0	0
18	x	1	1	1	0	0
18	AI	1	1	1	0	0

3 Residue-property plots (i)

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

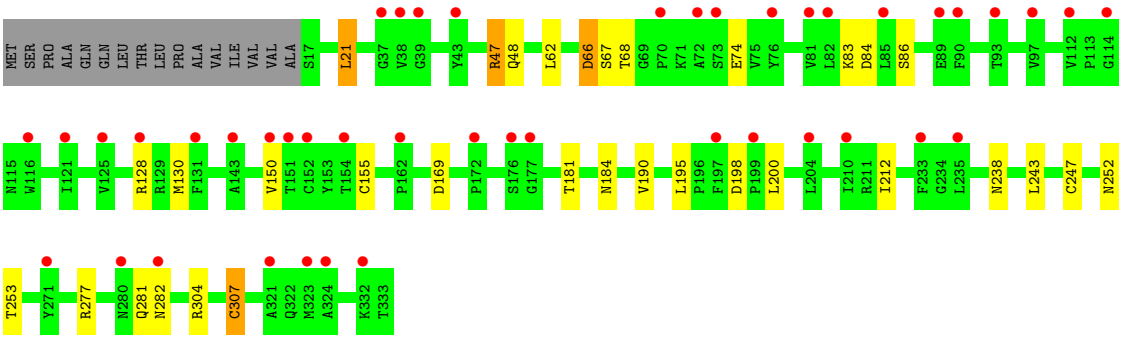
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



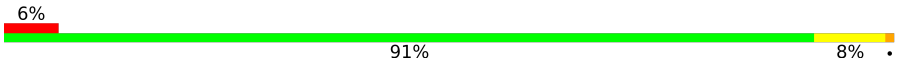
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

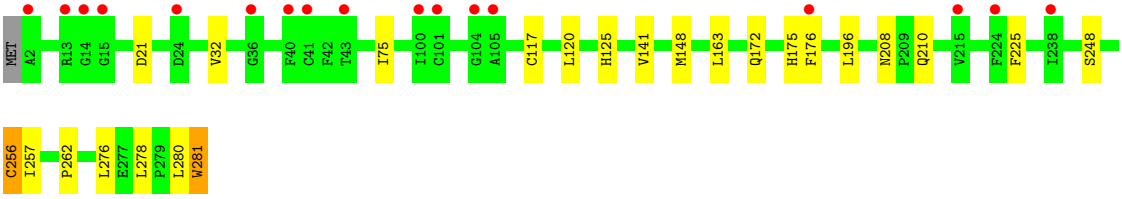
Chain o:



• Molecule 2: Photosynthetic reaction center L subunit

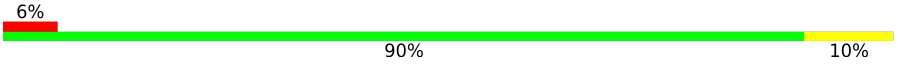
Chain L:

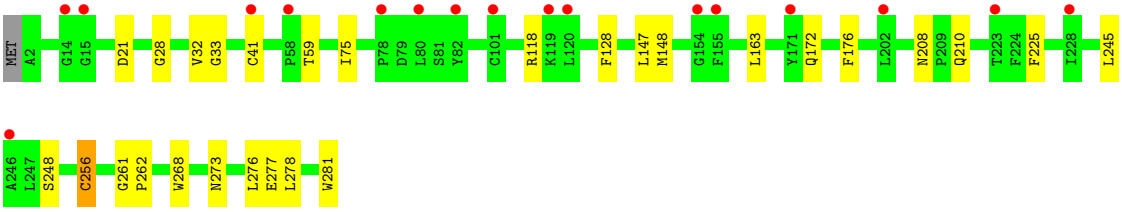




• Molecule 2: Photosynthetic reaction center L subunit

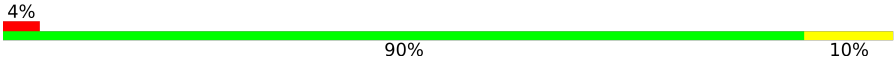
Chain x:

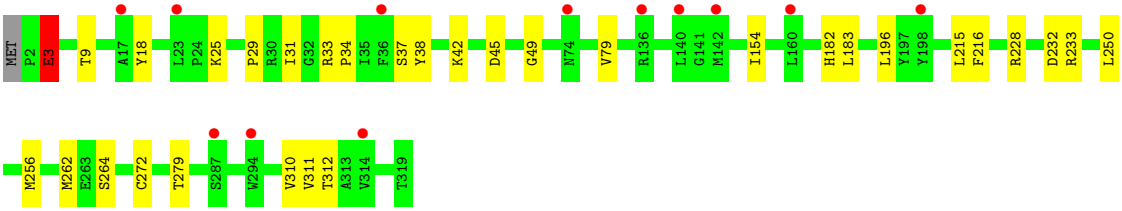




• Molecule 3: Photosynthetic reaction center M subunit

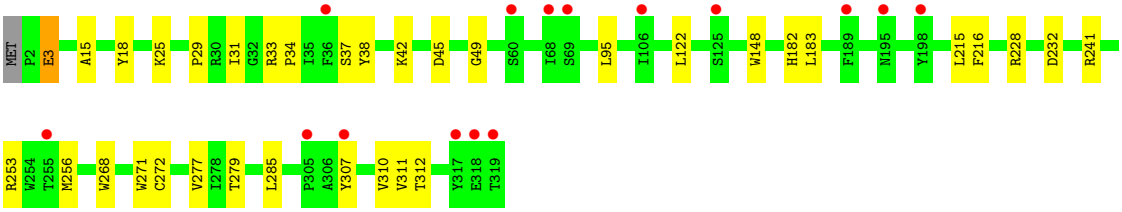
Chain M:





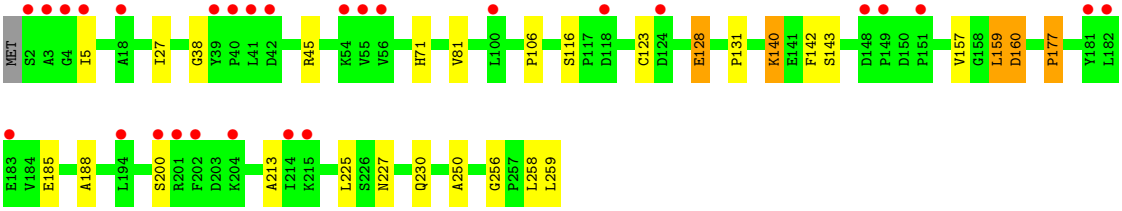
• Molecule 3: Photosynthetic reaction center M subunit

Chain y:



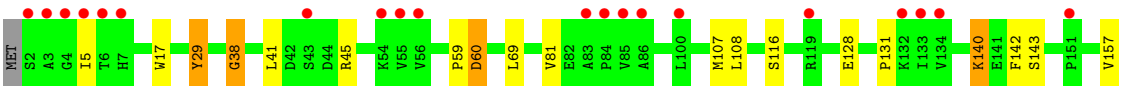
• Molecule 4: Photosynthetic reaction center H subunit

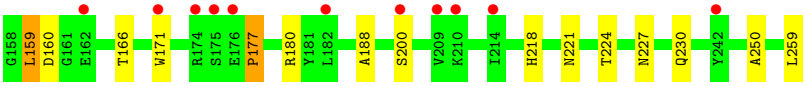
Chain H:



• Molecule 4: Photosynthetic reaction center H subunit

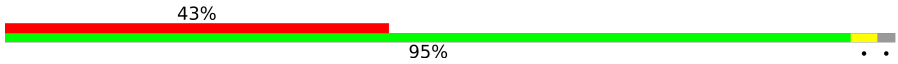
Chain t:

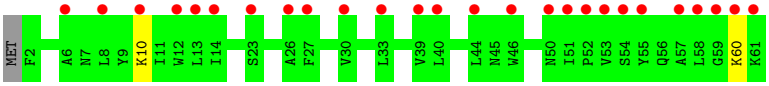




• Molecule 5: LH1 alpha polypeptide

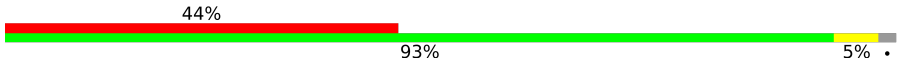
Chain A:

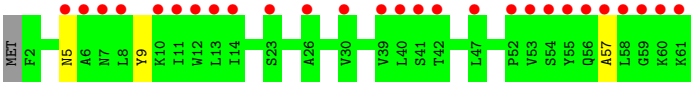




• Molecule 5: LH1 alpha polypeptide

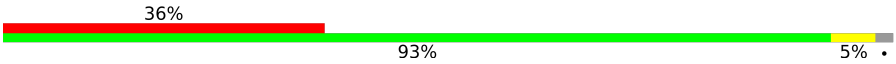
Chain D:

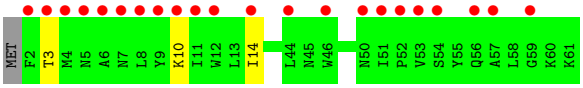




• Molecule 5: LH1 alpha polypeptide

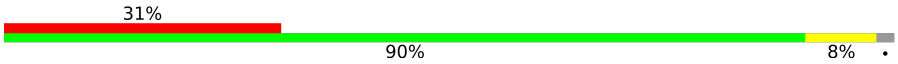
Chain F:

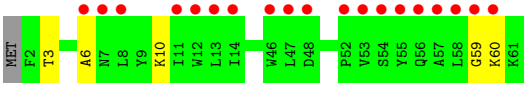




• Molecule 5: LH1 alpha polypeptide

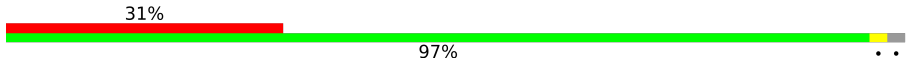
Chain I:

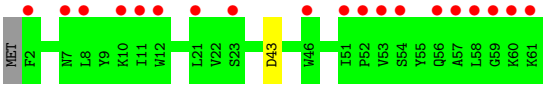




• Molecule 5: LH1 alpha polypeptide

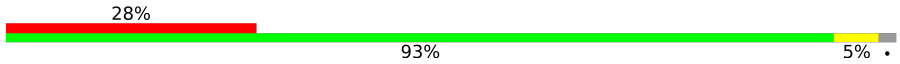
Chain K:

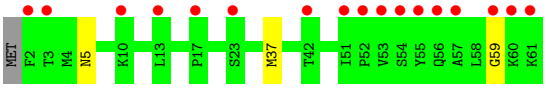




• Molecule 5: LH1 alpha polypeptide

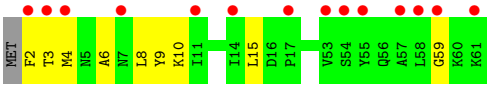
Chain O:





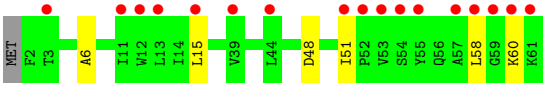
• Molecule 5: LH1 alpha polypeptide

Chain Q:



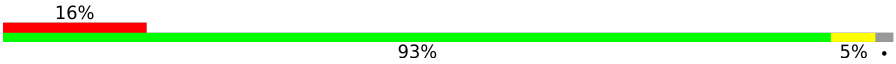
- Molecule 5: LH1 alpha polypeptide

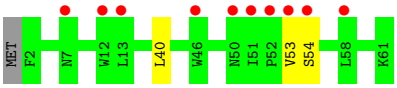
Chain S:



- Molecule 5: LH1 alpha polypeptide

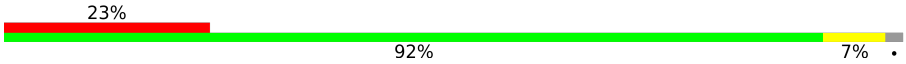
Chain U:

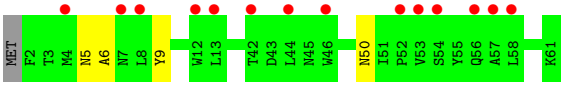




- Molecule 5: LH1 alpha polypeptide

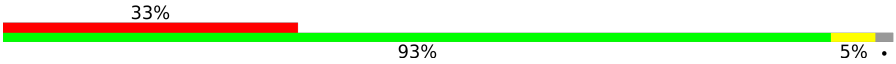
Chain W:

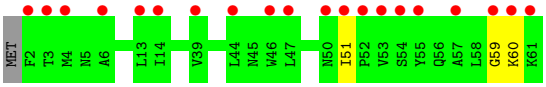




- Molecule 5: LH1 alpha polypeptide

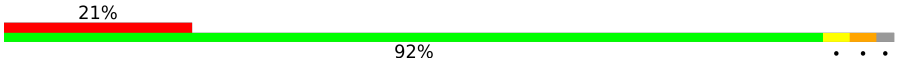
Chain Y:

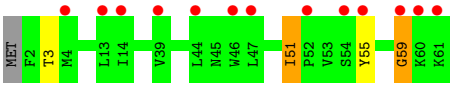




- Molecule 5: LH1 alpha polypeptide

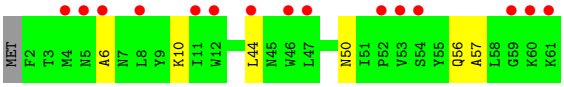
Chain 1:





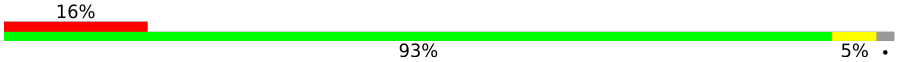
- Molecule 5: LH1 alpha polypeptide

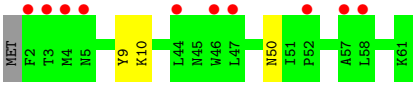
Chain 3:



• Molecule 5: LH1 alpha polypeptide

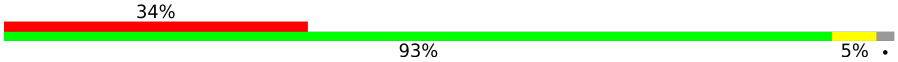
Chain 5:

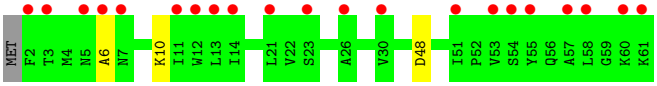




• Molecule 5: LH1 alpha polypeptide

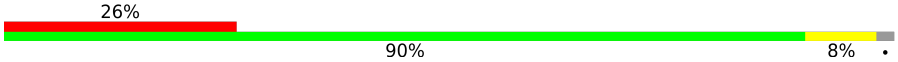
Chain 7:

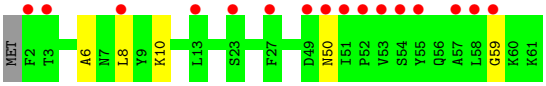




• Molecule 5: LH1 alpha polypeptide

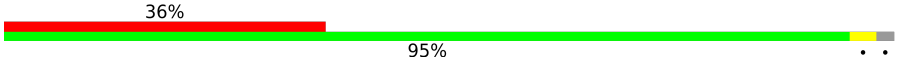
Chain 9:

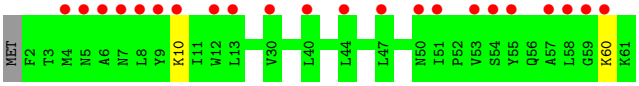




• Molecule 5: LH1 alpha polypeptide

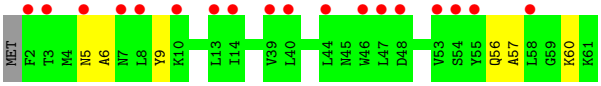
Chain m:





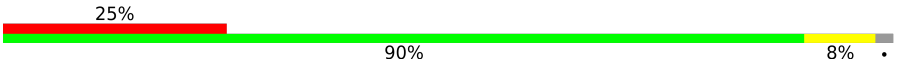
• Molecule 5: LH1 alpha polypeptide

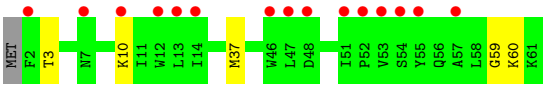
Chain p:



• Molecule 5: LH1 alpha polypeptide

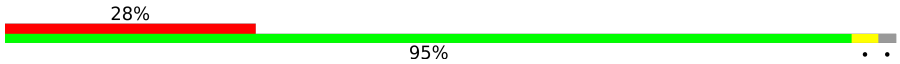
Chain r:

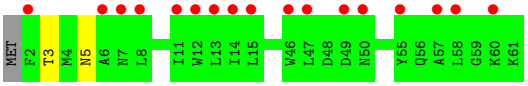




• Molecule 5: LH1 alpha polypeptide

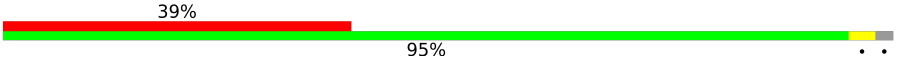
Chain u:

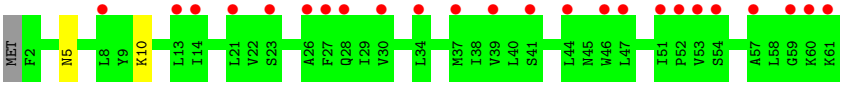




• Molecule 5: LH1 alpha polypeptide

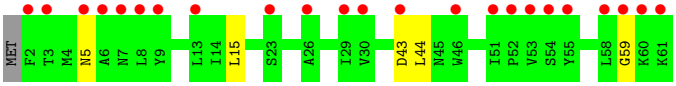
Chain w:





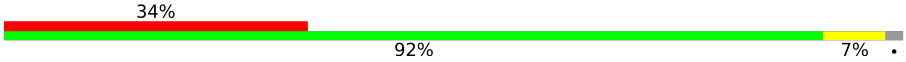
• Molecule 5: LH1 alpha polypeptide

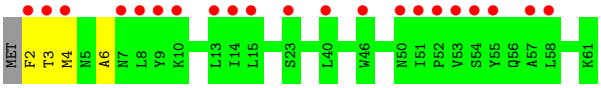
Chain AA:



• Molecule 5: LH1 alpha polypeptide

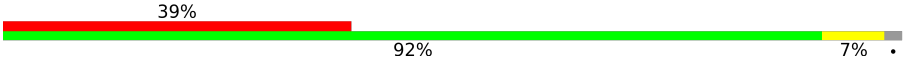
Chain AC:

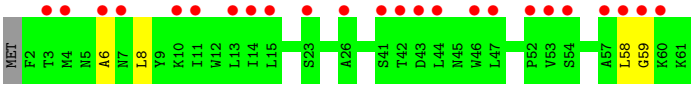




• Molecule 5: LH1 alpha polypeptide

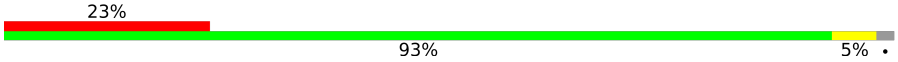
Chain AE:

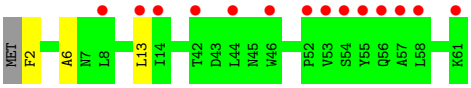




• Molecule 5: LH1 alpha polypeptide

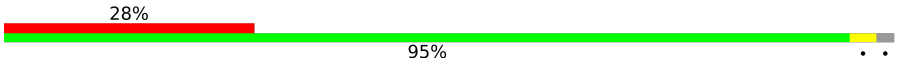
Chain AG:

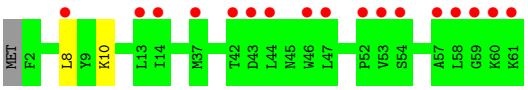




• Molecule 5: LH1 alpha polypeptide

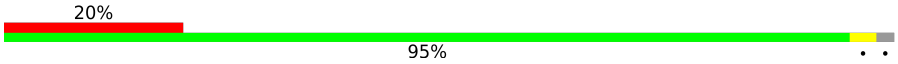
Chain AI:

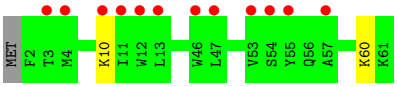




• Molecule 5: LH1 alpha polypeptide

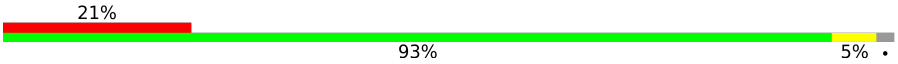
Chain AK:

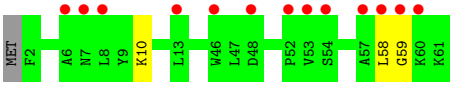




• Molecule 5: LH1 alpha polypeptide

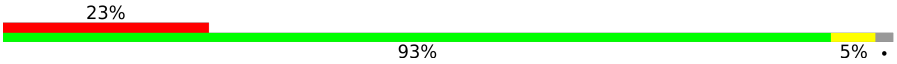
Chain d:

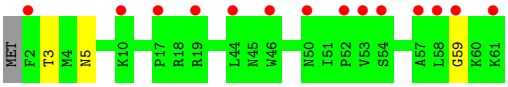




• Molecule 5: LH1 alpha polypeptide

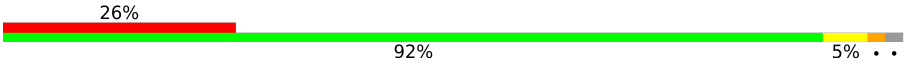
Chain f:

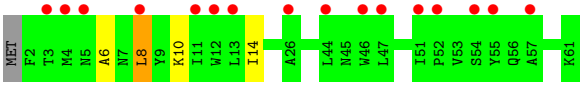




• Molecule 5: LH1 alpha polypeptide

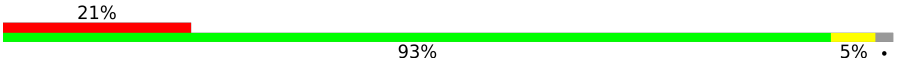
Chain h:

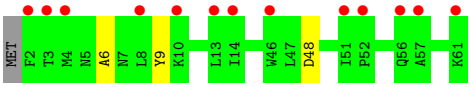




• Molecule 5: LH1 alpha polypeptide

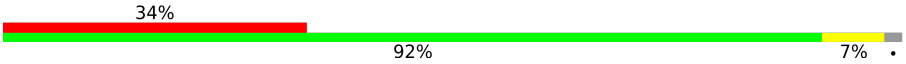
Chain j:

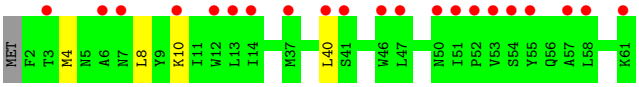




• Molecule 5: LH1 alpha polypeptide

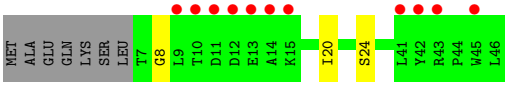
Chain l:





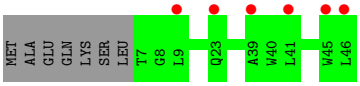
• Molecule 6: LH1 beta polypeptide

Chain B:



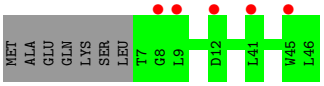
• Molecule 6: LH1 beta polypeptide

Chain E:



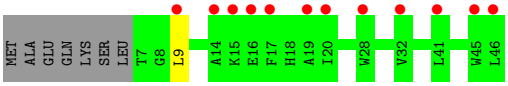
• Molecule 6: LH1 beta polypeptide

Chain G:



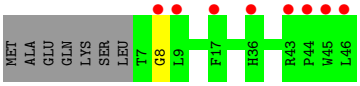
• Molecule 6: LH1 beta polypeptide

Chain J:



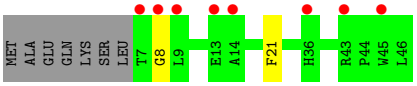
• Molecule 6: LH1 beta polypeptide

Chain N:



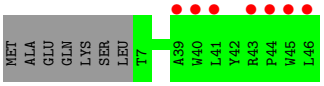
• Molecule 6: LH1 beta polypeptide

Chain P:



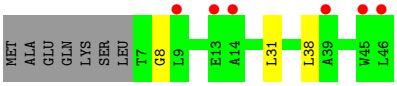
• Molecule 6: LH1 beta polypeptide

Chain R:



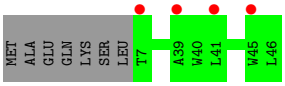
• Molecule 6: LH1 beta polypeptide

Chain T:



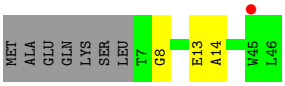
• Molecule 6: LH1 beta polypeptide

Chain V:



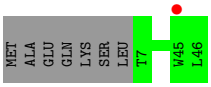
• Molecule 6: LH1 beta polypeptide

Chain X:



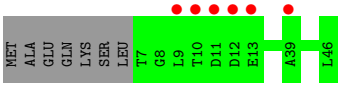
• Molecule 6: LH1 beta polypeptide

Chain Z:



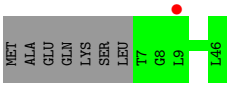
• Molecule 6: LH1 beta polypeptide

Chain 2:



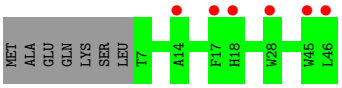
• Molecule 6: LH1 beta polypeptide

Chain 4:



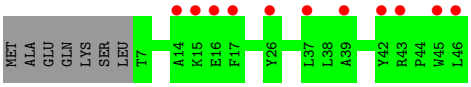
• Molecule 6: LH1 beta polypeptide

Chain 6:



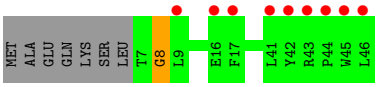
• Molecule 6: LH1 beta polypeptide

Chain 8:



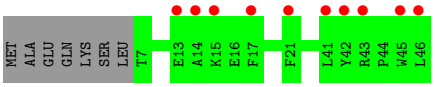
• Molecule 6: LH1 beta polypeptide

Chain 0:



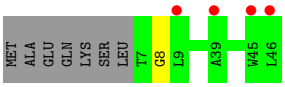
• Molecule 6: LH1 beta polypeptide

Chain n:



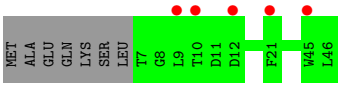
• Molecule 6: LH1 beta polypeptide

Chain q:



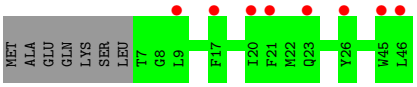
• Molecule 6: LH1 beta polypeptide

Chain s:



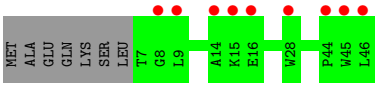
• Molecule 6: LH1 beta polypeptide

Chain v:



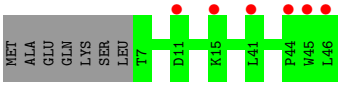
• Molecule 6: LH1 beta polypeptide

Chain z:



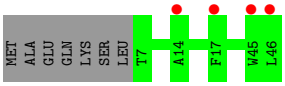
• Molecule 6: LH1 beta polypeptide

Chain AB:



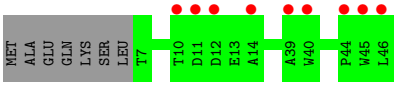
• Molecule 6: LH1 beta polypeptide

Chain AD:



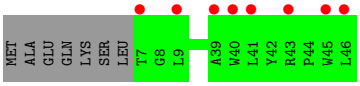
• Molecule 6: LH1 beta polypeptide

Chain AF:



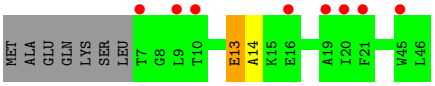
• Molecule 6: LH1 beta polypeptide

Chain AH:



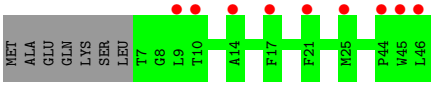
• Molecule 6: LH1 beta polypeptide

Chain AJ:



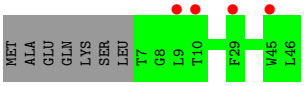
• Molecule 6: LH1 beta polypeptide

Chain AL:



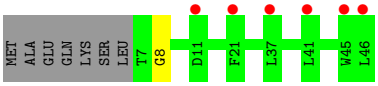
• Molecule 6: LH1 beta polypeptide

Chain e:



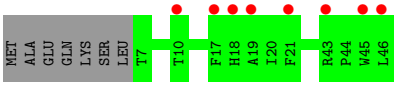
- Molecule 6: LH1 beta polypeptide

Chain g:



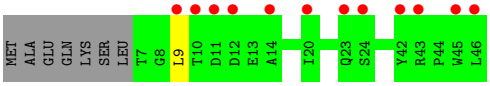
- Molecule 6: LH1 beta polypeptide

Chain i:



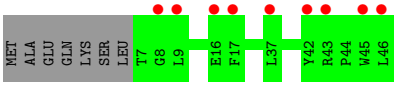
- Molecule 6: LH1 beta polypeptide

Chain k:



- Molecule 6: LH1 beta polypeptide

Chain c:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	164.89Å 148.95Å 210.23Å 90.00° 108.18° 90.00°	Depositor
Resolution (Å)	48.18 – 3.30 48.18 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.18-3.30) 98.3 (48.18-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.271 , 0.309 0.272 , 0.310	Depositor DCC
R_{free} test set	7034 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	107.8	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	51893	wwPDB-VP
Average B, all atoms (Å^2)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.86	2/2528 (0.1%)	1.17	10/3451 (0.3%)
1	o	0.83	2/2528 (0.1%)	1.14	10/3451 (0.3%)
2	L	0.90	3/2318 (0.1%)	1.16	7/3167 (0.2%)
2	x	0.89	4/2318 (0.2%)	1.13	8/3167 (0.3%)
3	M	0.83	1/2646 (0.0%)	1.11	10/3621 (0.3%)
3	y	0.83	1/2646 (0.0%)	1.08	10/3621 (0.3%)
4	H	0.83	2/2037 (0.1%)	1.13	7/2776 (0.3%)
4	t	0.91	2/2037 (0.1%)	1.22	10/2776 (0.4%)
5	1	0.58	0/485	0.91	0/664
5	3	0.53	0/485	0.82	0/664
5	5	0.53	0/485	0.77	0/664
5	7	0.47	0/485	0.69	0/664
5	9	0.46	0/485	0.76	0/664
5	A	0.45	0/485	0.76	0/664
5	AA	0.43	0/485	0.75	1/664 (0.2%)
5	AC	0.43	0/485	0.68	0/664
5	AE	0.38	0/491	0.65	0/672
5	AG	0.43	0/485	0.71	1/664 (0.2%)
5	AI	0.49	0/485	0.81	1/664 (0.2%)
5	AK	0.53	0/485	0.80	0/664
5	D	0.46	0/485	0.79	0/664
5	F	0.46	0/485	0.74	0/664
5	I	0.48	0/485	0.73	0/664
5	K	0.42	0/485	0.72	0/664
5	O	0.47	0/485	0.77	0/664
5	Q	0.49	0/485	0.81	1/664 (0.2%)
5	S	0.50	0/491	0.74	1/672 (0.1%)
5	U	0.53	0/485	0.84	1/664 (0.2%)
5	W	0.56	0/485	0.84	0/664
5	Y	0.68	0/485	0.84	1/664 (0.2%)
5	d	0.47	0/485	0.81	1/664 (0.2%)
5	f	0.52	0/485	0.77	0/664

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	h	0.51	0/485	0.76	1/664 (0.2%)
5	j	0.46	0/485	0.68	0/664
5	l	0.48	0/485	0.75	0/664
5	m	0.46	0/485	0.77	0/664
5	p	0.51	0/485	0.81	1/664 (0.2%)
5	r	0.57	0/485	0.75	0/664
5	u	0.49	0/485	0.80	0/664
5	w	0.43	0/485	0.76	0/664
6	0	0.41	0/350	0.70	1/476 (0.2%)
6	2	0.56	0/350	0.70	0/476
6	4	0.53	0/350	0.73	0/476
6	6	0.45	0/350	0.65	0/476
6	8	0.43	0/350	0.68	0/476
6	AB	0.39	0/350	0.67	0/476
6	AD	0.42	0/350	0.60	0/476
6	AF	0.42	0/350	0.62	0/476
6	AH	0.43	0/350	0.64	0/476
6	AJ	0.50	0/350	0.67	0/476
6	AL	0.47	0/350	0.68	0/476
6	B	0.43	0/350	0.65	0/476
6	E	0.47	0/350	0.75	0/476
6	G	0.48	0/350	0.67	0/476
6	J	0.48	0/350	0.71	1/476 (0.2%)
6	N	0.44	0/350	0.73	0/476
6	P	0.45	0/350	0.71	0/476
6	R	0.43	0/350	0.73	0/476
6	T	0.48	0/350	0.73	2/476 (0.4%)
6	V	0.43	0/350	0.64	0/476
6	X	0.56	0/350	0.81	0/476
6	Z	0.51	0/350	0.74	0/476
6	c	0.36	0/350	0.61	0/476
6	e	0.45	0/350	0.66	0/476
6	g	0.44	0/350	0.62	1/476 (0.2%)
6	i	0.50	0/350	0.70	0/476
6	k	0.38	0/350	0.63	1/476 (0.2%)
6	n	0.43	0/350	0.60	0/476
6	q	0.46	0/350	0.75	1/476 (0.2%)
6	s	0.51	0/350	0.79	0/476
6	v	0.46	0/350	0.75	0/476
6	z	0.41	0/350	0.67	0/476
All	All	0.66	17/45790 (0.0%)	0.93	89/62526 (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	3
2	x	0	1
3	M	0	2
3	y	0	3
4	t	0	1
5	1	0	2
6	AJ	0	2
6	X	0	1
All	All	0	15

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	CYS	CB-SG	-7.73	1.69	1.82
2	L	256	CYS	CB-SG	-7.49	1.69	1.82
3	y	268	TRP	CB-CG	-7.36	1.36	1.50
2	x	41	CYS	CB-SG	-7.27	1.69	1.82
1	C	100	TRP	CB-CG	-6.91	1.37	1.50

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	o	247	CYS	CA-CB-SG	-10.24	95.56	114.00
1	C	247	CYS	CA-CB-SG	-8.96	97.86	114.00
1	C	195	LEU	CB-CG-CD2	-8.93	95.81	111.00
4	t	29	TYR	CA-CB-CG	8.57	129.69	113.40
1	o	47	ARG	NE-CZ-NH1	8.44	124.52	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	189	THR	Mainchain
1	C	246	GLY	Mainchain
1	C	57	GLN	Sidechain
3	M	272	CYS	Mainchain
3	M	9	THR	Mainchain

5.2 Too-close contacts (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%)	276 (88%)	32 (10%)	7 (2%)	6	30
1	o	315/333 (95%)	277 (88%)	30 (10%)	8 (2%)	5	27
2	L	278/281 (99%)	247 (89%)	27 (10%)	4 (1%)	11	38
2	x	278/281 (99%)	248 (89%)	27 (10%)	3 (1%)	14	45
3	M	316/319 (99%)	282 (89%)	30 (10%)	4 (1%)	12	40
3	y	316/319 (99%)	284 (90%)	28 (9%)	4 (1%)	12	40
4	H	256/259 (99%)	213 (83%)	34 (13%)	9 (4%)	3	21
4	t	256/259 (99%)	214 (84%)	33 (13%)	9 (4%)	3	21
5	1	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	22
5	3	58/61 (95%)	44 (76%)	10 (17%)	4 (7%)	1	8
5	5	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	22
5	7	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	22
5	9	58/61 (95%)	49 (84%)	5 (9%)	4 (7%)	1	8
5	A	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	22
5	AA	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	9	35
5	AC	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	22
5	AE	59/61 (97%)	50 (85%)	6 (10%)	3 (5%)	2	13
5	AG	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	35
5	AI	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	9	35
5	AK	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	22
5	D	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	22
5	I	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	8
5	K	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
5	O	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	9	35
5	Q	58/61 (95%)	47 (81%)	6 (10%)	5 (9%)	1	5
5	S	59/61 (97%)	48 (81%)	8 (14%)	3 (5%)	2	13
5	U	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	9	35
5	W	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	22
5	Y	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	22
5	d	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	22
5	f	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	22
5	h	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	13
5	j	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	9	35
5	l	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	22
5	m	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	22
5	p	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	1	5
5	r	58/61 (95%)	45 (78%)	9 (16%)	4 (7%)	1	8
5	u	58/61 (95%)	47 (81%)	10 (17%)	1 (2%)	9	35
5	w	58/61 (95%)	46 (79%)	11 (19%)	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%)	38 (100%)	0	0	100	100
6	AD	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AF	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	AH	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	AJ	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	AL	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	B	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	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%)	37 (97%)	1 (3%)	0	100	100
6	N	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	5	27
6	P	38/47 (81%)	37 (97%)	0	1 (3%)	5	27
6	R	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	T	38/47 (81%)	37 (97%)	0	1 (3%)	5	27
6	V	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	X	38/47 (81%)	36 (95%)	1 (3%)	1 (3%)	5	27
6	Z	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	c	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	e	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	g	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	i	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	k	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
6	n	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	q	38/47 (81%)	38 (100%)	0	0	100	100
6	s	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	v	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	z	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
All	All	5404/5840 (92%)	4736 (88%)	543 (10%)	125 (2%)	6	29

5 of 125 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	265/278 (95%)	245 (92%)	20 (8%)	13	39
1	o	265/278 (95%)	246 (93%)	19 (7%)	14	41
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%)	238 (93%)	18 (7%)	15	43
3	y	256/257 (100%)	238 (93%)	18 (7%)	15	43
4	H	210/211 (100%)	194 (92%)	16 (8%)	13	39
4	t	210/211 (100%)	191 (91%)	19 (9%)	9	32
5	1	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	3	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	5	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	7	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	9	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	A	52/56 (93%)	52 (100%)	0	100	100
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%)	51 (98%)	1 (2%)	57	77
5	AI	52/56 (93%)	52 (100%)	0	100	100
5	AK	52/56 (93%)	52 (100%)	0	100	100
5	D	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	F	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	I	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	K	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	O	52/56 (93%)	50 (96%)	2 (4%)	33	62
5	Q	52/56 (93%)	49 (94%)	3 (6%)	20	50
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%)	50 (96%)	2 (4%)	33	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Y	52/56 (93%)	52 (100%)	0	100	100
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%)	50 (96%)	2 (4%)	33	62
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%)	52 (100%)	0	100	100
5	r	52/56 (93%)	51 (98%)	1 (2%)	57	77
5	u	52/56 (93%)	51 (98%)	1 (2%)	57	77
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%)	33 (100%)	0	100	100
6	G	33/39 (85%)	33 (100%)	0	100	100
6	J	33/39 (85%)	33 (100%)	0	100	100
6	N	33/39 (85%)	33 (100%)	0	100	100
6	P	33/39 (85%)	32 (97%)	1 (3%)	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%)	4462 (96%)	178 (4%)	33	62

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	x	163	LEU
4	t	60	ASP
2	x	210	GLN
3	y	45	ASP
4	t	157	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	x	273	ASN
5	m	7	ASN
3	y	301	HIS
5	w	50	ASN
6	X	36	HIS

5.3.3 RNA (i)

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	$\#\|Z\| > 2$
12	PEF	H	301	-	18,18,46	1.57	2 (11%)	21,23,51	1.74	3 (14%)
16	PO4	H	302	-	4,4,4	0.75	0	6,6,6	0.54	0
12	PEF	A	101	-	18,18,46	1.54	2 (11%)	21,23,51	1.74	3 (14%)
9	BCL	R	102	-	64,74,74	1.64	11 (17%)	78,115,115	2.35	27 (34%)
9	BCL	1	101	-	64,74,74	1.66	12 (18%)	78,115,115	2.27	23 (29%)
9	BCL	f	101	-	64,74,74	1.75	14 (21%)	78,115,115	2.30	24 (30%)
15	CRT	J	101	-	41,43,43	0.76	0	50,54,54	3.78	19 (38%)
16	PO4	y	405	-	4,4,4	0.81	0	6,6,6	0.52	0
15	CRT	N	101	-	41,43,43	0.81	0	50,54,54	4.01	19 (38%)
12	PEF	t	301	-	18,18,46	1.50	2 (11%)	21,23,51	1.32	4 (19%)
15	CRT	AJ	101	-	41,43,43	0.75	0	50,54,54	1.94	15 (30%)
15	CRT	6	101	-	41,43,43	0.81	0	50,54,54	3.60	18 (36%)
7	HEM	C	504	1	41,50,50	1.99	8 (19%)	45,82,82	1.87	10 (22%)
7	HEM	o	503	1	41,50,50	2.00	8 (19%)	45,82,82	2.09	17 (37%)
12	PEF	y	407	-	18,18,46	1.82	2 (11%)	21,23,51	1.58	3 (14%)
15	CRT	f	102	-	41,43,43	0.89	0	50,54,54	3.95	21 (42%)
7	HEM	o	504	1	41,50,50	1.98	9 (21%)	45,82,82	1.72	11 (24%)
9	BCL	z	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.35	32 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	BCL	L	303	-	64,74,74	1.76	13 (20%)	78,115,115	2.55	29 (37%)
17	PGW	S	101	-	20,20,50	1.06	1 (5%)	23,26,56	1.24	3 (13%)
9	BCL	L	301	-	64,74,74	1.83	15 (23%)	78,115,115	2.46	28 (35%)
15	CRT	R	101	-	41,43,43	0.75	0	50,54,54	3.43	19 (38%)
9	BCL	s	102	-	64,74,74	1.74	12 (18%)	78,115,115	2.39	26 (33%)
7	HEM	o	502	1	41,50,50	1.91	8 (19%)	45,82,82	2.21	14 (31%)
9	BCL	B	101	-	64,74,74	1.64	10 (15%)	78,115,115	2.22	27 (34%)
9	BCL	AK	101	-	64,74,74	1.73	9 (14%)	78,115,115	2.33	29 (37%)
9	BCL	W	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.20	25 (32%)
15	CRT	k	101	-	41,43,43	0.79	1 (2%)	50,54,54	3.63	15 (30%)
9	BCL	AH	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.31	27 (34%)
9	BCL	d	101	-	64,74,74	1.75	13 (20%)	78,115,115	2.32	30 (38%)
9	BCL	9	103	-	64,74,74	1.73	14 (21%)	78,115,115	2.30	29 (37%)
9	BCL	4	102	-	64,74,74	1.76	14 (21%)	78,115,115	2.43	31 (39%)
9	BCL	v	102	-	64,74,74	1.76	13 (20%)	78,115,115	2.39	29 (37%)
9	BCL	5	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.37	28 (35%)
12	PEF	y	408	-	18,18,46	1.75	3 (16%)	21,23,51	2.02	5 (23%)
9	BCL	P	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.37	32 (41%)
7	HEM	C	503	1	41,50,50	1.97	7 (17%)	45,82,82	2.15	14 (31%)
14	MQ8	M	403	-	54,54,54	1.10	5 (9%)	66,69,69	1.61	14 (21%)
15	CRT	AH	102	-	41,43,43	0.75	0	50,54,54	3.44	16 (32%)
15	CRT	M	404	-	41,43,43	0.85	0	50,54,54	3.73	13 (26%)
15	CRT	z	101	-	41,43,43	0.72	0	50,54,54	3.71	15 (30%)
15	CRT	i	101	-	41,43,43	0.81	0	50,54,54	3.50	14 (28%)
9	BCL	x	305	-	64,74,74	1.87	13 (20%)	78,115,115	2.50	31 (39%)
17	PGW	AE	101	-	20,20,50	1.04	1 (5%)	23,26,56	1.36	2 (8%)
9	BCL	U	101	-	64,74,74	1.76	12 (18%)	78,115,115	2.24	23 (29%)
9	BCL	AJ	102	-	64,74,74	1.67	11 (17%)	78,115,115	2.29	23 (29%)
9	BCL	M	401	-	64,74,74	1.85	17 (26%)	78,115,115	2.55	32 (41%)
9	BCL	Z	102	-	64,74,74	1.73	11 (17%)	78,115,115	2.37	27 (34%)
9	BCL	AA	101	-	64,74,74	1.74	11 (17%)	78,115,115	2.24	25 (32%)
9	BCL	x	301	-	64,74,74	1.82	16 (25%)	78,115,115	2.64	27 (34%)
14	MQ8	y	403	-	54,54,54	1.20	6 (11%)	66,69,69	1.67	16 (24%)
12	PEF	t	303	-	18,18,46	1.49	2 (11%)	21,23,51	2.40	8 (38%)
15	CRT	A	103	-	41,43,43	0.80	0	50,54,54	3.51	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	BCL	e	102	-	64,74,74	1.66	10 (15%)	78,115,115	2.24	29 (37%)
15	CRT	9	102	-	41,43,43	0.77	0	50,54,54	3.68	17 (34%)
7	HEM	o	501	1	41,50,50	1.95	8 (19%)	45,82,82	2.11	11 (24%)
9	BCL	y	401	-	64,74,74	1.78	13 (20%)	78,115,115	2.47	35 (44%)
9	BCL	O	101	-	64,74,74	1.70	10 (15%)	78,115,115	2.45	32 (41%)
10	BPH	x	302	-	51,70,70	0.81	1 (1%)	52,101,101	1.75	8 (15%)
15	CRT	e	101	-	41,43,43	0.78	0	50,54,54	1.78	12 (24%)
12	PEF	M	406	-	18,18,46	1.44	2 (11%)	21,23,51	2.24	4 (19%)
15	CRT	n	101	-	41,43,43	0.80	0	50,54,54	3.87	15 (30%)
16	PO4	M	405	-	4,4,4	0.60	0	6,6,6	1.05	0
9	BCL	S	102	-	64,74,74	1.76	13 (20%)	78,115,115	2.33	30 (38%)
9	BCL	X	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.21	31 (39%)
15	CRT	c	101	-	41,43,43	0.78	0	50,54,54	3.47	18 (36%)
9	BCL	AI	101	-	64,74,74	1.71	12 (18%)	78,115,115	2.24	27 (34%)
7	HEM	C	502	1	41,50,50	1.91	7 (17%)	45,82,82	2.39	13 (28%)
15	CRT	s	101	-	41,43,43	0.71	0	50,54,54	3.49	16 (32%)
12	PEF	y	406	-	18,18,46	1.56	2 (11%)	21,23,51	1.73	3 (14%)
9	BCL	r	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.22	26 (33%)
9	BCL	T	102	-	64,74,74	1.75	13 (20%)	78,115,115	2.35	27 (34%)
9	BCL	D	102	-	64,74,74	1.66	9 (14%)	78,115,115	2.39	32 (41%)
9	BCL	x	303	-	64,74,74	1.96	12 (18%)	78,115,115	2.42	28 (35%)
10	BPH	y	402	-	51,70,70	0.83	3 (5%)	52,101,101	1.27	6 (11%)
11	UQ8	x	304	-	53,53,53	1.52	3 (5%)	64,67,67	2.29	27 (42%)
9	BCL	g	101	-	64,74,74	1.69	11 (17%)	78,115,115	2.29	30 (38%)
9	BCL	h	101	-	64,74,74	1.81	14 (21%)	78,115,115	2.25	28 (35%)
9	BCL	3	101	-	64,74,74	1.73	13 (20%)	78,115,115	2.37	29 (37%)
10	BPH	M	402	-	51,70,70	0.84	3 (5%)	52,101,101	1.69	9 (17%)
9	BCL	m	102	-	64,74,74	1.74	13 (20%)	78,115,115	2.31	22 (28%)
15	CRT	y	404	-	41,43,43	0.94	1 (2%)	50,54,54	3.64	17 (34%)
15	CRT	Z	101	-	41,43,43	0.87	0	50,54,54	1.80	12 (24%)
16	PO4	t	302	-	4,4,4	0.52	0	6,6,6	1.95	2 (33%)
9	BCL	AE	102	-	64,74,74	1.66	10 (15%)	78,115,115	2.25	28 (35%)
9	BCL	p	104	-	64,74,74	1.71	12 (18%)	78,115,115	2.39	31 (39%)
9	BCL	i	102	-	64,74,74	1.69	11 (17%)	78,115,115	2.26	25 (32%)
9	BCL	K	101	-	64,74,74	1.73	15 (23%)	78,115,115	2.30	30 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	BCL	8	102	-	64,74,74	1.66	10 (15%)	78,115,115	2.26	27 (34%)
10	BPH	L	302	-	51,70,70	0.66	1 (1%)	52,101,101	1.53	11 (21%)
15	CRT	G	101	-	41,43,43	0.73	0	50,54,54	3.74	17 (34%)
15	CRT	p	103	-	41,43,43	0.71	0	50,54,54	3.75	16 (32%)
9	BCL	Q	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.33	29 (37%)
15	CRT	T	101	-	41,43,43	0.83	0	50,54,54	4.20	23 (46%)
11	UQ8	L	304	-	53,53,53	1.50	6 (11%)	64,67,67	1.81	19 (29%)
9	BCL	1	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.20	21 (26%)
9	BCL	AE	104	-	64,74,74	1.68	11 (17%)	78,115,115	2.37	28 (35%)
9	BCL	N	102	-	64,74,74	1.72	13 (20%)	78,115,115	2.32	27 (34%)
9	BCL	V	101	-	64,74,74	1.76	14 (21%)	78,115,115	2.29	25 (32%)
15	CRT	X	101	-	41,43,43	0.87	0	50,54,54	1.89	11 (22%)
12	PEF	H	304	-	18,18,46	1.59	2 (11%)	21,23,51	1.80	5 (23%)
15	CRT	AE	103	-	41,43,43	0.75	0	50,54,54	3.69	15 (30%)
9	BCL	l	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.39	32 (41%)
15	CRT	AC	101	-	41,43,43	0.74	0	50,54,54	1.78	11 (22%)
12	PEF	M	408	-	18,18,46	1.65	2 (11%)	21,23,51	1.95	3 (14%)
9	BCL	7	101	-	64,74,74	1.67	11 (17%)	78,115,115	2.21	28 (35%)
9	BCL	k	102	-	64,74,74	1.72	11 (17%)	78,115,115	2.44	30 (38%)
15	CRT	2	101	-	41,43,43	0.75	0	50,54,54	1.81	16 (32%)
15	CRT	v	101	-	41,43,43	0.77	0	50,54,54	3.93	18 (36%)
9	BCL	Y	101	-	64,74,74	1.77	12 (18%)	78,115,115	2.43	25 (32%)
15	CRT	E	101	-	41,43,43	0.80	0	50,54,54	3.46	16 (32%)
9	BCL	5	102	-	64,74,74	1.76	13 (20%)	78,115,115	2.44	33 (42%)
9	BCL	w	101	-	64,74,74	1.80	14 (21%)	78,115,115	2.35	28 (35%)
9	BCL	AD	101	-	64,74,74	1.72	10 (15%)	78,115,115	2.21	28 (35%)
15	CRT	AL	101	-	41,43,43	0.76	0	50,54,54	1.55	13 (26%)
9	BCL	p	102	-	64,74,74	1.68	10 (15%)	78,115,115	2.31	26 (33%)
12	PEF	m	101	-	18,18,46	1.64	2 (11%)	21,23,51	1.56	3 (14%)
15	CRT	U	102	-	41,43,43	0.73	0	50,54,54	3.26	19 (38%)
9	BCL	A	102	-	64,74,74	1.71	9 (14%)	78,115,115	2.32	28 (35%)
12	PEF	p	101	-	15,15,46	0.93	1 (6%)	17,19,51	0.84	1 (5%)
15	CRT	P	102	-	41,43,43	0.78	0	50,54,54	1.88	15 (30%)
15	CRT	AD	102	-	41,43,43	0.78	0	50,54,54	3.55	15 (30%)
9	BCL	I	101	-	64,74,74	1.80	12 (18%)	78,115,115	2.32	27 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	PEF	x	306	-	18,18,46	1.72	2 (11%)	21,23,51	1.41	3 (14%)
15	CRT	8	101	-	41,43,43	0.85	0	50,54,54	3.56	9 (18%)
9	BCL	j	101	-	64,74,74	1.67	9 (14%)	78,115,115	2.29	27 (34%)
9	BCL	L	305	-	64,74,74	1.71	11 (17%)	78,115,115	2.31	30 (38%)
9	BCL	c	102	-	64,74,74	1.67	9 (14%)	78,115,115	2.36	29 (37%)
7	HEM	C	501	1	41,50,50	2.11	8 (19%)	45,82,82	2.60	16 (35%)
9	BCL	u	101	-	64,74,74	1.71	12 (18%)	78,115,115	2.21	26 (33%)
9	BCL	AB	101	-	64,74,74	1.78	13 (20%)	78,115,115	2.31	29 (37%)
9	BCL	J	102	-	64,74,74	1.69	14 (21%)	78,115,115	2.33	31 (39%)
9	BCL	m	103	-	64,74,74	1.67	12 (18%)	78,115,115	2.33	27 (34%)
12	PEF	H	303	-	18,18,46	1.51	2 (11%)	21,23,51	1.34	2 (9%)
12	PEF	M	407	-	15,15,46	1.05	1 (6%)	17,19,51	1.31	2 (11%)
9	BCL	AC	102	-	64,74,74	1.67	12 (18%)	78,115,115	2.27	27 (34%)
15	CRT	4	101	-	41,43,43	0.73	0	50,54,54	4.06	21 (42%)
9	BCL	G	102	-	64,74,74	1.70	10 (15%)	78,115,115	2.35	33 (42%)
9	BCL	0	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.24	28 (35%)
9	BCL	F	101	-	64,74,74	1.66	13 (20%)	78,115,115	2.27	32 (41%)
9	BCL	AH	103	-	64,74,74	1.71	13 (20%)	78,115,115	2.35	30 (38%)
9	BCL	AL	102	-	64,74,74	1.75	13 (20%)	78,115,115	2.35	26 (33%)
12	PEF	L	306	-	10,11,46	0.73	0	11,14,51	1.46	1 (9%)
9	BCL	D	101	-	64,74,74	1.74	10 (15%)	78,115,115	2.35	24 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEF	H	301	-	-	7/20/20/50	-
12	PEF	A	101	-	-	9/20/20/50	-
9	BCL	R	102	-	-	15/37/137/137	-
9	BCL	1	101	-	-	19/37/137/137	-
9	BCL	f	101	-	-	19/37/137/137	-
15	CRT	J	101	-	-	10/51/51/51	-
15	CRT	N	101	-	-	10/51/51/51	-
12	PEF	t	301	-	-	7/20/20/50	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	AJ	101	-	-	7/51/51/51	-
15	CRT	6	101	-	-	8/51/51/51	-
7	HEM	C	504	1	-	5/12/54/54	-
7	HEM	o	503	1	-	4/12/54/54	-
12	PEF	y	407	-	-	7/20/20/50	-
15	CRT	f	102	-	-	9/51/51/51	-
7	HEM	o	504	1	-	2/12/54/54	-
9	BCL	z	102	-	-	17/37/137/137	-
9	BCL	L	303	-	-	18/37/137/137	-
17	PGW	S	101	-	-	13/23/23/55	-
9	BCL	L	301	-	-	12/37/137/137	-
15	CRT	R	101	-	-	12/51/51/51	-
9	BCL	s	102	-	-	17/37/137/137	-
7	HEM	o	502	1	-	5/12/54/54	-
9	BCL	B	101	-	-	13/37/137/137	-
9	BCL	AK	101	-	-	15/37/137/137	-
9	BCL	W	101	-	-	19/37/137/137	-
15	CRT	k	101	-	-	6/51/51/51	-
9	BCL	AH	101	-	-	21/37/137/137	-
9	BCL	d	101	-	-	16/37/137/137	-
9	BCL	9	103	-	-	14/37/137/137	-
9	BCL	4	102	-	-	17/37/137/137	-
9	BCL	v	102	-	-	13/37/137/137	-
9	BCL	5	101	-	-	16/37/137/137	-
12	PEF	y	408	-	-	9/20/20/50	-
9	BCL	P	101	-	-	17/37/137/137	-
7	HEM	C	503	1	-	4/12/54/54	-
14	MQ8	M	403	-	-	21/47/67/67	0/2/2/2
15	CRT	AH	102	-	-	14/51/51/51	-
15	CRT	M	404	-	-	11/51/51/51	-
15	CRT	z	101	-	-	3/51/51/51	-
15	CRT	i	101	-	-	11/51/51/51	-
9	BCL	x	305	-	-	17/37/137/137	-
17	PGW	AE	101	-	-	12/23/23/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	U	101	-	-	15/37/137/137	-
9	BCL	AJ	102	-	-	17/37/137/137	-
9	BCL	M	401	-	-	10/37/137/137	-
9	BCL	Z	102	-	-	16/37/137/137	-
9	BCL	AA	101	-	-	17/37/137/137	-
9	BCL	x	301	-	-	10/37/137/137	-
14	MQ8	y	403	-	-	26/47/67/67	0/2/2/2
12	PEF	t	303	-	-	7/20/20/50	-
15	CRT	A	103	-	-	6/51/51/51	-
9	BCL	e	102	-	-	18/37/137/137	-
15	CRT	9	102	-	-	9/51/51/51	-
7	HEM	o	501	1	-	6/12/54/54	-
9	BCL	y	401	-	-	13/37/137/137	-
9	BCL	O	101	-	-	18/37/137/137	-
10	BPH	x	302	-	-	16/37/105/105	0/5/6/6
15	CRT	e	101	-	-	8/51/51/51	-
12	PEF	M	406	-	-	11/20/20/50	-
15	CRT	n	101	-	-	19/51/51/51	-
9	BCL	S	102	-	-	14/37/137/137	-
9	BCL	X	102	-	-	23/37/137/137	-
15	CRT	c	101	-	-	8/51/51/51	-
9	BCL	AI	101	-	-	19/37/137/137	-
7	HEM	C	502	1	-	5/12/54/54	-
15	CRT	s	101	-	-	8/51/51/51	-
12	PEF	y	406	-	-	2/20/20/50	-
9	BCL	r	101	-	-	18/37/137/137	-
9	BCL	T	102	-	-	17/37/137/137	-
9	BCL	D	102	-	-	12/37/137/137	-
9	BCL	x	303	-	-	15/37/137/137	-
10	BPH	y	402	-	-	15/37/105/105	0/5/6/6
11	UQ8	x	304	-	-	7/51/75/75	0/1/1/1
9	BCL	g	101	-	-	19/37/137/137	-
9	BCL	h	101	-	-	9/37/137/137	-
9	BCL	3	101	-	-	13/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BPH	M	402	-	-	22/37/105/105	0/5/6/6
9	BCL	m	102	-	-	16/37/137/137	-
15	CRT	y	404	-	-	9/51/51/51	-
15	CRT	Z	101	-	-	11/51/51/51	-
9	BCL	AE	102	-	-	13/37/137/137	-
9	BCL	p	104	-	-	16/37/137/137	-
9	BCL	i	102	-	-	19/37/137/137	-
9	BCL	K	101	-	-	13/37/137/137	-
9	BCL	8	102	-	-	26/37/137/137	-
10	BPH	L	302	-	-	16/37/105/105	0/5/6/6
15	CRT	G	101	-	-	6/51/51/51	-
15	CRT	p	103	-	-	9/51/51/51	-
9	BCL	Q	101	-	-	22/37/137/137	-
15	CRT	T	101	-	-	7/51/51/51	-
11	UQ8	L	304	-	-	9/51/75/75	0/1/1/1
9	BCL	1	102	-	-	13/37/137/137	-
9	BCL	AE	104	-	-	11/37/137/137	-
9	BCL	N	102	-	-	18/37/137/137	-
9	BCL	V	101	-	-	15/37/137/137	-
15	CRT	X	101	-	-	13/51/51/51	-
12	PEF	H	304	-	-	11/20/20/50	-
15	CRT	AE	103	-	-	5/51/51/51	-
9	BCL	l	101	-	-	15/37/137/137	-
15	CRT	AC	101	-	-	5/51/51/51	-
12	PEF	M	408	-	-	12/20/20/50	-
9	BCL	7	101	-	-	17/37/137/137	-
9	BCL	k	102	-	-	21/37/137/137	-
15	CRT	2	101	-	-	7/51/51/51	-
15	CRT	v	101	-	-	9/51/51/51	-
9	BCL	Y	101	-	-	20/37/137/137	-
15	CRT	E	101	-	-	8/51/51/51	-
9	BCL	5	102	-	-	17/37/137/137	-
9	BCL	w	101	-	-	15/37/137/137	-
9	BCL	AD	101	-	-	21/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	AL	101	-	-	9/51/51/51	-
9	BCL	p	102	-	-	17/37/137/137	-
12	PEF	m	101	-	-	7/20/20/50	-
15	CRT	U	102	-	-	10/51/51/51	-
9	BCL	A	102	-	-	12/37/137/137	-
12	PEF	p	101	-	-	6/16/16/50	-
15	CRT	P	102	-	-	7/51/51/51	-
15	CRT	AD	102	-	-	11/51/51/51	-
9	BCL	I	101	-	-	10/37/137/137	-
12	PEF	x	306	-	-	15/20/20/50	-
15	CRT	8	101	-	-	6/51/51/51	-
9	BCL	j	101	-	-	21/37/137/137	-
9	BCL	L	305	-	-	14/37/137/137	-
9	BCL	c	102	-	-	18/37/137/137	-
7	HEM	C	501	1	-	6/12/54/54	-
9	BCL	u	101	-	-	17/37/137/137	-
9	BCL	AB	101	-	-	19/37/137/137	-
9	BCL	J	102	-	-	14/37/137/137	-
9	BCL	m	103	-	-	19/37/137/137	-
12	PEF	H	303	-	-	13/20/20/50	-
12	PEF	M	407	-	-	8/16/16/50	-
9	BCL	AC	102	-	-	15/37/137/137	-
15	CRT	4	101	-	-	13/51/51/51	-
9	BCL	G	102	-	-	16/37/137/137	-
9	BCL	0	101	-	-	12/37/137/137	-
9	BCL	F	101	-	-	20/37/137/137	-
9	BCL	AH	103	-	-	24/37/137/137	-
9	BCL	AL	102	-	-	15/37/137/137	-
12	PEF	L	306	-	-	8/11/11/50	-
9	BCL	D	101	-	-	11/37/137/137	-

The worst 5 of 988 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	504	HEM	FE-NB	8.64	2.39	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	o	503	HEM	FE-NB	8.54	2.39	1.96
7	C	503	HEM	FE-NB	8.46	2.38	1.96
7	C	504	HEM	FE-NB	8.21	2.37	1.96
7	o	502	HEM	FE-NB	8.06	2.36	1.96

The worst 5 of 2844 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 1807 torsion outliers are listed below:

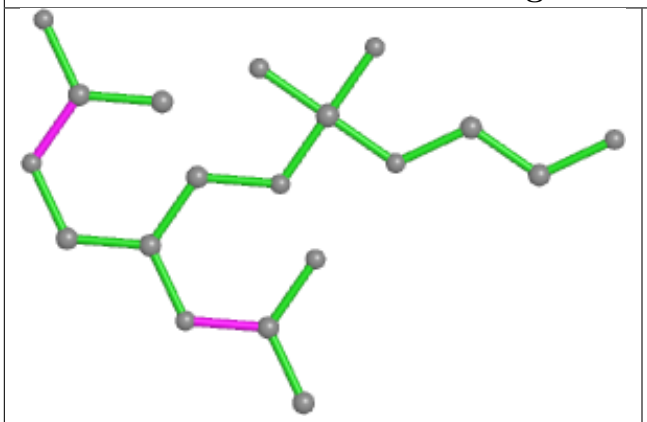
Mol	Chain	Res	Type	Atoms
7	C	503	HEM	C2B-C3B-CAB-CBB
7	C	503	HEM	C4B-C3B-CAB-CBB
7	o	501	HEM	C2B-C3B-CAB-CBB
7	o	502	HEM	C2B-C3B-CAB-CBB
7	o	502	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

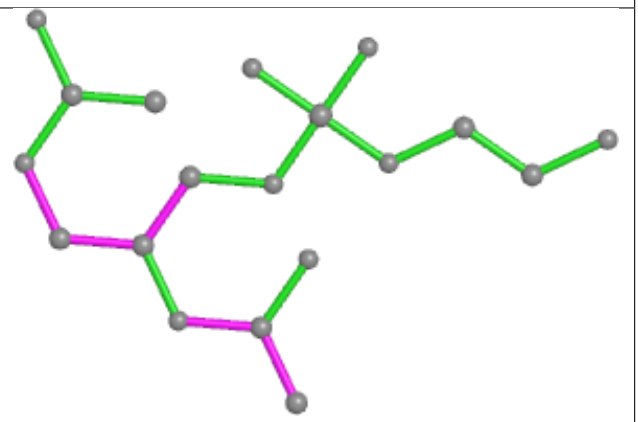
No monomer is involved in short contacts.

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 then 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.

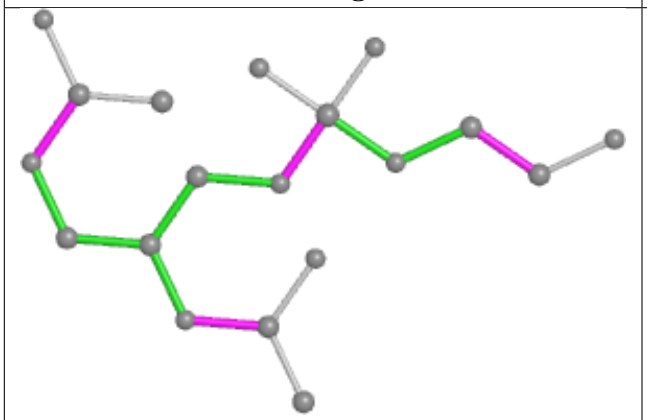
Ligand PEF H 301



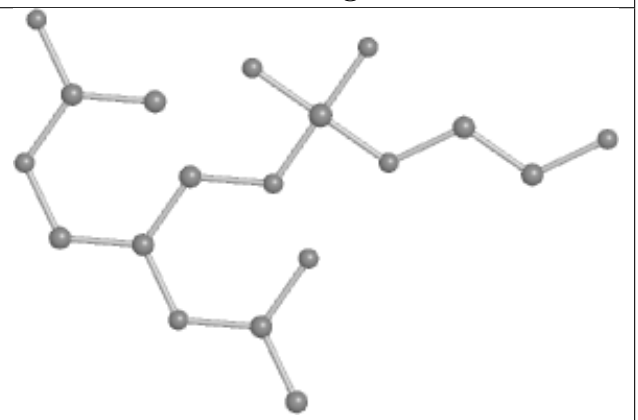
Bond lengths



Bond angles

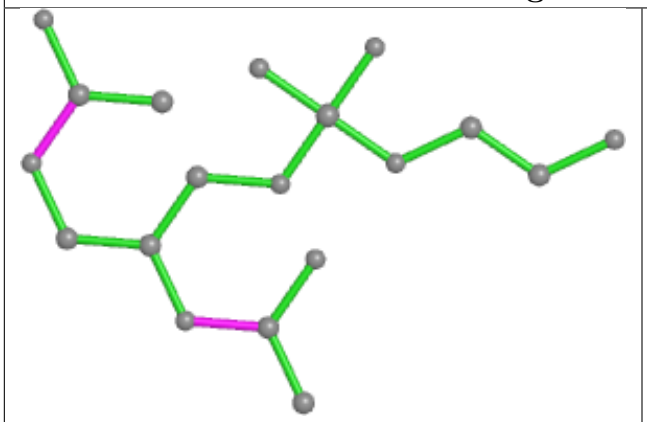


Torsions

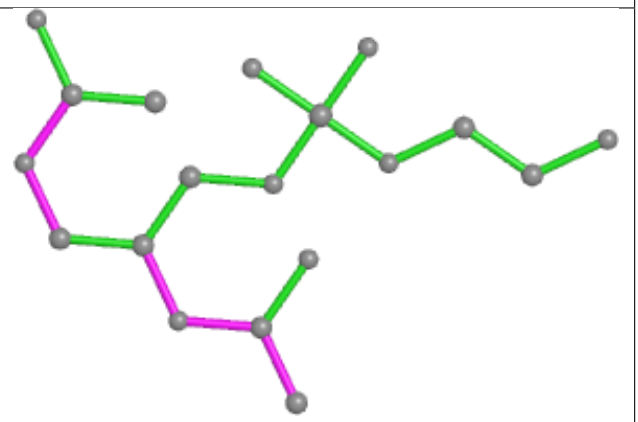


Rings

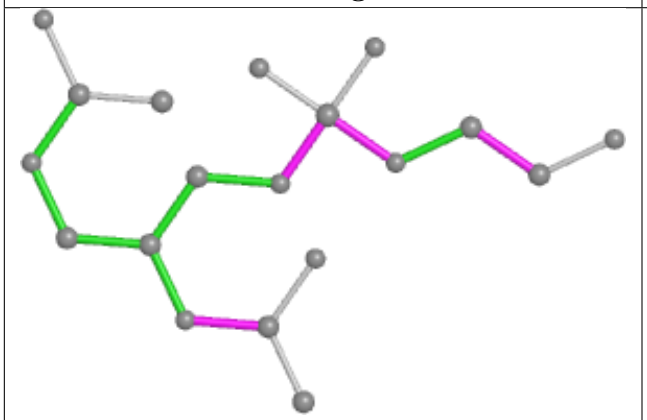
Ligand PEF A 101



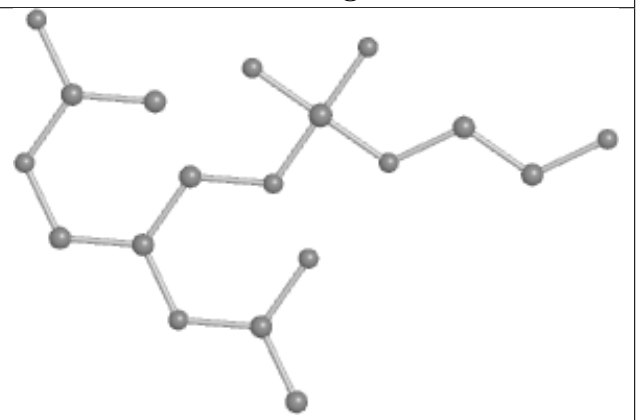
Bond lengths



Bond angles

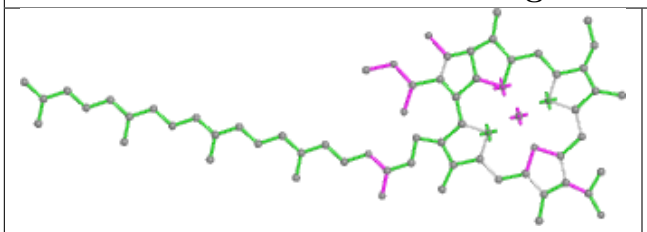


Torsions

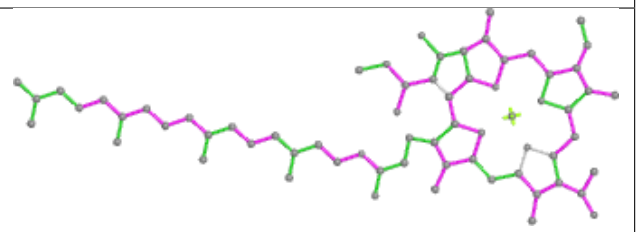


Rings

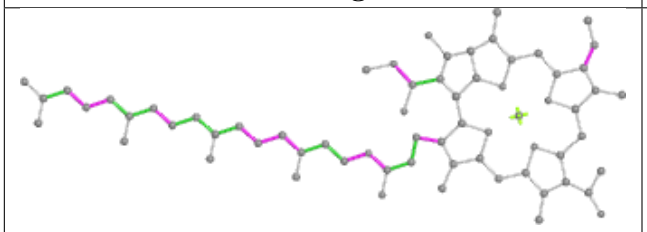
Ligand BCL R 102



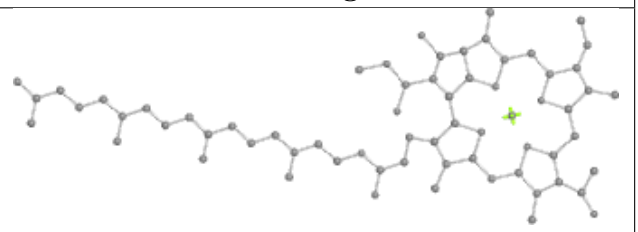
Bond lengths



Bond angles

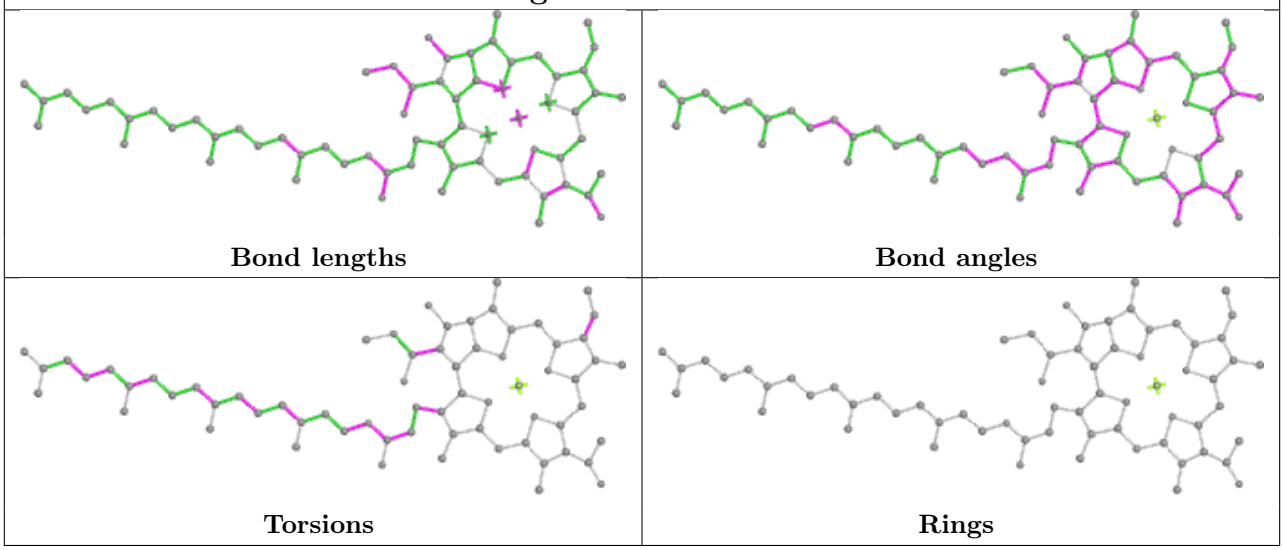


Torsions

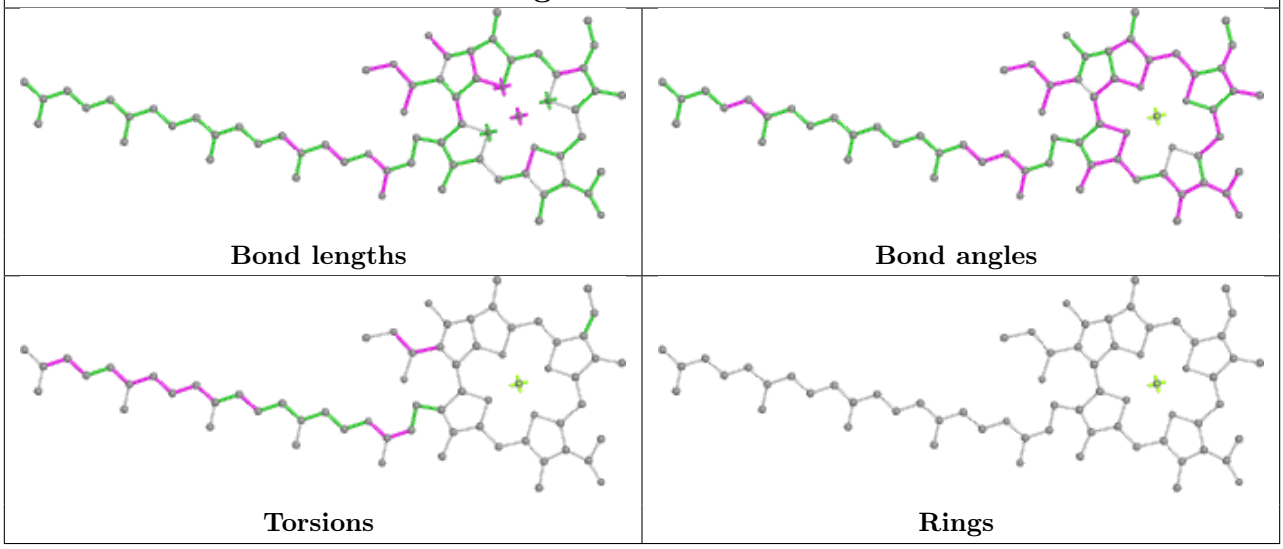


Rings

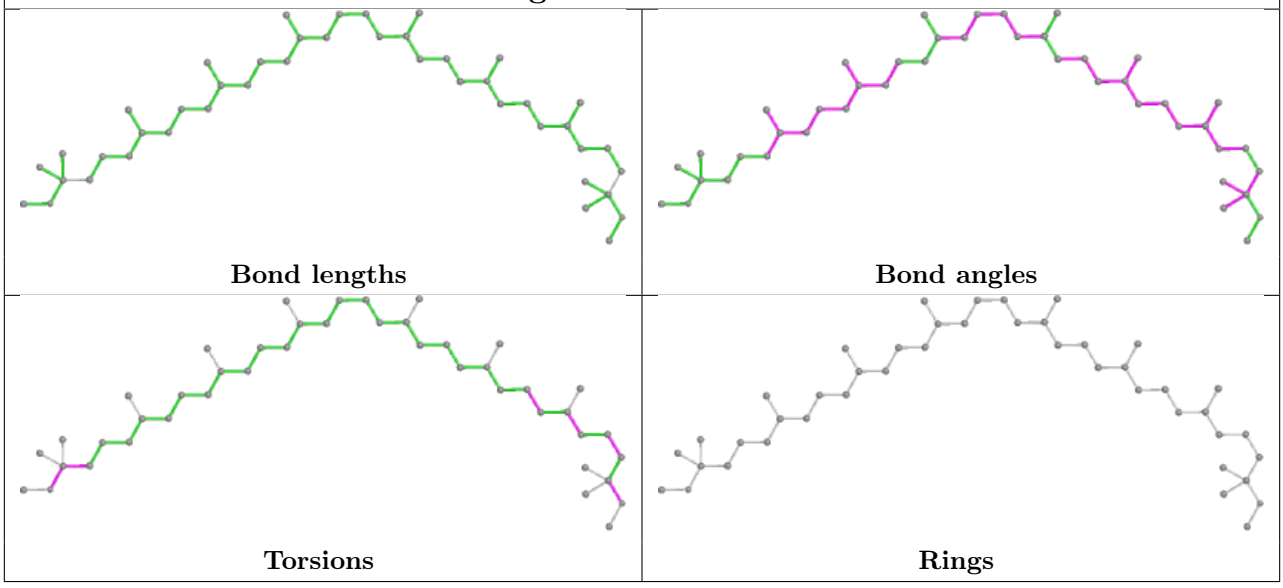
Ligand BCL 1 101



Ligand BCL f 101



Ligand CRT J 101



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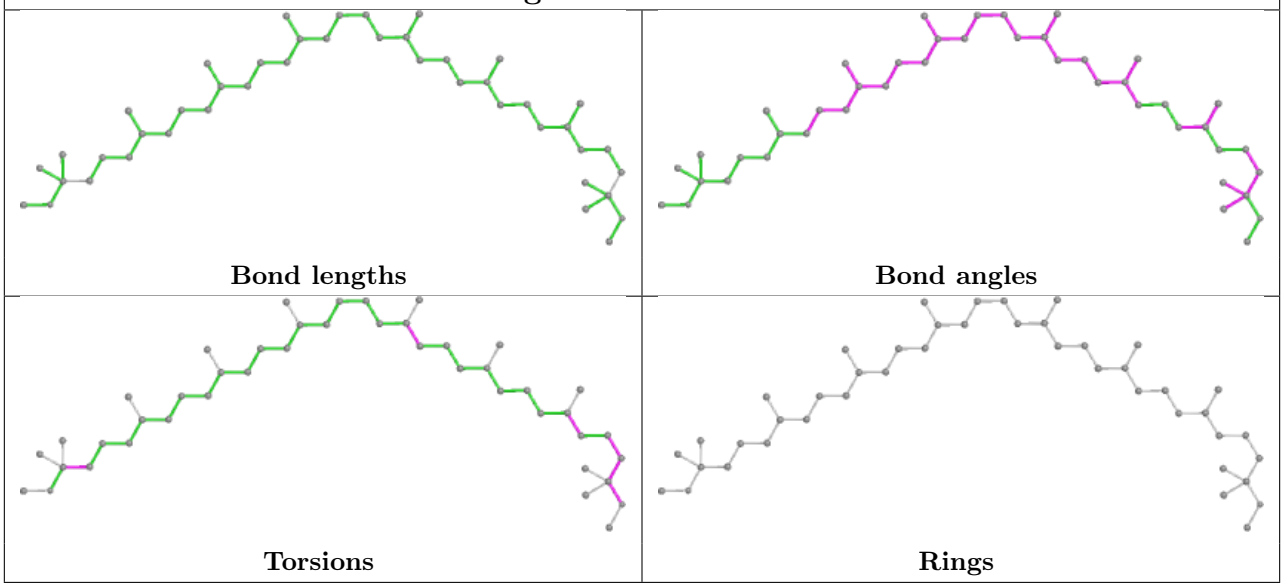
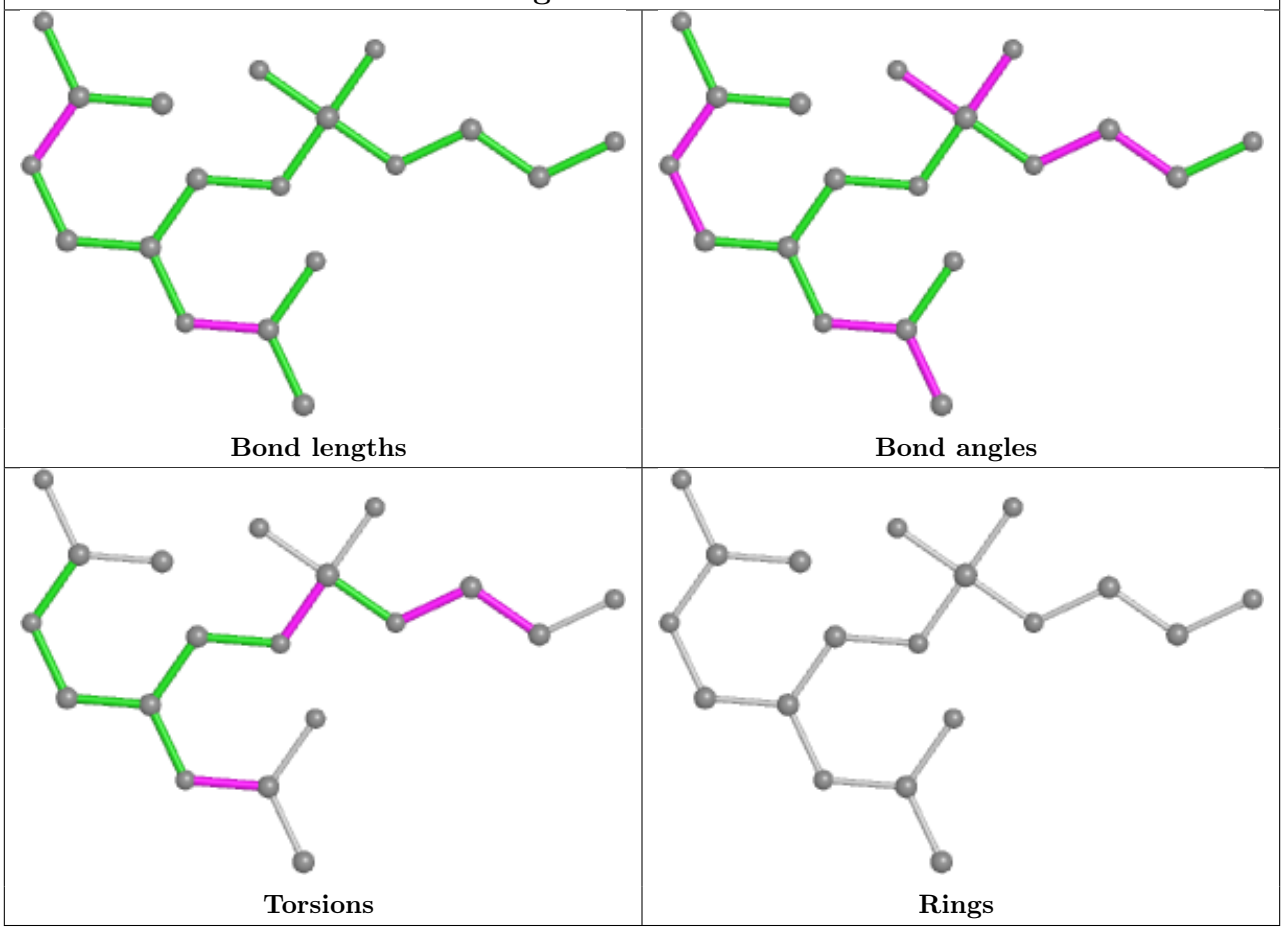


Ligand PEF t 301



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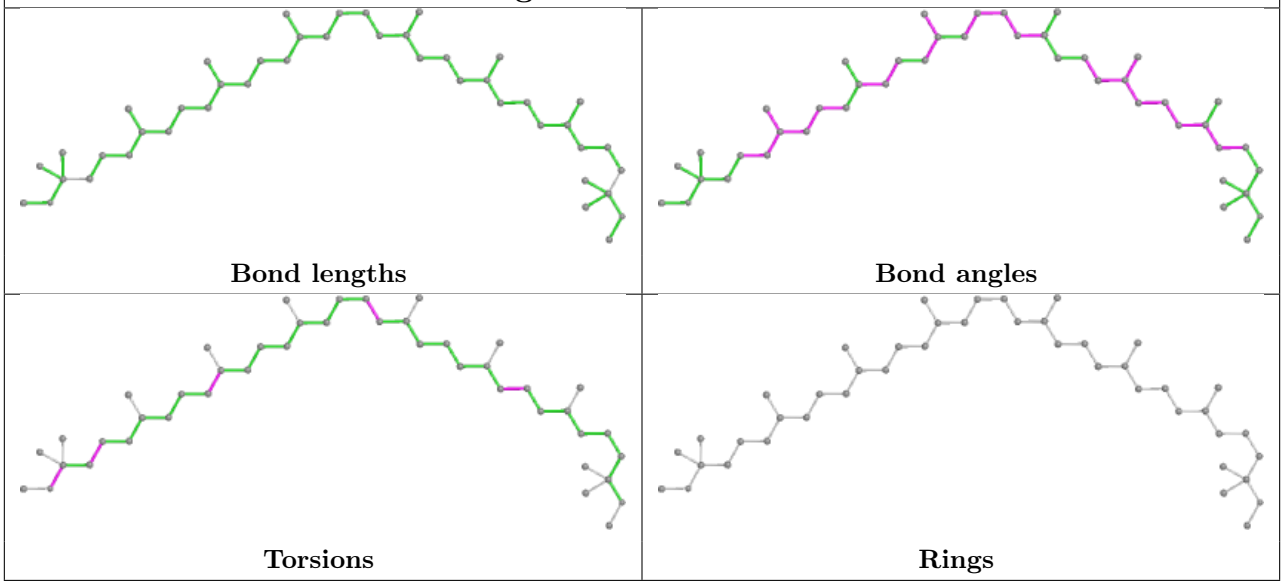
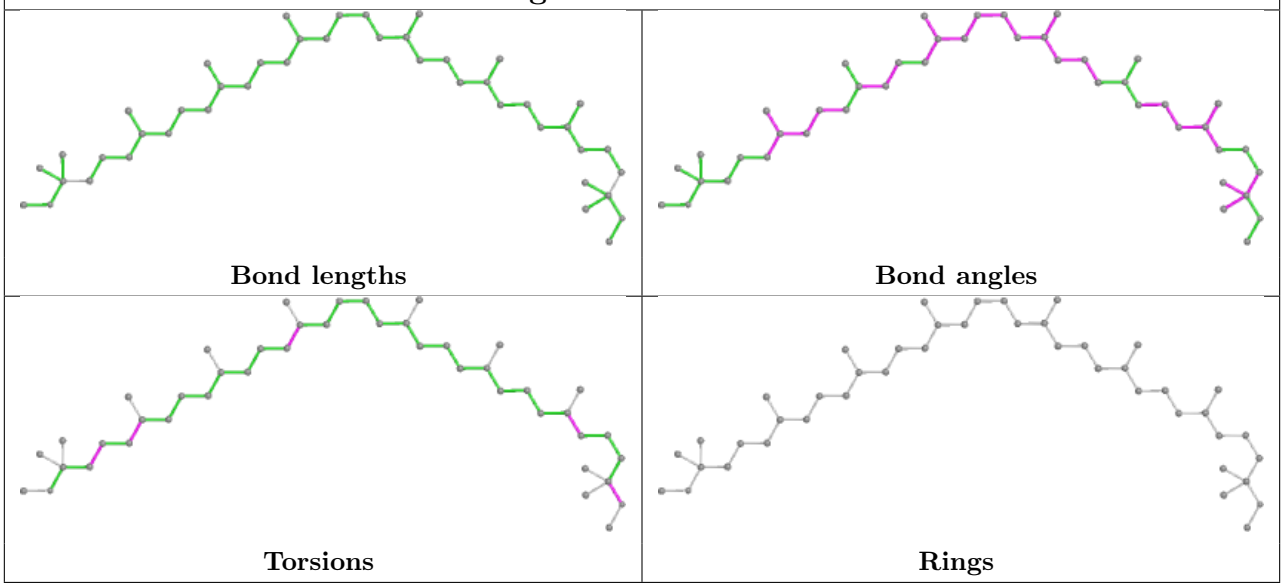
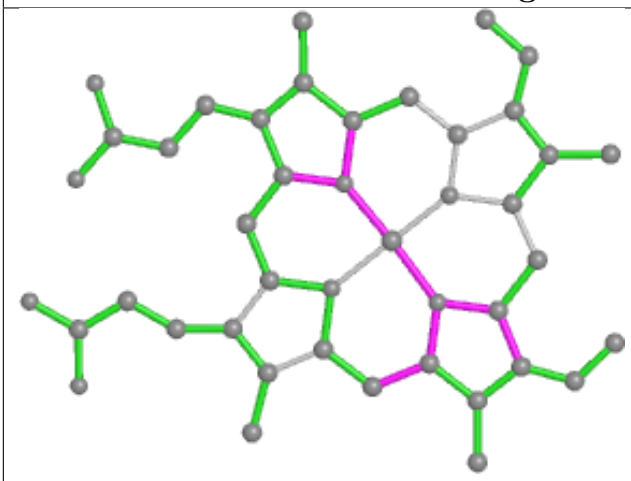


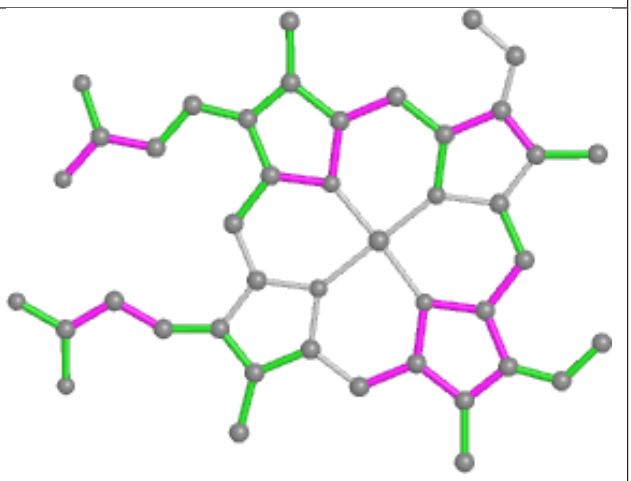
Ligand CRT 6 101



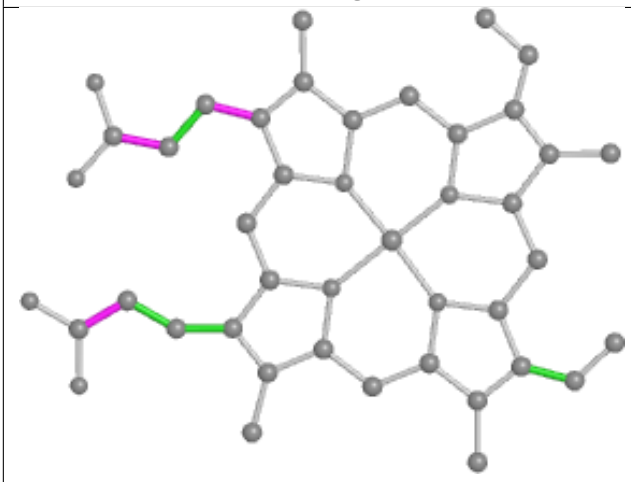
Ligand HEM C 504



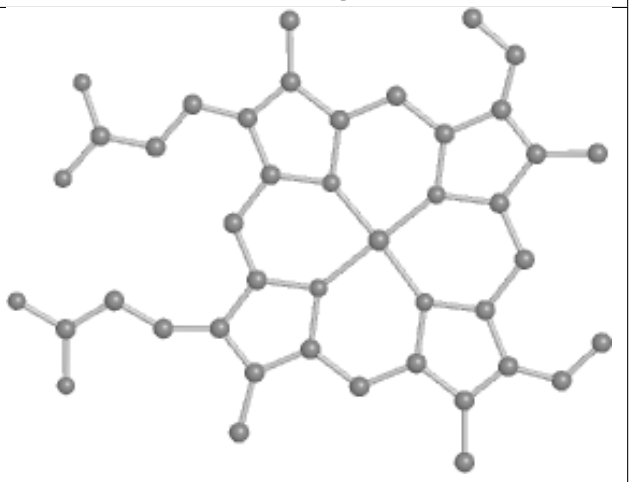
Bond lengths



Bond angles

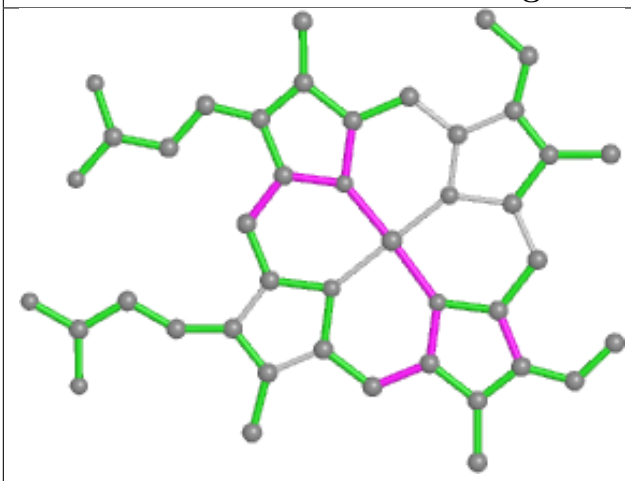


Torsions



Rings

Ligand HEM o 503



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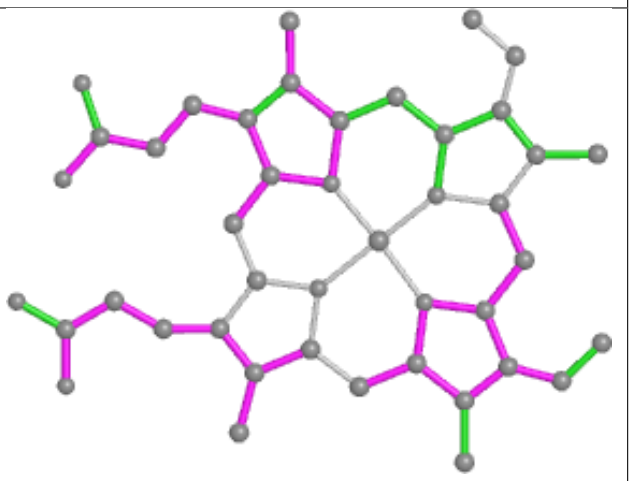
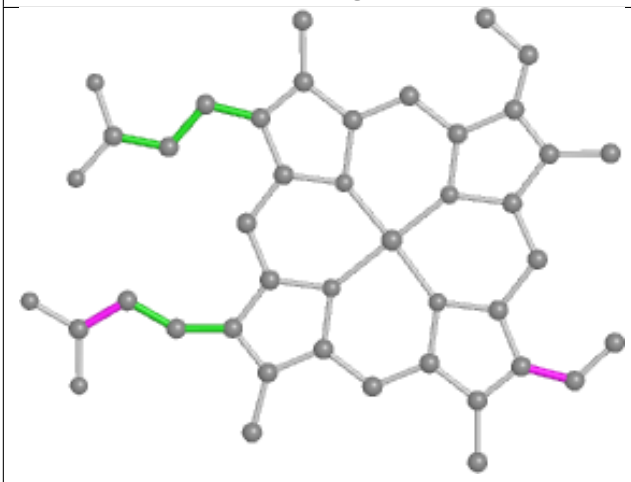


Bond angles



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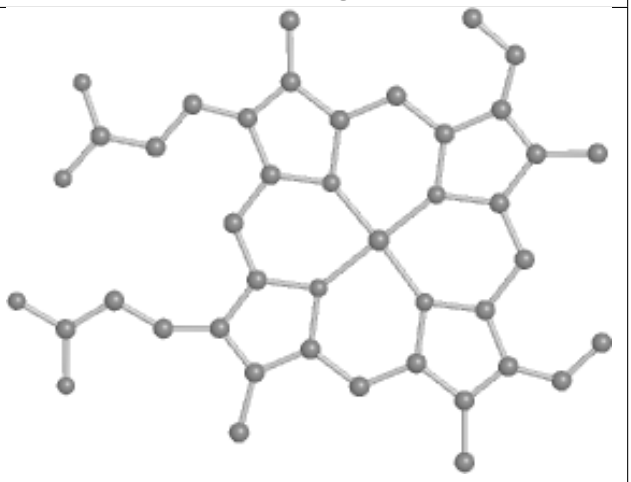
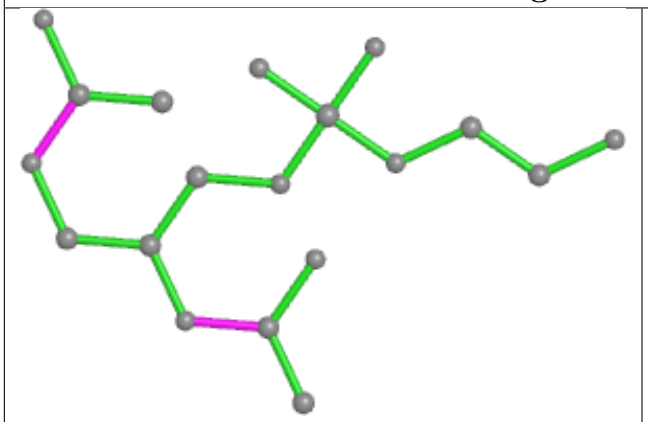


Rings

Ligand PEF y 407



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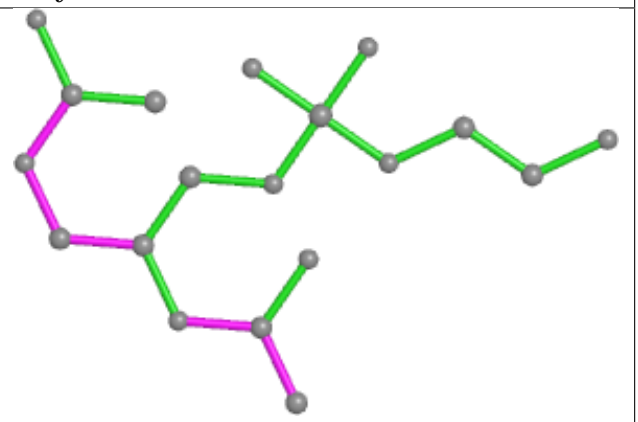

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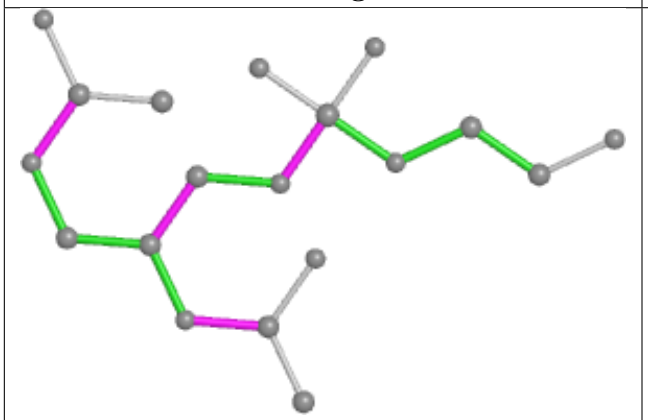

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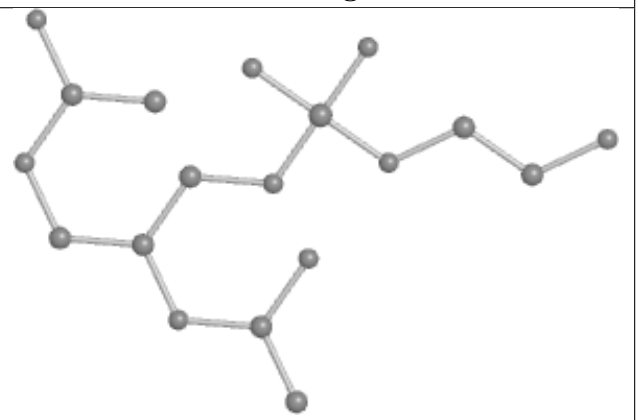
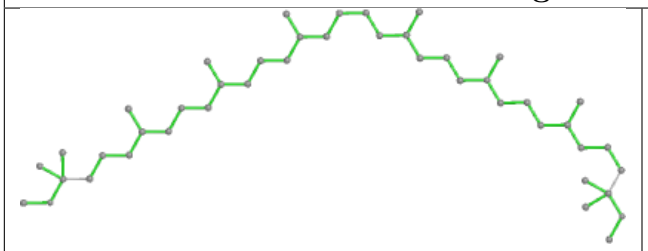


Rings

Ligand CRT f 102



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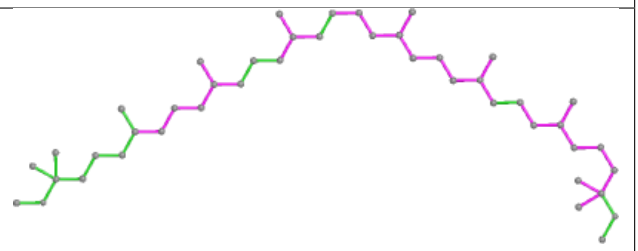

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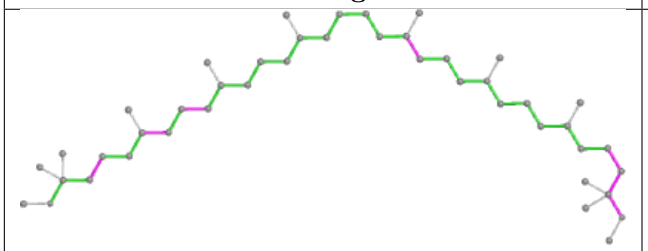

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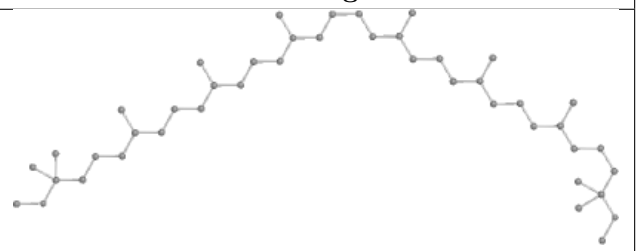
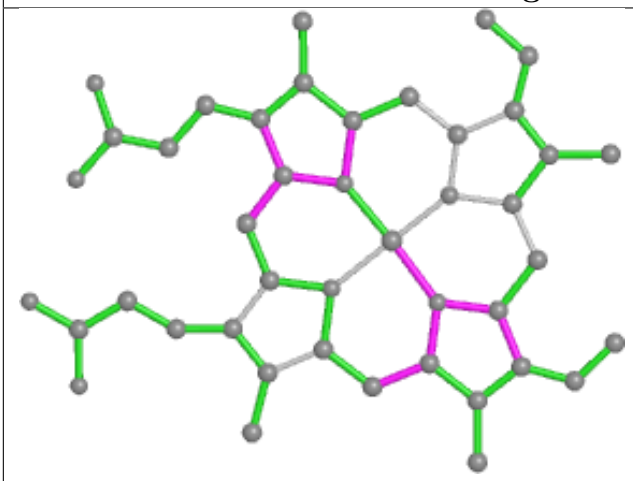


Rings

Ligand HEM o 504



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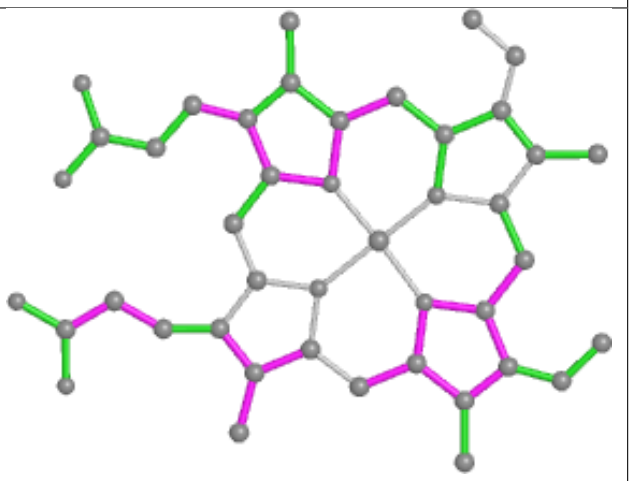
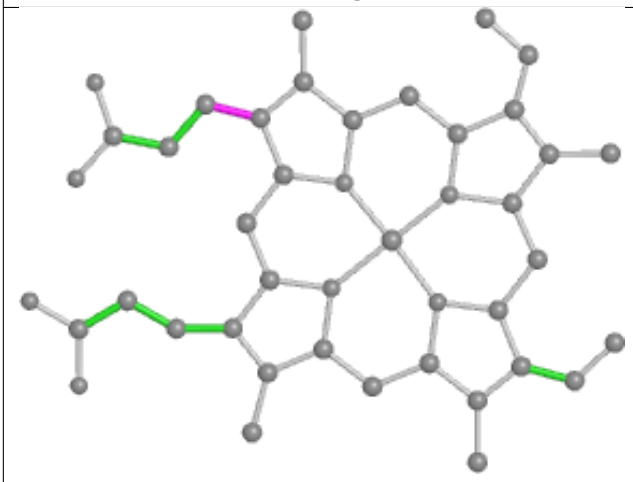


Bond angles



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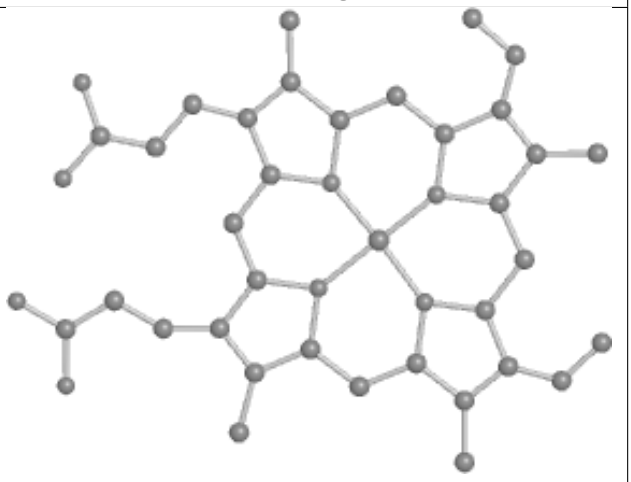
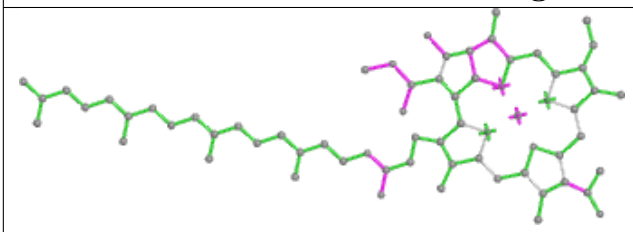


Rings

Ligand BCL z 102



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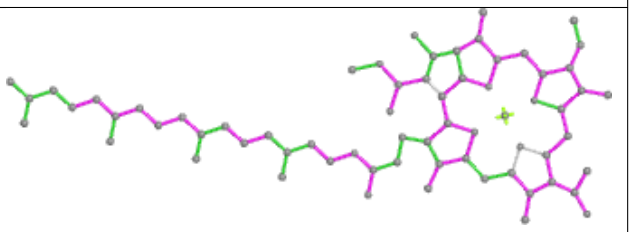
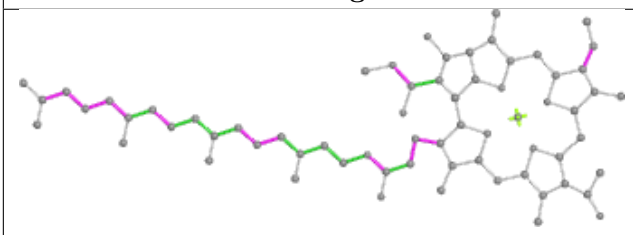


Bond angles



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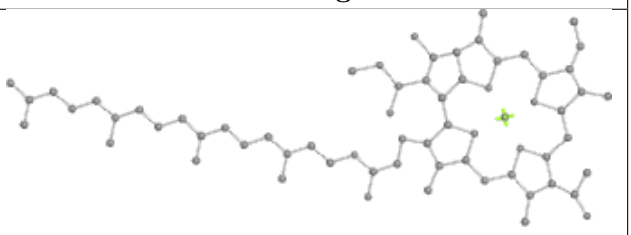
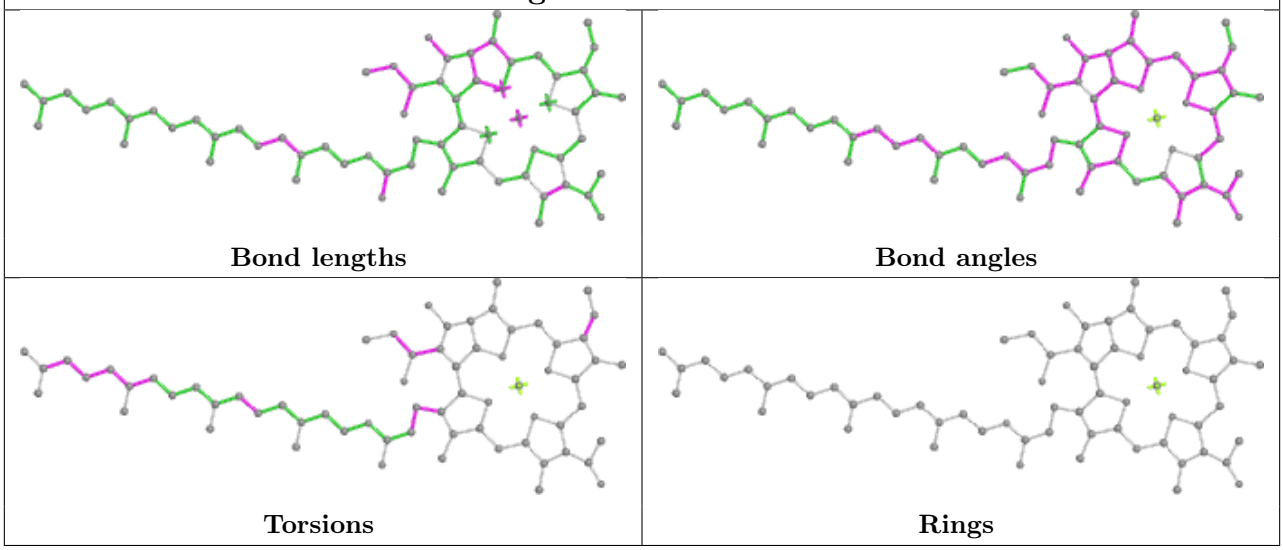
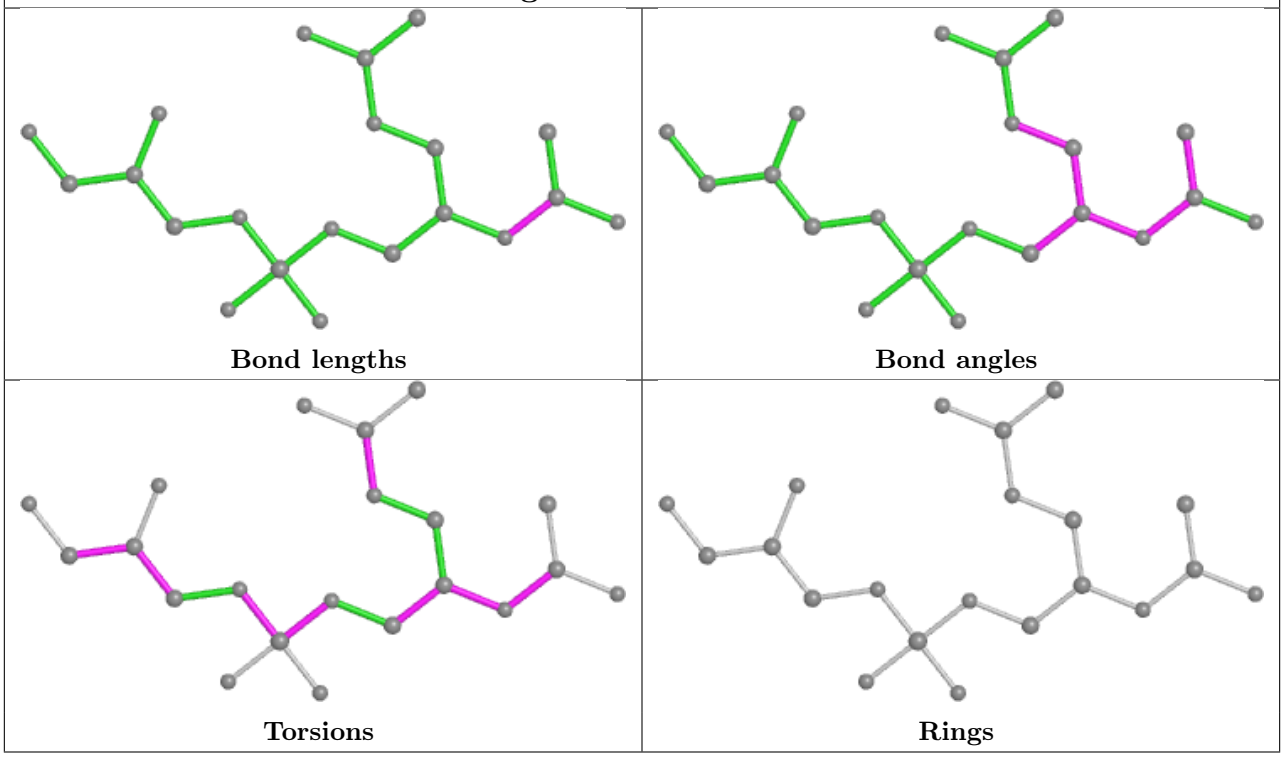


Rings

Ligand BCL L 303



Ligand PGW S 101



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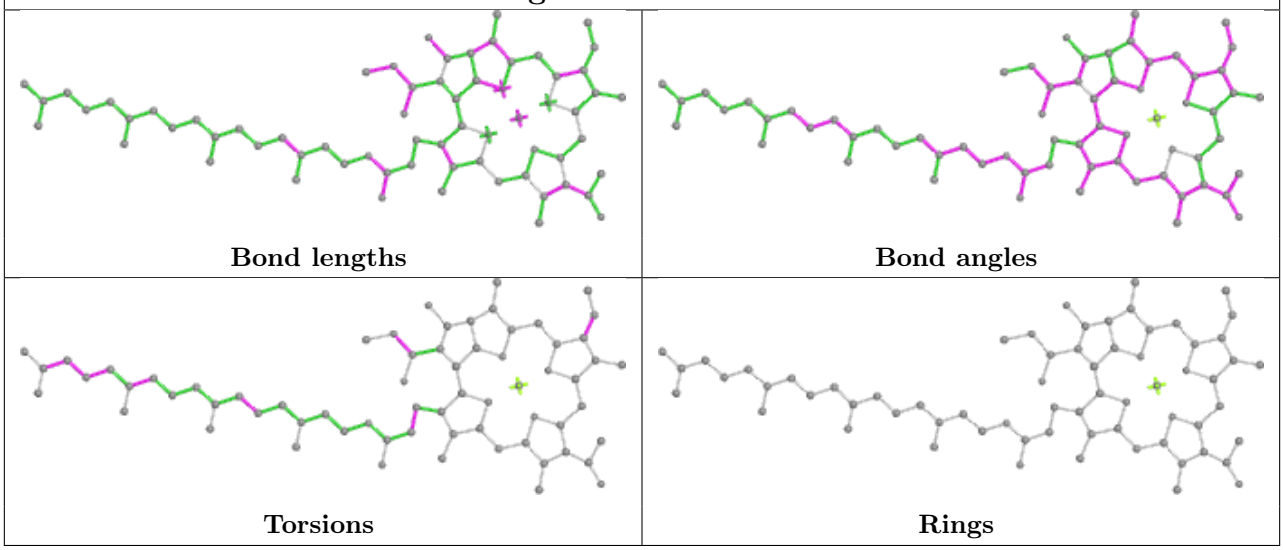

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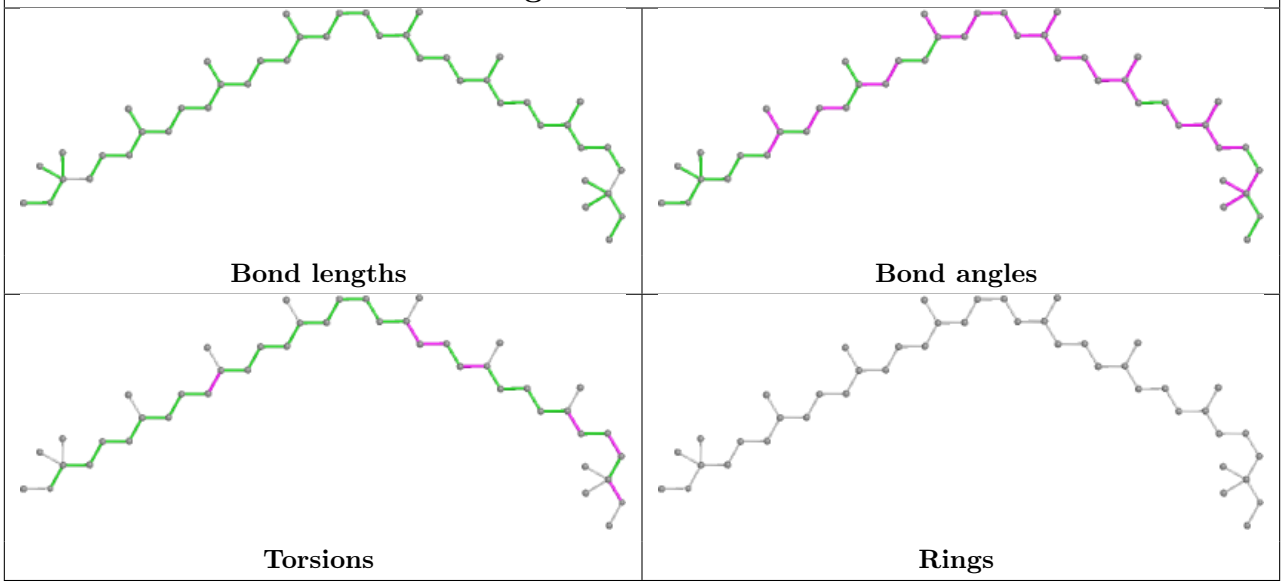

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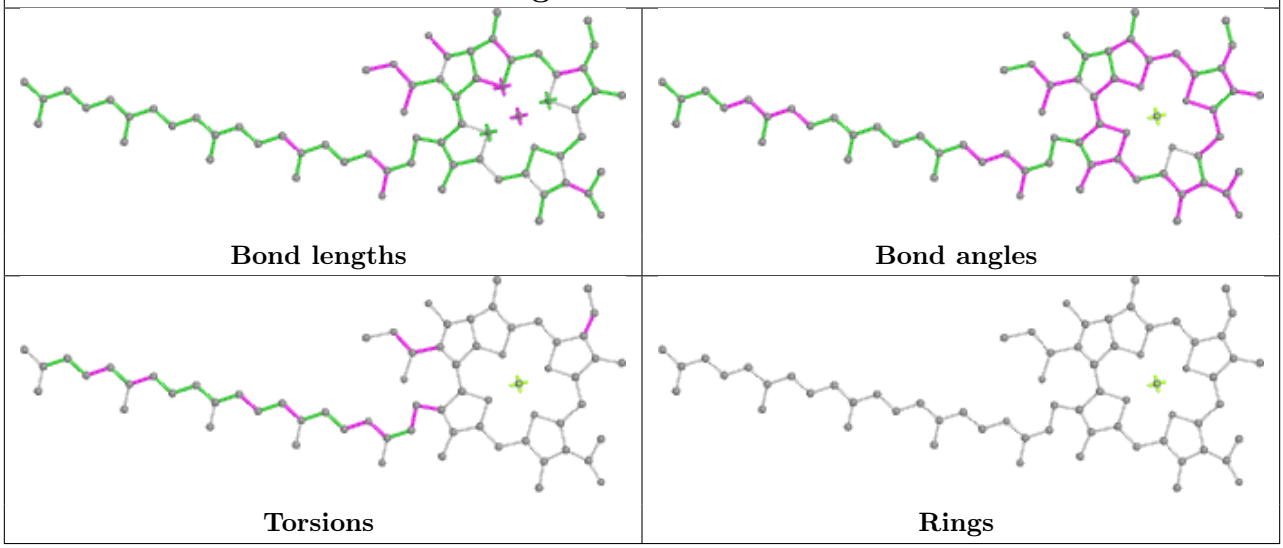
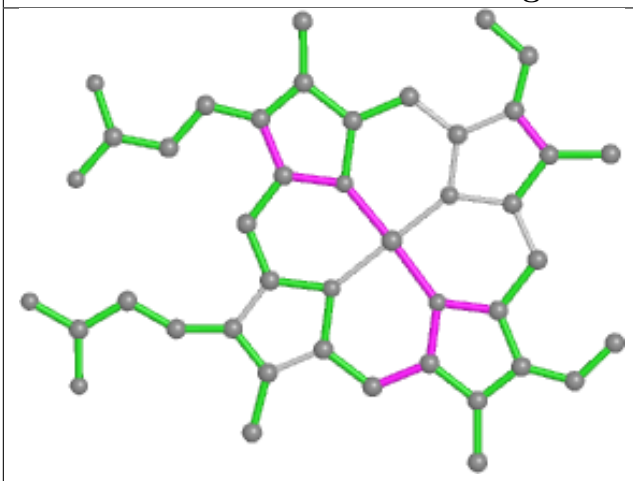
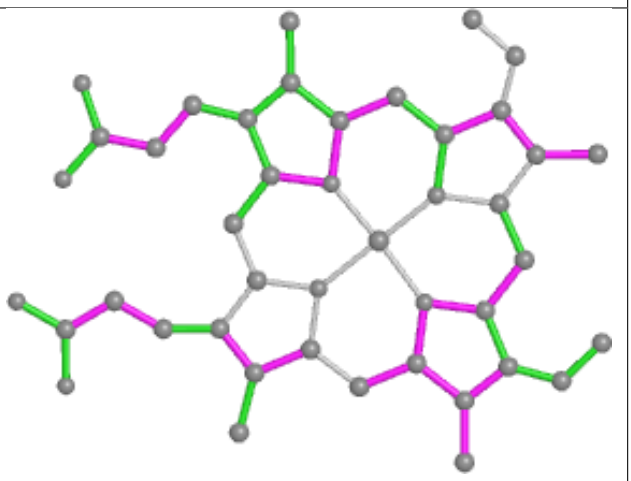


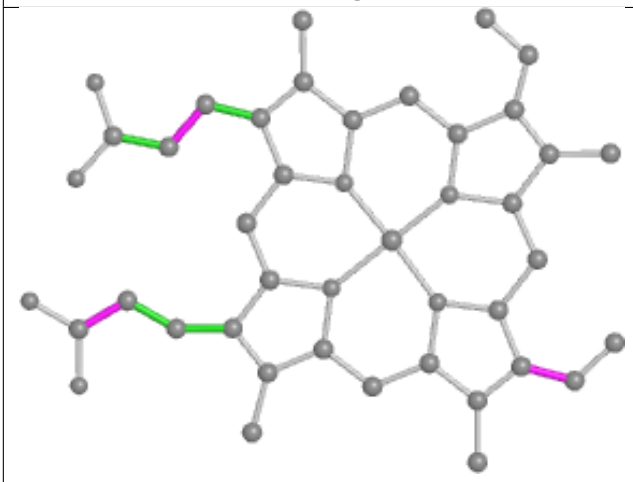
Ligand HEM o 502



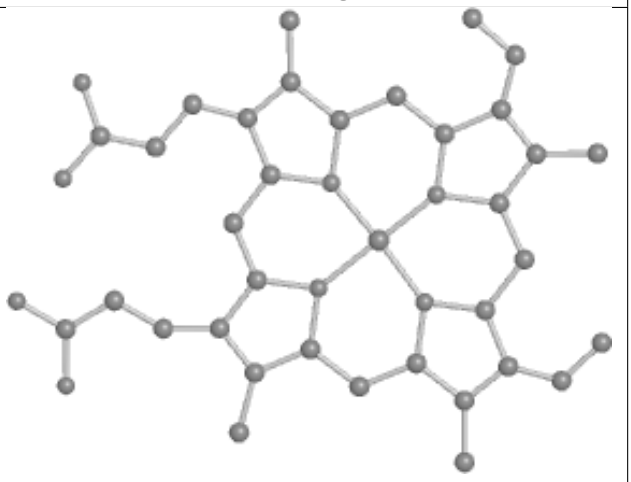
Bond lengths



Bond angles

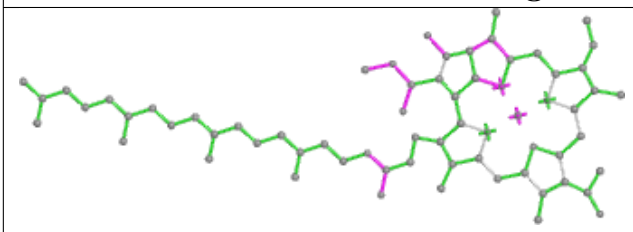


Torsions



Rings

Ligand BCL B 101



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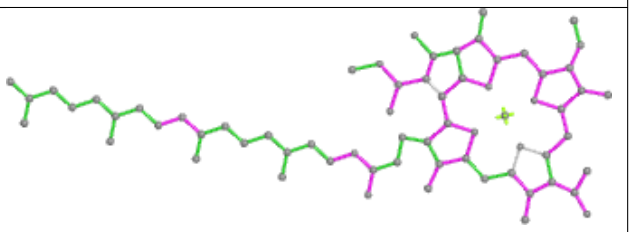
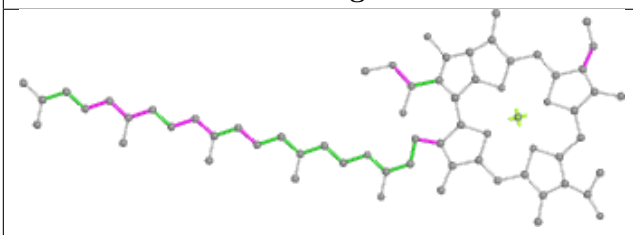


Bond angles



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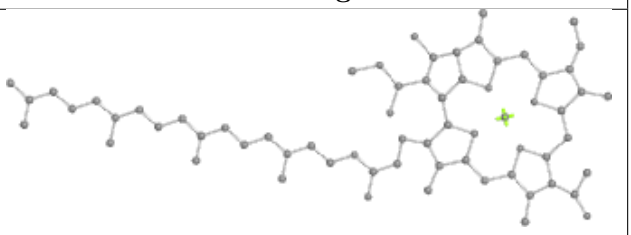

Rings

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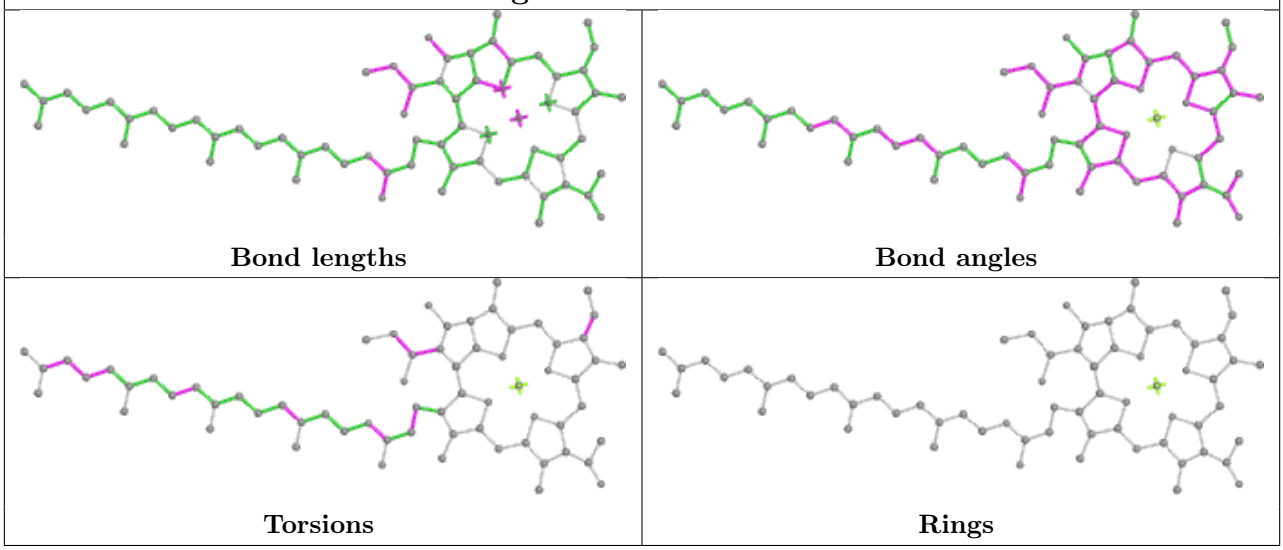
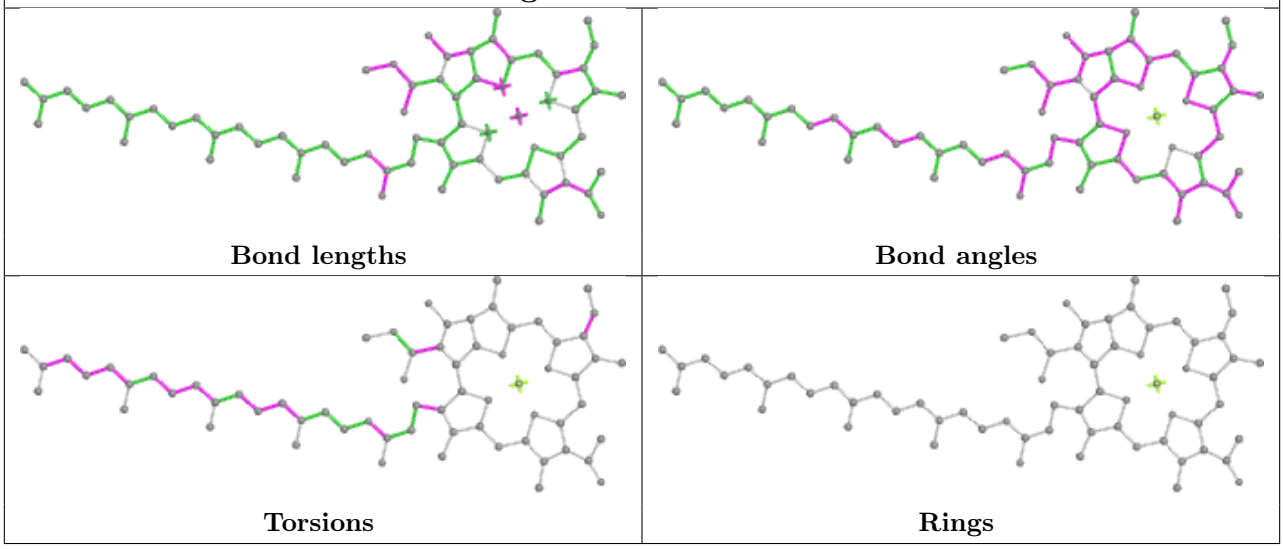
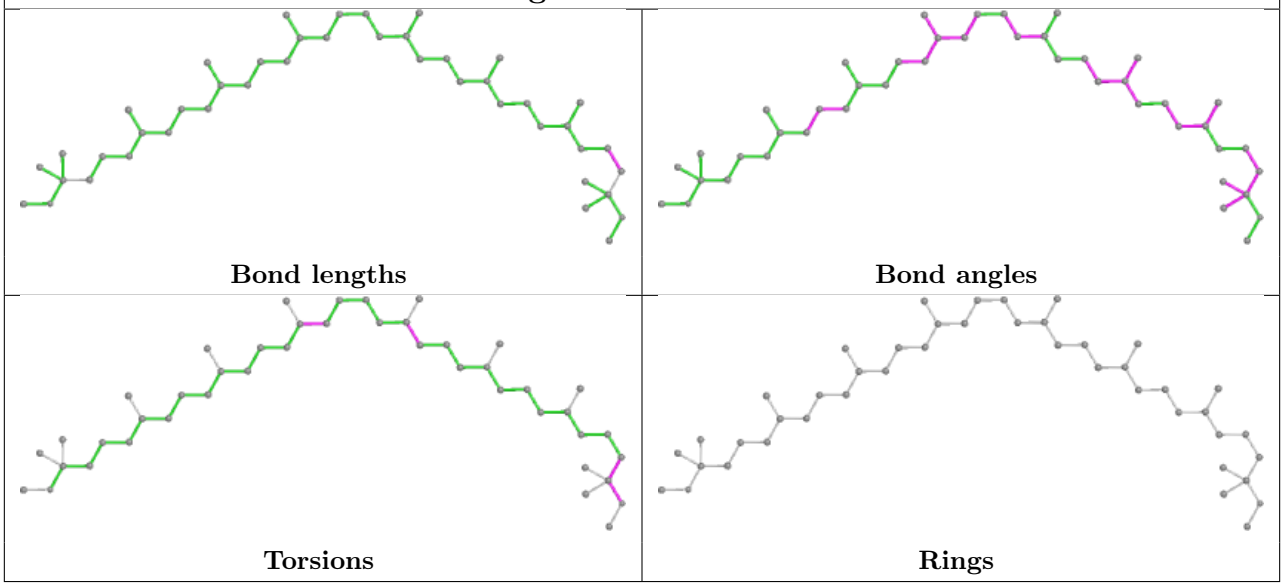


Ligand BCL W 101



Ligand CRT k 101



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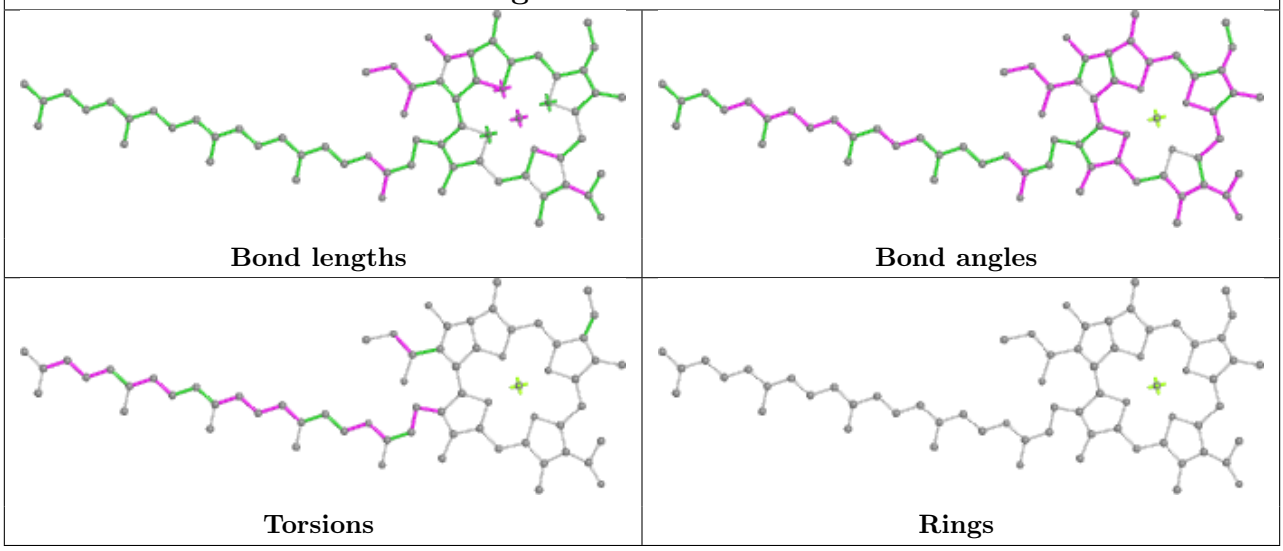

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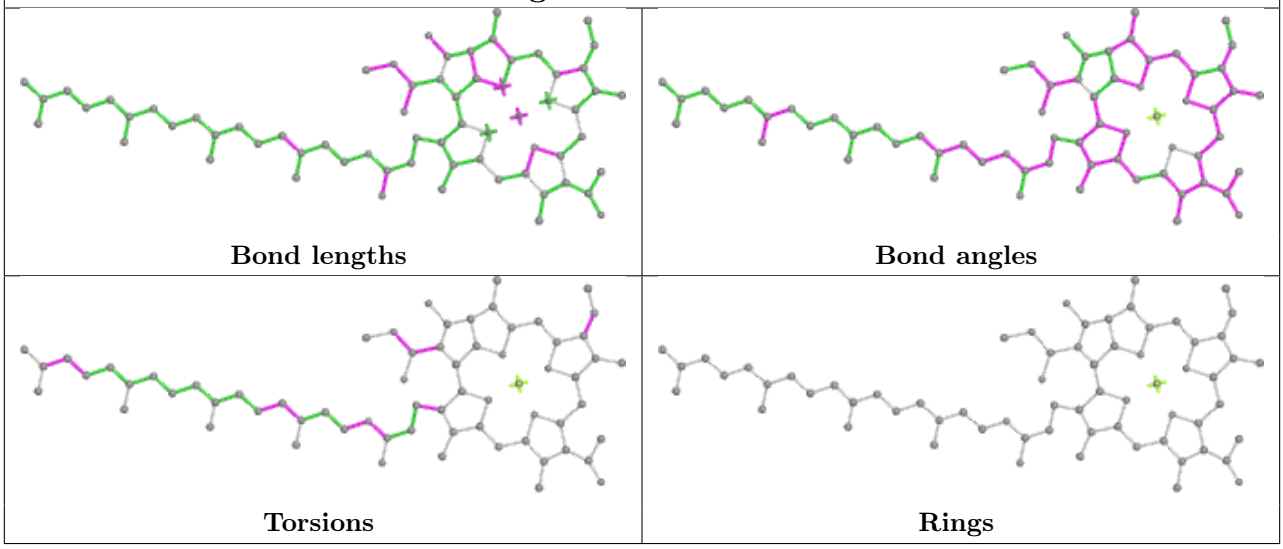
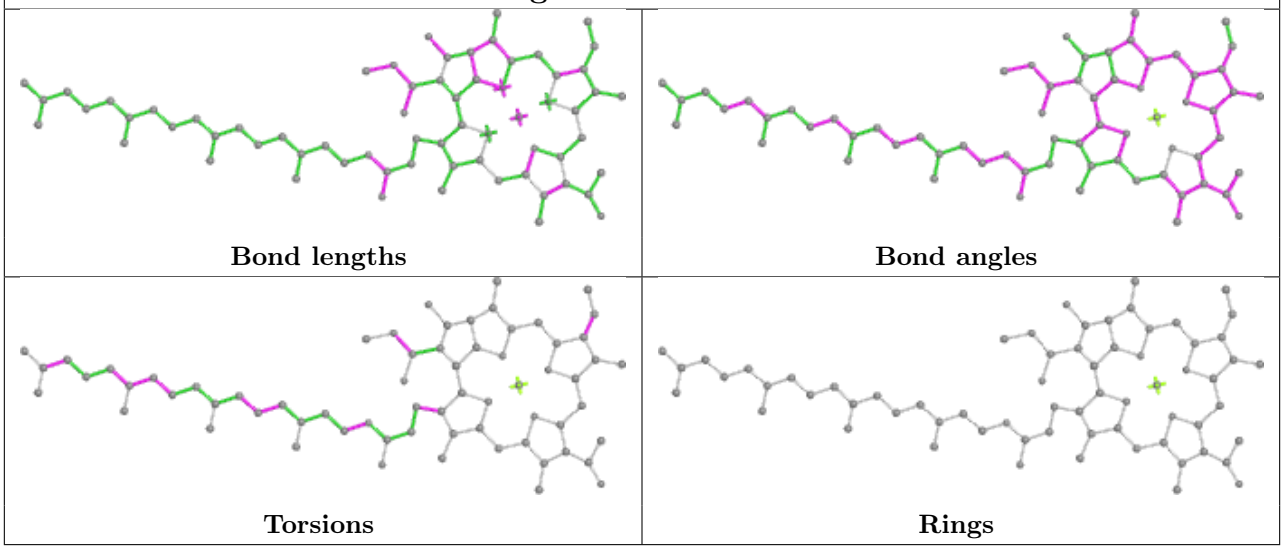
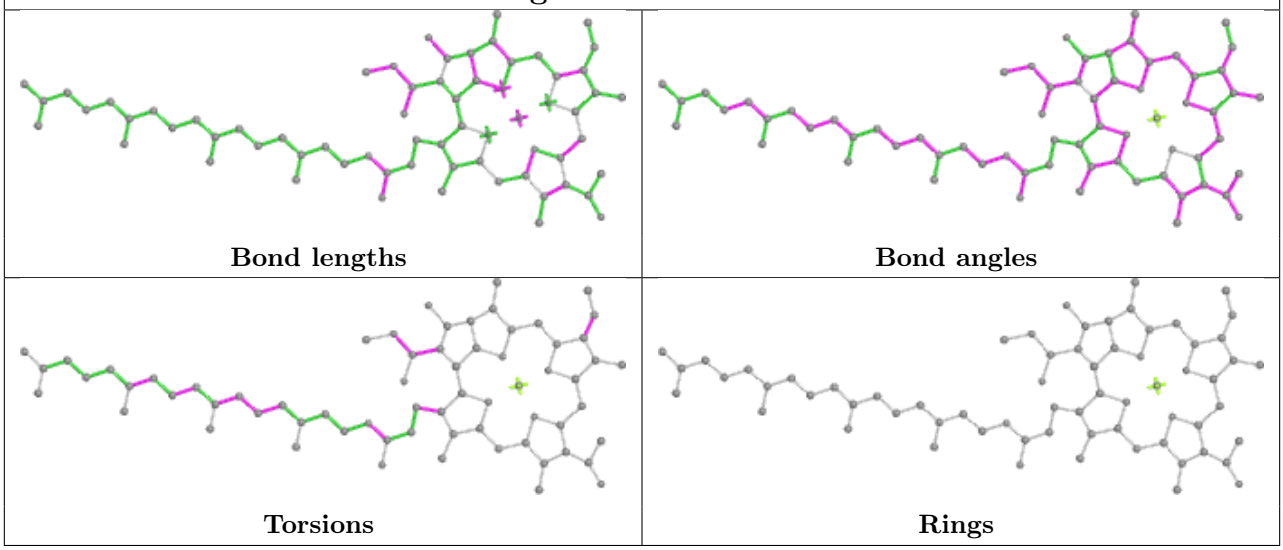


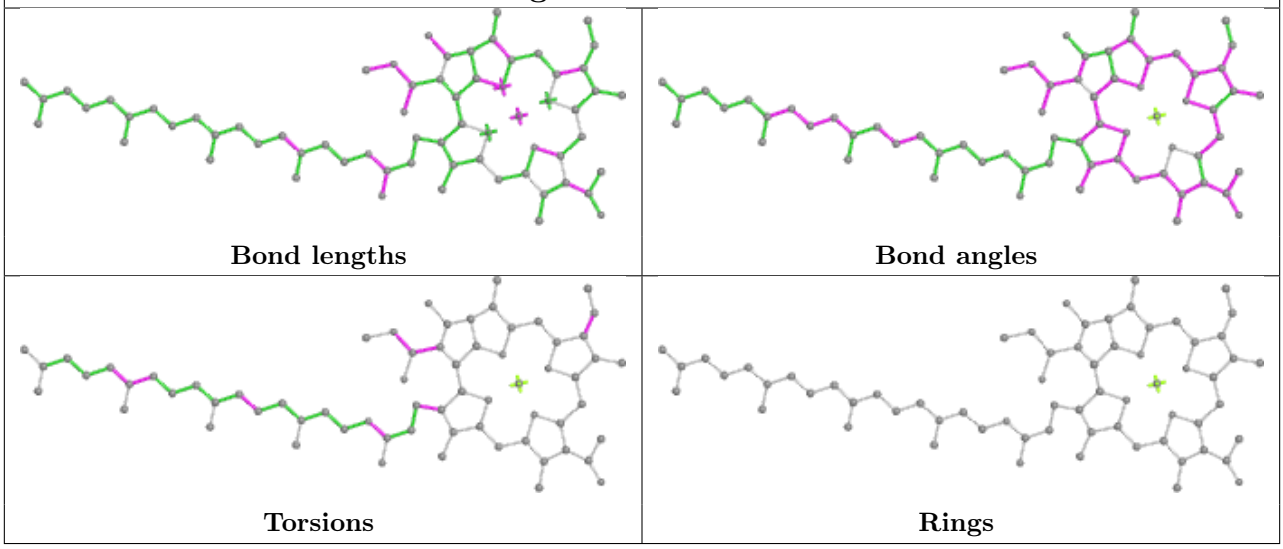
Ligand BCL 9 103



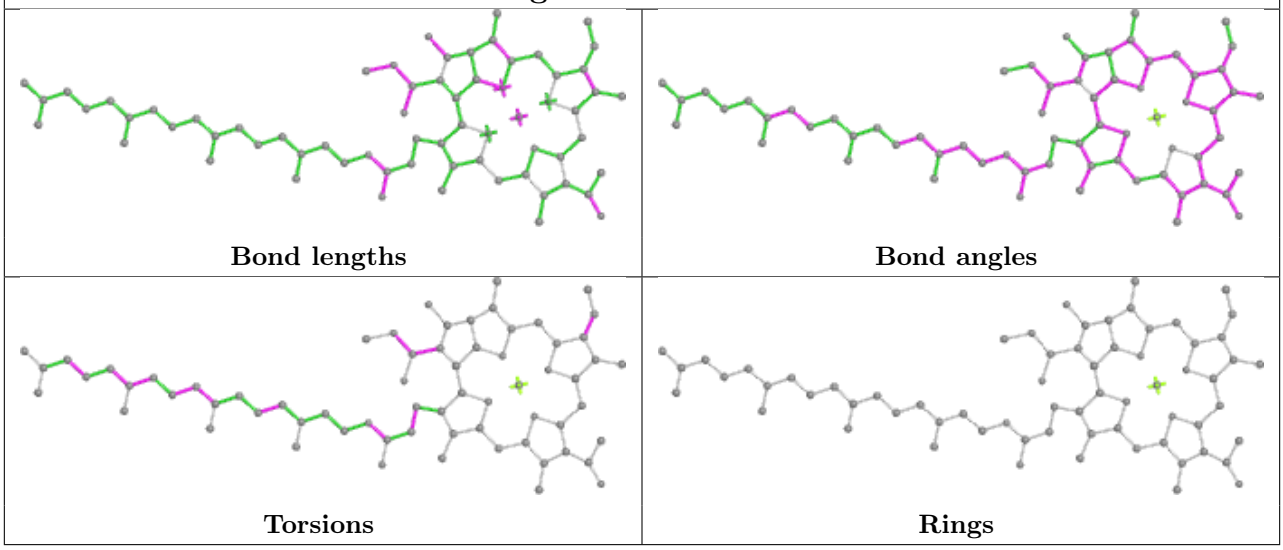
Ligand BCL 4 102



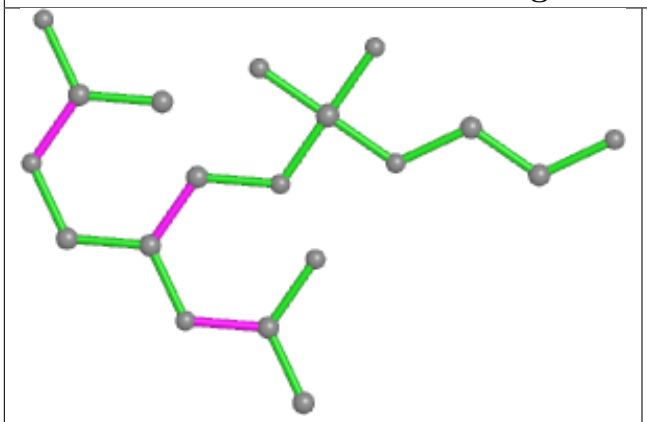
Ligand BCL v 102



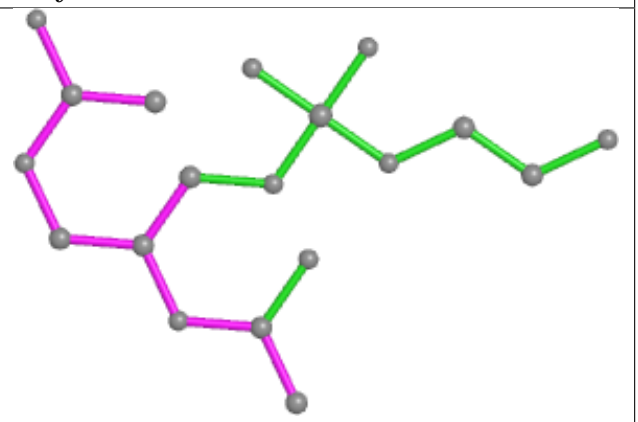
Ligand BCL 5 101



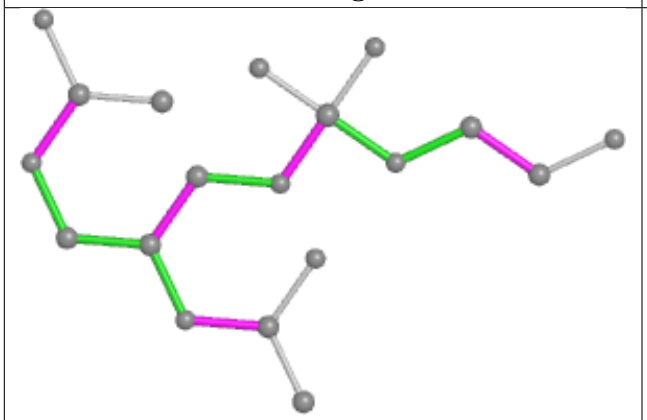
Ligand PEF y 408



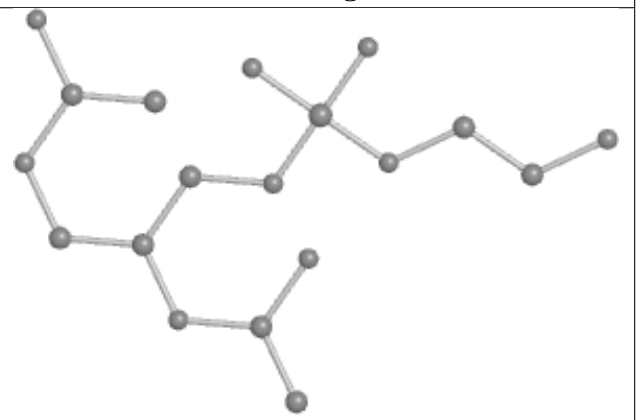
Bond lengths



Bond angles

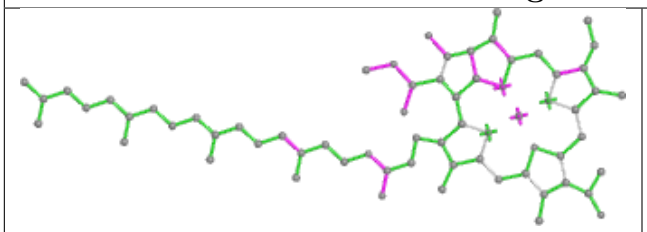


Torsions



Rings

Ligand BCL P 101



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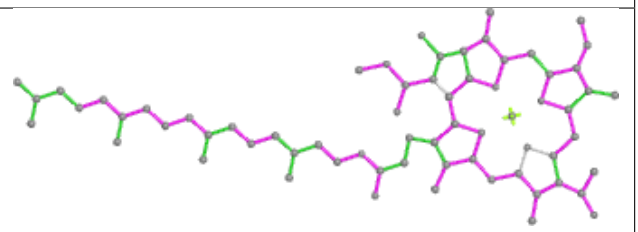
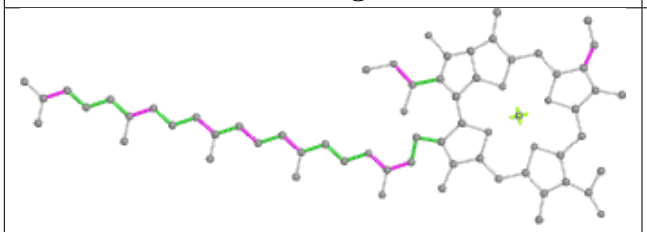
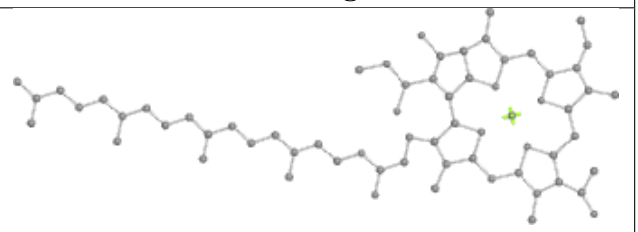


Bond angles

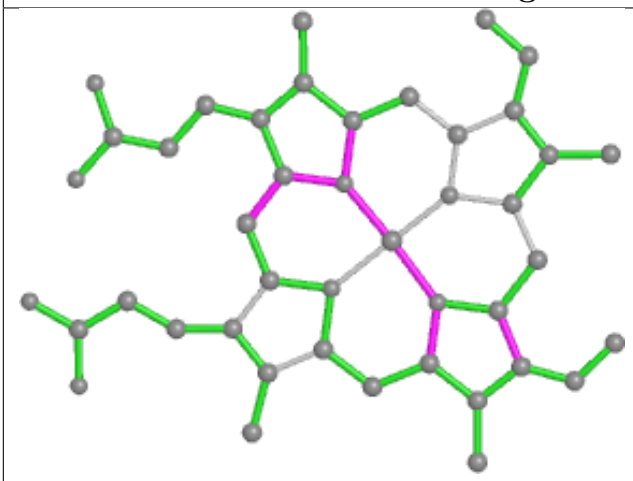


Torsions



Rings

Ligand HEM C 503



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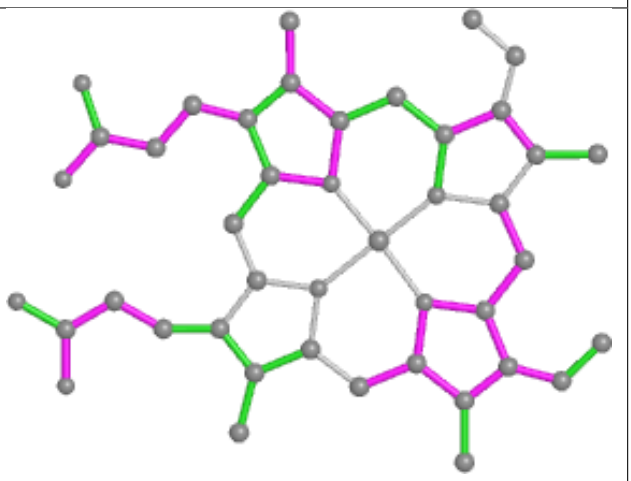
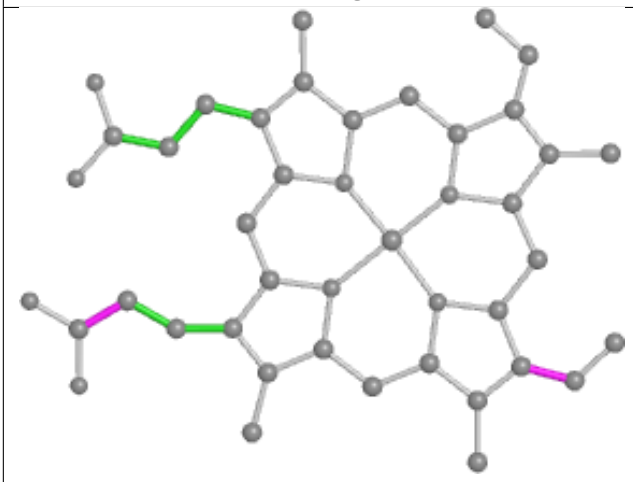
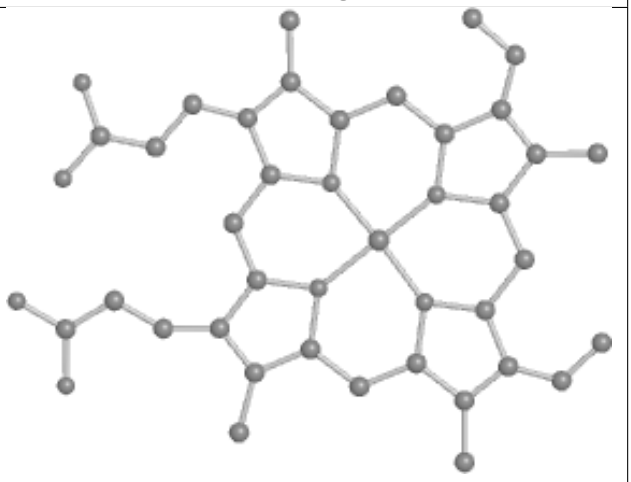


Bond angles

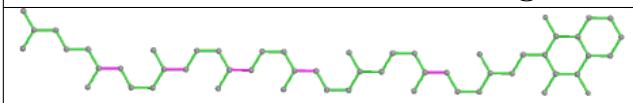


Torsions

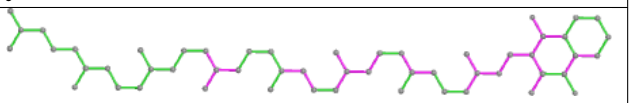


Rings

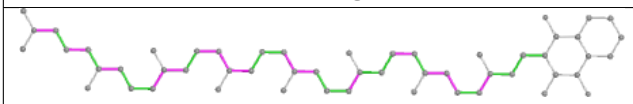
Ligand MQ8 M 403



Bond lengths



Bond angles



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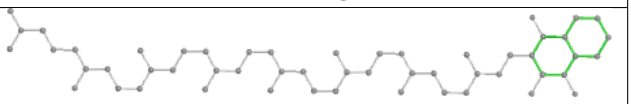
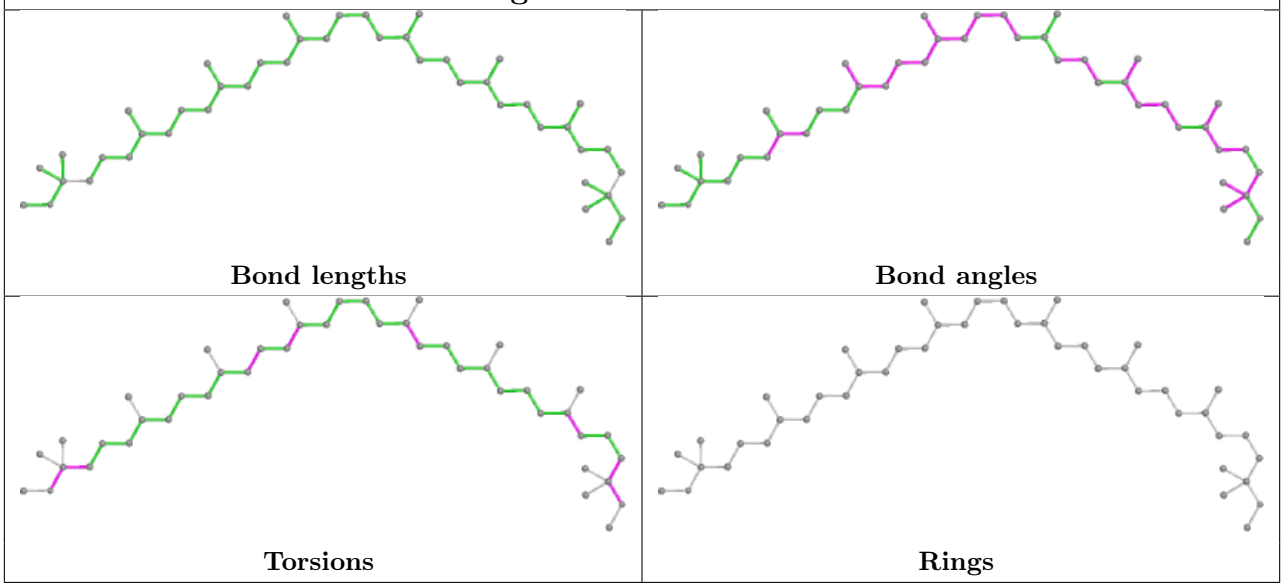
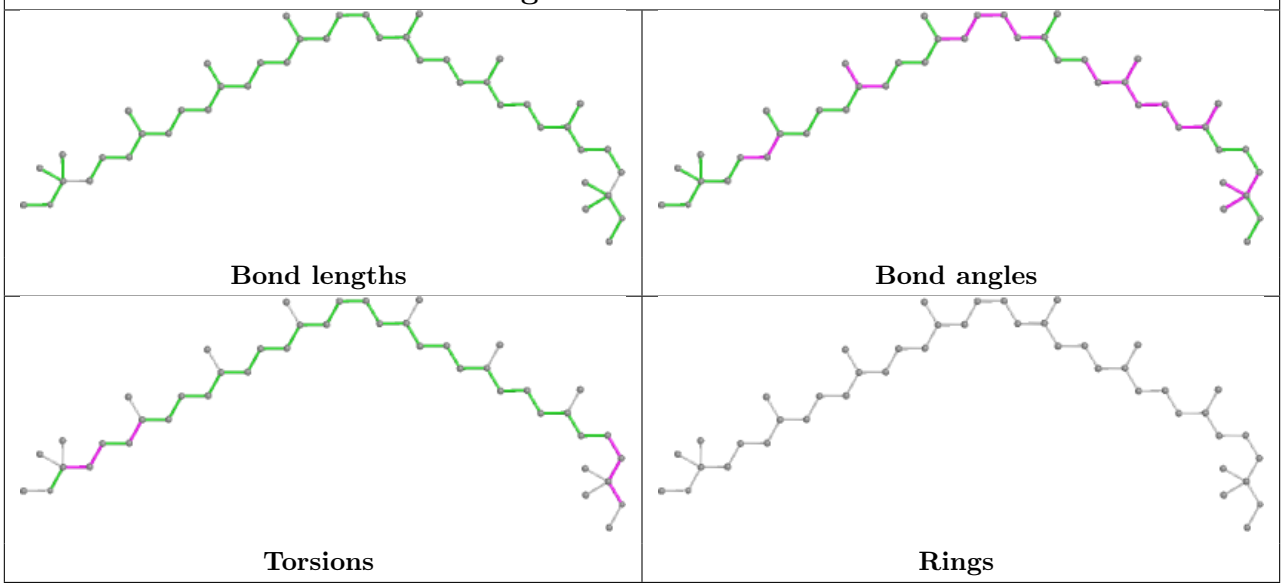


Rings

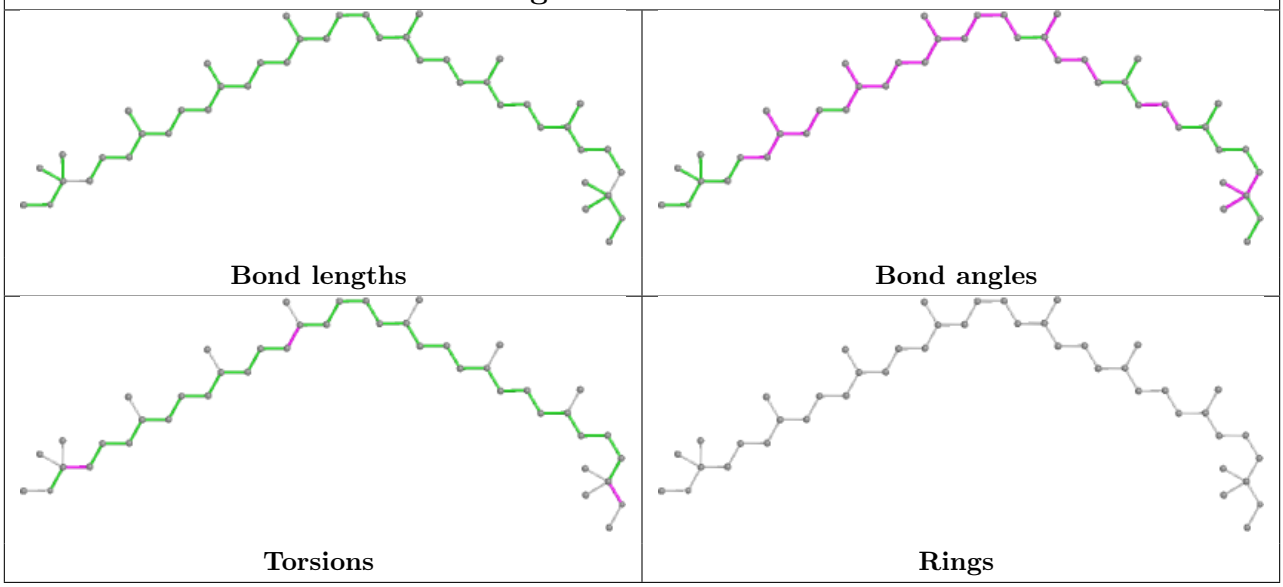
Ligand CRT AH 102



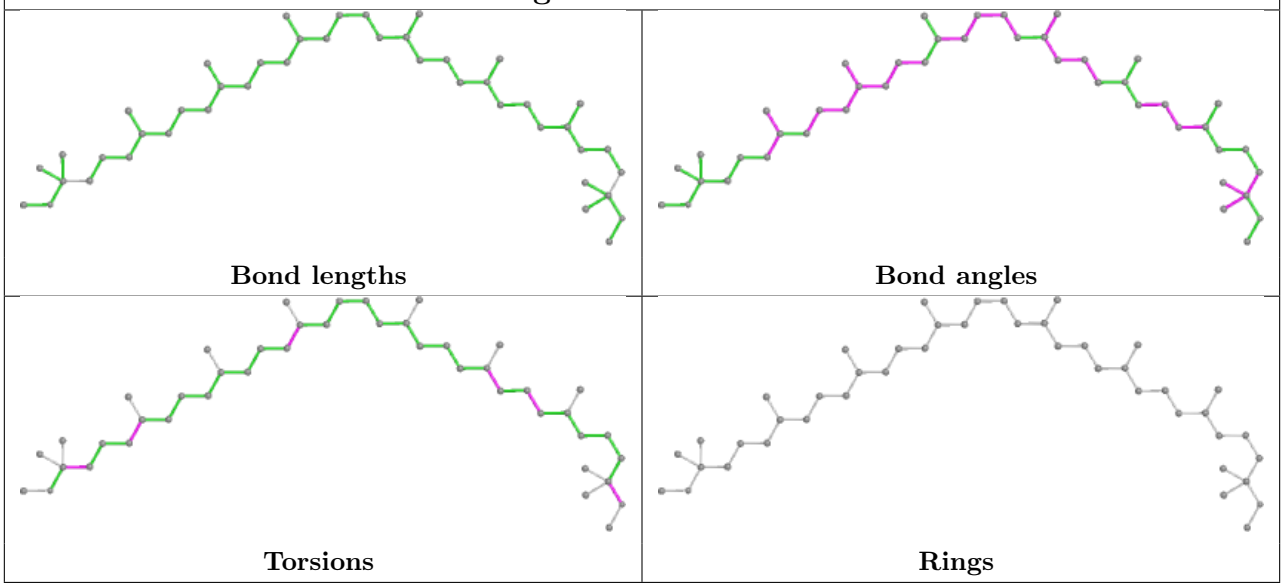
Ligand CRT M 404



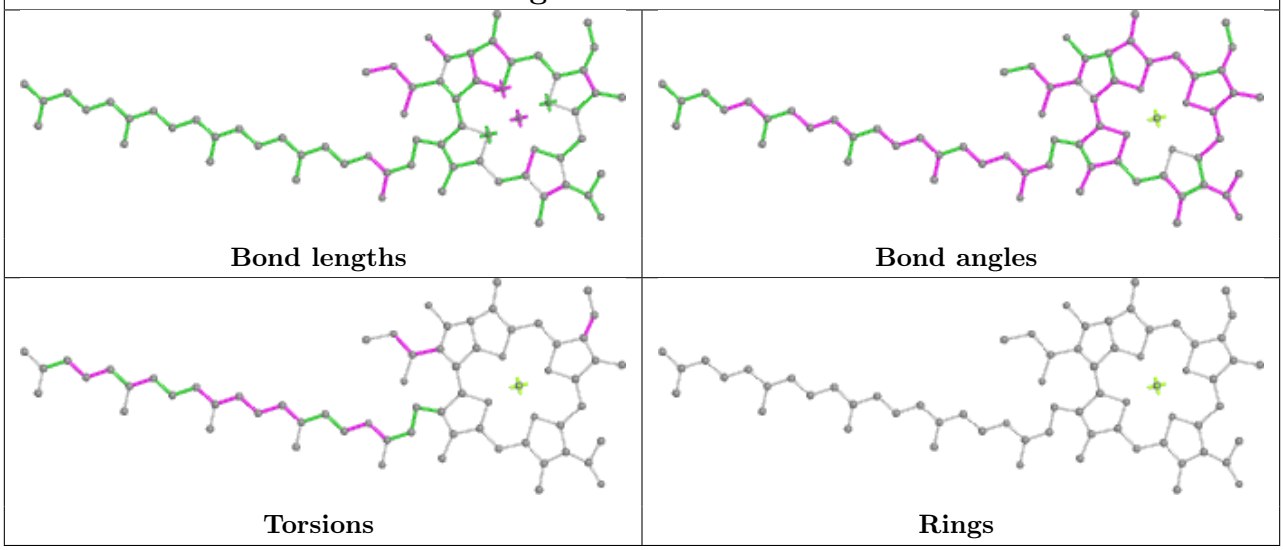
Ligand CRT z 101



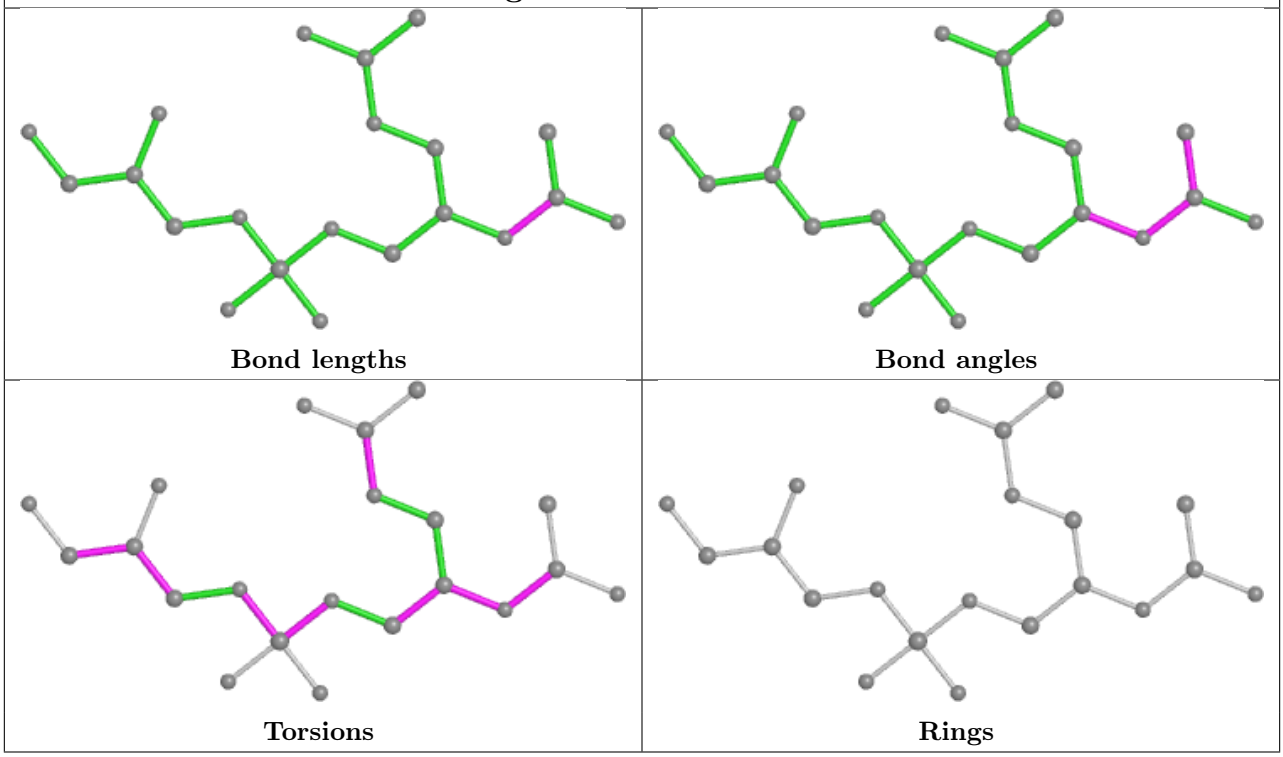
Ligand CRT i 101



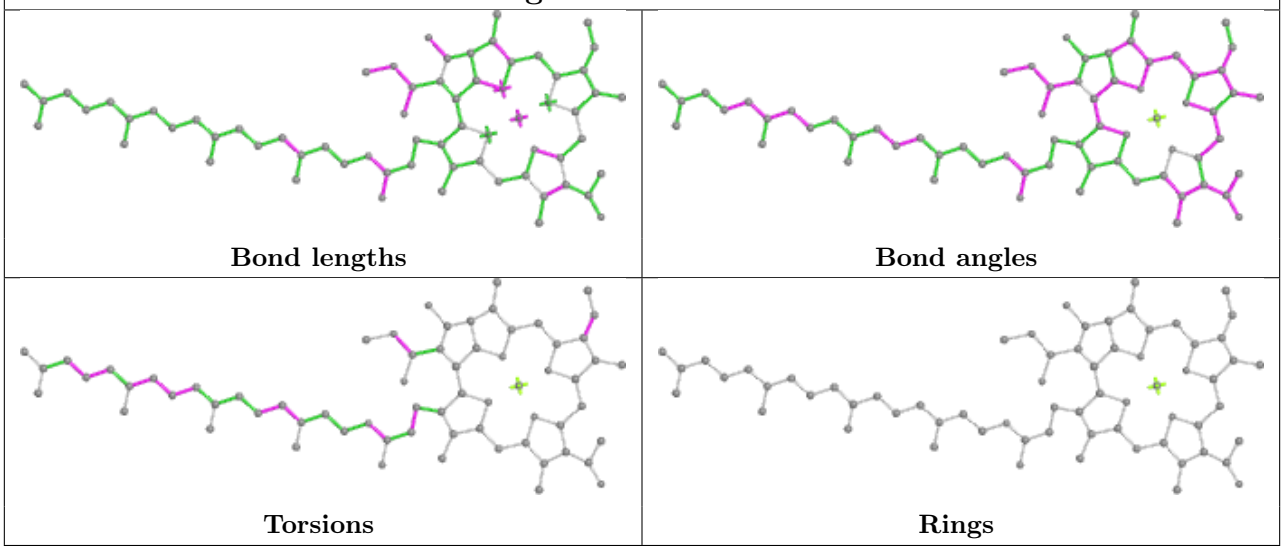
Ligand BCL x 305



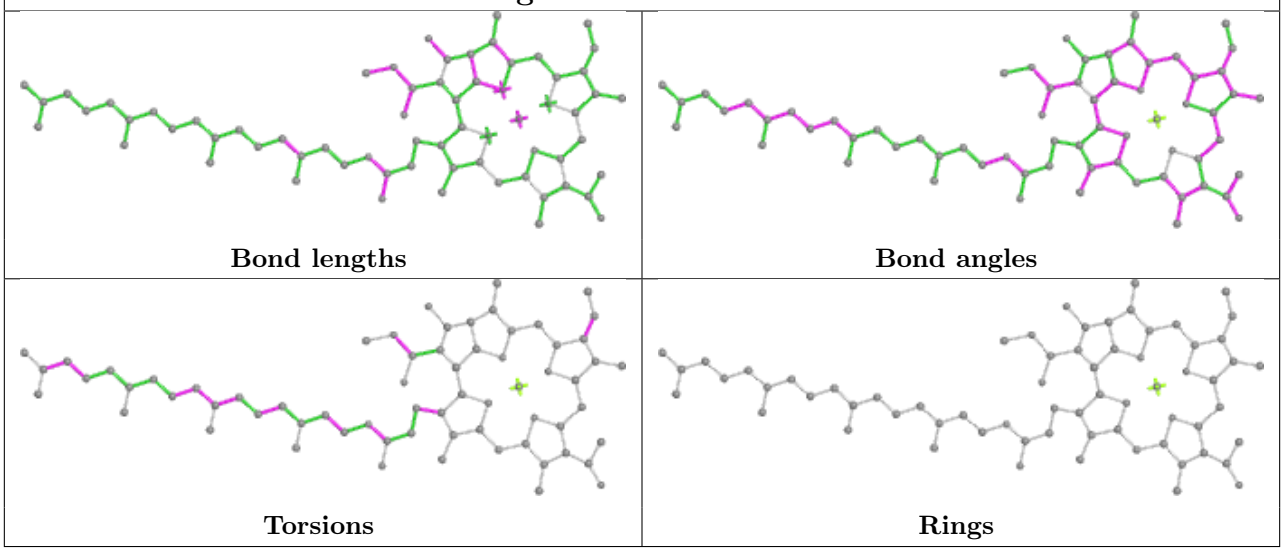
Ligand PGW AE 101



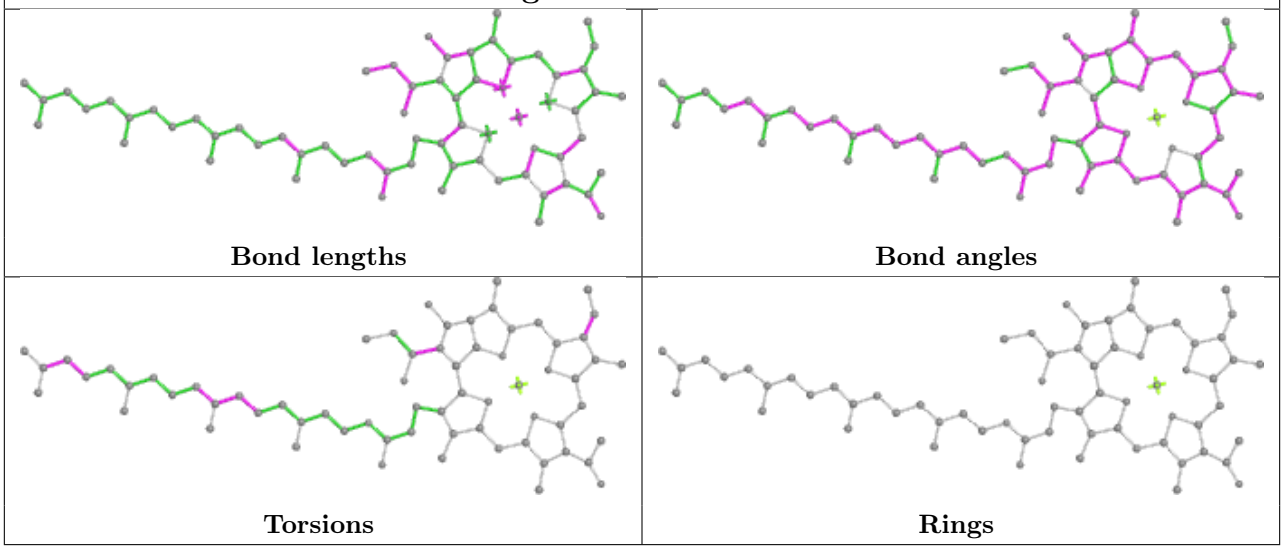
Ligand BCL U 101



Ligand BCL AJ 102



Ligand BCL M 401



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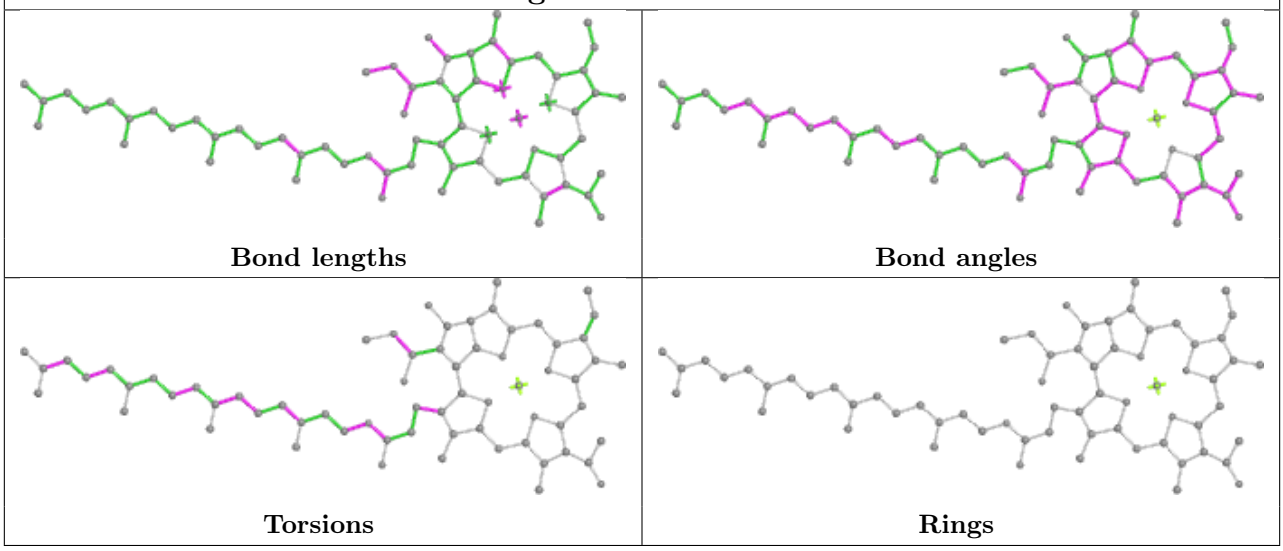

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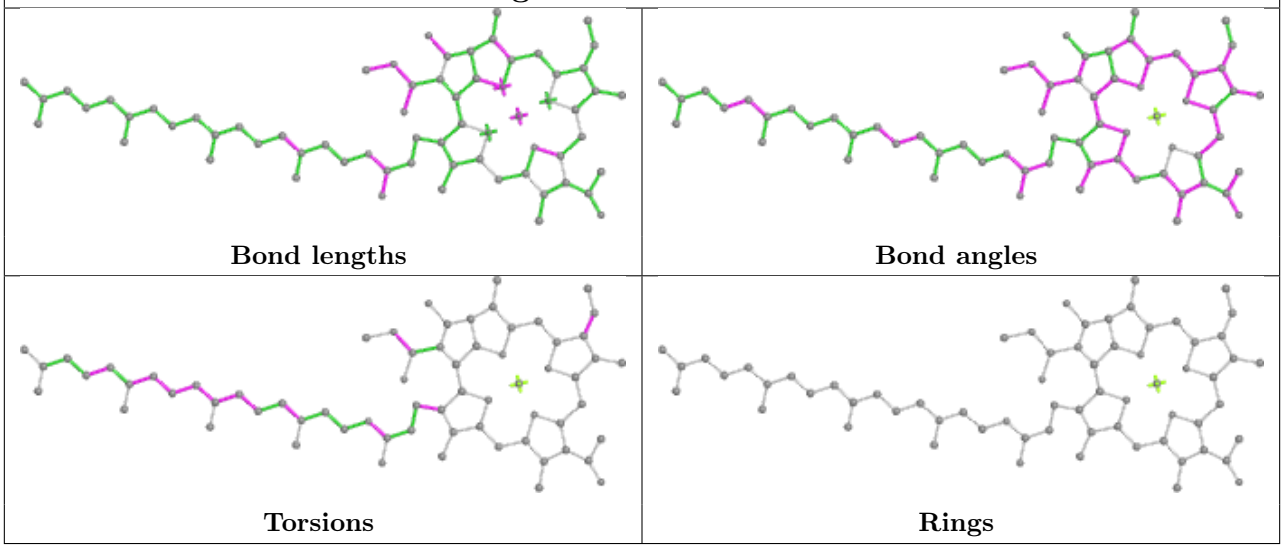
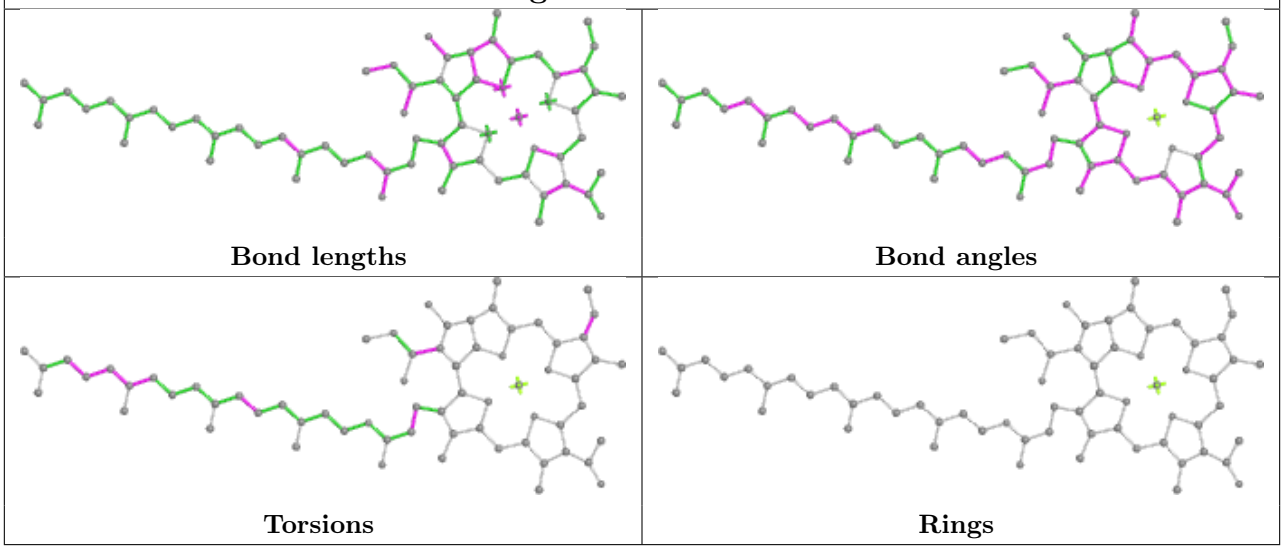
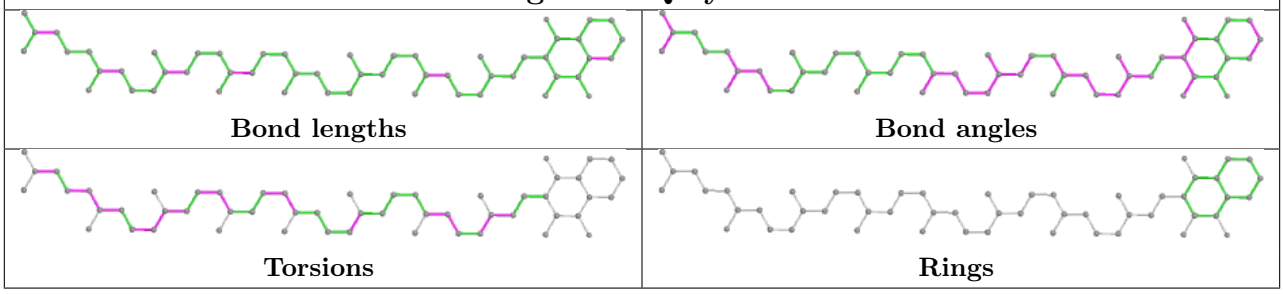


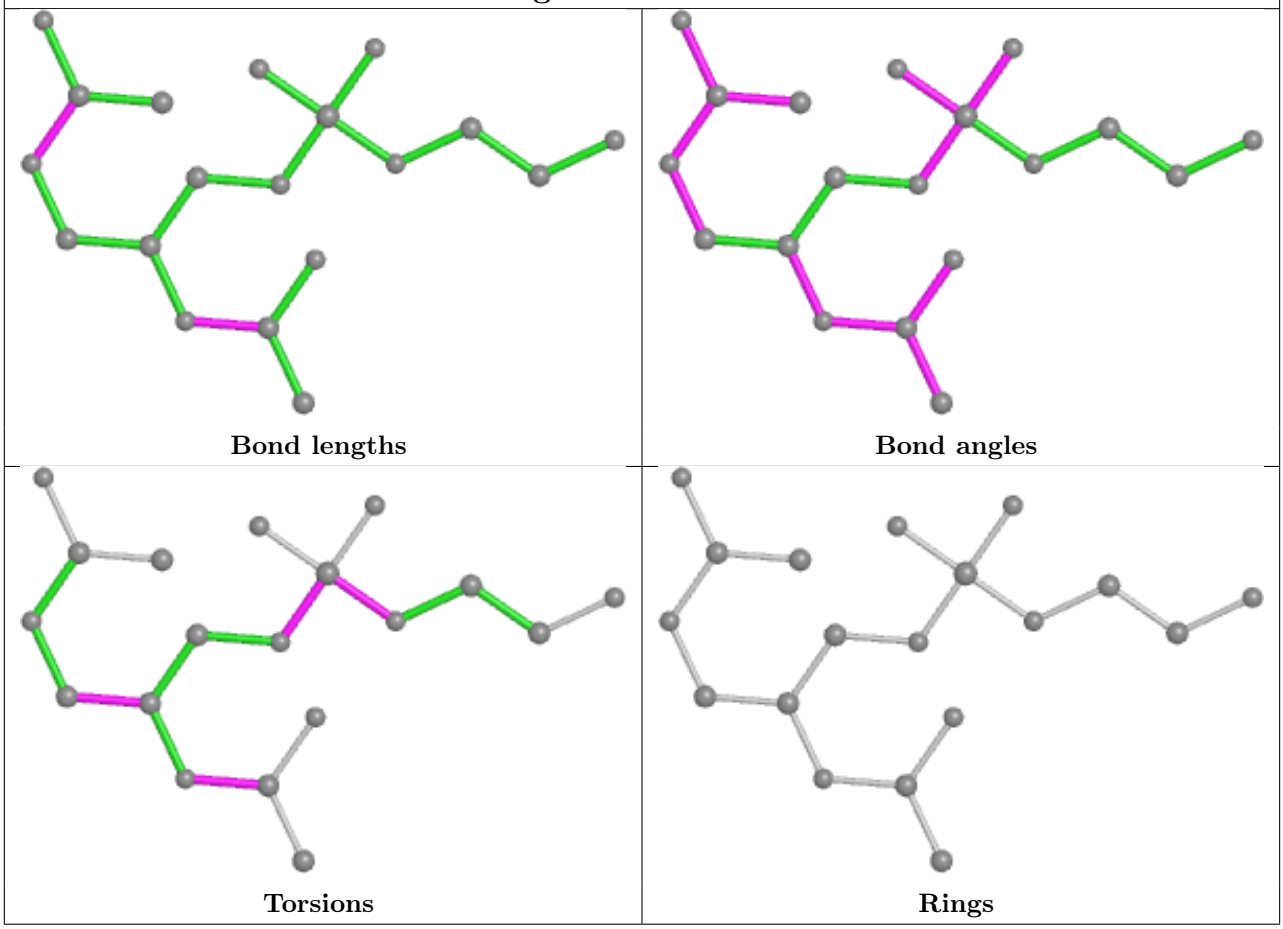
Ligand BCL x 301



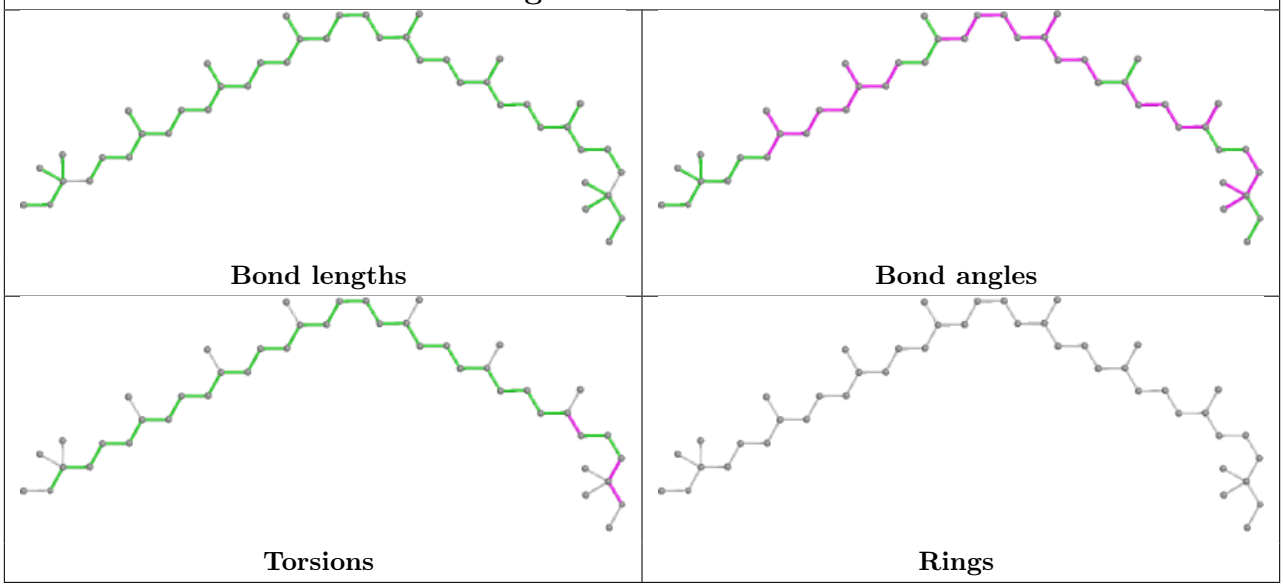
Ligand MQ8 y 403



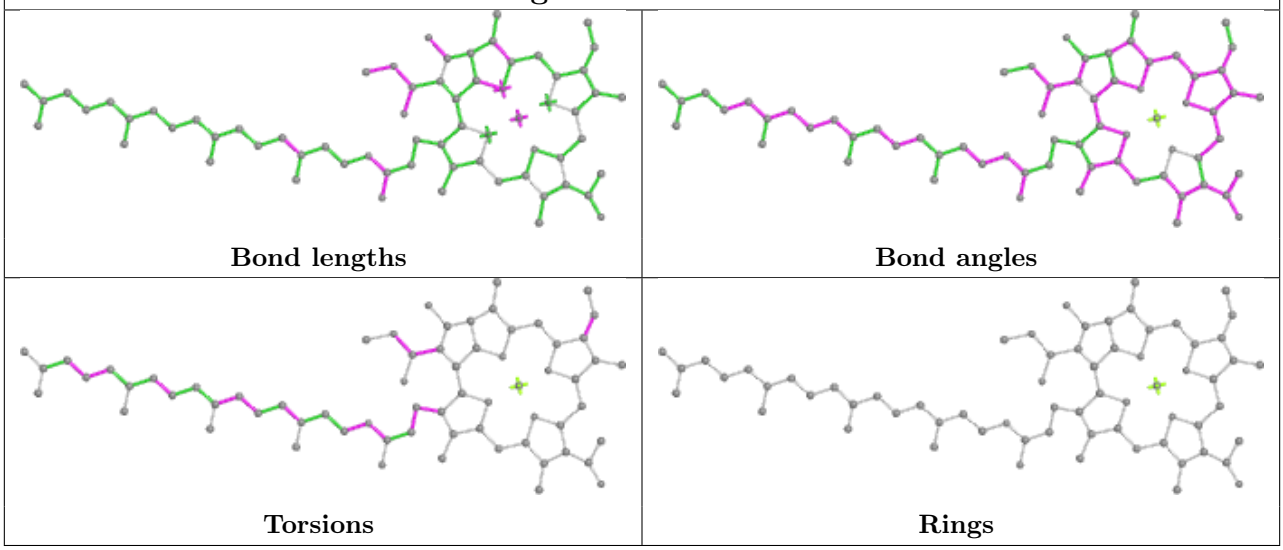
Ligand PEF t 303



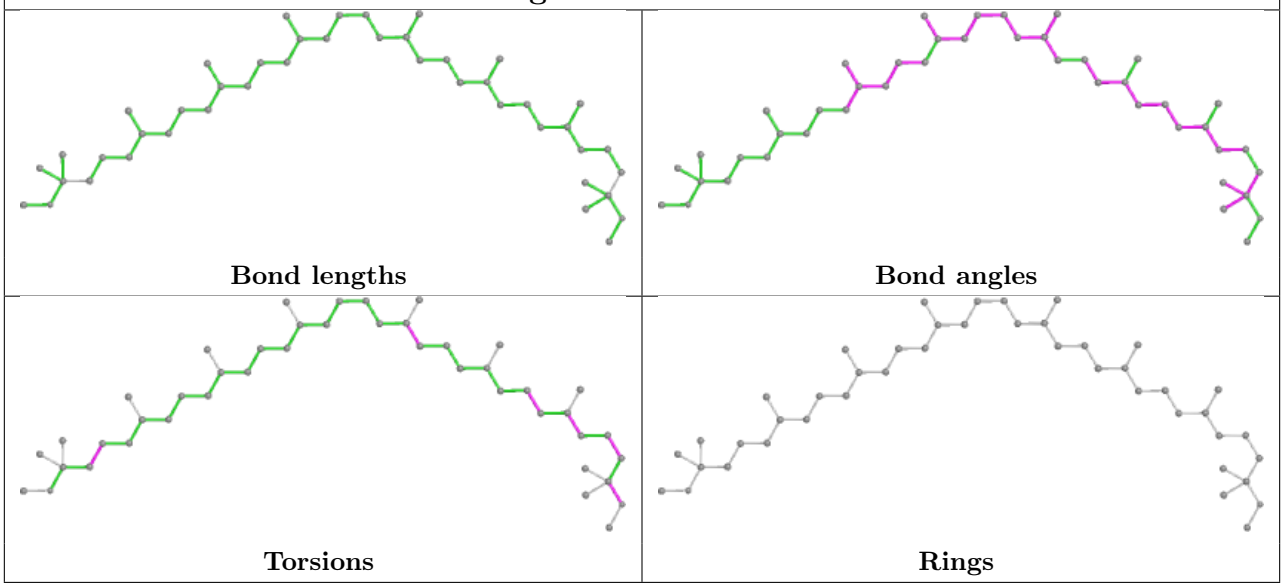
Ligand CRT A 103



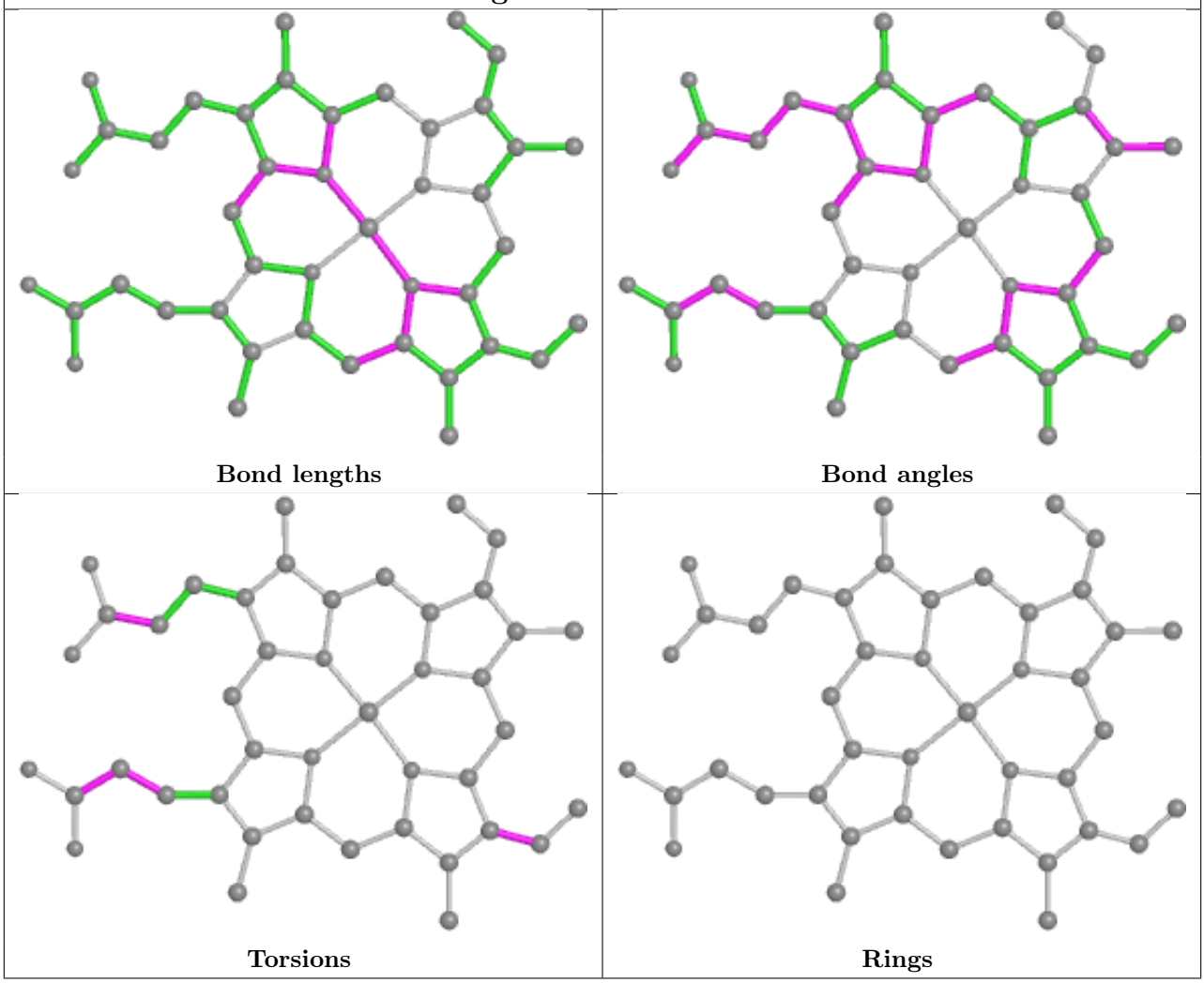
Ligand BCL e 102

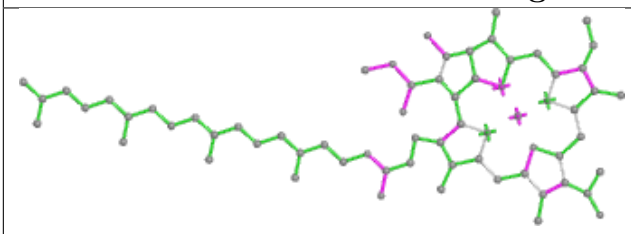
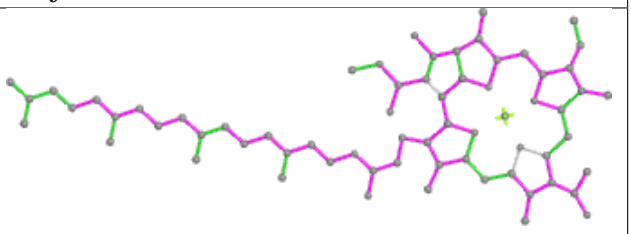
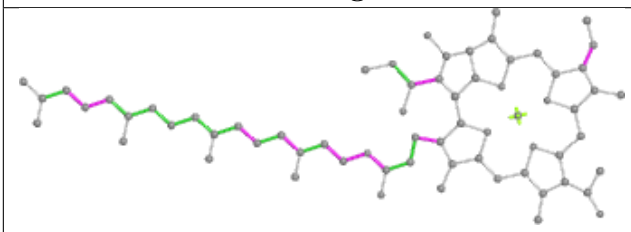
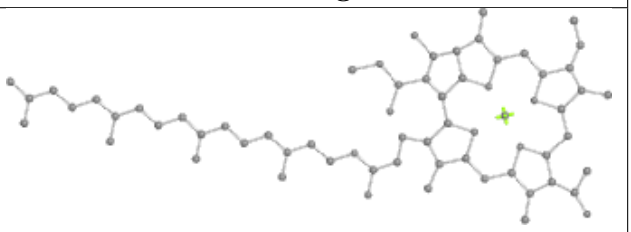


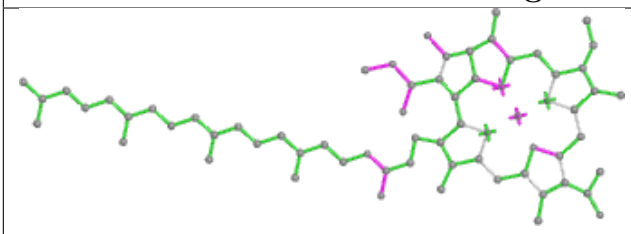
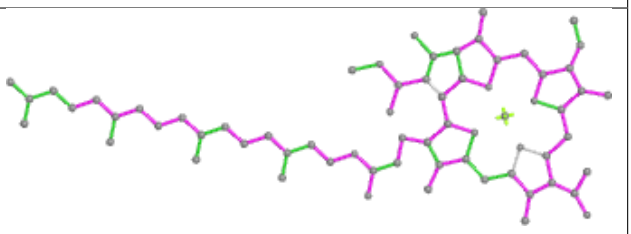
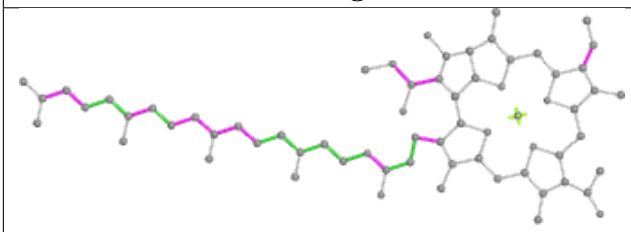
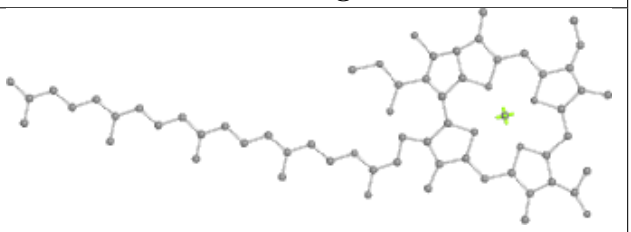
Ligand CRT 9 102



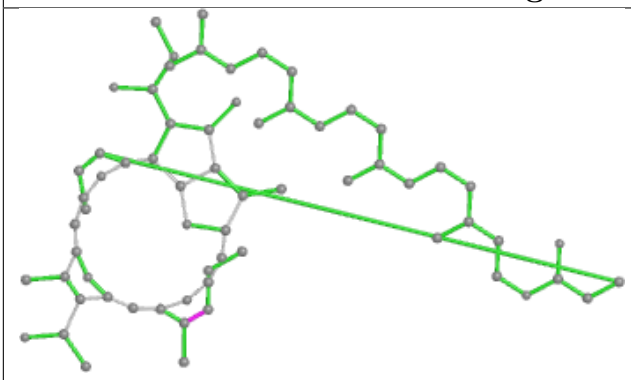
Ligand HEM o 501



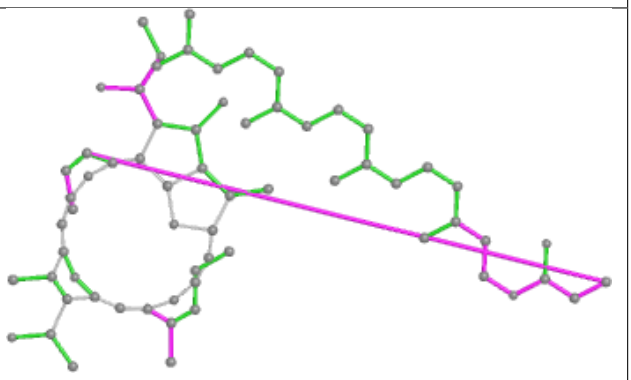
Ligand BCL y 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL O 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

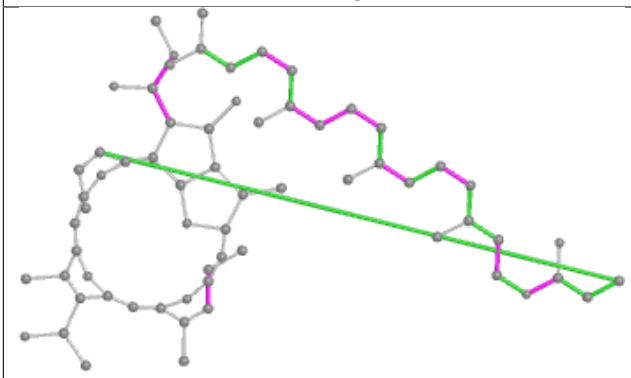
Ligand BPH x 302



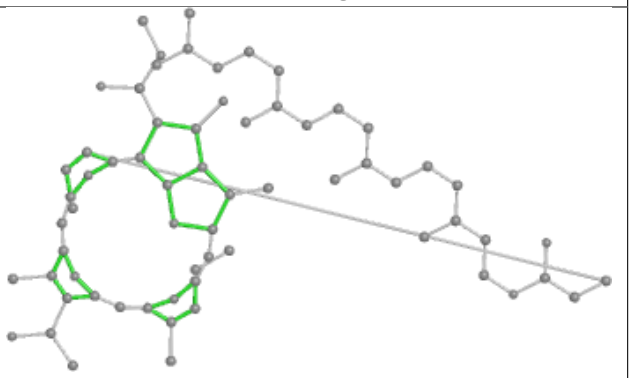
Bond lengths



Bond angles

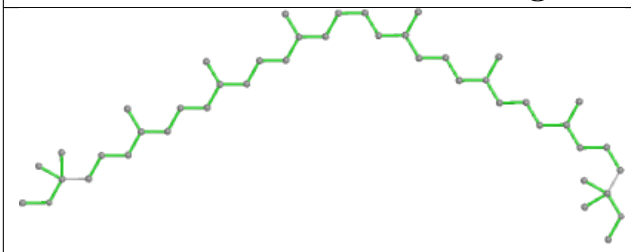


Torsions



Rings

Ligand CRT e 101



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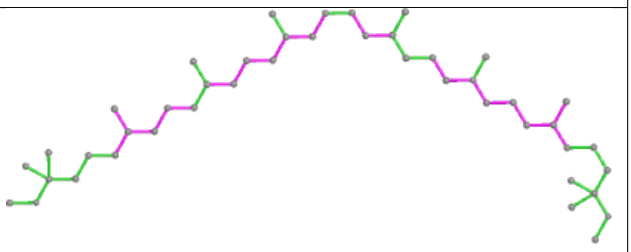

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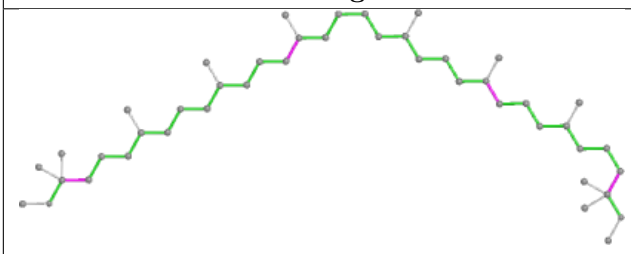

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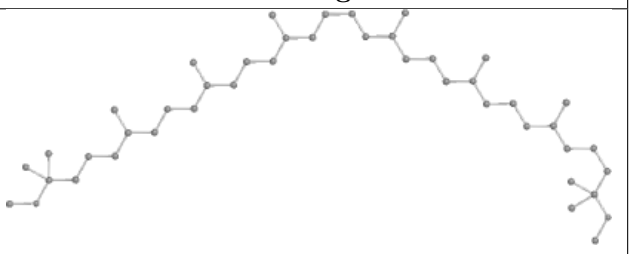
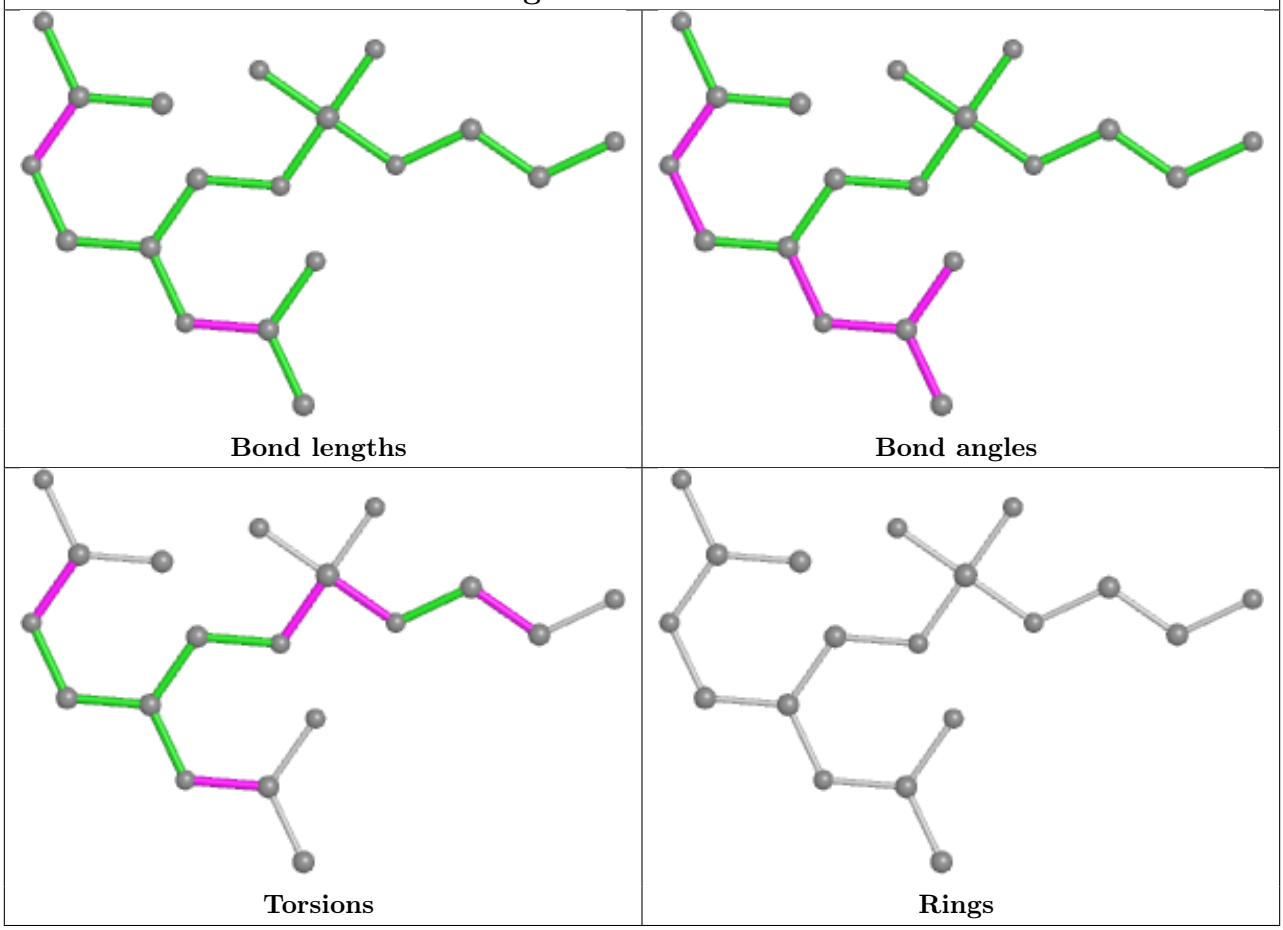
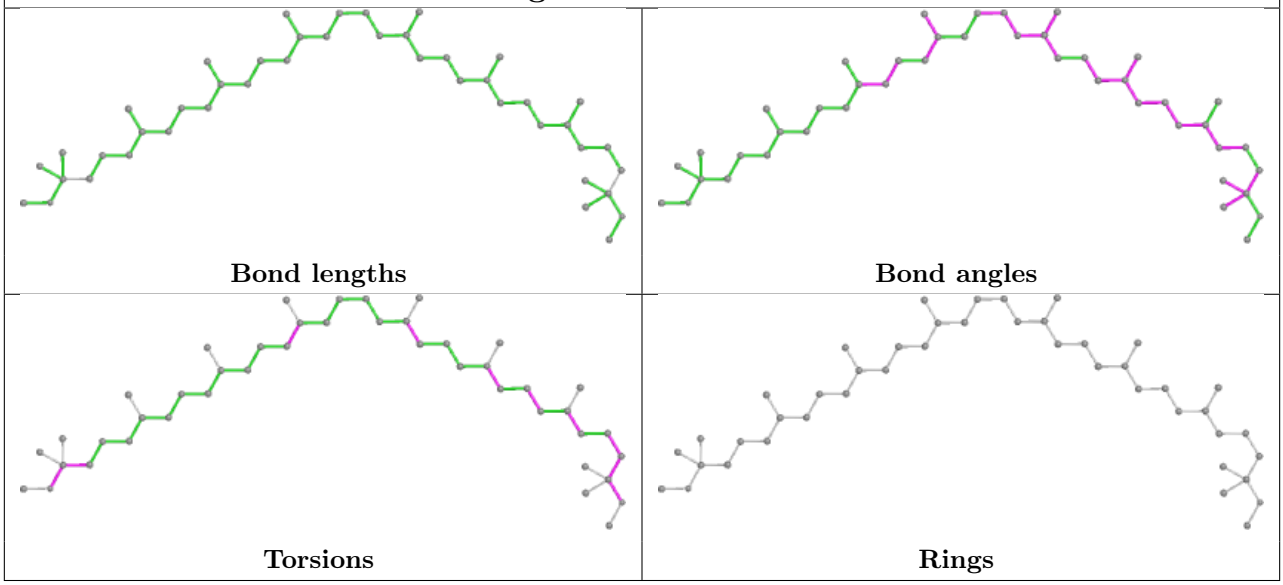


Rings

Ligand PEF M 406



Ligand CRT n 101



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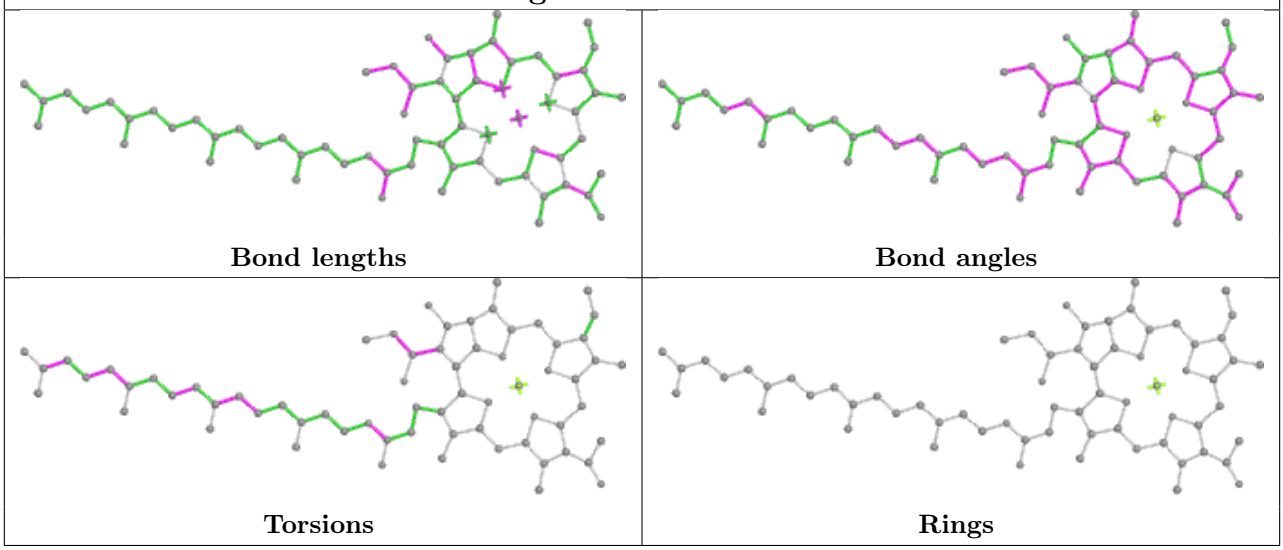

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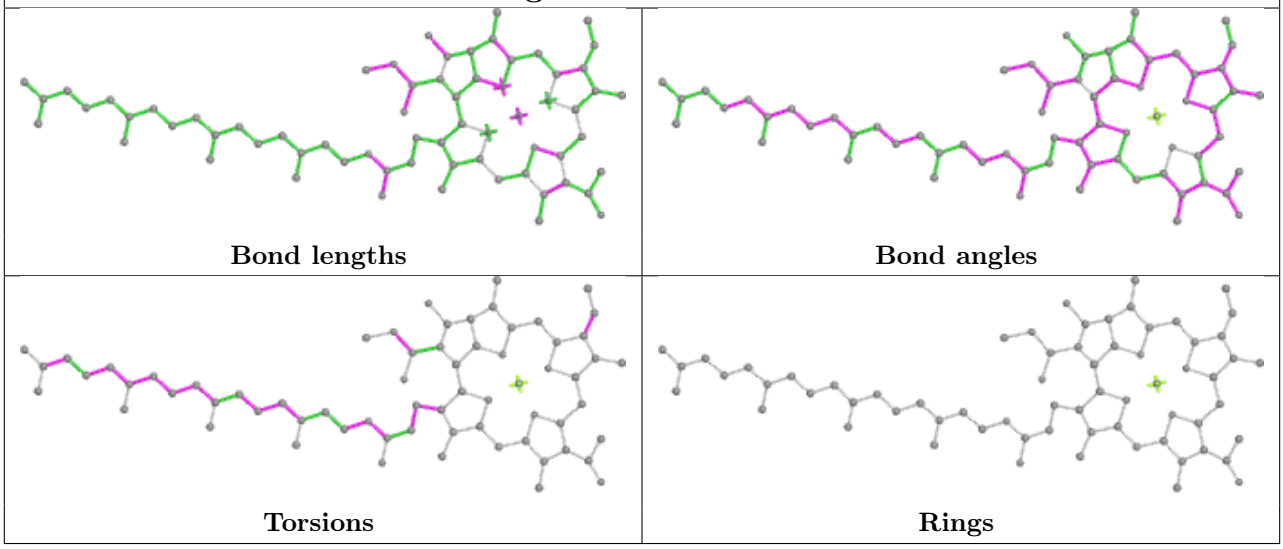

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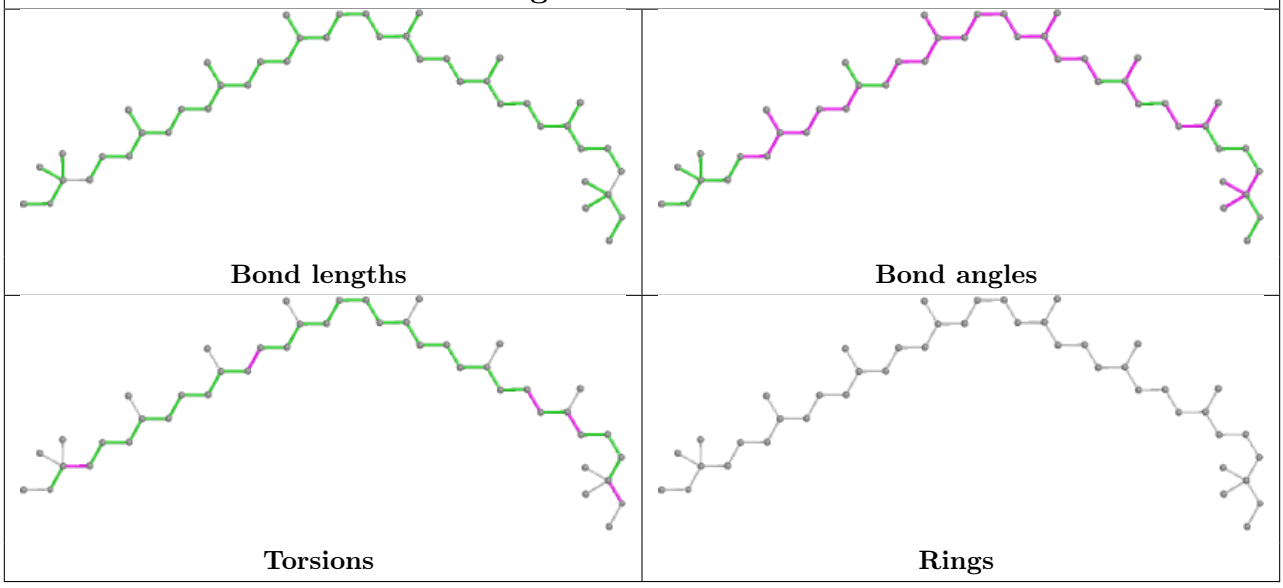

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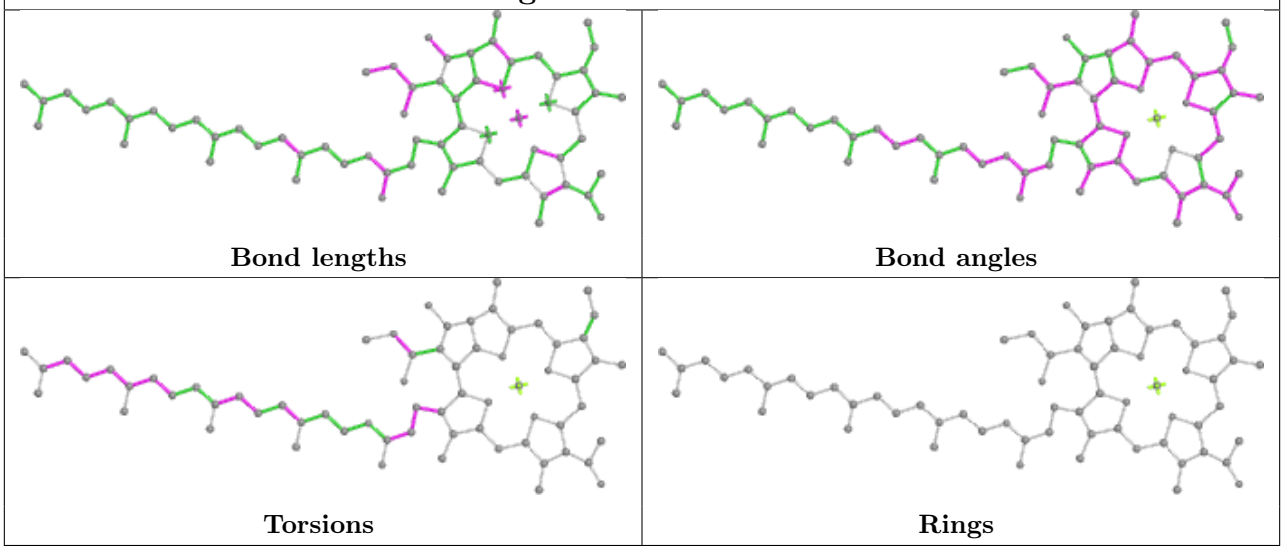

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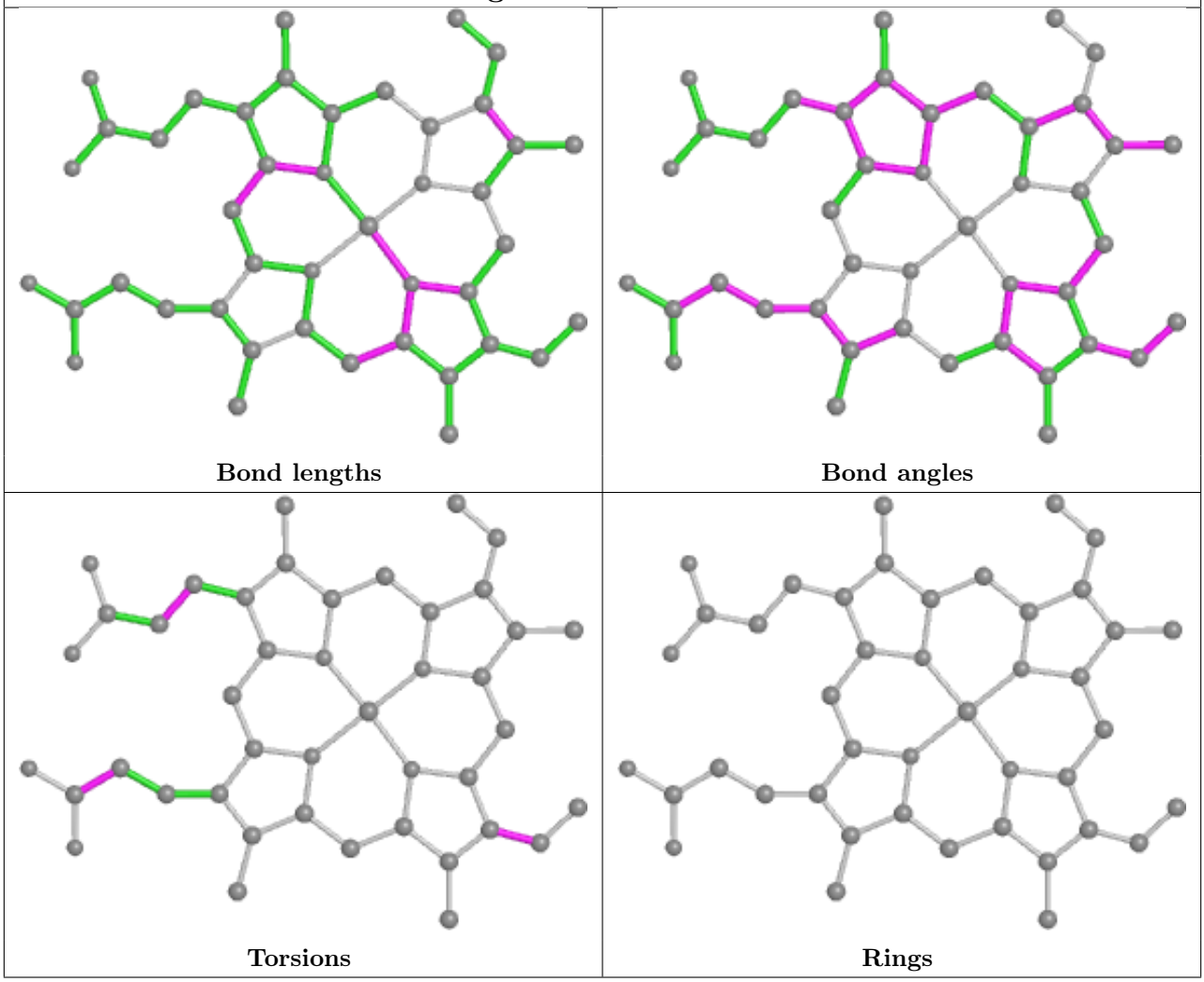

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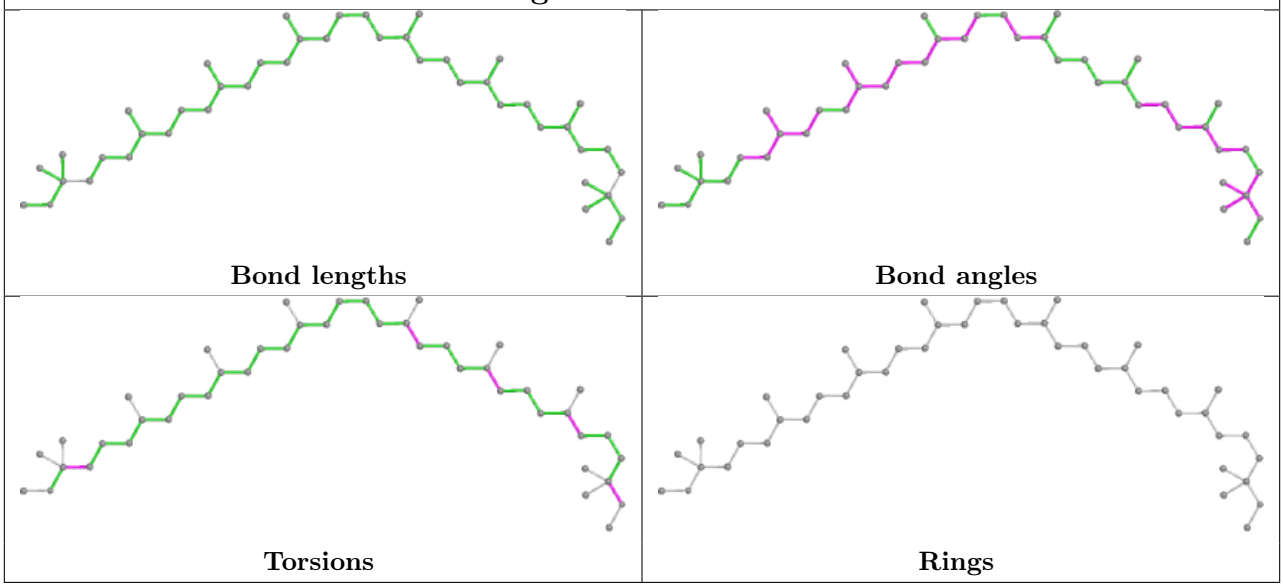

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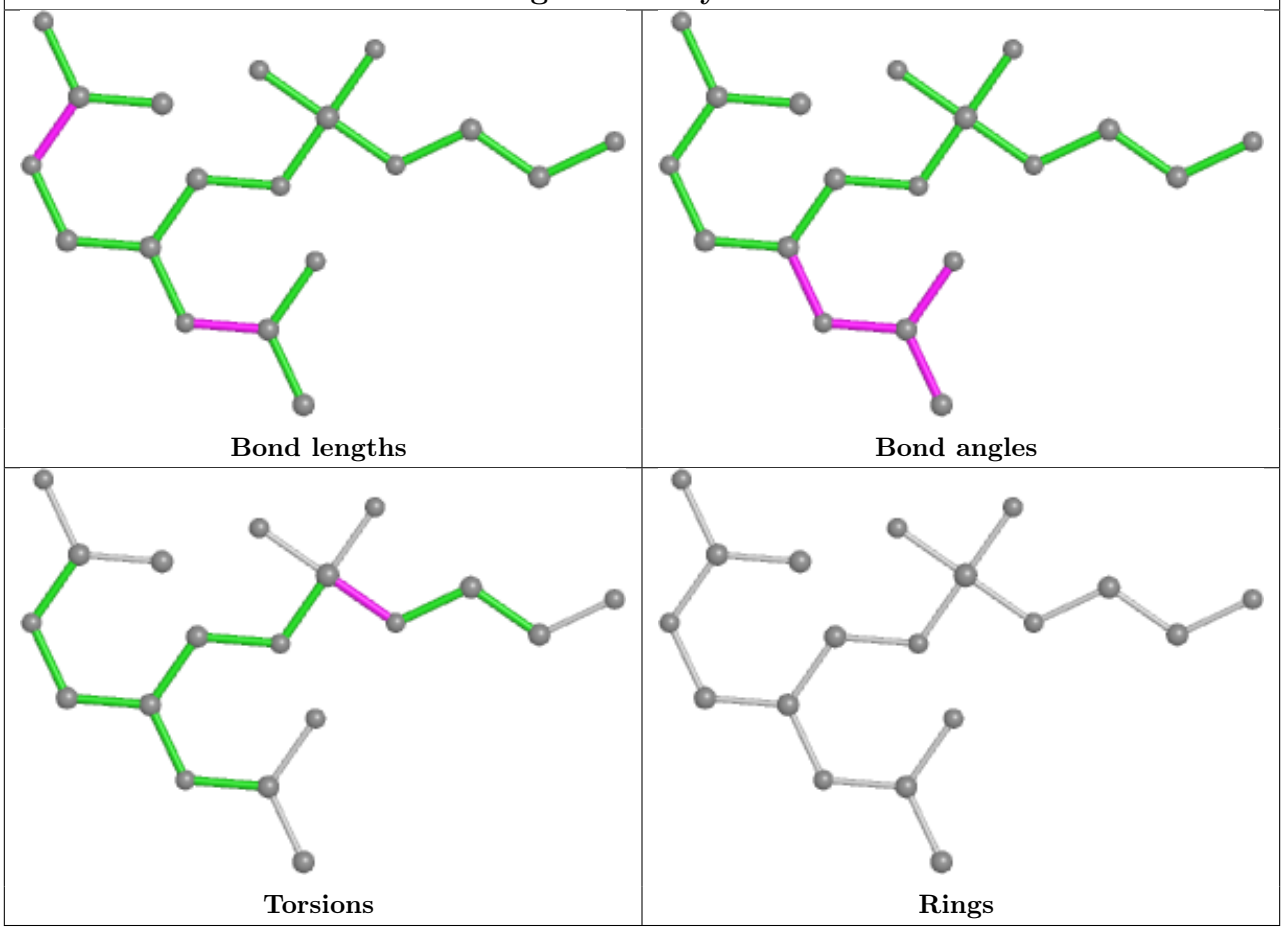

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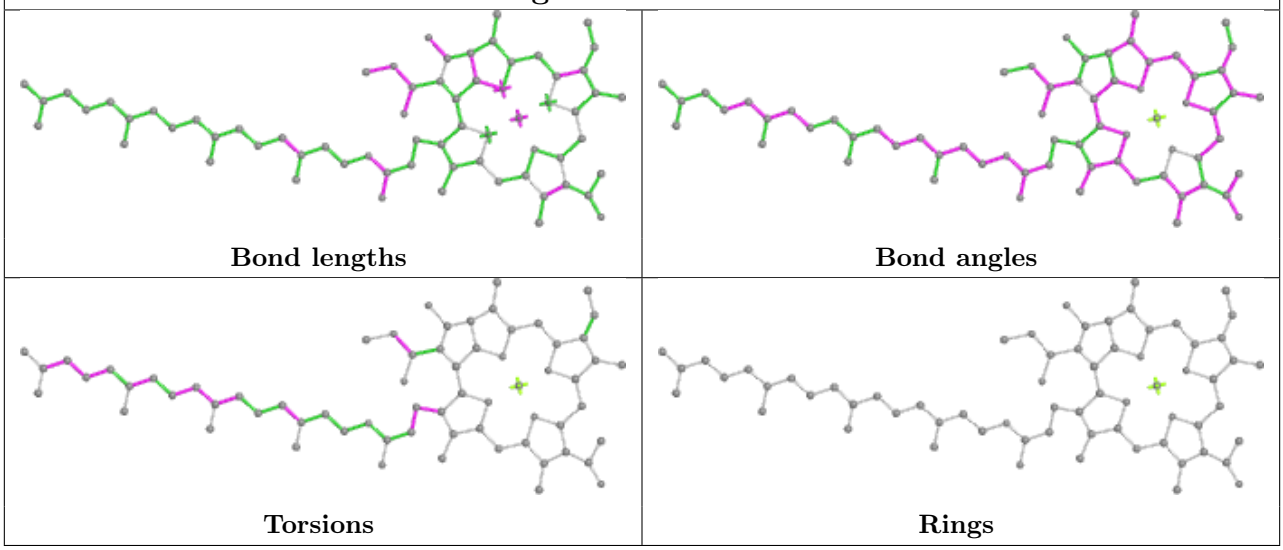

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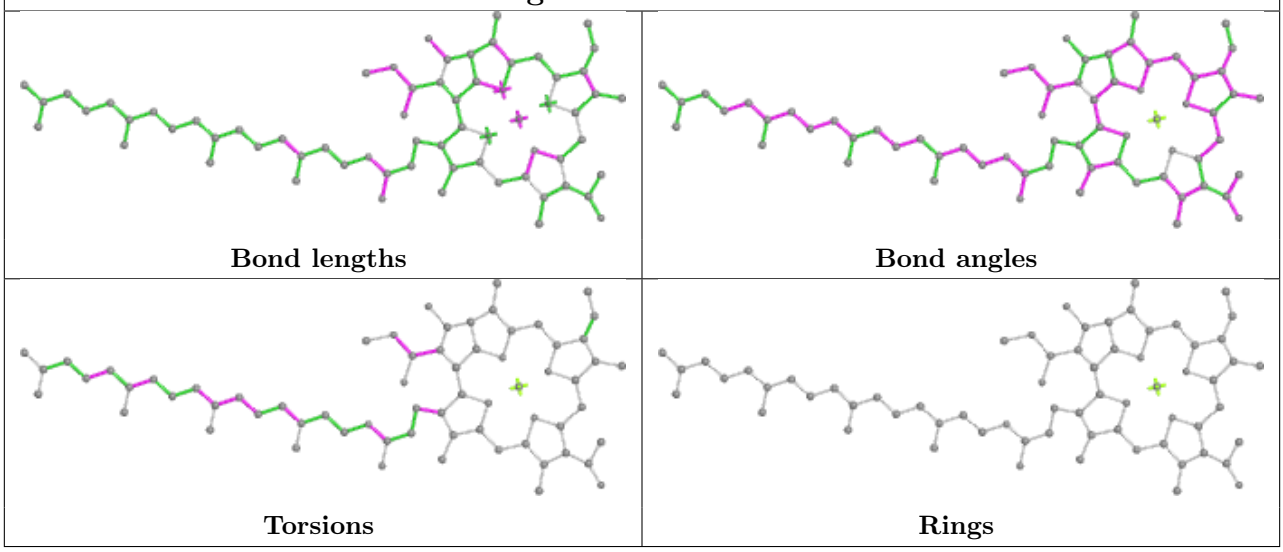

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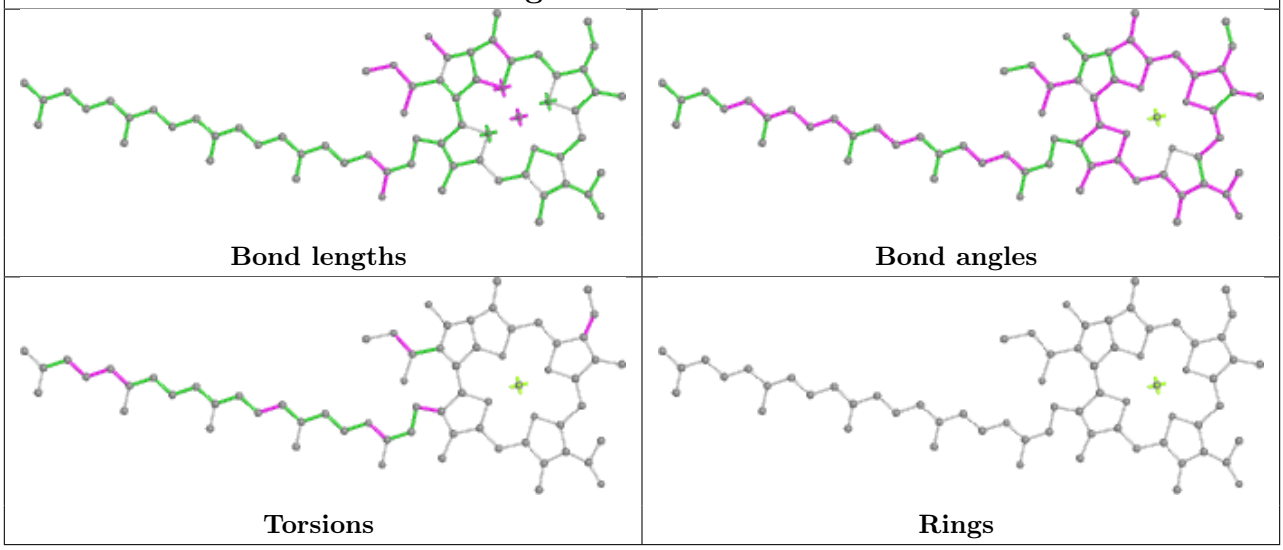

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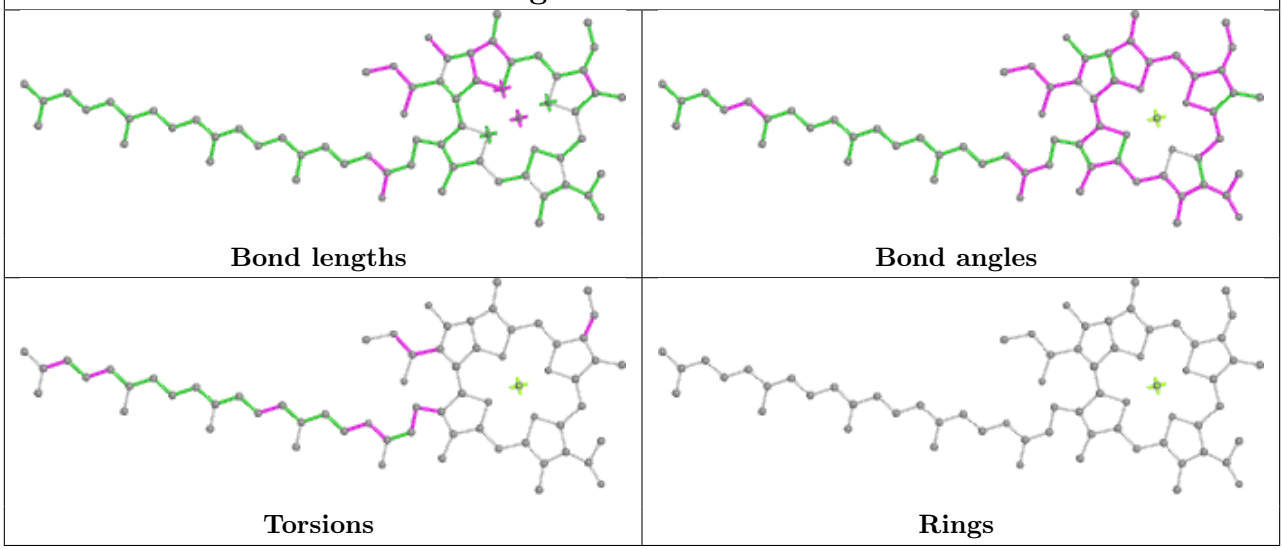

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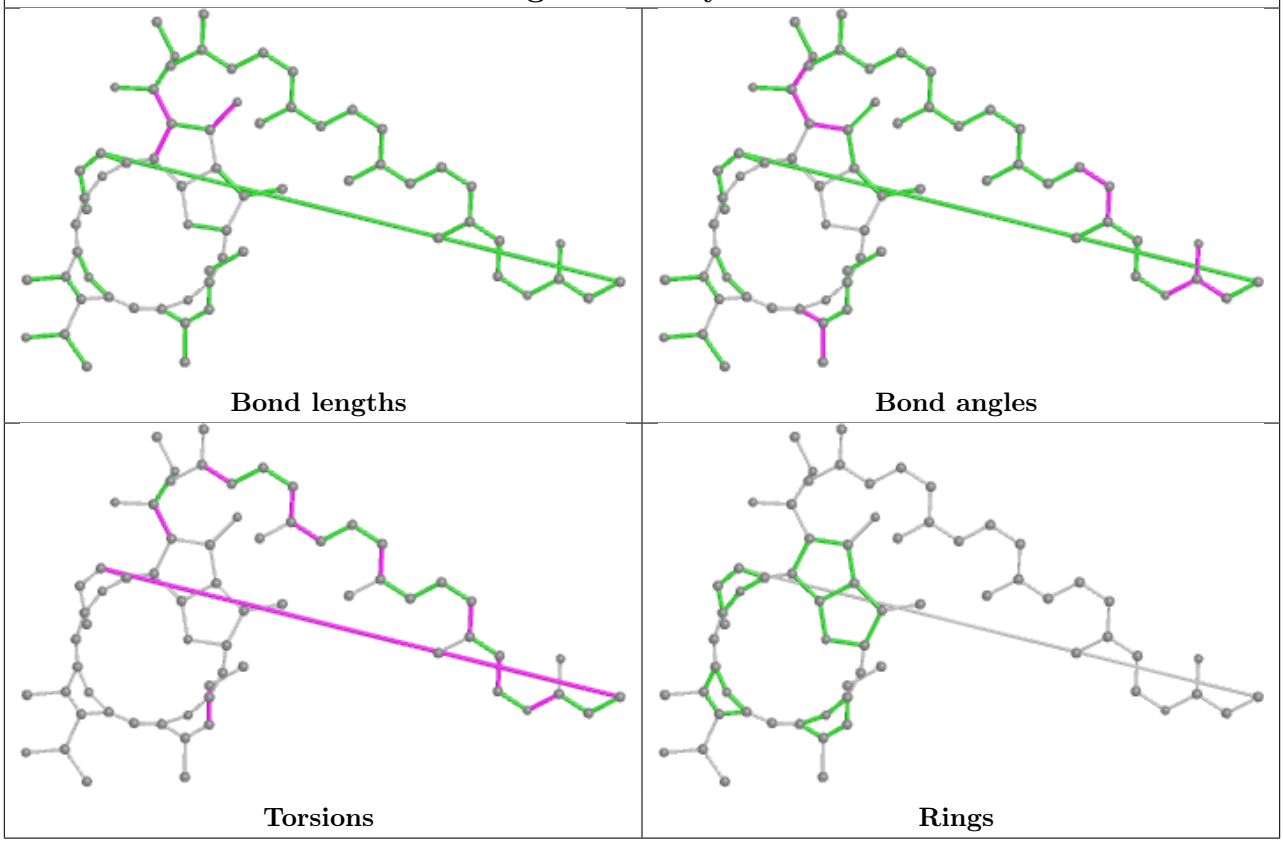

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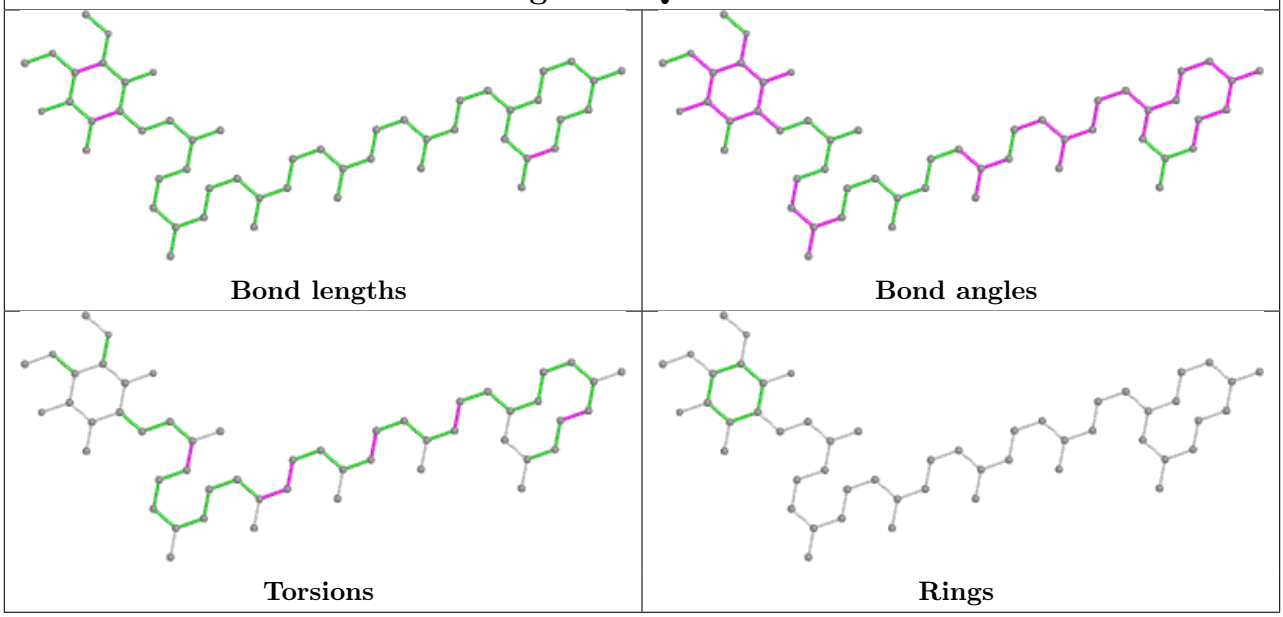

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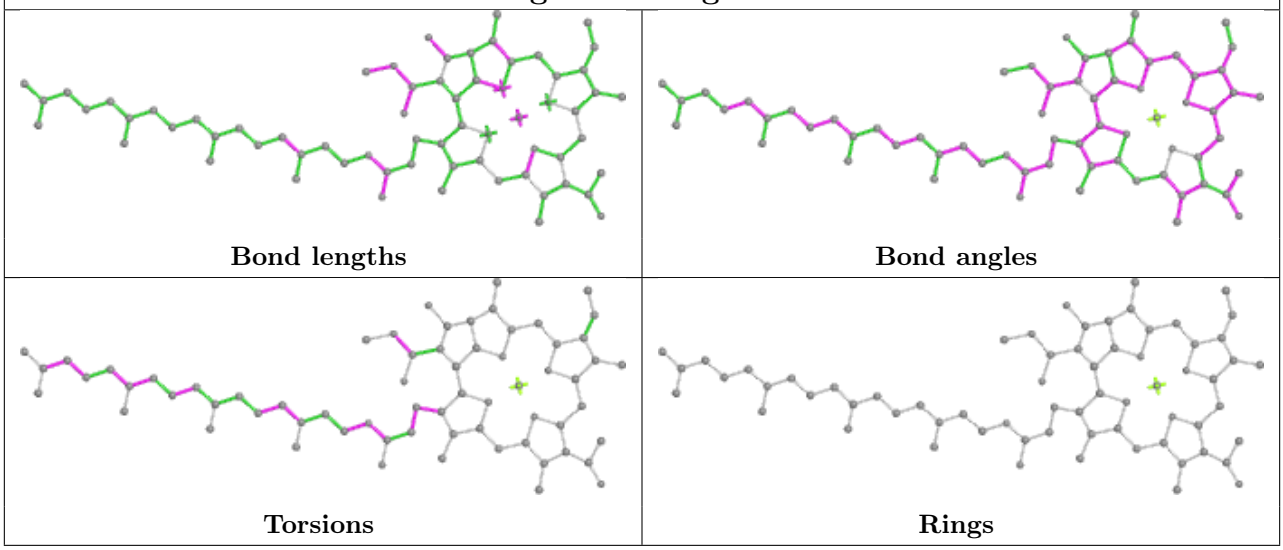

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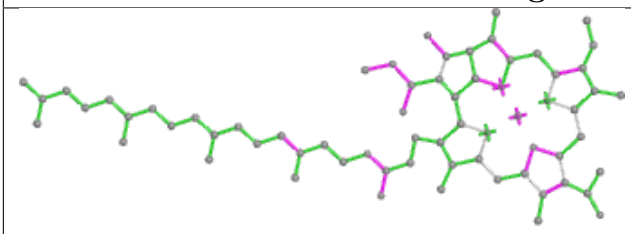
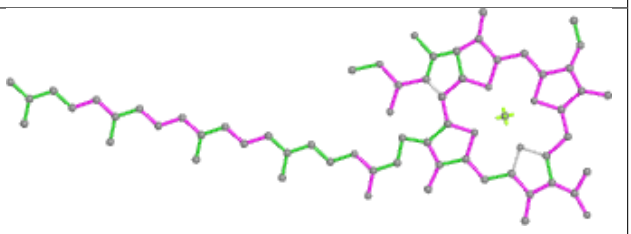
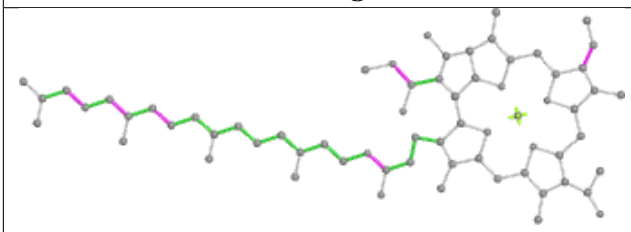
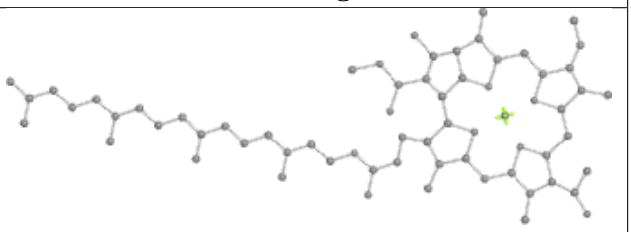
 Bond lengths	 Bond angles
 Torsions	 Rings

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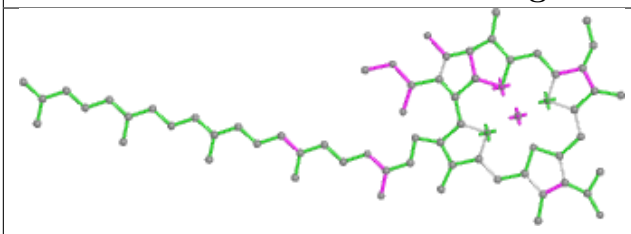
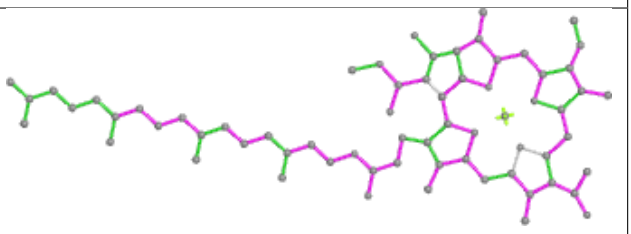
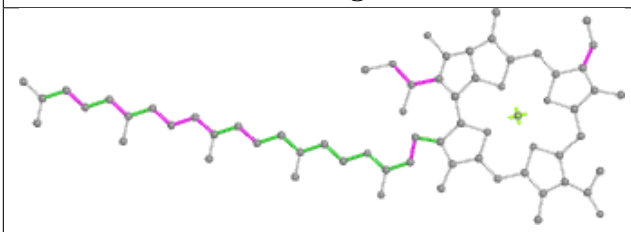
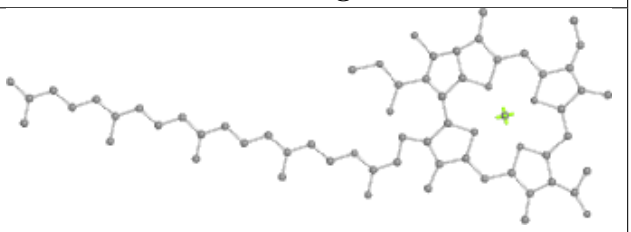
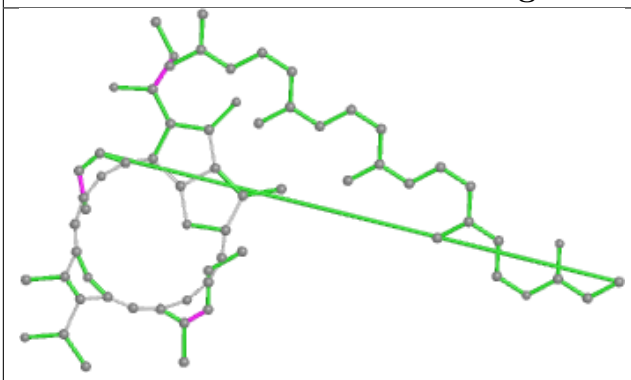
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPH M 402



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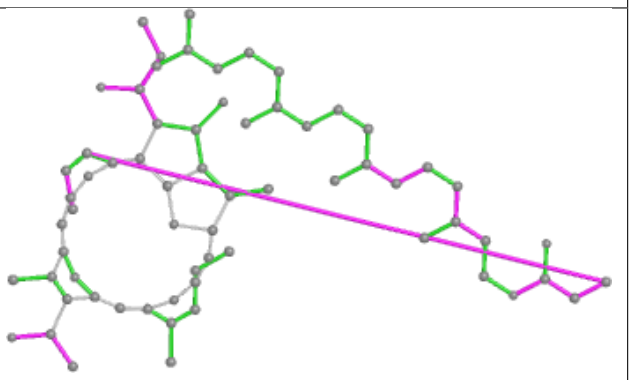
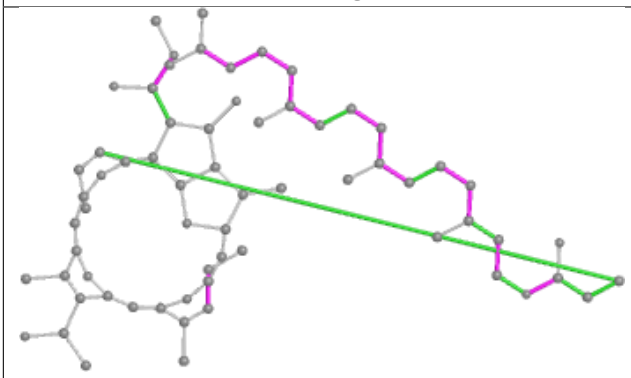


Bond angles



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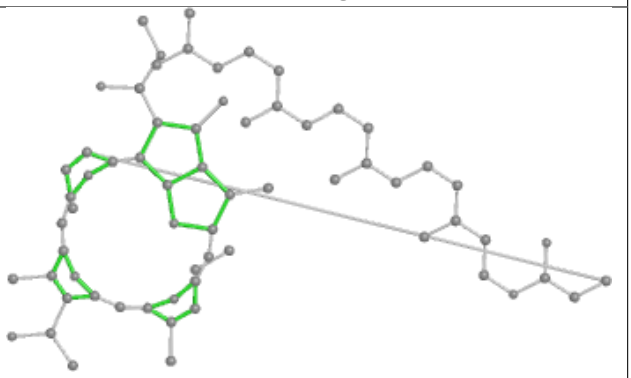
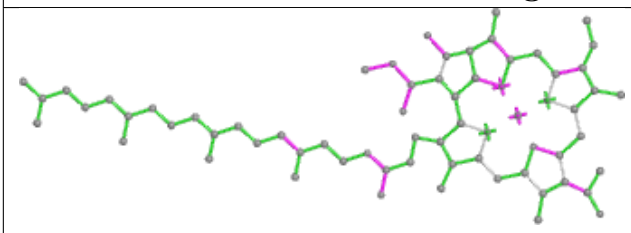


Rings

Ligand BCL m 102



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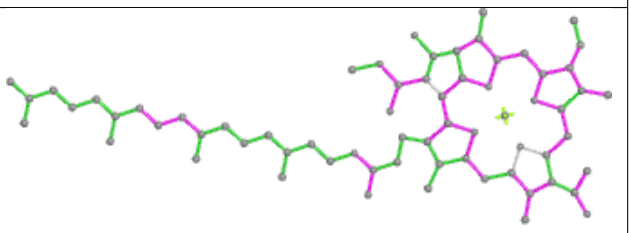

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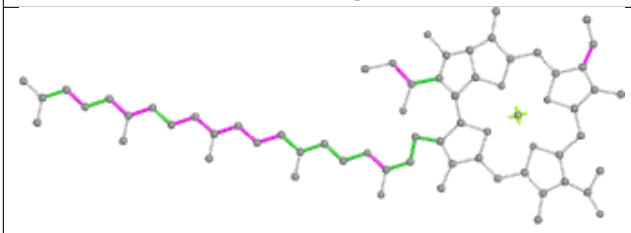

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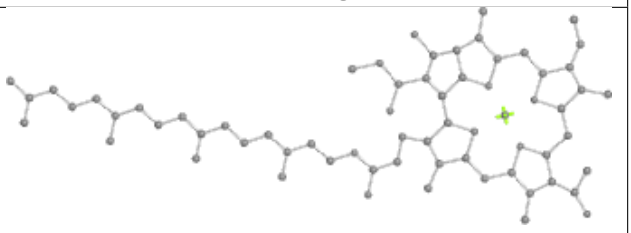
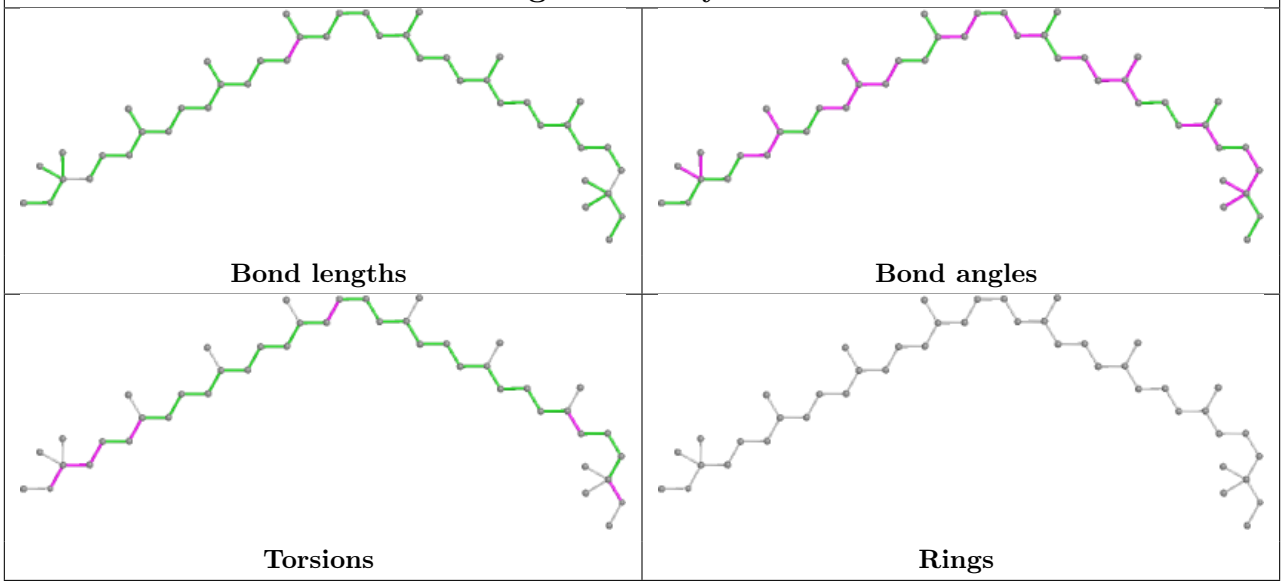
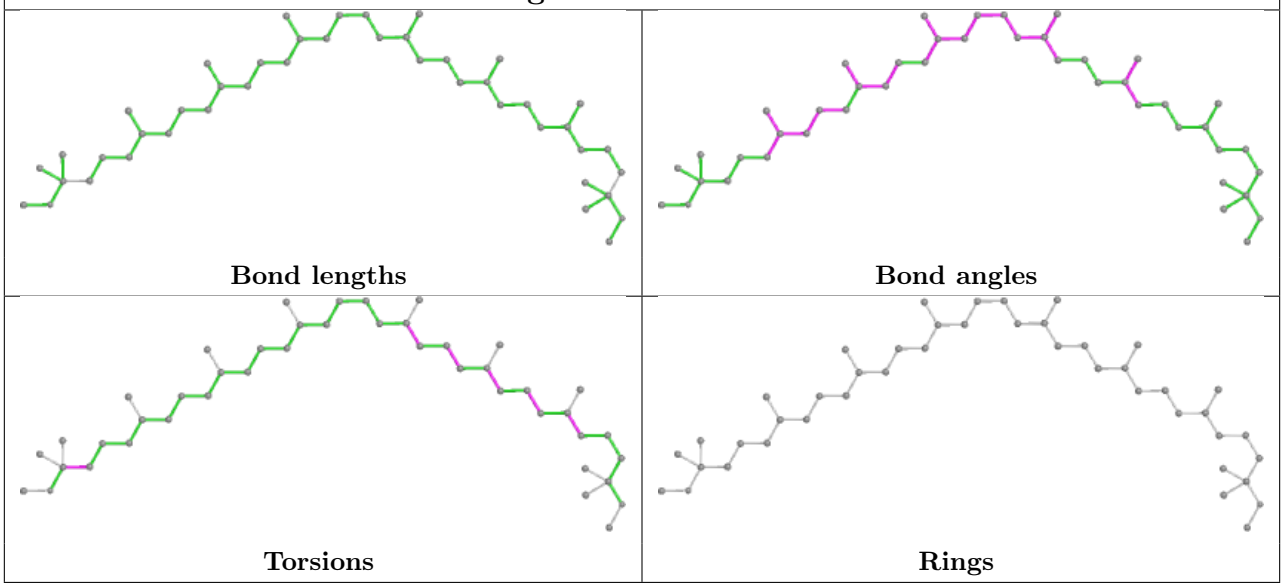


Rings

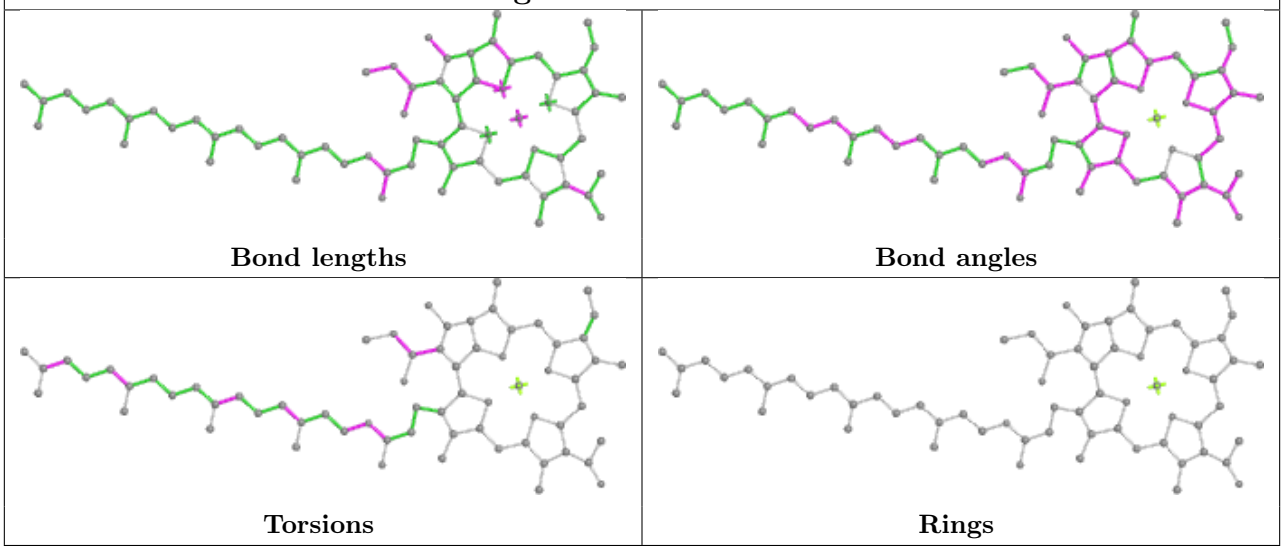
Ligand CRT y 404



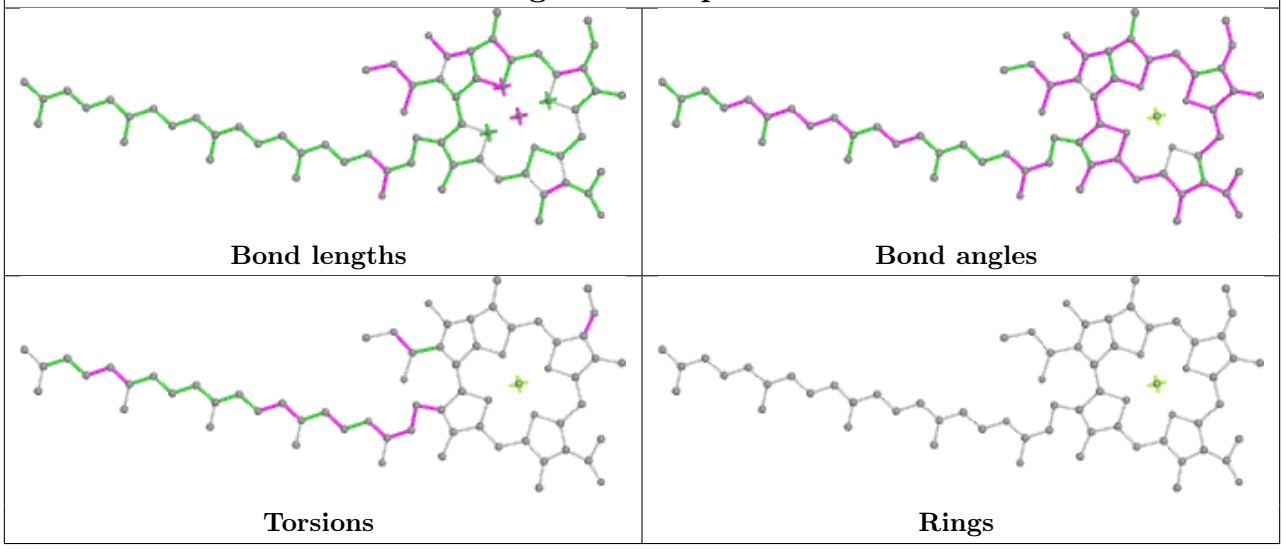
Ligand CRT Z 101



Ligand BCL AE 102



Ligand BCL p 104



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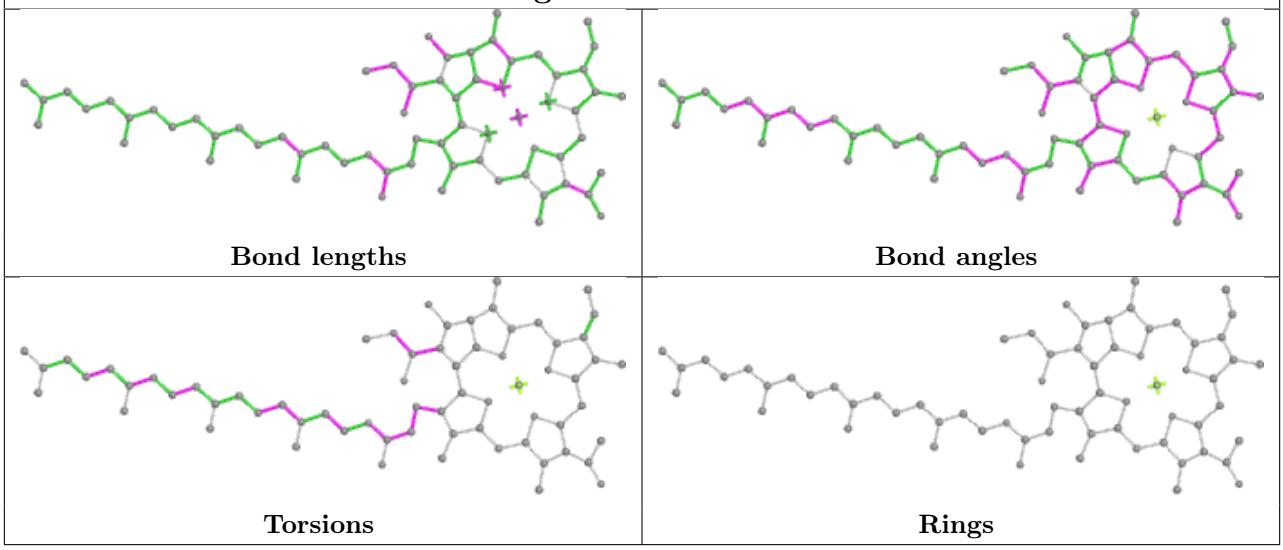

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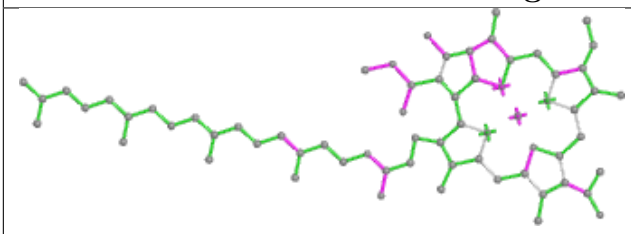
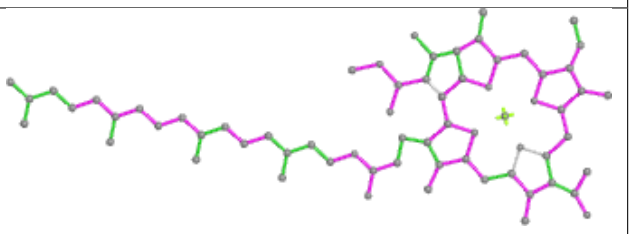
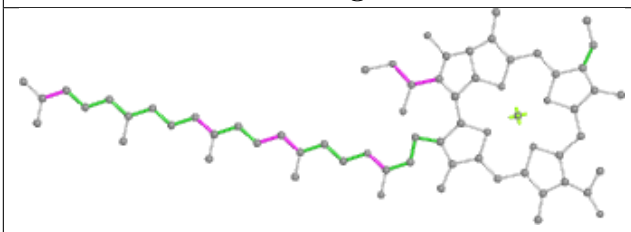
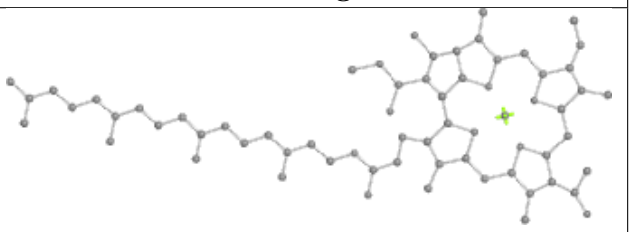
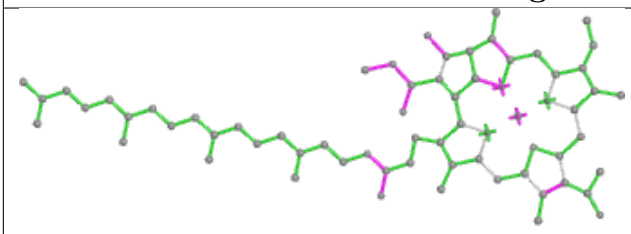
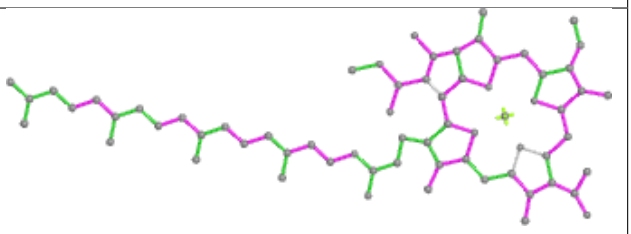
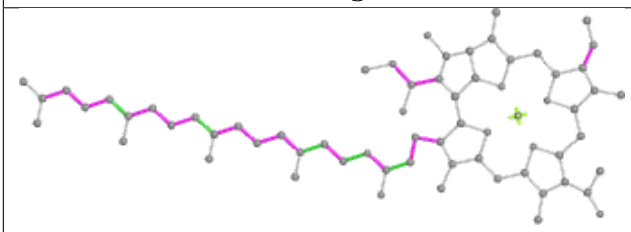
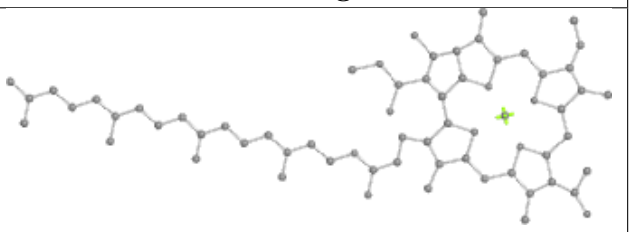
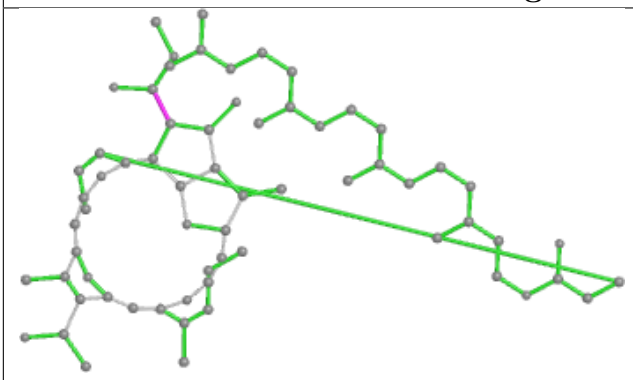
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 8 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPH L 302



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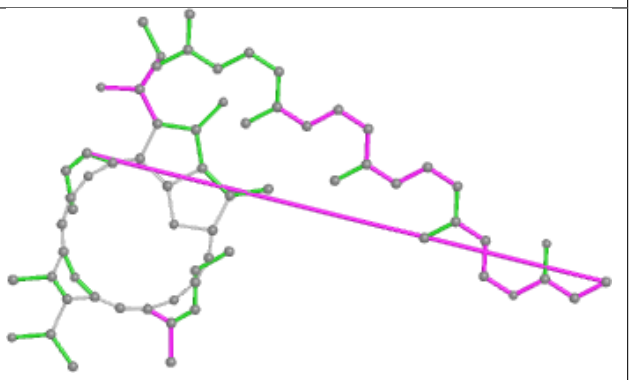
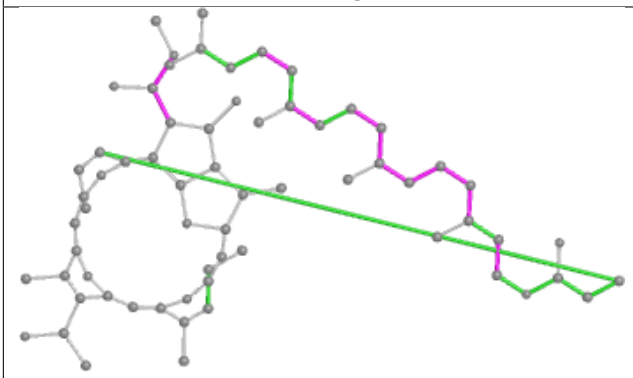


Bond angles



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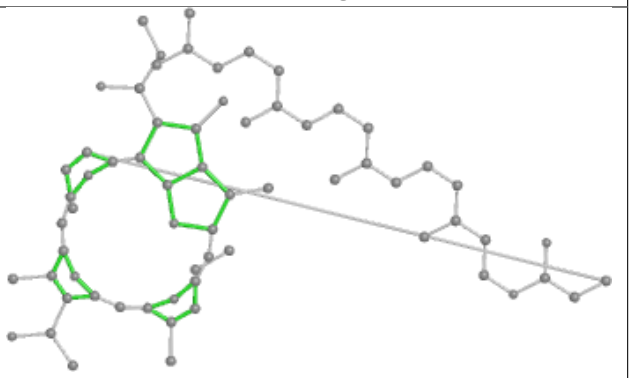
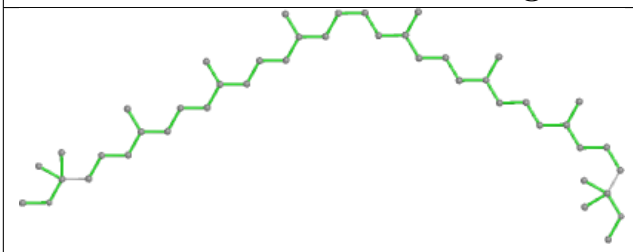


Rings

Ligand CRT G 101



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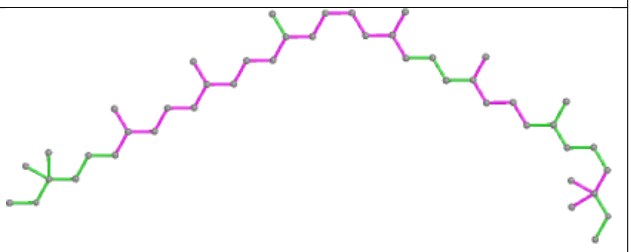

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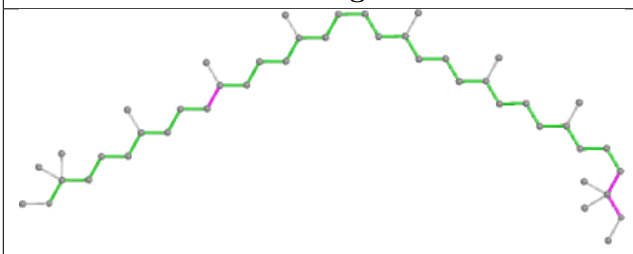

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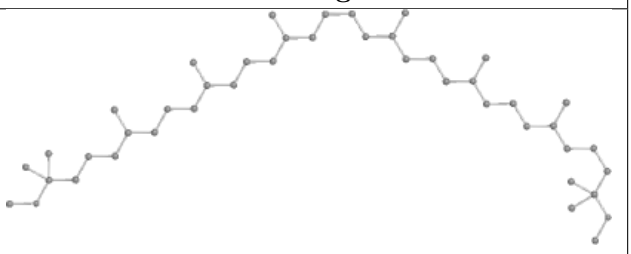
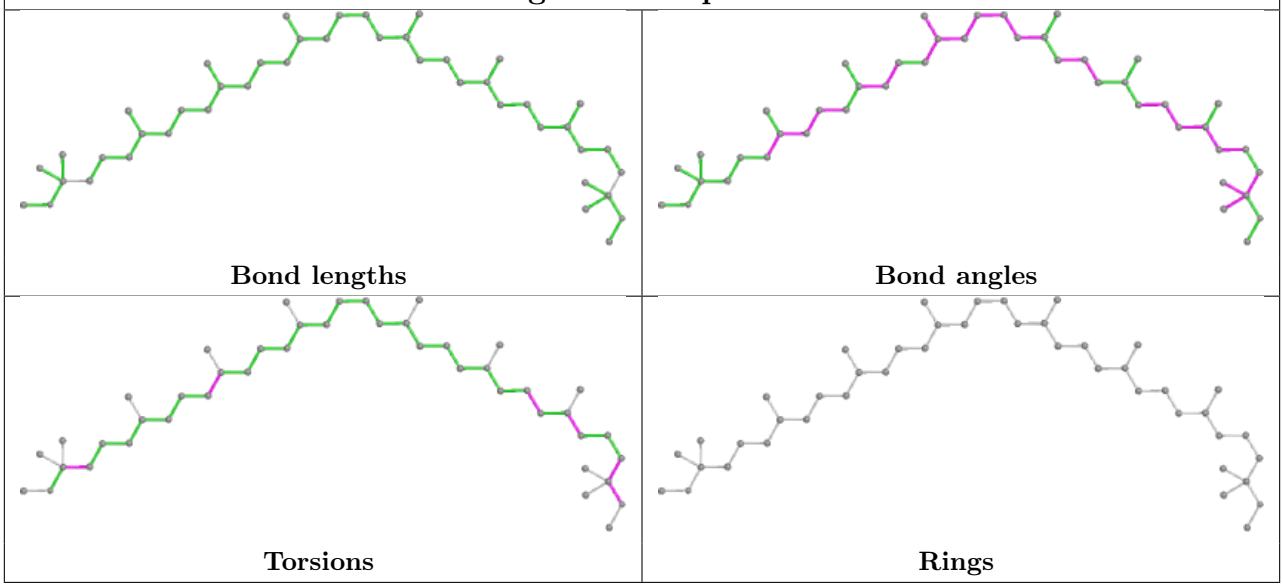
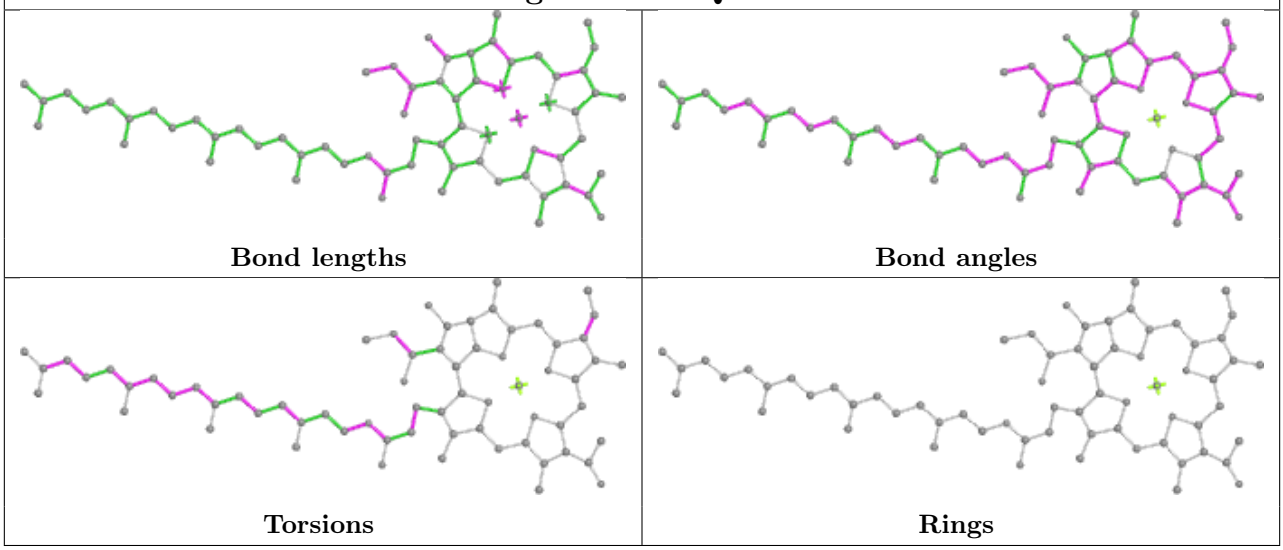


Rings

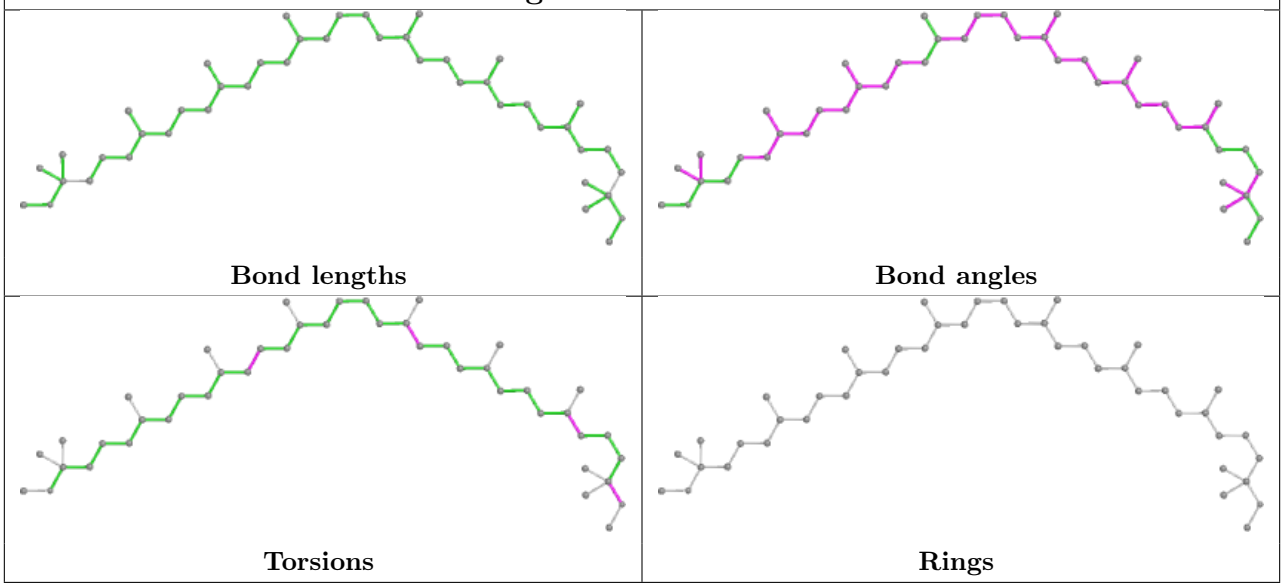
Ligand CRT p 103



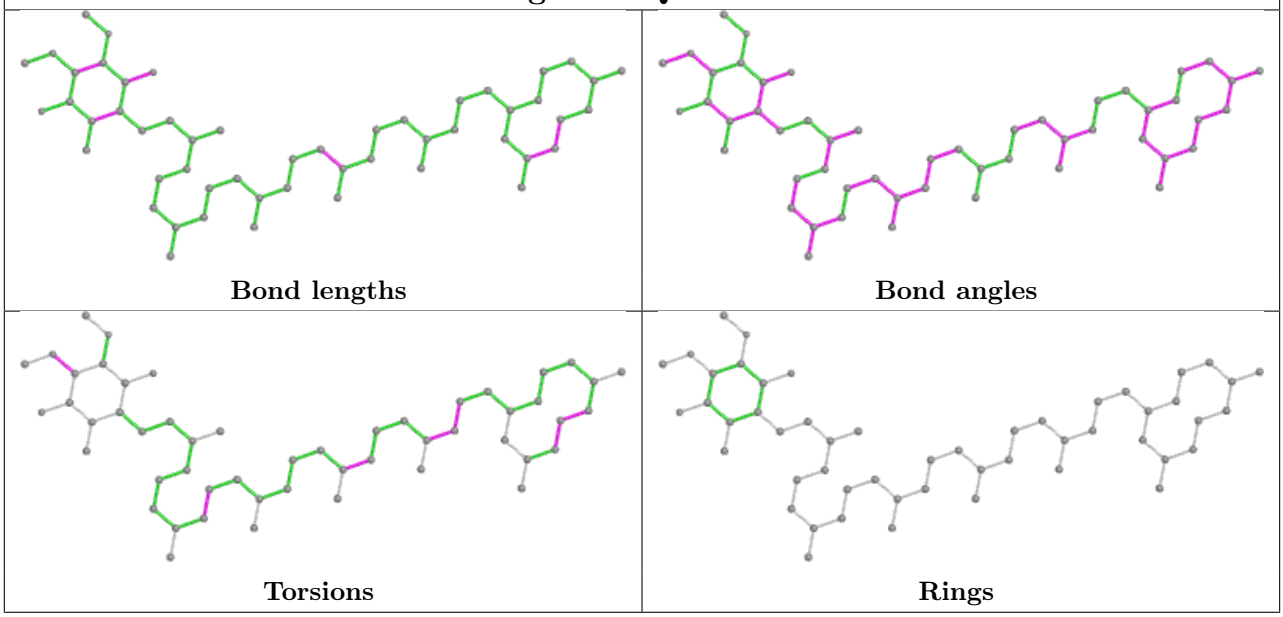
Ligand BCL Q 101



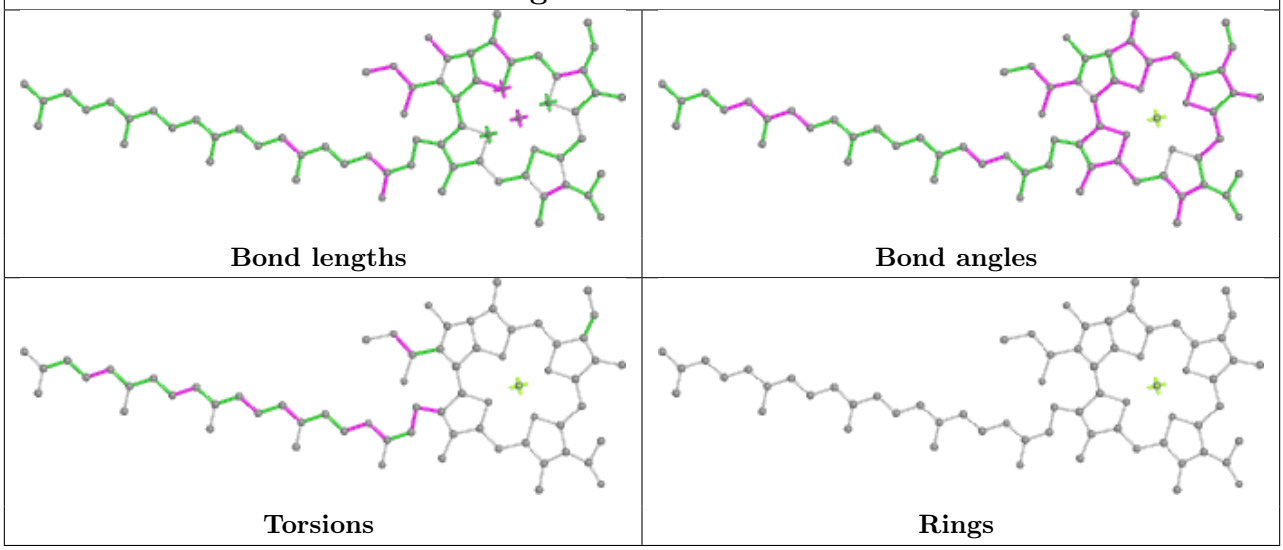
Ligand CRT T 101



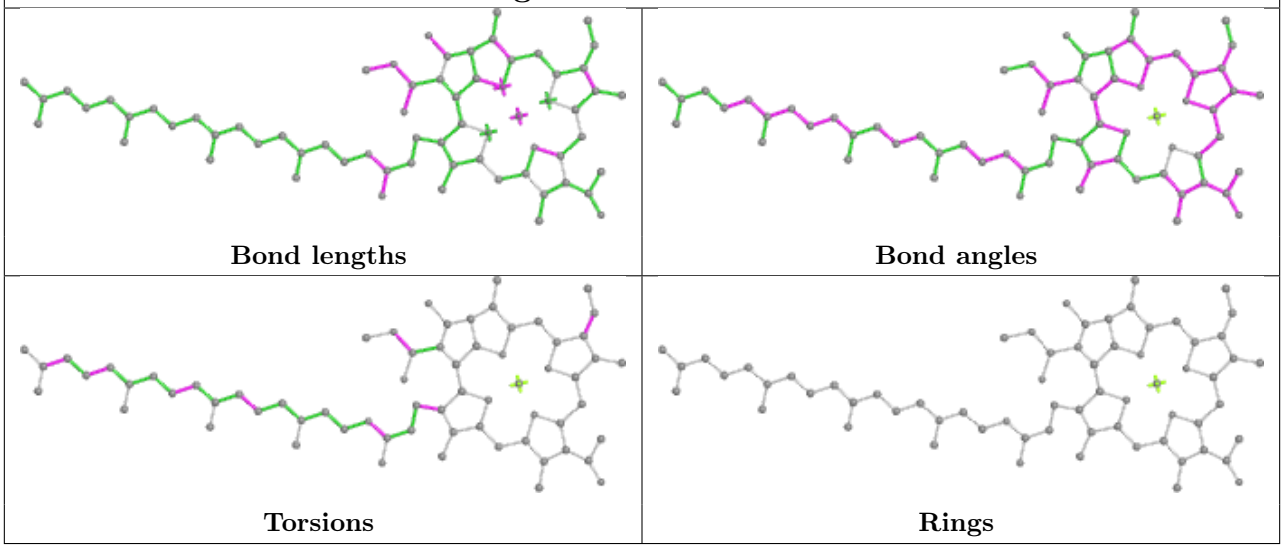
Ligand UQ8 L 304



Ligand BCL 1 102



Ligand BCL AE 104



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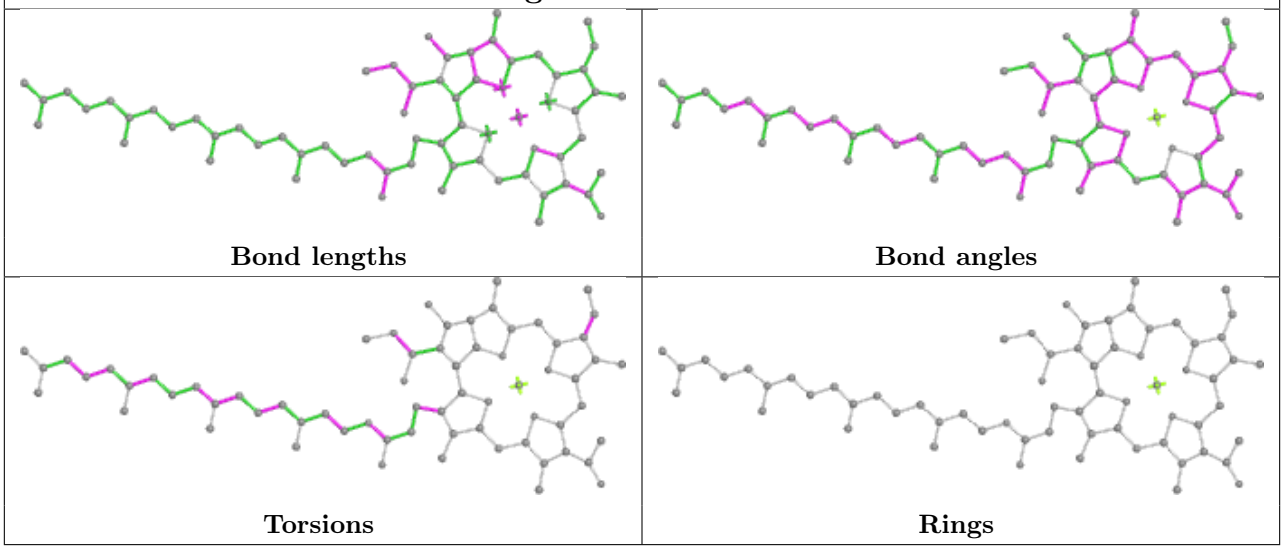
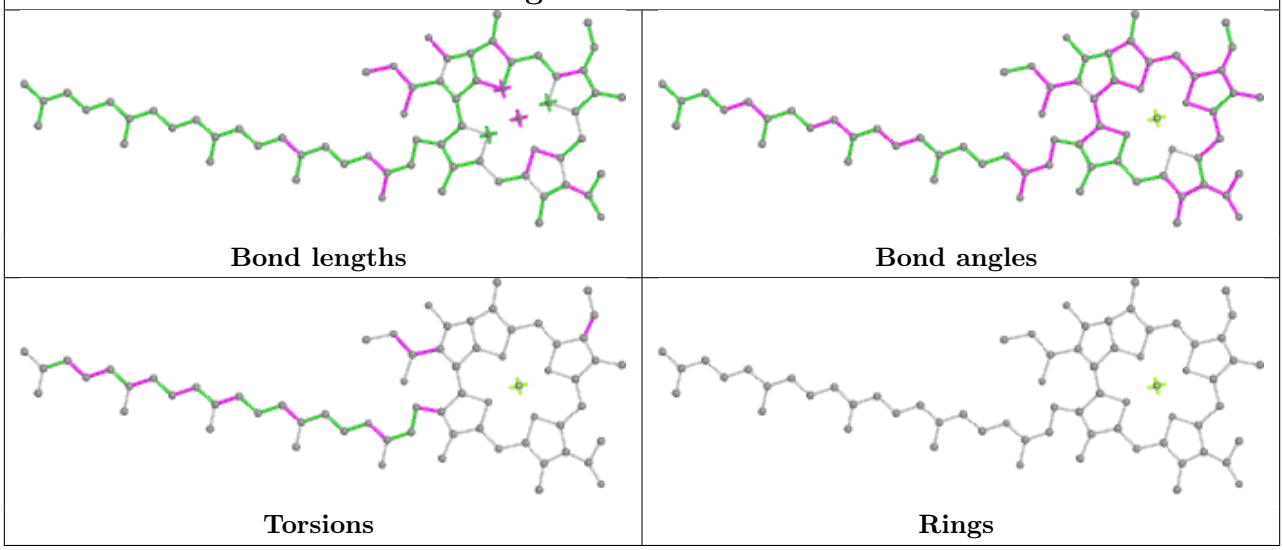


Ligand BCL V 101



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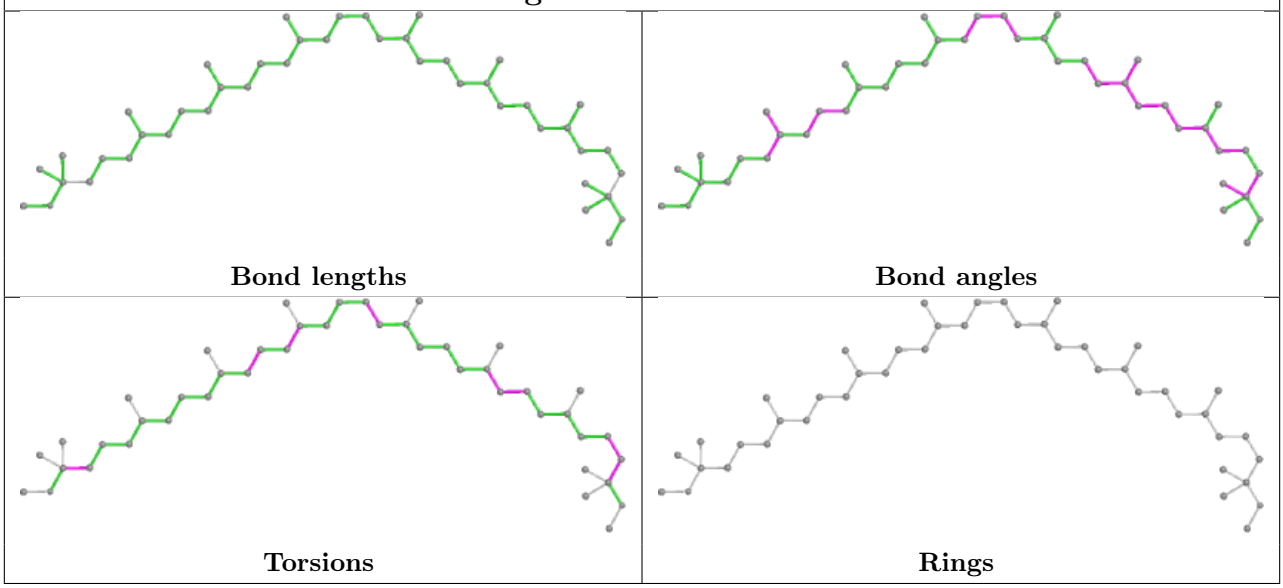
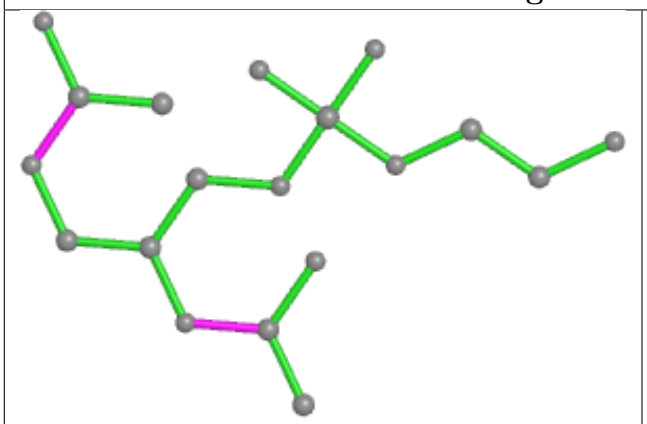
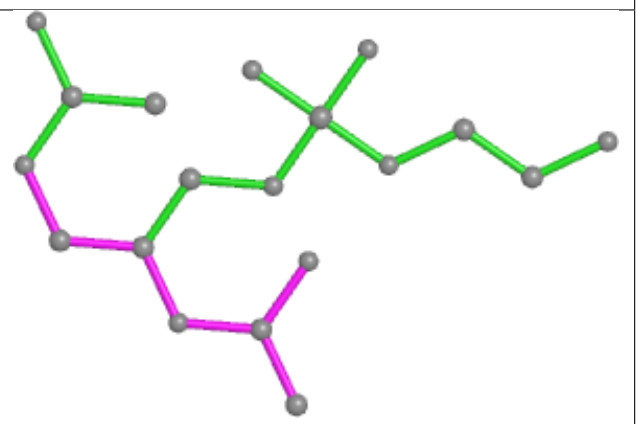


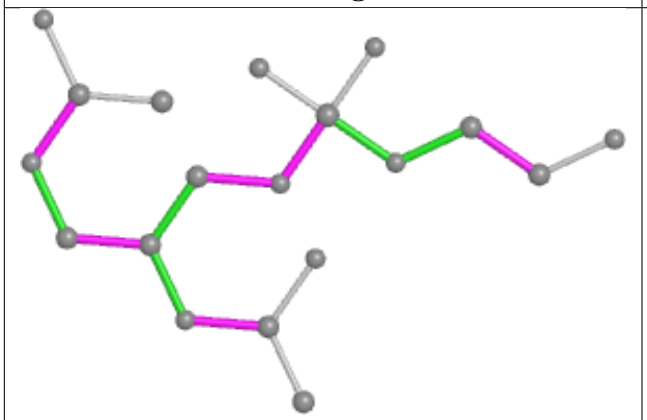
Ligand PEF H 304



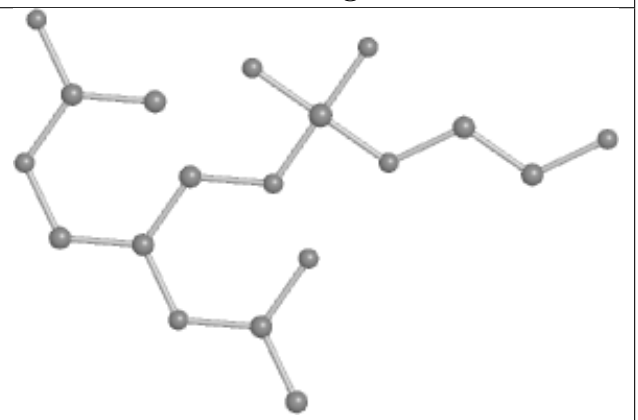
Bond lengths



Bond angles

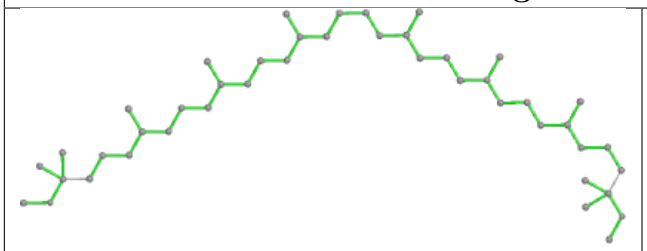


Torsions



Rings

Ligand CRT AE 103



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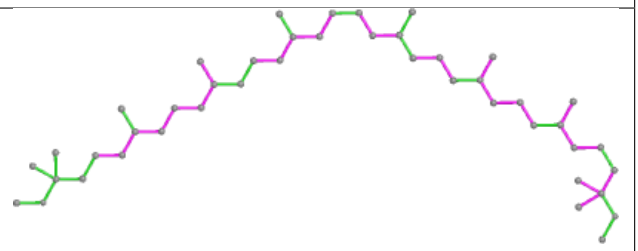
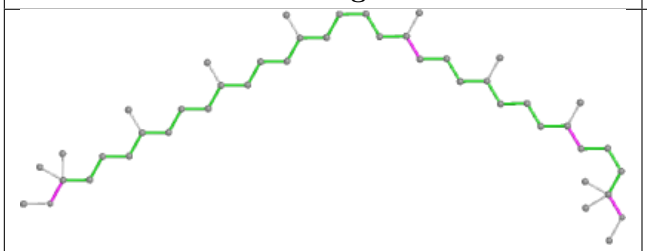
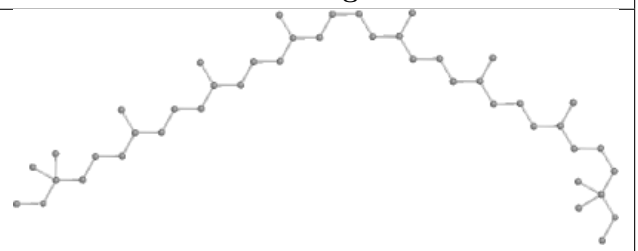


Bond angles

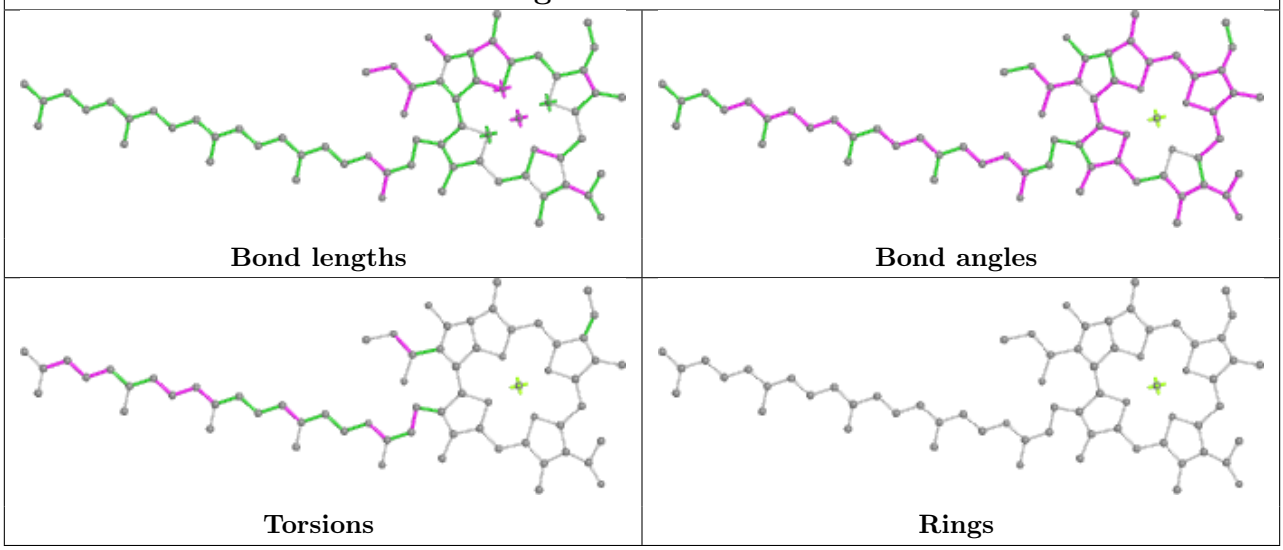


Torsions

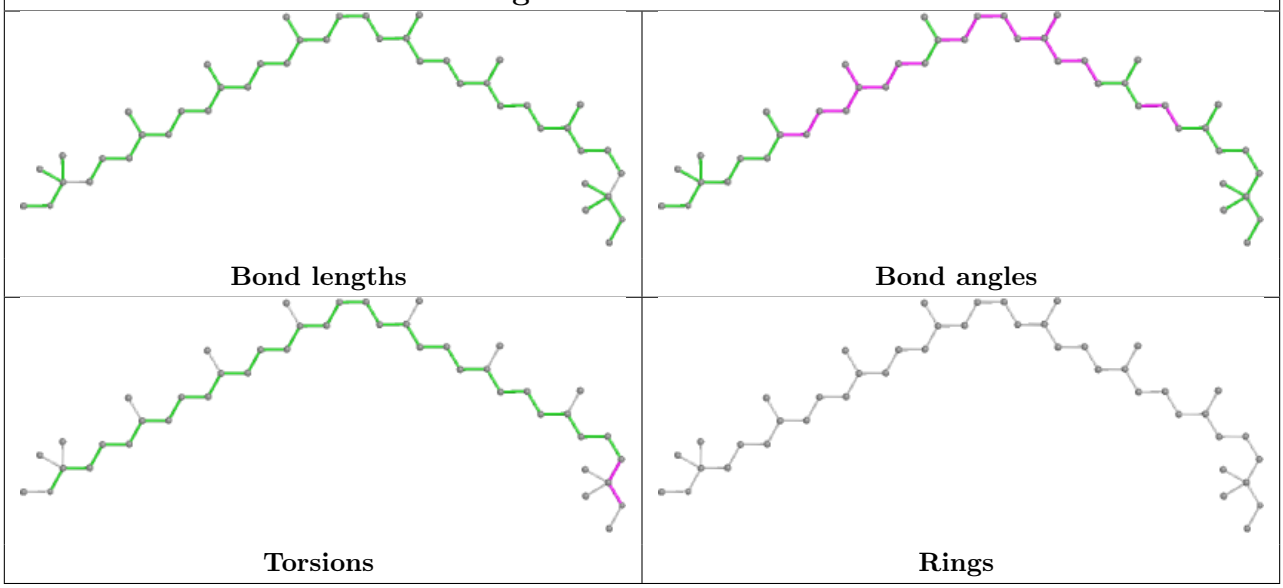


Rings

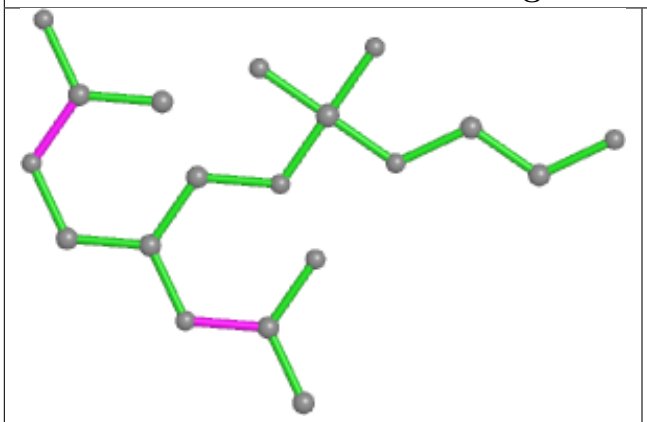
Ligand BCL l 101



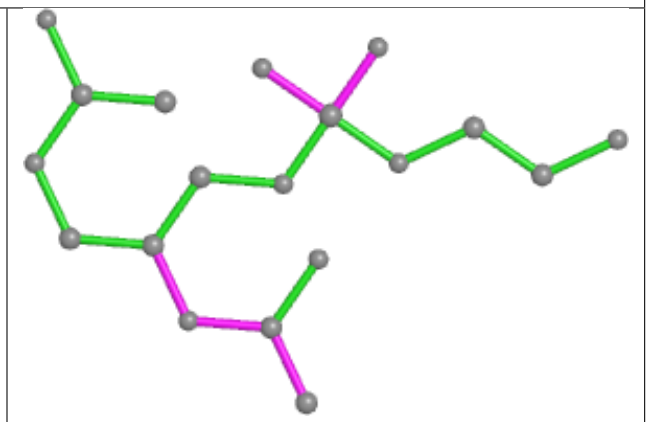
Ligand CRT AC 101



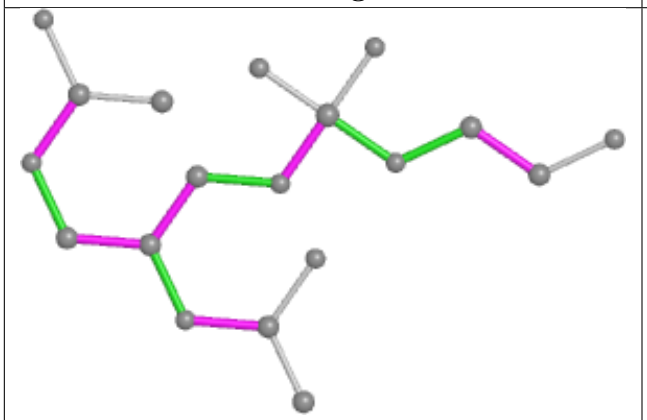
Ligand PEF M 408



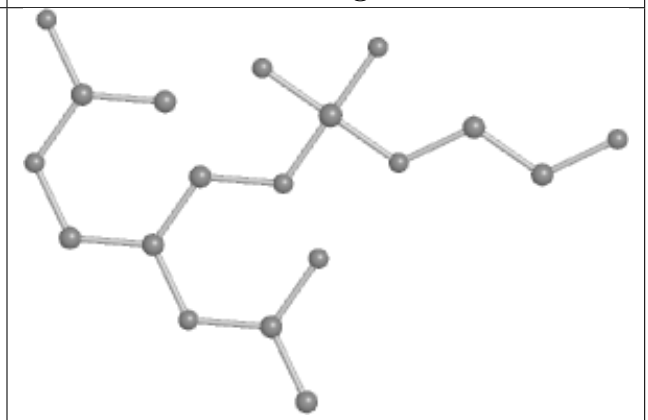
Bond lengths



Bond angles

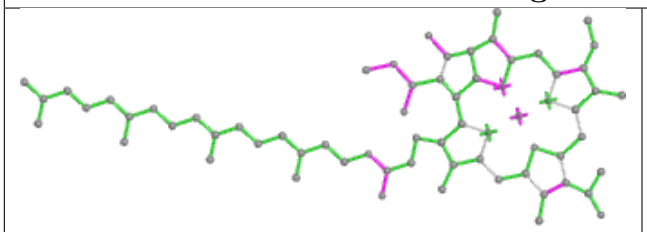


Torsions

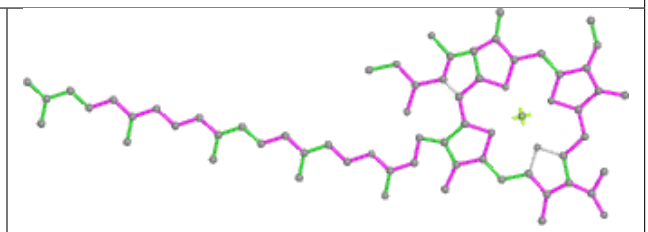


Rings

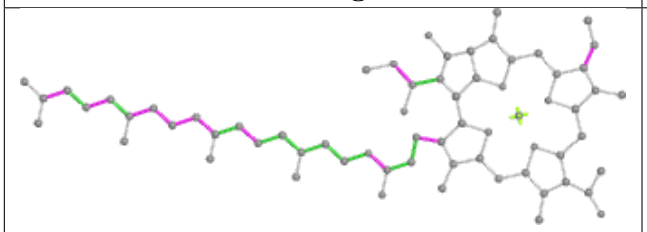
Ligand BCL 7 101



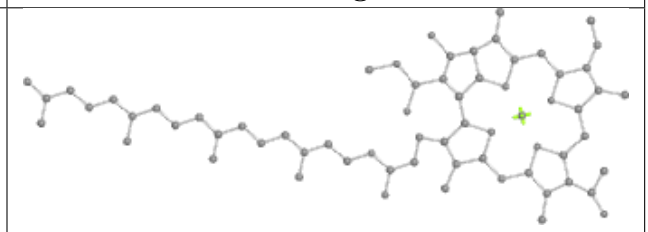
Bond lengths



Bond angles

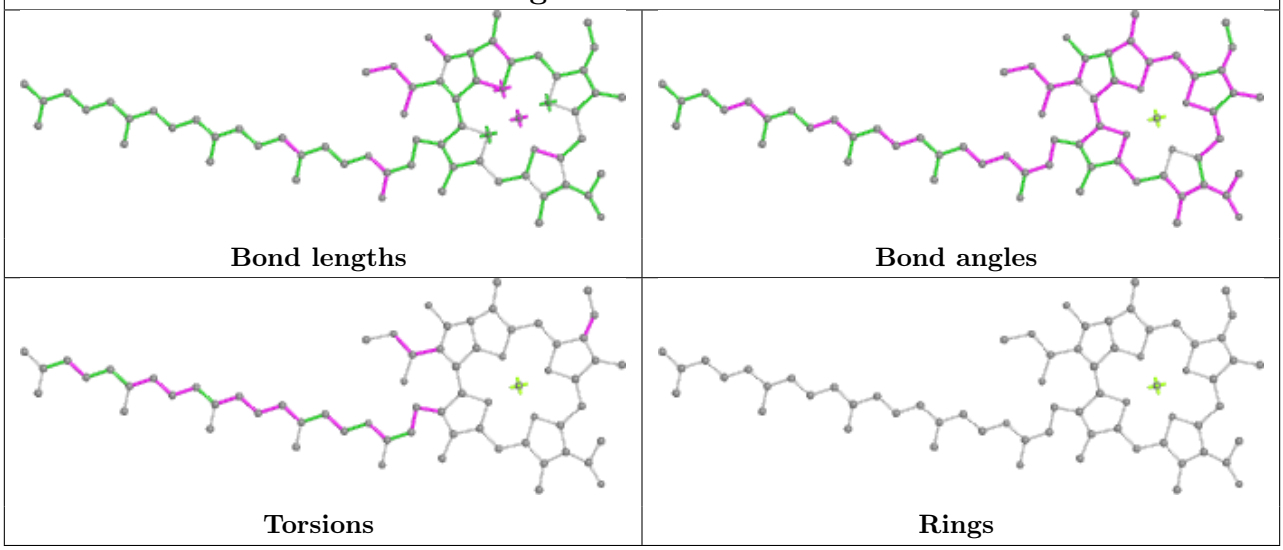


Torsions

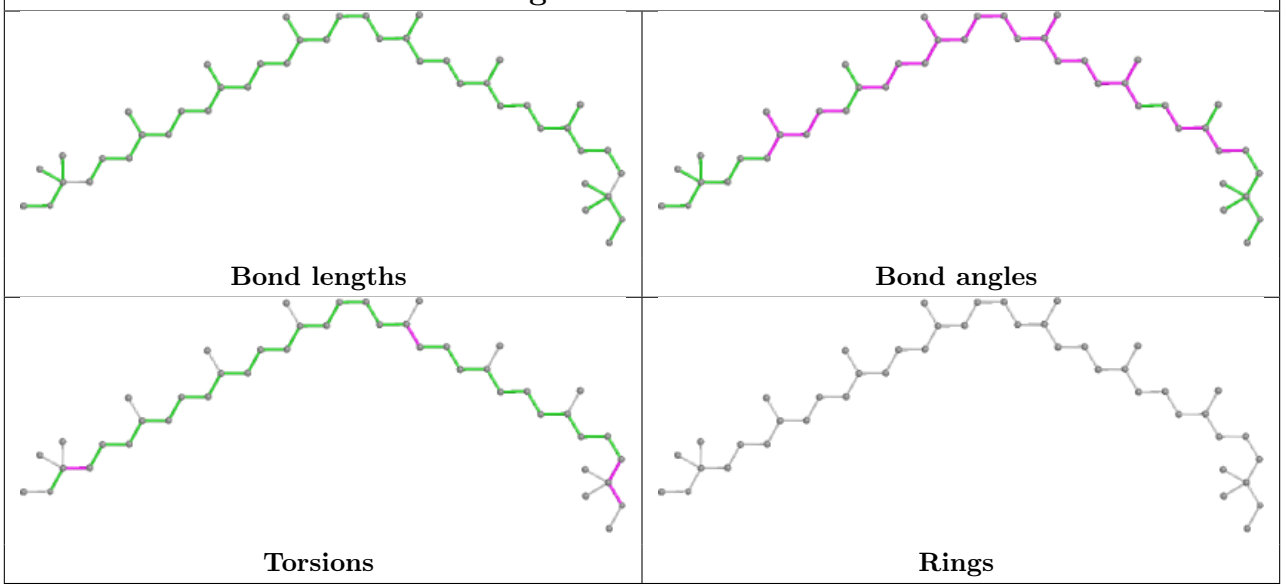


Rings

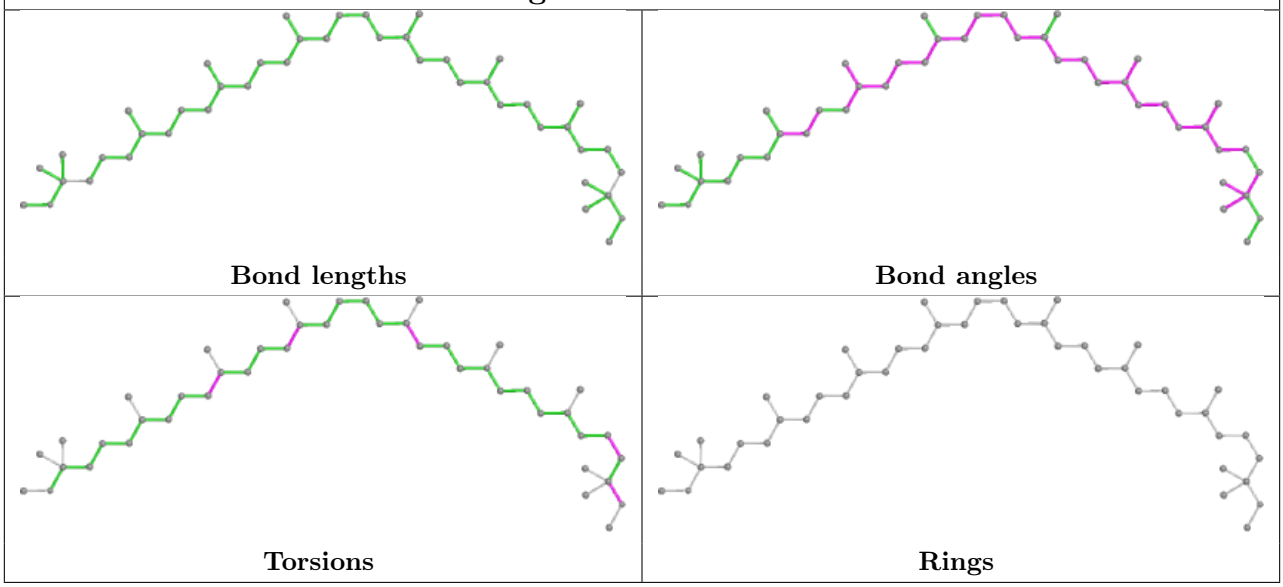
Ligand BCL k 102



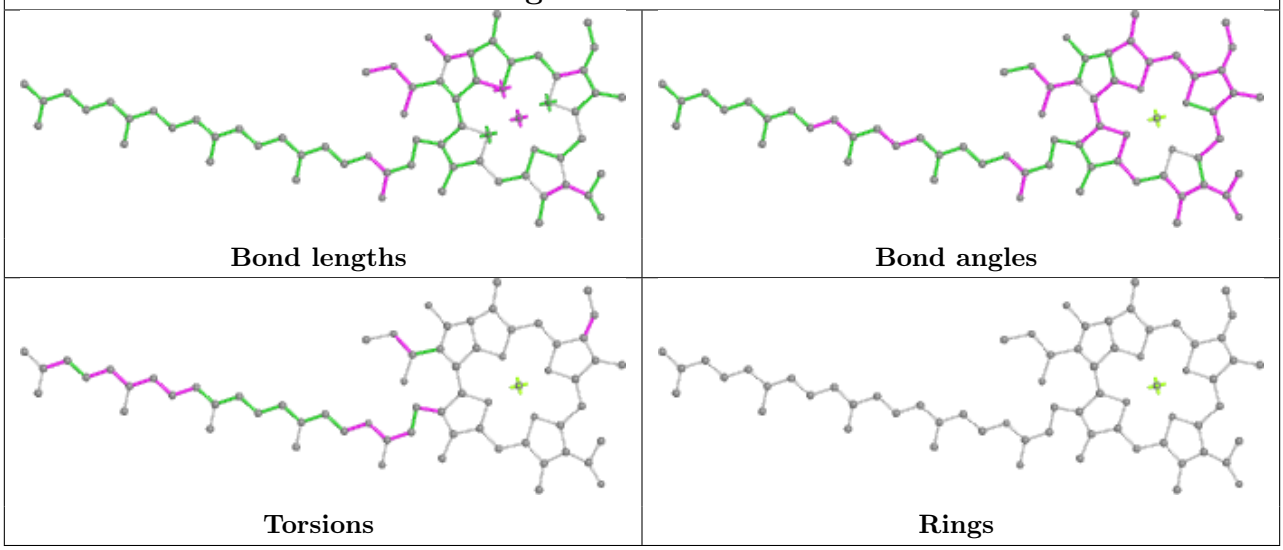
Ligand CRT 2 101



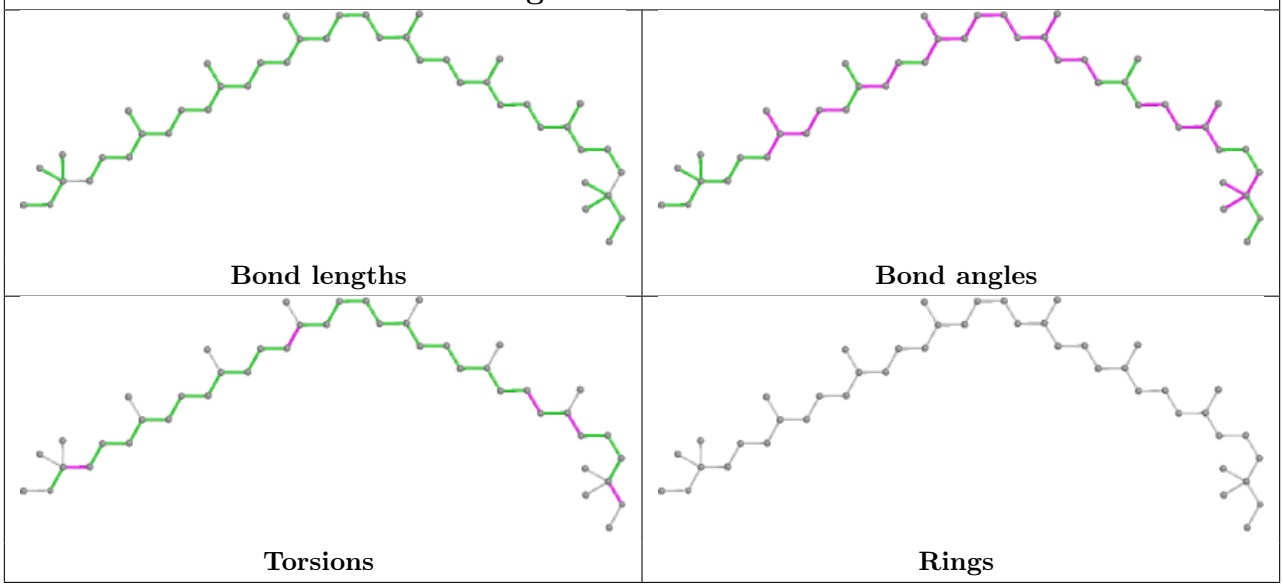
Ligand CRT v 101



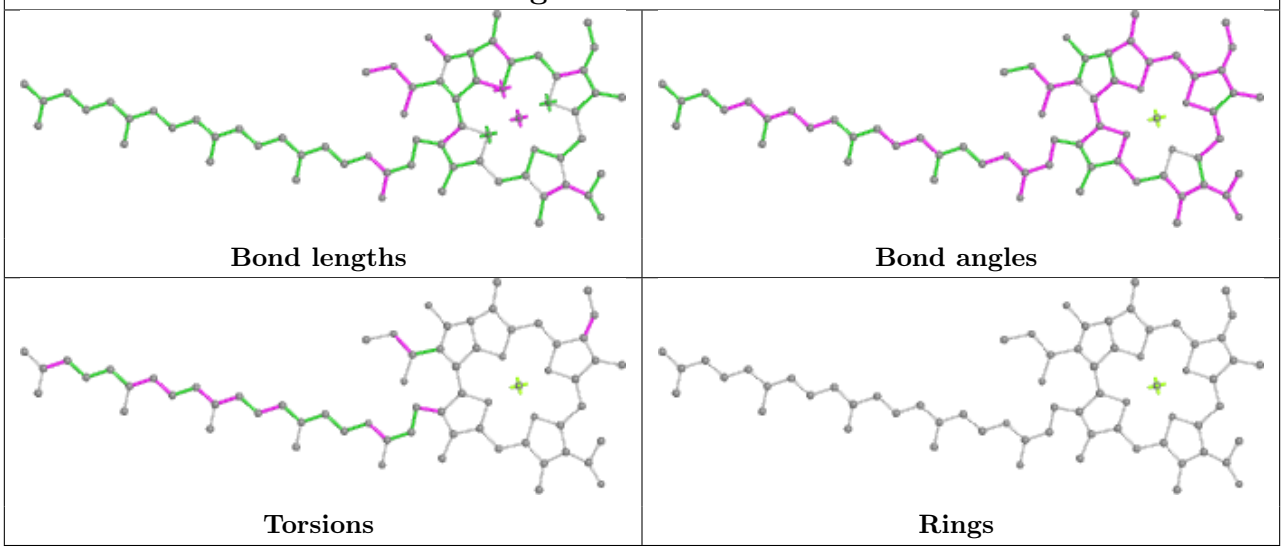
Ligand BCL Y 101



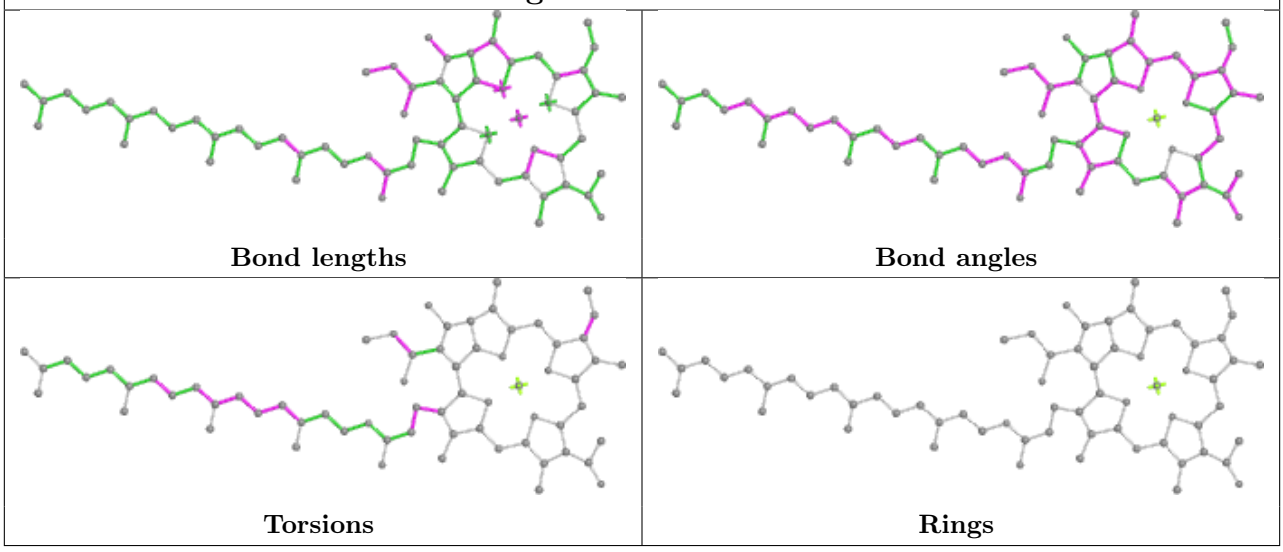
Ligand CRT E 101



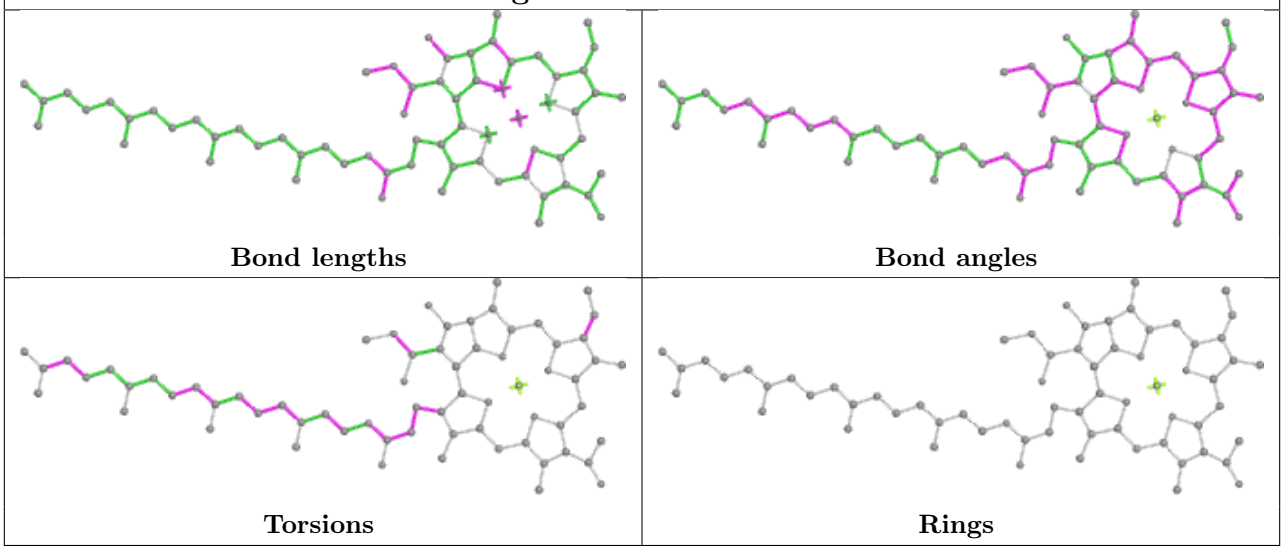
Ligand BCL 5 102



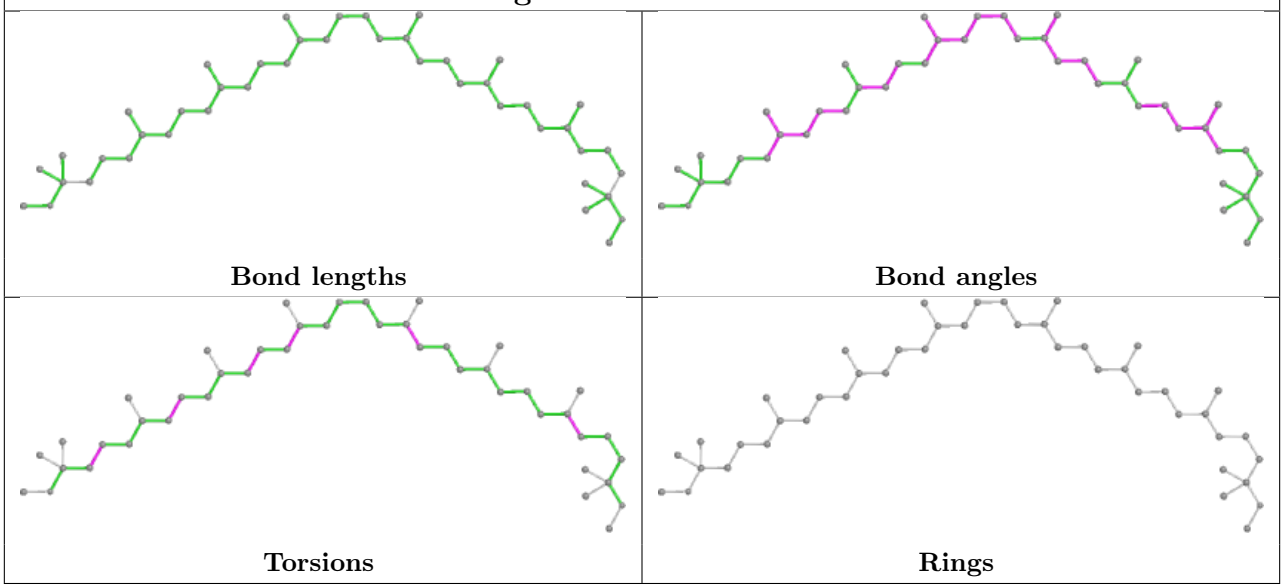
Ligand BCL w 101



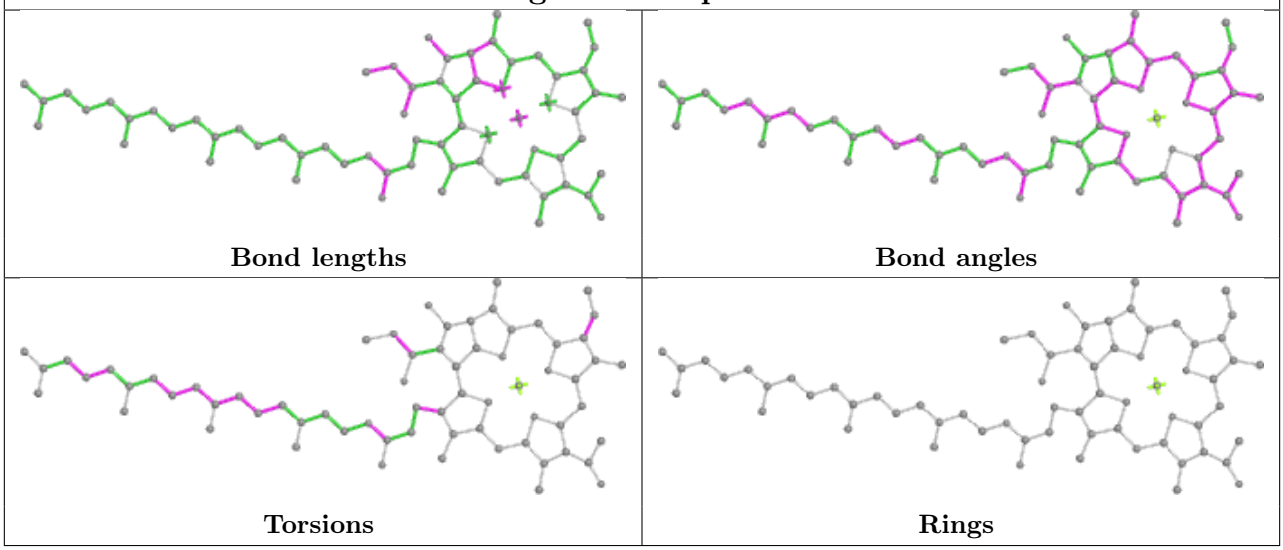
Ligand BCL AD 101



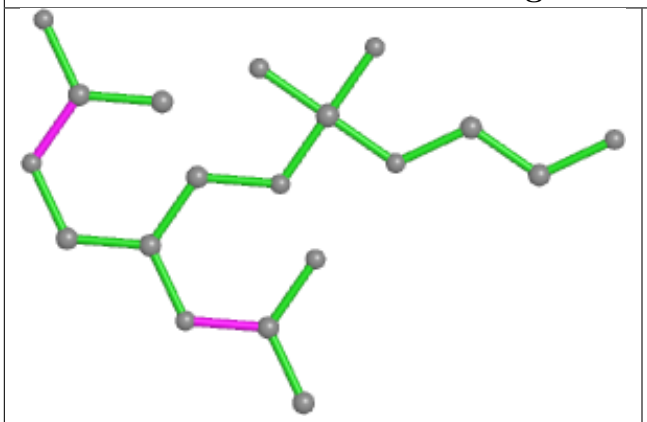
Ligand CRT AL 101



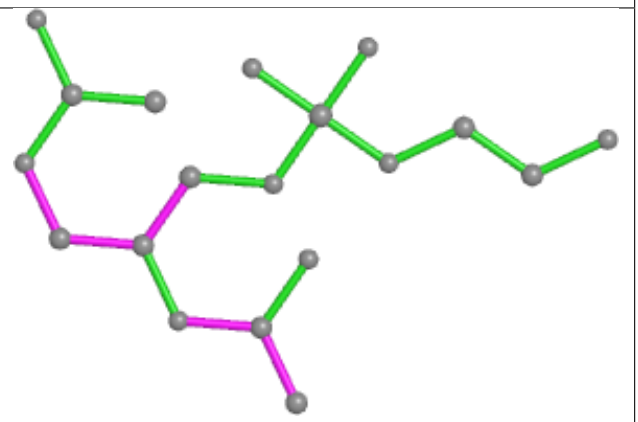
Ligand BCL p 102



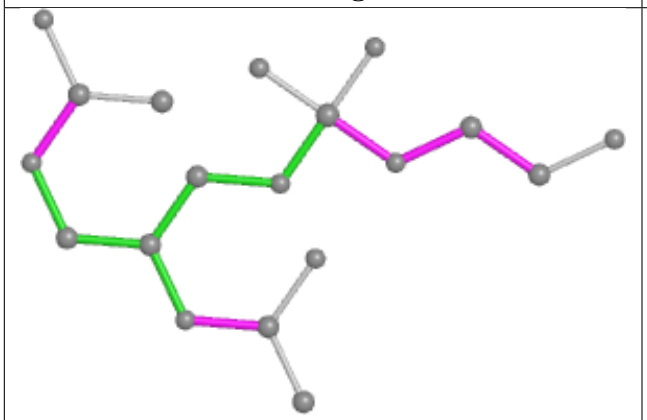
Ligand PEF m 101



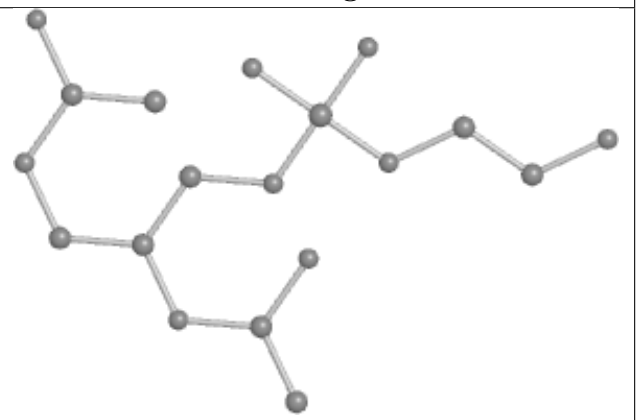
Bond lengths



Bond angles

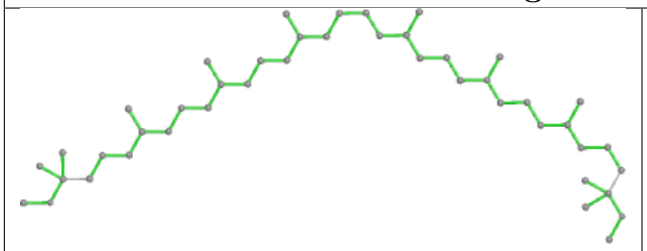


Torsions

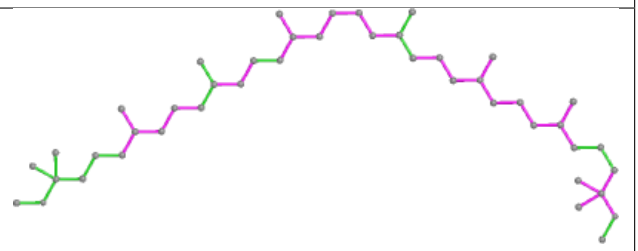


Rings

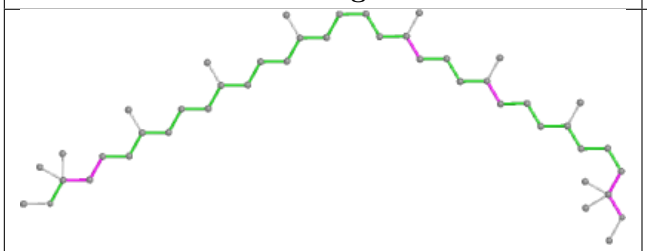
Ligand CRT U 102



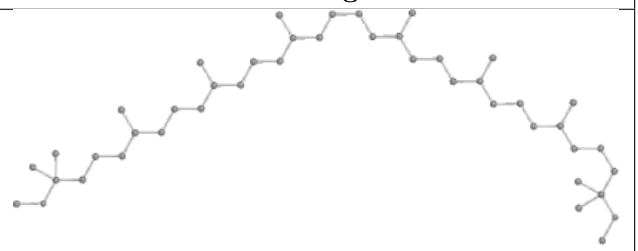
Bond lengths



Bond angles

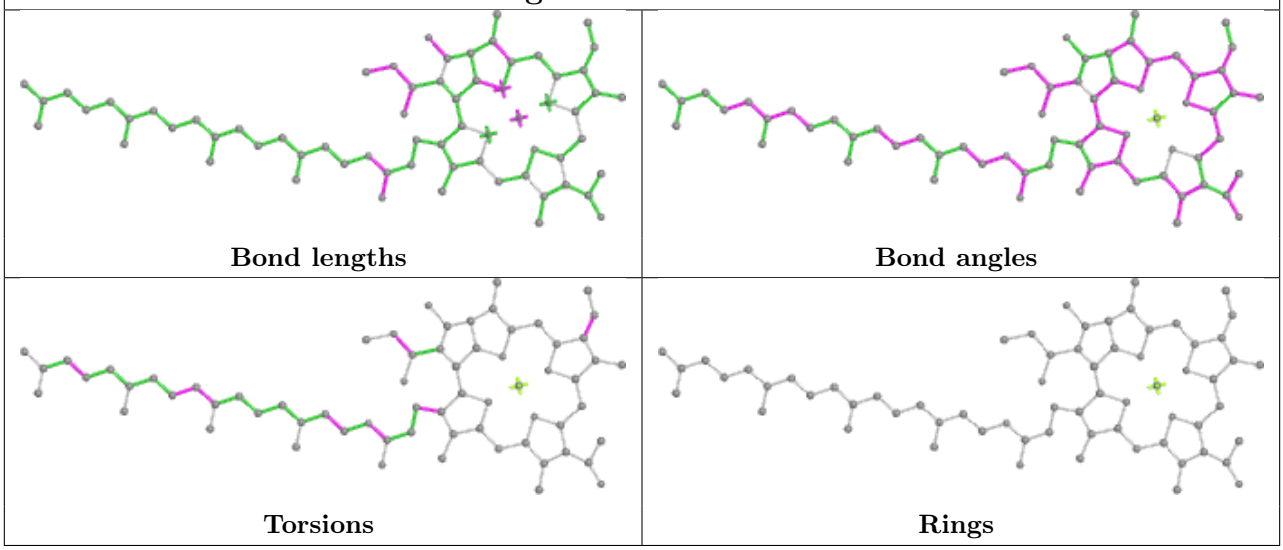


Torsions

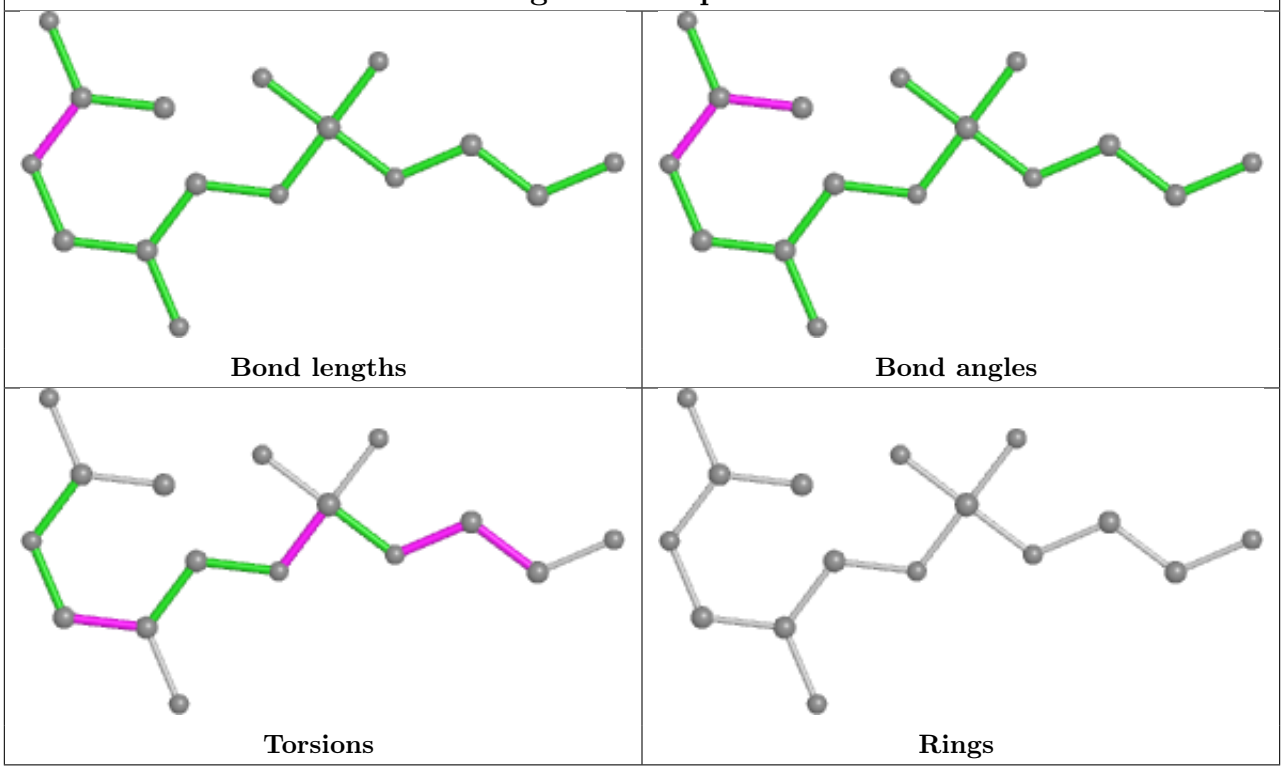


Rings

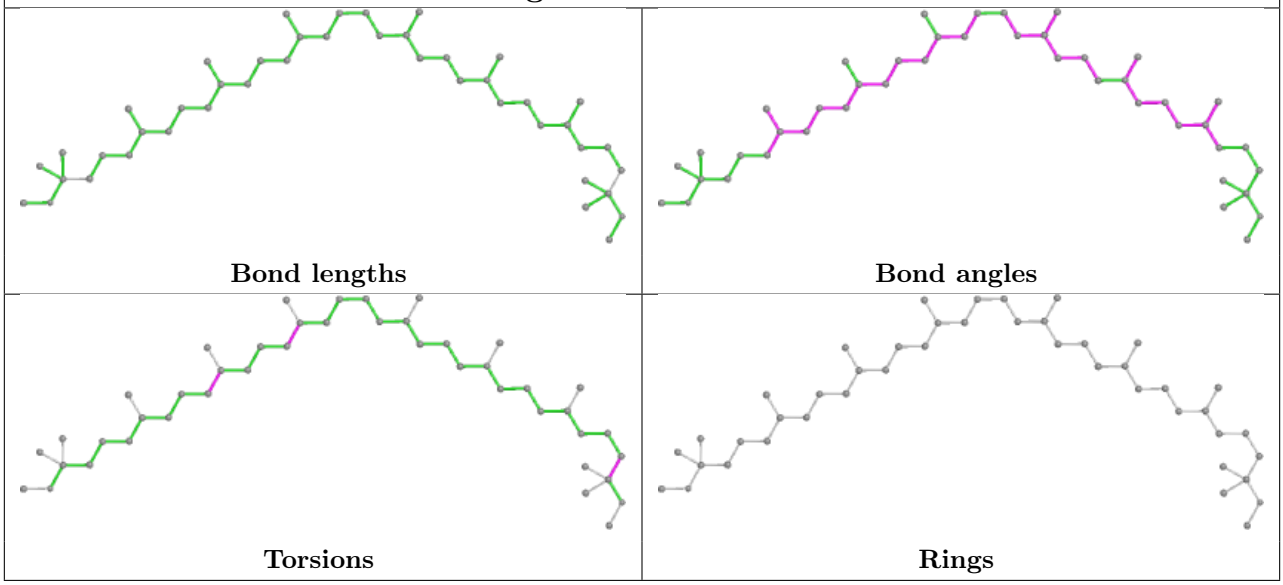
Ligand BCL A 102



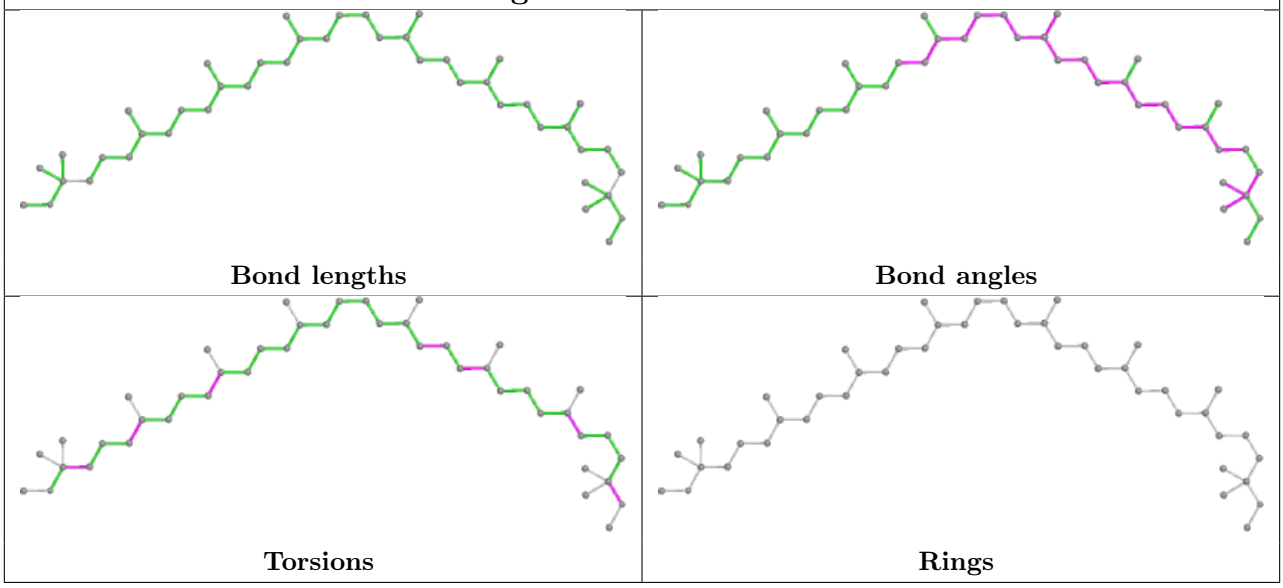
Ligand PEF p 101



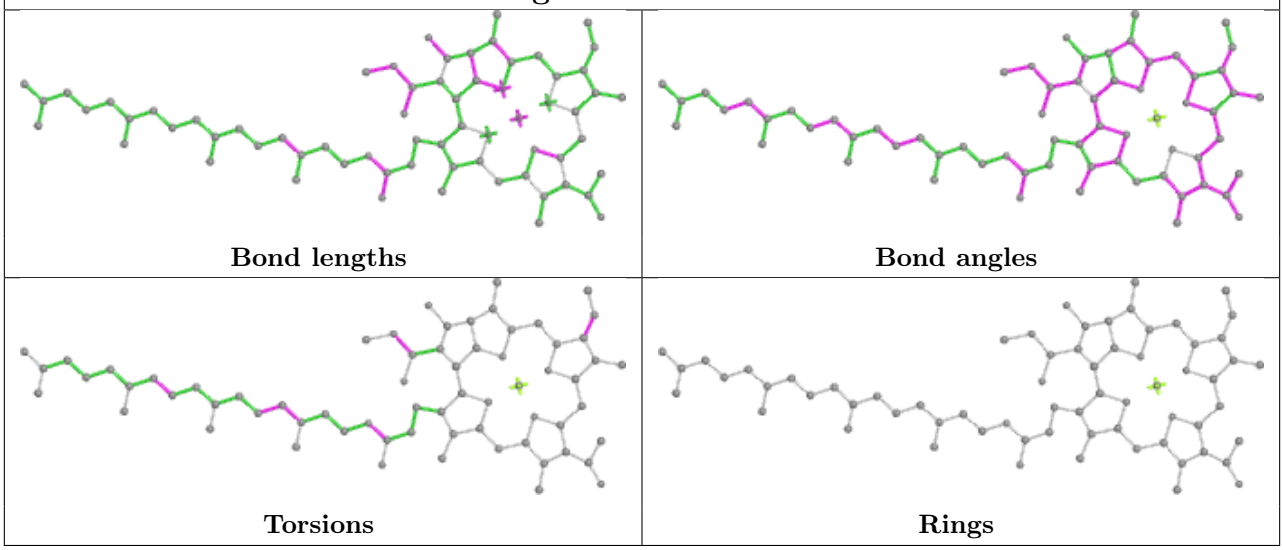
Ligand CRT P 102



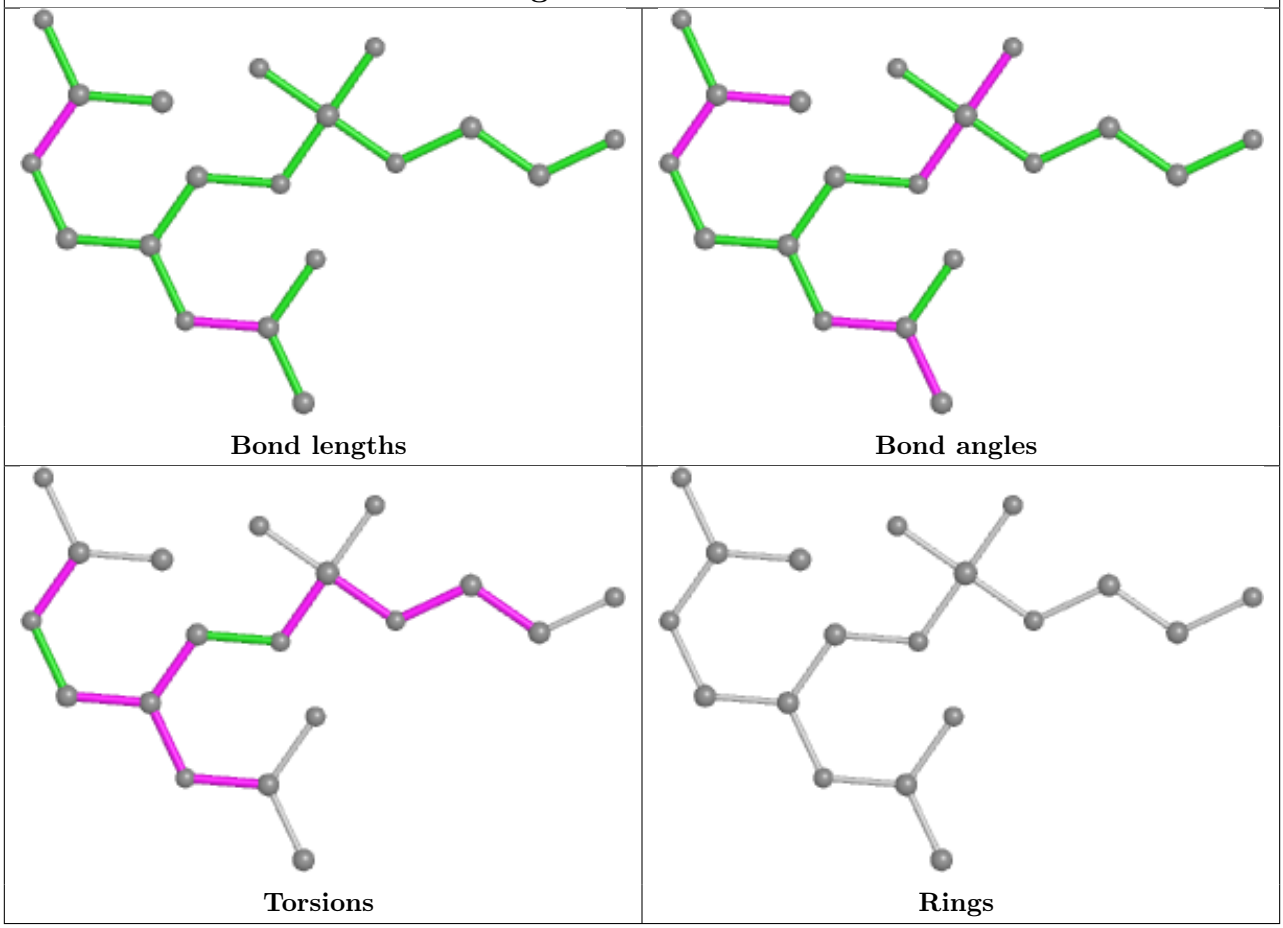
Ligand CRT AD 102



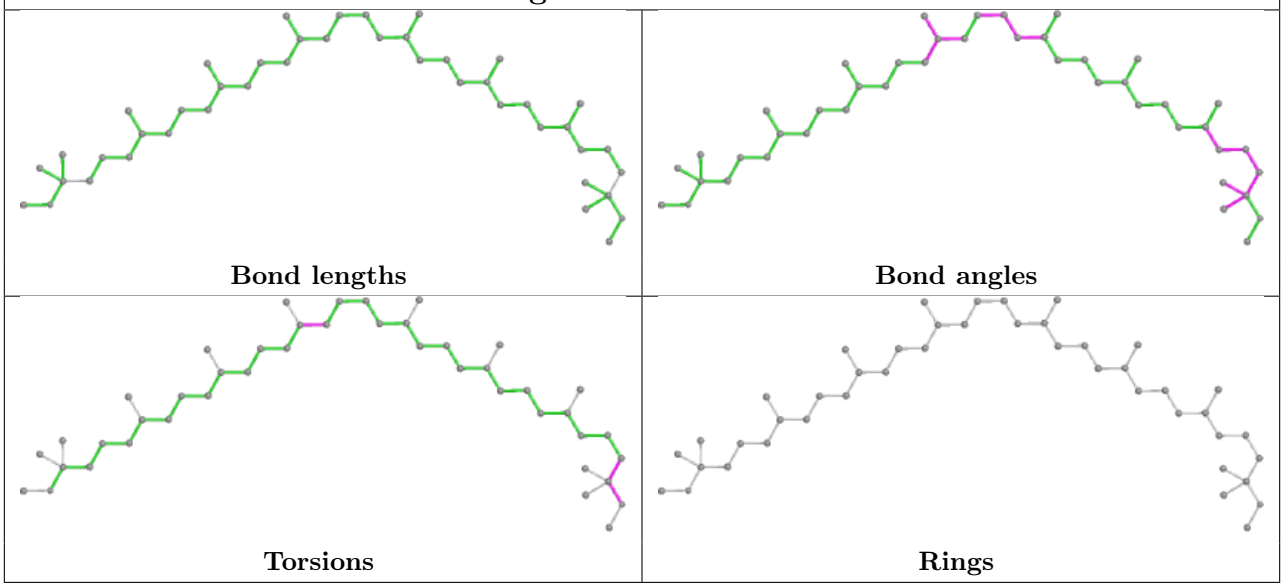
Ligand BCL I 101



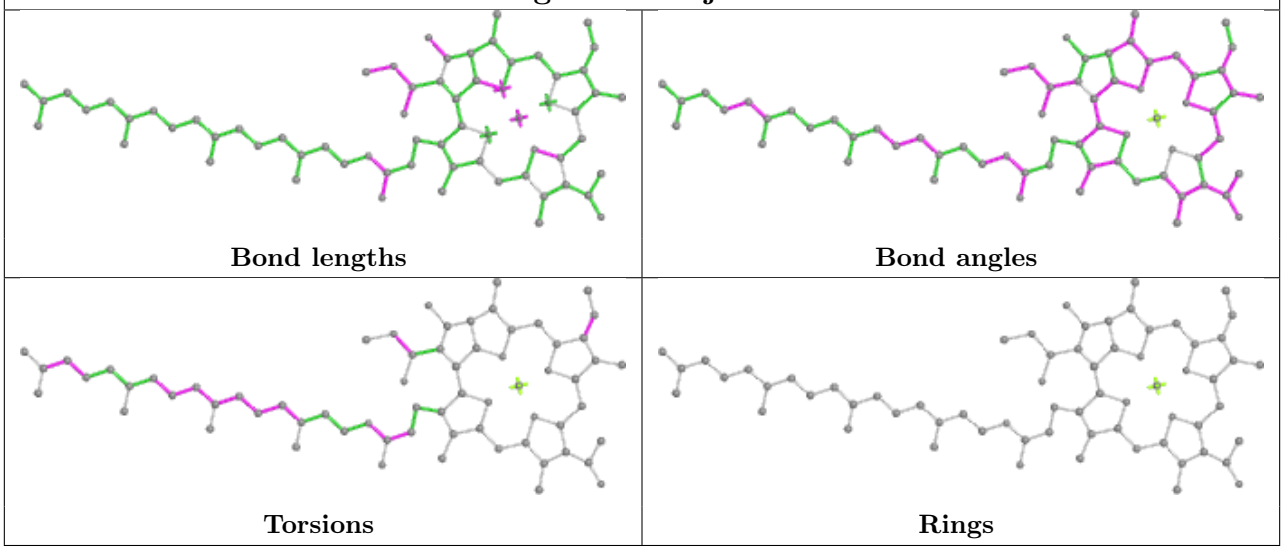
Ligand PEF x 306



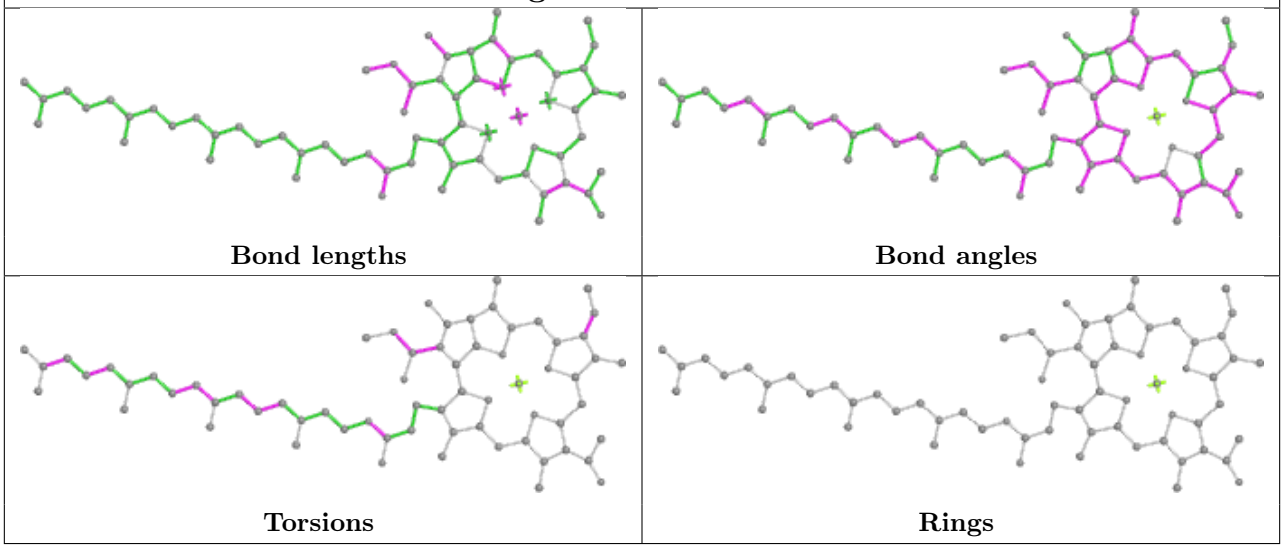
Ligand CRT 8 101



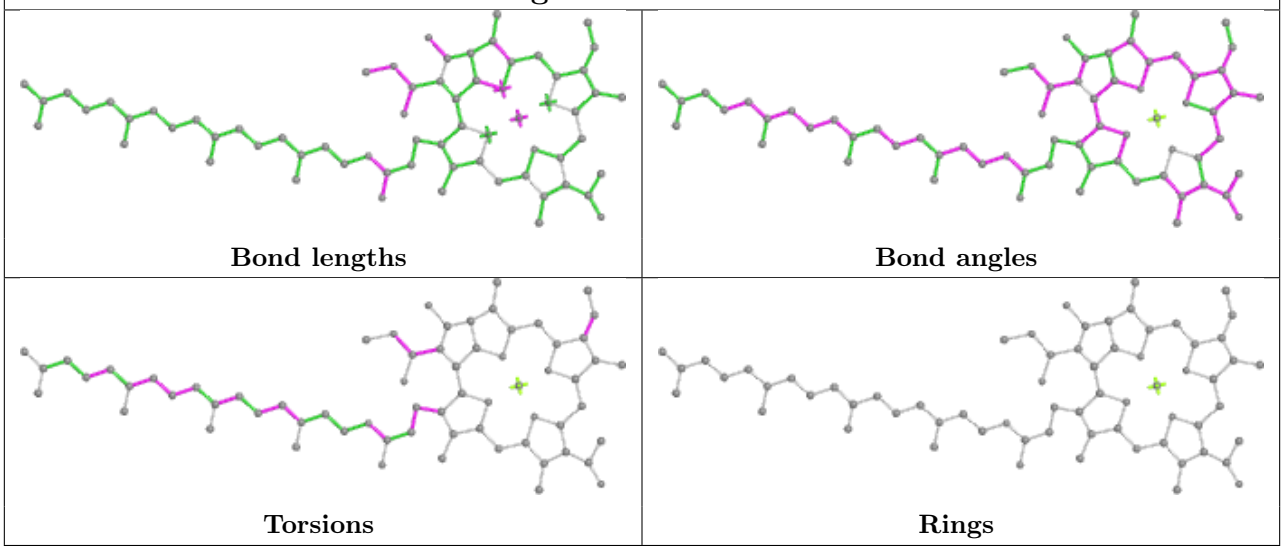
Ligand BCL j 101



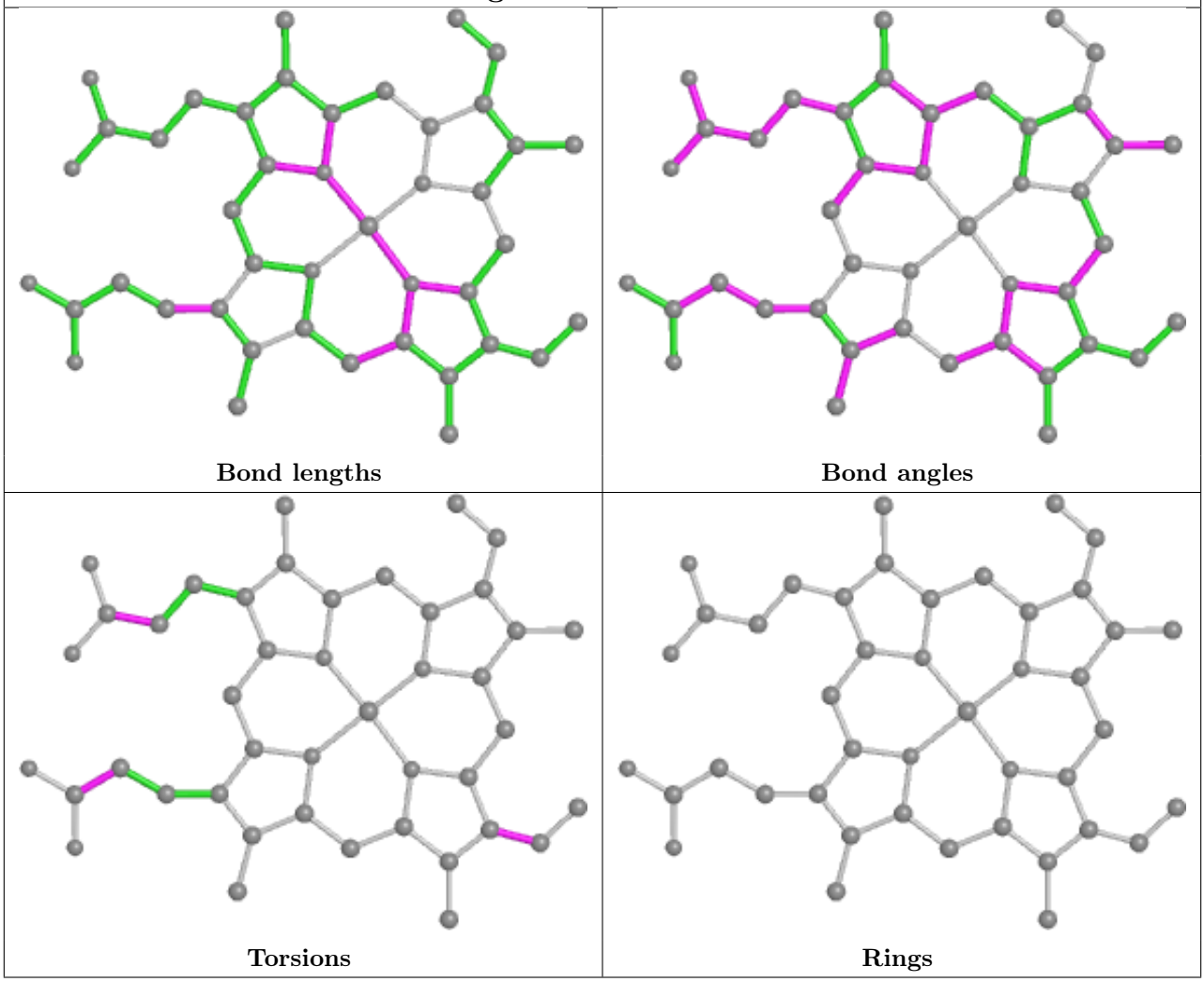
Ligand BCL L 305



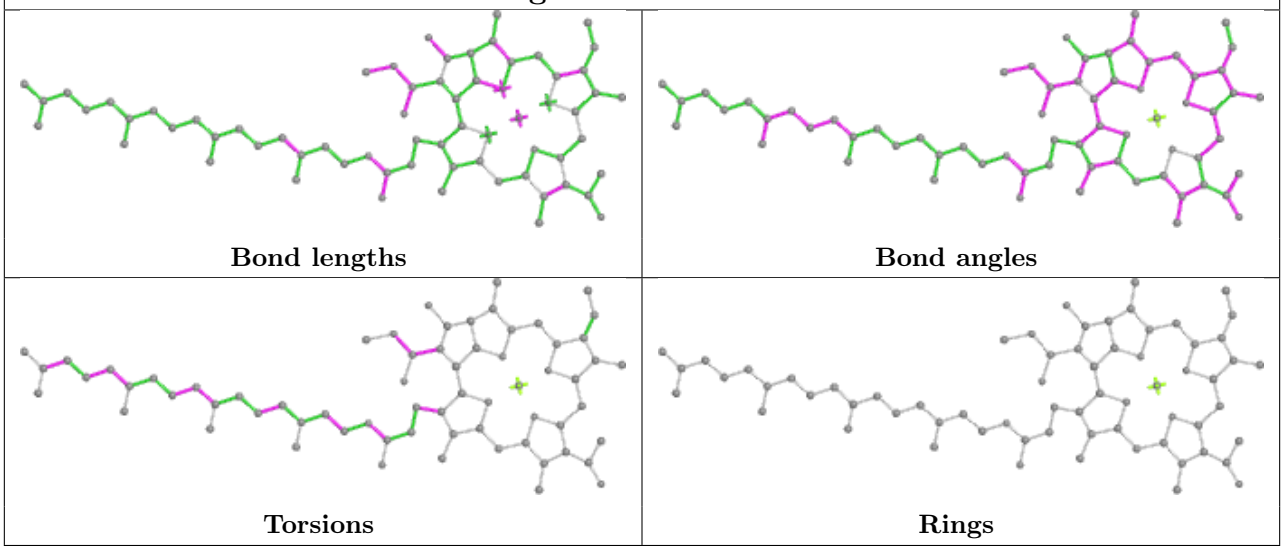
Ligand BCL c 102



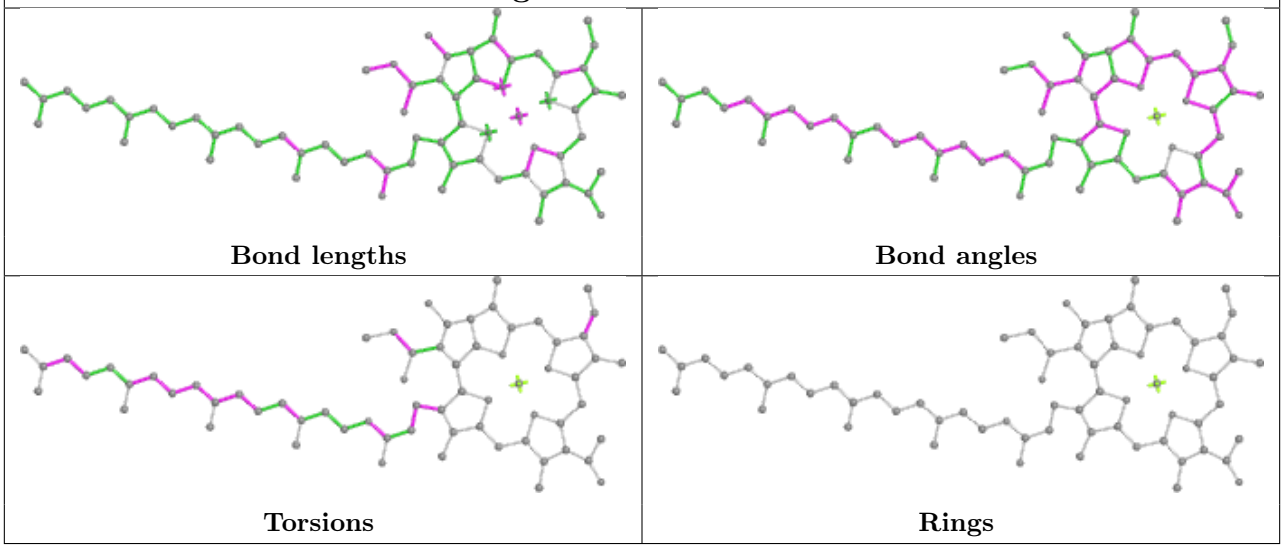
Ligand HEM C 501



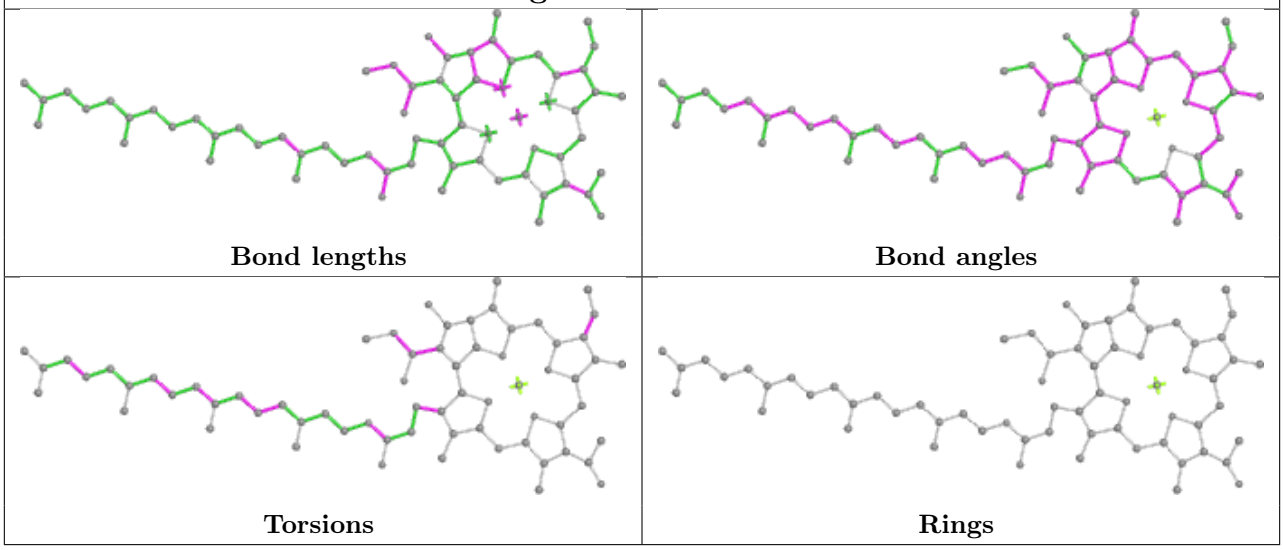
Ligand BCL u 101



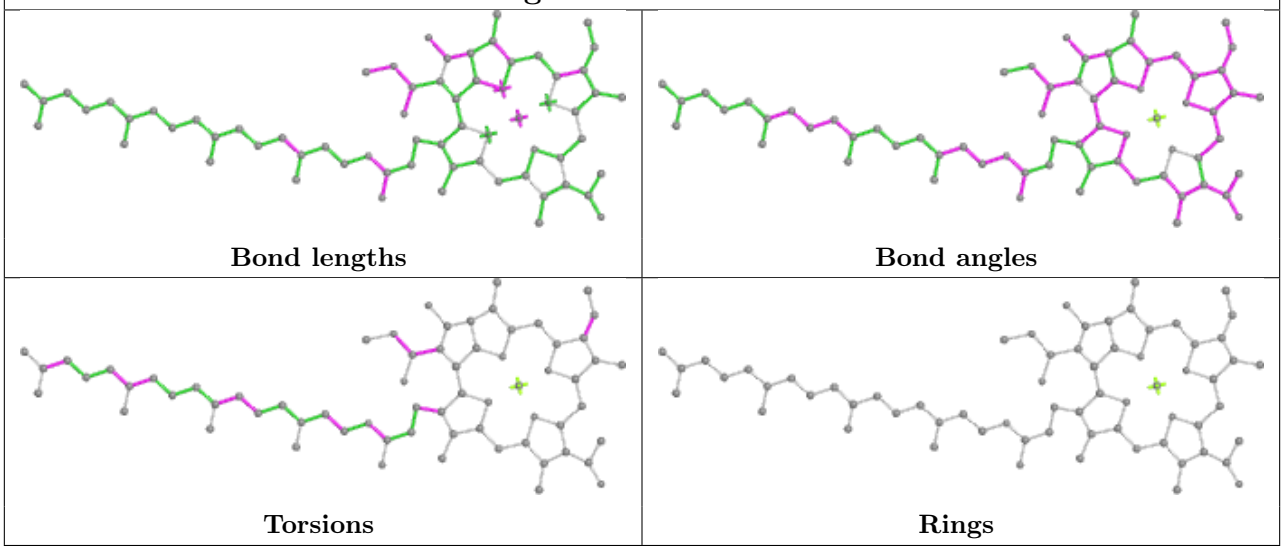
Ligand BCL AB 101



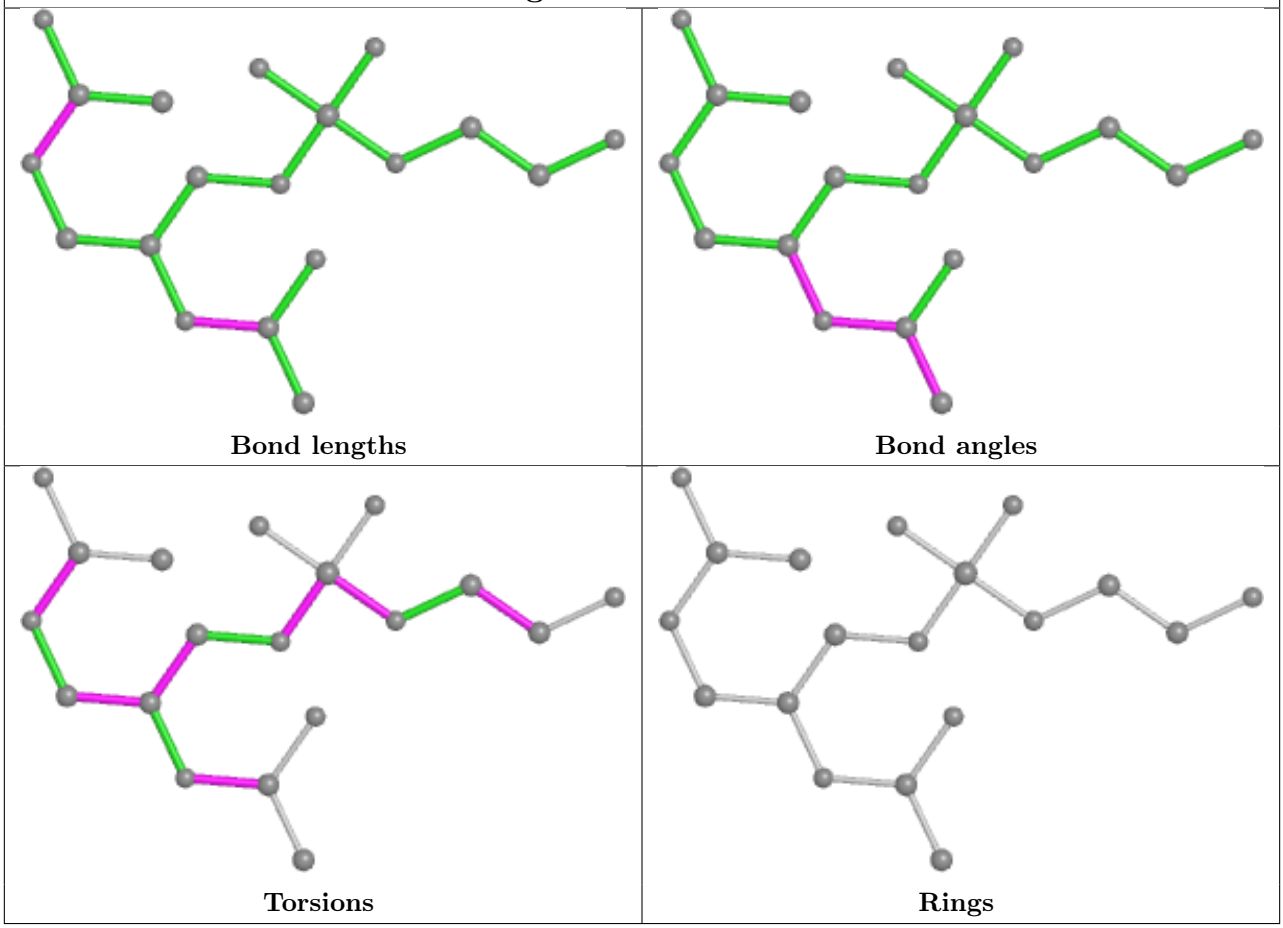
Ligand BCL J 102



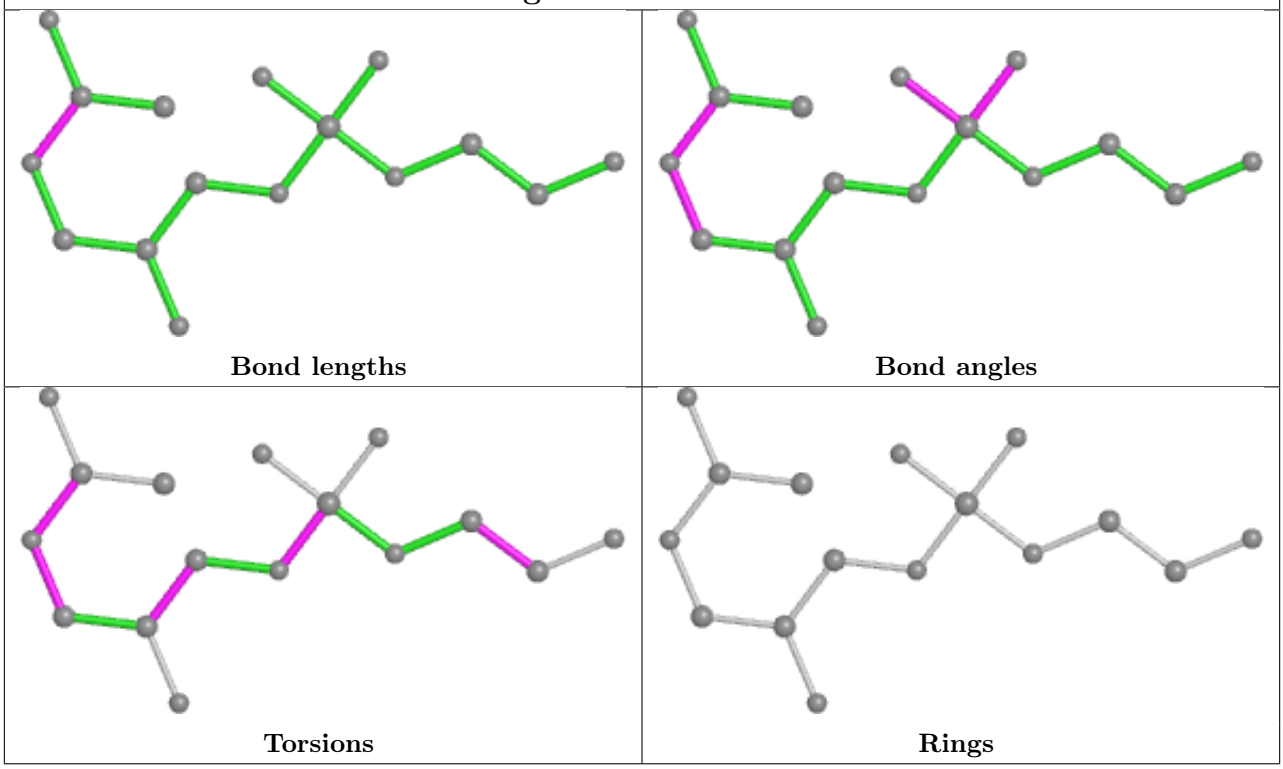
Ligand BCL m 103



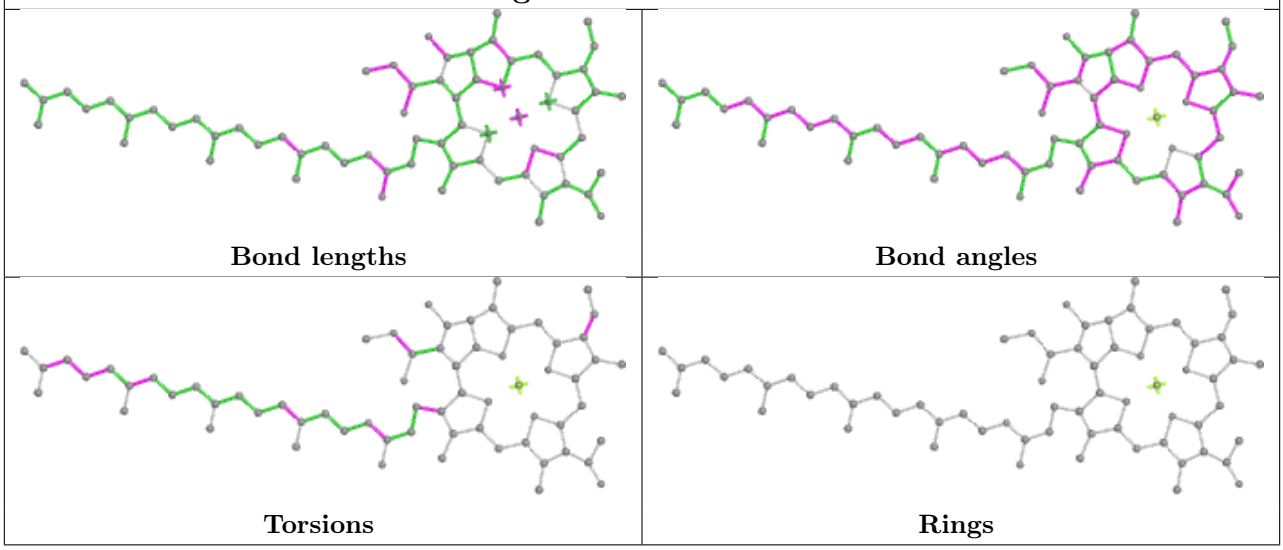
Ligand PEF H 303



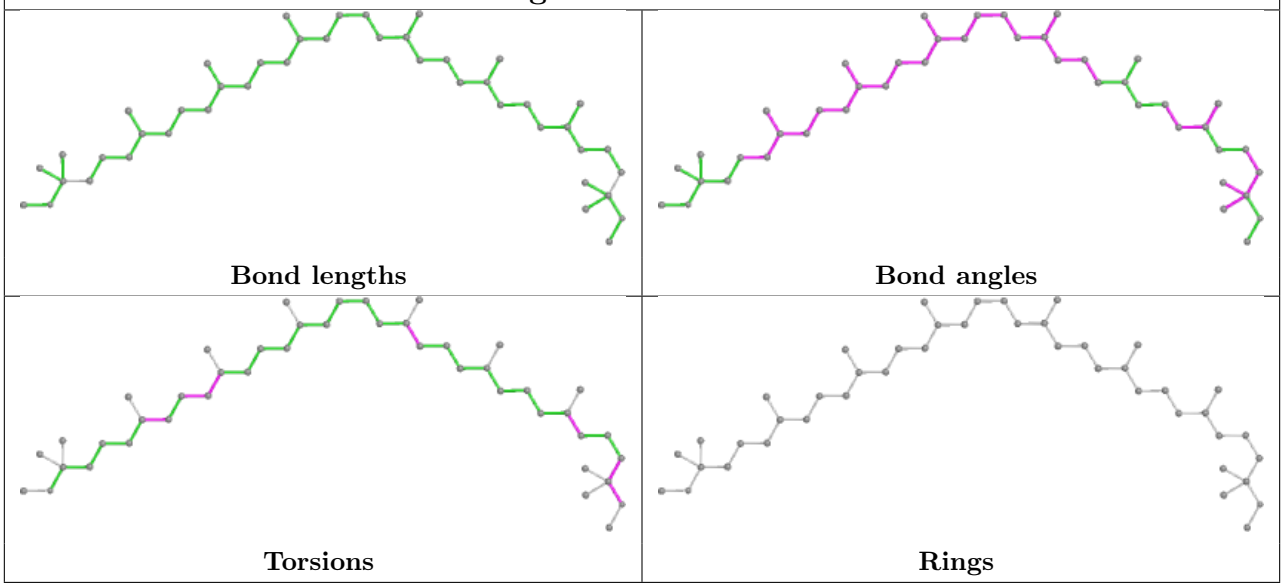
Ligand PEF M 407



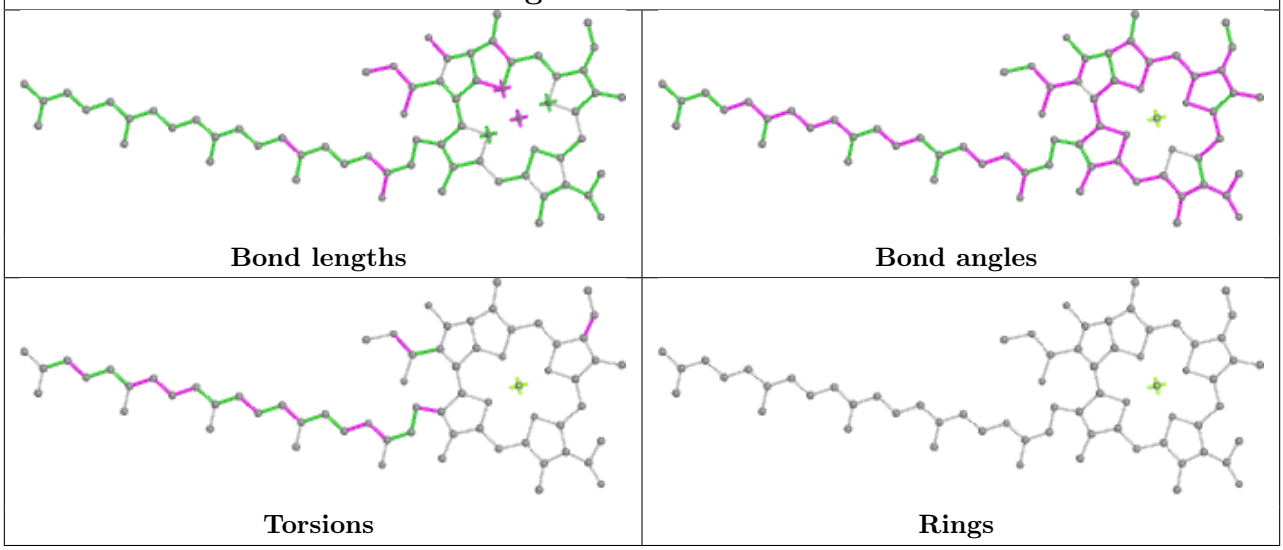
Ligand BCL AC 102



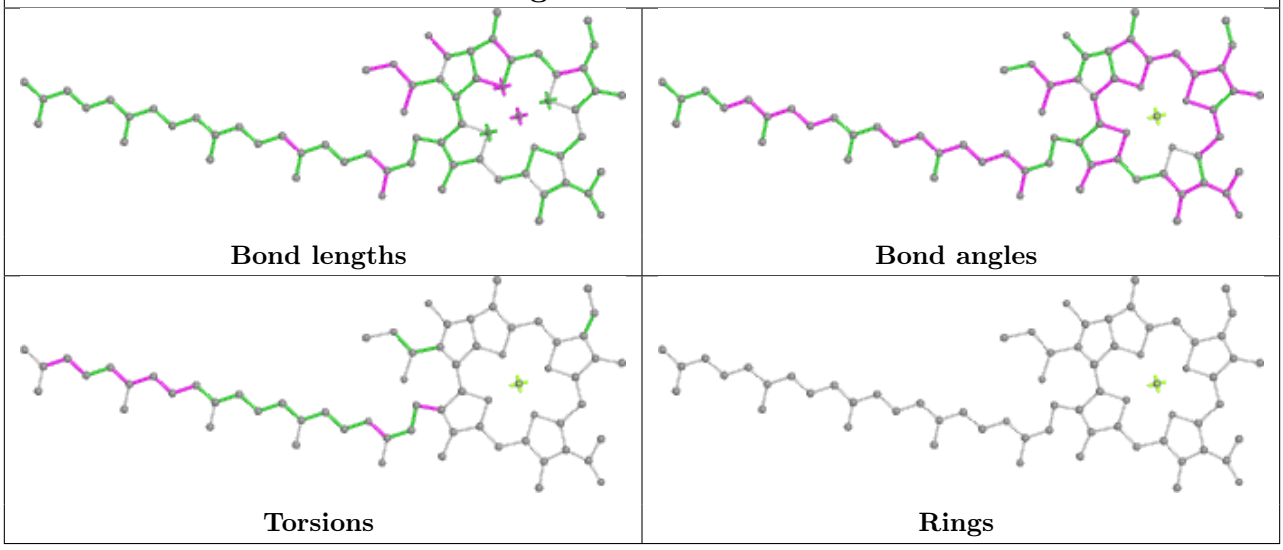
Ligand CRT 4 101



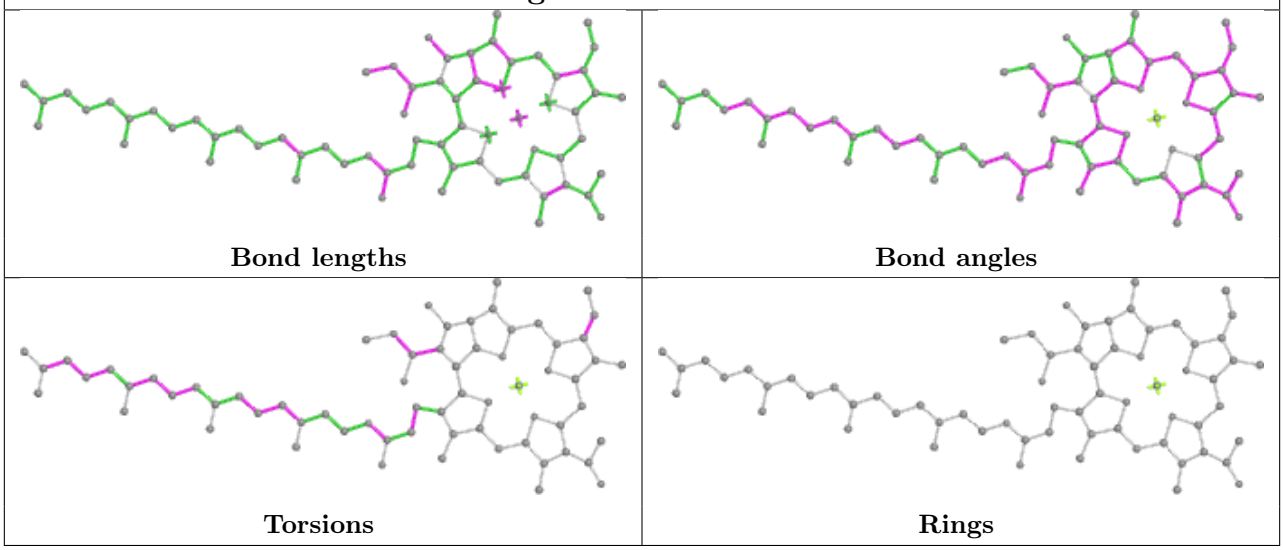
Ligand BCL G 102



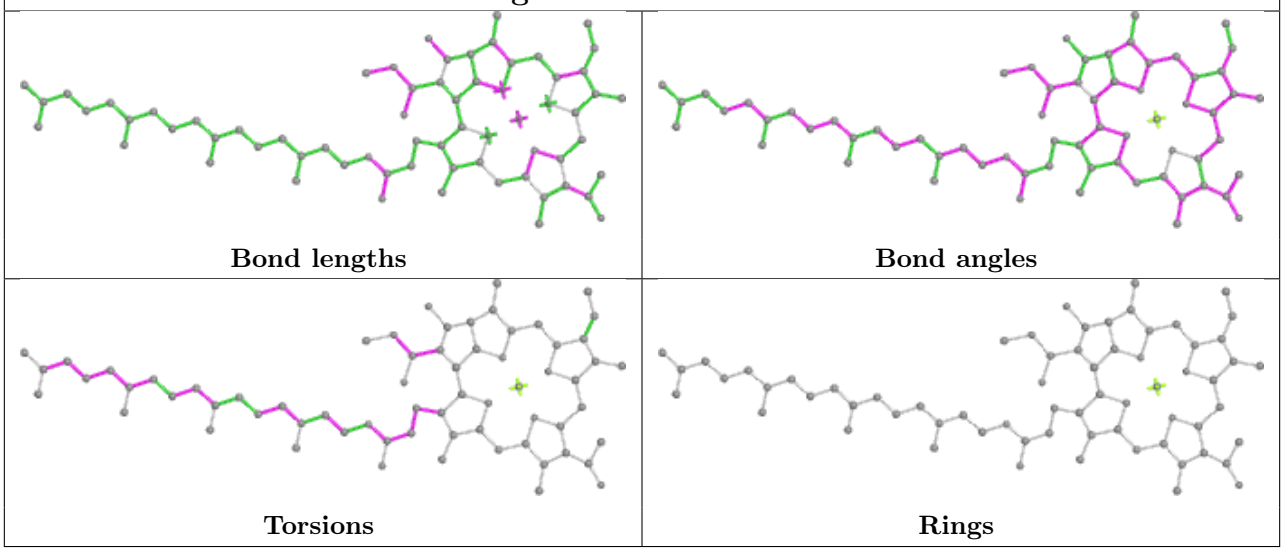
Ligand BCL 0 101



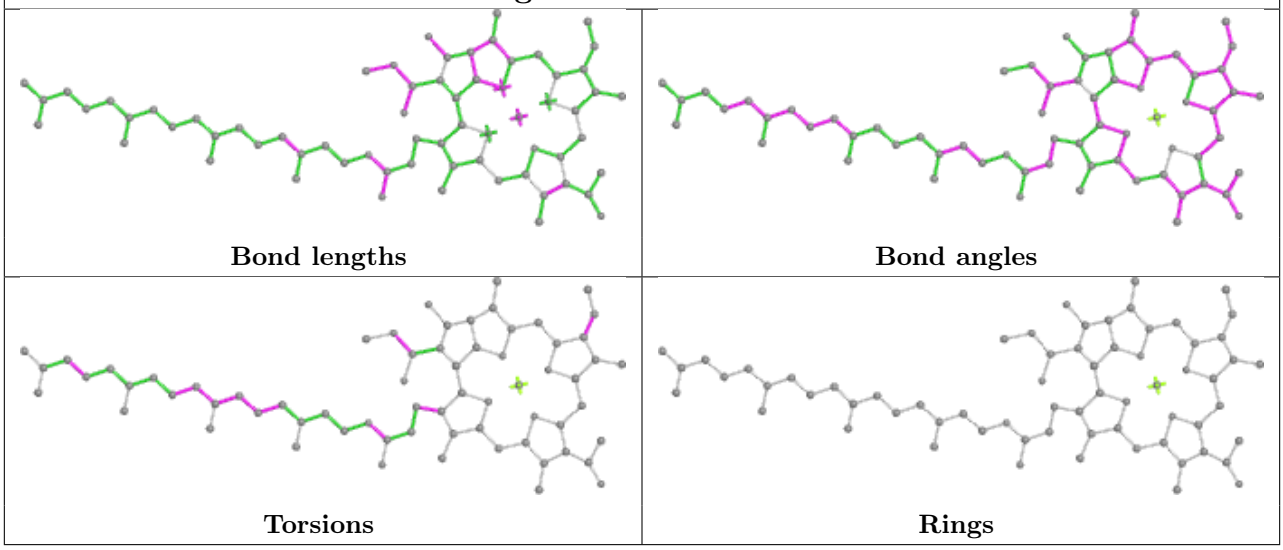
Ligand BCL F 101



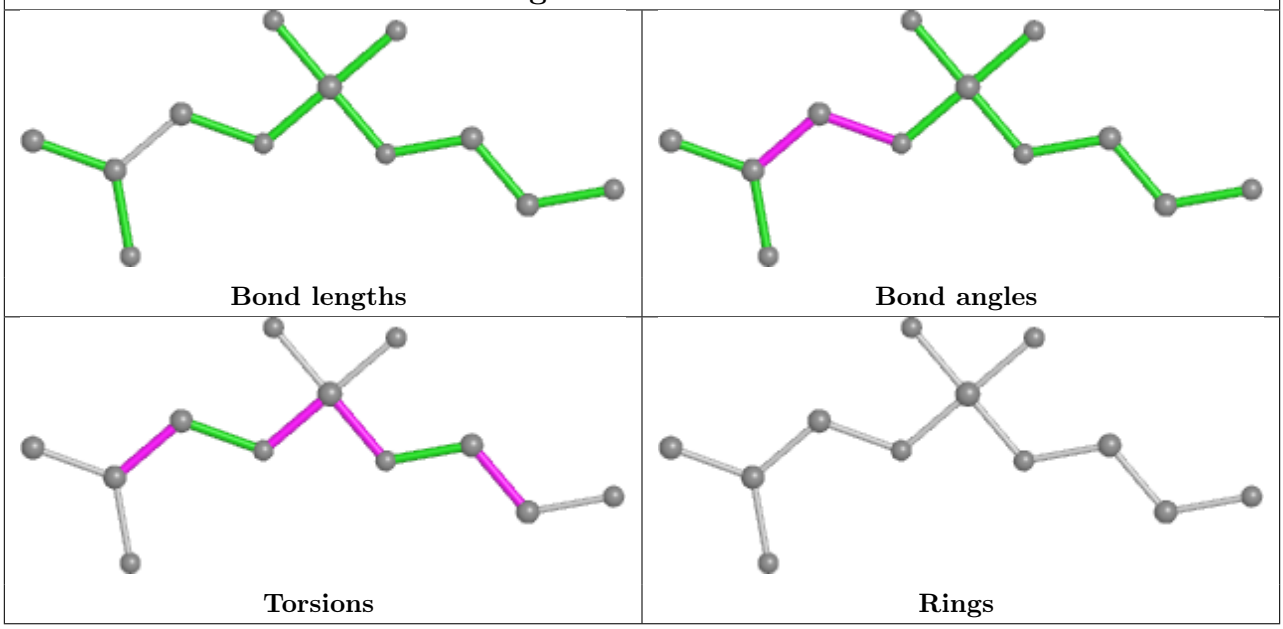
Ligand BCL AH 103



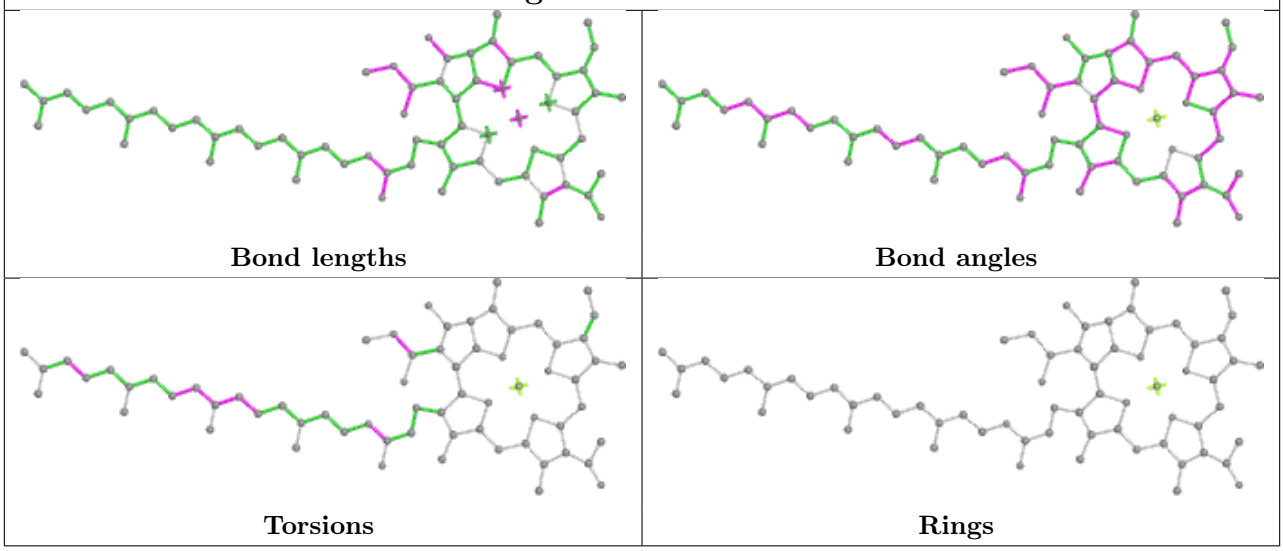
Ligand BCL AL 102



Ligand PEF L 306



Ligand BCL D 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.53	40 (12%)	3	3	79, 112, 143, 161	0
1	o	317/333 (95%)	0.64	44 (13%)	2	2	96, 133, 172, 190	0
2	L	280/281 (99%)	0.36	17 (6%)	21	20	60, 95, 154, 189	0
2	x	280/281 (99%)	0.36	17 (6%)	21	20	63, 97, 147, 181	0
3	M	318/319 (99%)	0.29	12 (3%)	40	37	65, 100, 140, 160	0
3	y	318/319 (99%)	0.30	15 (4%)	31	29	61, 111, 158, 187	0
4	H	258/259 (99%)	0.41	28 (10%)	5	5	77, 105, 171, 274	0
4	t	258/259 (99%)	0.54	31 (12%)	4	3	77, 106, 143, 251	0
5	1	60/61 (98%)	0.89	13 (21%)	0	1	130, 158, 212, 237	0
5	3	60/61 (98%)	1.31	15 (25%)	0	0	129, 157, 225, 232	0
5	5	60/61 (98%)	0.98	10 (16%)	1	1	137, 174, 239, 244	0
5	7	60/61 (98%)	1.98	21 (35%)	0	0	159, 188, 259, 272	0
5	9	60/61 (98%)	1.80	16 (26%)	0	0	163, 204, 239, 243	0
5	A	60/61 (98%)	2.56	26 (43%)	0	0	170, 210, 257, 260	0
5	AA	60/61 (98%)	2.13	23 (38%)	0	0	165, 216, 280, 292	0
5	AC	60/61 (98%)	2.00	21 (35%)	0	0	176, 225, 276, 279	0
5	AE	60/61 (98%)	2.00	24 (40%)	0	0	191, 230, 263, 270	0
5	AG	60/61 (98%)	1.15	14 (23%)	0	1	177, 216, 274, 278	0
5	AI	60/61 (98%)	1.45	17 (28%)	0	0	159, 194, 255, 261	0
5	AK	60/61 (98%)	0.87	12 (20%)	1	1	151, 180, 247, 264	0
5	D	60/61 (98%)	2.21	27 (45%)	0	0	170, 217, 266, 269	0
5	F	60/61 (98%)	1.92	22 (36%)	0	0	174, 215, 261, 264	0
5	I	60/61 (98%)	1.77	19 (31%)	0	0	179, 222, 268, 269	0
5	K	60/61 (98%)	2.40	19 (31%)	0	0	164, 214, 288, 303	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
5	O	60/61 (98%)	1.75	17 (28%)	0	0	143, 195, 279, 284	0
5	Q	60/61 (98%)	1.26	14 (23%)	0	1	139, 185, 264, 270	0
5	S	60/61 (98%)	2.25	17 (28%)	0	0	153, 193, 256, 260	0
5	U	60/61 (98%)	1.08	10 (16%)	1	1	138, 179, 250, 256	0
5	W	60/61 (98%)	1.11	14 (23%)	0	1	126, 164, 228, 235	0
5	Y	60/61 (98%)	2.00	20 (33%)	0	0	123, 153, 233, 264	0
5	d	60/61 (98%)	1.17	13 (21%)	0	1	147, 181, 240, 252	0
5	f	60/61 (98%)	1.25	14 (23%)	0	1	157, 180, 247, 253	0
5	h	60/61 (98%)	1.56	16 (26%)	0	0	154, 189, 257, 267	0
5	j	60/61 (98%)	1.34	13 (21%)	0	1	157, 191, 243, 257	0
5	l	60/61 (98%)	1.82	21 (35%)	0	0	147, 187, 241, 251	0
5	m	60/61 (98%)	1.98	22 (36%)	0	0	146, 186, 255, 259	0
5	p	60/61 (98%)	1.58	18 (30%)	0	0	135, 189, 258, 262	0
5	r	60/61 (98%)	1.47	15 (25%)	0	0	139, 186, 274, 280	0
5	u	60/61 (98%)	1.69	17 (28%)	0	0	156, 202, 257, 263	0
5	w	60/61 (98%)	1.62	24 (40%)	0	0	168, 218, 271, 277	0
6	0	40/47 (85%)	0.75	9 (22%)	0	1	178, 236, 246, 250	0
6	2	40/47 (85%)	0.54	6 (15%)	2	2	164, 177, 210, 219	0
6	4	40/47 (85%)	-0.14	1 (2%)	57	54	166, 181, 200, 210	0
6	6	40/47 (85%)	0.48	6 (15%)	2	2	178, 203, 222, 224	0
6	8	40/47 (85%)	0.99	11 (27%)	0	0	194, 230, 240, 241	0
6	AB	40/47 (85%)	0.56	6 (15%)	2	2	198, 237, 255, 258	0
6	AD	40/47 (85%)	0.51	4 (10%)	7	7	210, 245, 256, 257	0
6	AF	40/47 (85%)	0.71	9 (22%)	0	1	230, 249, 257, 257	0
6	AH	40/47 (85%)	0.72	8 (20%)	1	1	224, 241, 251, 254	0
6	AJ	40/47 (85%)	0.53	8 (20%)	1	1	199, 230, 241, 243	0
6	AL	40/47 (85%)	0.77	9 (22%)	0	1	190, 211, 236, 238	0
6	B	40/47 (85%)	0.81	11 (27%)	0	0	188, 239, 250, 254	0
6	E	40/47 (85%)	0.35	6 (15%)	2	2	193, 239, 251, 252	0
6	G	40/47 (85%)	0.49	5 (12%)	3	3	187, 239, 252, 255	0
6	J	40/47 (85%)	0.82	12 (30%)	0	0	191, 243, 258, 262	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
6	N	40/47 (85%)	0.92	8 (20%)	1	1	175, 225, 247, 254	0
6	P	40/47 (85%)	0.81	8 (20%)	1	1	170, 220, 241, 245	0
6	R	40/47 (85%)	0.58	7 (17%)	1	1	170, 223, 236, 236	0
6	T	40/47 (85%)	0.55	6 (15%)	2	2	184, 218, 236, 237	0
6	V	40/47 (85%)	0.18	4 (10%)	7	7	171, 205, 226, 234	0
6	X	40/47 (85%)	-0.38	1 (2%)	57	54	160, 186, 205, 209	0
6	Z	40/47 (85%)	-0.01	1 (2%)	57	54	159, 173, 197, 202	0
6	c	40/47 (85%)	0.79	9 (22%)	0	1	160, 217, 245, 247	0
6	e	40/47 (85%)	0.55	4 (10%)	7	7	189, 204, 236, 240	0
6	g	40/47 (85%)	0.26	6 (15%)	2	2	195, 213, 235, 239	0
6	i	40/47 (85%)	0.73	8 (20%)	1	1	199, 223, 240, 241	0
6	k	40/47 (85%)	0.91	12 (30%)	0	0	195, 233, 251, 255	0
6	n	40/47 (85%)	1.02	10 (25%)	0	0	153, 214, 249, 253	0
6	q	40/47 (85%)	0.28	4 (10%)	7	7	156, 199, 239, 246	0
6	s	40/47 (85%)	0.47	5 (12%)	3	3	151, 198, 236, 238	0
6	v	40/47 (85%)	0.81	8 (20%)	1	1	182, 205, 244, 247	0
6	z	40/47 (85%)	1.04	9 (22%)	0	1	184, 224, 266, 271	0
All	All	5546/5840 (94%)	0.88	989 (17%)	1	1	60, 169, 252, 303	0

The worst 5 of 989 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	S	59	GLY	25.9
5	AC	54	SER	20.4
5	7	2	PHE	18.2
5	AA	52	PRO	17.6
5	S	60	LYS	15.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	CRT	J	101	44/44	0.08	1.33	196,214,220,222	0
15	CRT	c	101	44/44	0.12	1.10	179,196,203,207	0
15	CRT	N	101	44/44	0.27	1.01	179,199,209,214	0
15	CRT	8	101	44/44	0.29	0.86	174,203,220,223	0
15	CRT	n	101	44/44	0.37	1.15	173,188,197,201	0
15	CRT	A	103	44/44	0.38	0.89	186,214,224,225	0
15	CRT	v	101	44/44	0.39	1.01	165,192,198,200	0
8	SR	AI	102	1/1	0.40	0.07	245,245,245,245	0
15	CRT	p	103	44/44	0.40	1.11	158,177,182,187	0
15	CRT	AC	101	44/44	0.44	0.80	195,211,216,218	0
15	CRT	k	101	44/44	0.45	0.77	172,200,217,220	0
15	CRT	R	101	44/44	0.46	0.89	157,189,197,198	0
8	SR	w	103	1/1	0.46	0.26	260,260,260,260	0
8	SR	S	103	1/1	0.49	0.12	235,235,235,235	0
15	CRT	z	101	44/44	0.51	0.81	179,205,209,210	0
14	MQ8	M	403	53/53	0.52	0.65	75,98,159,170	0
15	CRT	i	101	44/44	0.56	0.78	163,197,220,226	0
15	CRT	M	404	44/44	0.58	0.61	75,96,139,150	0
15	CRT	E	101	44/44	0.58	0.76	182,217,225,226	0
12	PEF	H	301	19/47	0.63	0.26	140,163,175,180	0
8	SR	p	105	1/1	0.64	0.19	265,265,265,265	0
8	SR	I	102	1/1	0.64	0.14	284,284,284,284	0
15	CRT	G	101	44/44	0.65	0.95	187,217,225,228	0
15	CRT	AH	102	44/44	0.66	1.14	163,220,243,244	0
15	CRT	6	101	44/44	0.66	0.95	153,180,198,203	0
8	SR	d	102	1/1	0.66	0.06	198,198,198,198	0
15	CRT	s	101	44/44	0.66	1.01	155,177,181,183	0
15	CRT	f	102	44/44	0.67	0.95	152,190,223,230	0
15	CRT	AE	103	44/44	0.68	0.93	182,236,248,249	0
12	PEF	A	101	19/47	0.68	0.46	141,149,161,165	0
15	CRT	P	102	44/44	0.69	0.57	169,193,199,202	0
15	CRT	e	101	44/44	0.69	1.24	149,194,237,241	0
15	CRT	T	101	44/44	0.70	0.93	145,187,206,207	0
15	CRT	y	404	44/44	0.70	0.49	96,117,155,166	0
15	CRT	AJ	101	44/44	0.70	1.24	147,203,240,241	0
15	CRT	AD	102	44/44	0.70	0.49	192,225,232,234	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	PGW	AE	101	21/51	0.70	0.34	149,167,181,187	0
16	PO4	t	302	5/5	0.71	0.40	138,140,144,147	0
8	SR	K	102	1/1	0.73	0.29	270,270,270,270	0
12	PEF	p	101	16/47	0.73	0.24	132,144,152,156	0
9	BCL	AC	102	66/66	0.73	0.48	205,236,259,261	0
8	SR	w	102	1/1	0.73	0.07	263,263,263,263	0
16	PO4	H	302	5/5	0.74	0.62	170,172,178,179	0
8	SR	5	103	1/1	0.74	0.13	197,197,197,197	0
15	CRT	U	102	44/44	0.74	1.16	132,179,205,208	0
12	PEF	m	101	19/47	0.75	0.32	124,130,143,146	0
14	MQ8	y	403	53/53	0.75	0.40	71,88,135,144	0
10	BPH	y	402	65/65	0.75	0.37	80,90,143,155	0
11	UQ8	L	304	53/53	0.76	0.57	75,80,82,83	0
15	CRT	AL	101	44/44	0.77	1.22	140,190,233,236	0
8	SR	m	104	1/1	0.78	0.19	253,253,253,253	0
15	CRT	2	101	44/44	0.78	0.98	128,165,195,200	0
17	PGW	S	101	21/51	0.78	0.23	118,132,142,148	0
8	SR	O	102	1/1	0.78	0.14	254,254,254,254	0
10	BPH	x	302	65/65	0.79	0.39	71,78,102,105	0
8	SR	AI	103	1/1	0.79	0.23	228,228,228,228	0
15	CRT	9	102	44/44	0.79	0.87	188,217,226,230	0
15	CRT	4	101	44/44	0.79	0.74	136,169,192,198	0
12	PEF	L	306	12/47	0.80	0.32	113,119,126,127	0
8	SR	9	101	1/1	0.80	0.15	236,236,236,236	0
15	CRT	X	101	44/44	0.80	0.86	118,164,193,198	0
15	CRT	Z	101	44/44	0.80	1.20	114,157,190,195	0
11	UQ8	x	304	53/53	0.80	0.57	73,85,92,93	0
7	HEM	o	501	43/43	0.81	0.46	142,155,165,169	0
8	SR	l	102	1/1	0.81	0.14	245,245,245,245	0
12	PEF	y	406	19/47	0.81	0.23	124,132,141,146	0
8	SR	x	307	1/1	0.82	0.25	168,168,168,168	0
9	BCL	j	101	66/66	0.82	0.34	177,199,217,223	0
9	BCL	0	101	66/66	0.82	0.45	190,224,244,245	0
9	BCL	AB	101	66/66	0.82	0.55	197,232,260,262	0
8	SR	AK	102	1/1	0.83	0.04	203,203,203,203	0
8	SR	5	104	1/1	0.83	0.16	206,206,206,206	0
9	BCL	AD	101	66/66	0.83	0.34	193,224,242,252	0
9	BCL	O	101	66/66	0.84	0.43	179,211,234,235	0
10	BPH	M	402	65/65	0.84	0.30	72,77,113,123	0
8	SR	AA	102	1/1	0.84	0.14	273,273,273,273	0
9	BCL	m	102	66/66	0.84	0.39	160,202,221,229	0
9	BCL	K	101	66/66	0.85	0.45	181,215,235,242	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	l	101	66/66	0.85	0.27	161,201,221,228	0
10	BPH	L	302	65/65	0.85	0.33	68,81,108,115	0
9	BCL	AE	104	66/66	0.85	0.46	208,235,262,264	0
9	BCL	AH	103	66/66	0.85	0.29	195,211,245,252	0
9	BCL	d	101	66/66	0.85	0.36	138,175,187,197	0
12	PEF	t	303	19/47	0.85	0.22	83,87,94,95	0
8	SR	F	102	1/1	0.86	0.20	262,262,262,262	0
12	PEF	y	407	19/47	0.86	0.20	91,96,102,105	0
8	SR	r	102	1/1	0.86	0.09	252,252,252,252	0
9	BCL	z	102	66/66	0.86	0.45	193,228,269,271	0
9	BCL	V	101	66/66	0.86	0.36	159,175,219,232	0
12	PEF	M	408	19/47	0.87	0.28	87,92,97,100	0
9	BCL	c	102	66/66	0.87	0.38	177,211,249,251	0
9	BCL	9	103	66/66	0.87	0.35	169,202,226,235	0
9	BCL	5	102	66/66	0.87	0.44	150,176,224,240	0
9	BCL	8	102	66/66	0.87	0.32	177,207,239,244	0
12	PEF	y	408	19/47	0.87	0.46	93,103,113,116	0
12	PEF	M	407	16/47	0.87	0.19	79,83,87,89	0
9	BCL	7	101	66/66	0.88	0.36	162,184,202,209	0
9	BCL	N	102	66/66	0.88	0.49	187,219,242,244	0
12	PEF	H	304	19/47	0.88	0.17	92,98,106,108	0
7	HEM	C	501	43/43	0.88	0.33	110,120,129,134	0
9	BCL	T	102	66/66	0.88	0.36	164,188,236,238	0
9	BCL	D	102	66/66	0.88	0.46	202,232,246,247	0
9	BCL	m	103	66/66	0.88	0.37	178,209,237,245	0
9	BCL	u	101	66/66	0.88	0.37	120,199,218,223	0
9	BCL	k	102	66/66	0.88	0.35	181,211,246,260	0
8	SR	x	308	1/1	0.88	0.15	196,196,196,196	0
9	BCL	AH	101	66/66	0.89	0.39	199,218,233,243	0
9	BCL	p	102	66/66	0.89	0.36	124,199,217,224	0
8	SR	Q	102	1/1	0.89	0.19	256,256,256,256	0
8	SR	AE	105	1/1	0.89	0.15	257,257,257,257	0
9	BCL	I	101	66/66	0.89	0.38	141,226,243,247	0
9	BCL	x	301	66/66	0.89	0.35	75,81,87,90	0
12	PEF	t	301	19/47	0.89	0.22	94,98,103,104	0
12	PEF	M	406	19/47	0.89	0.29	107,115,119,124	0
8	SR	D	103	1/1	0.89	0.19	269,269,269,269	0
8	SR	f	103	1/1	0.89	0.07	208,208,208,208	0
9	BCL	y	401	66/66	0.90	0.42	78,88,101,108	0
12	PEF	H	303	19/47	0.90	0.35	164,173,184,191	0
9	BCL	AE	102	66/66	0.90	0.35	169,228,244,254	0
9	BCL	1	101	66/66	0.90	0.32	115,148,161,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	PEF	x	306	19/47	0.90	0.18	96,102,108,108	0
8	SR	L	308	1/1	0.90	0.27	145,145,145,145	0
9	BCL	P	101	66/66	0.90	0.37	171,205,223,228	0
9	BCL	R	102	66/66	0.90	0.34	174,203,233,235	0
9	BCL	f	101	66/66	0.90	0.35	157,181,196,203	0
9	BCL	g	101	66/66	0.90	0.41	169,190,234,245	0
9	BCL	S	102	66/66	0.90	0.32	129,190,203,213	0
9	BCL	B	101	66/66	0.90	0.34	187,218,239,241	0
8	SR	h	102	1/1	0.90	0.14	220,220,220,220	0
8	SR	W	102	1/1	0.91	0.25	205,205,205,205	0
9	BCL	J	102	66/66	0.91	0.41	202,233,255,257	0
9	BCL	L	303	66/66	0.91	0.29	62,70,78,83	0
9	BCL	L	305	66/66	0.91	0.28	76,88,106,115	0
8	SR	7	102	1/1	0.91	0.32	221,221,221,221	0
9	BCL	D	101	66/66	0.91	0.33	149,221,243,245	0
9	BCL	AI	101	66/66	0.91	0.39	177,195,210,216	0
9	BCL	AK	101	66/66	0.91	0.40	168,180,199,220	0
9	BCL	AL	102	66/66	0.91	0.37	167,178,209,221	0
16	PO4	M	405	5/5	0.91	0.15	120,126,128,129	0
9	BCL	v	102	66/66	0.91	0.36	182,211,260,262	0
9	BCL	w	101	66/66	0.91	0.40	174,206,228,234	0
8	SR	U	103	1/1	0.91	0.35	233,233,233,233	0
9	BCL	F	101	66/66	0.91	0.42	184,220,238,242	0
9	BCL	e	102	66/66	0.92	0.45	166,180,213,225	0
9	BCL	L	301	66/66	0.92	0.31	67,74,92,98	0
9	BCL	3	101	66/66	0.92	0.39	134,153,169,173	0
16	PO4	y	405	5/5	0.92	0.16	138,141,147,148	0
9	BCL	h	101	66/66	0.92	0.32	168,188,207,212	0
9	BCL	i	102	66/66	0.92	0.38	173,197,242,261	0
9	BCL	AJ	102	66/66	0.92	0.29	177,189,226,232	0
7	HEM	o	504	43/43	0.93	0.41	112,116,123,124	0
9	BCL	W	101	66/66	0.93	0.34	146,162,172,181	0
9	BCL	x	303	66/66	0.93	0.35	73,82,94,98	0
9	BCL	Y	101	66/66	0.93	0.36	139,149,163,175	0
9	BCL	Z	102	66/66	0.93	0.46	141,150,181,191	0
7	HEM	C	504	43/43	0.93	0.39	97,99,104,107	0
9	BCL	1	102	66/66	0.93	0.35	140,153,192,205	0
9	BCL	r	101	66/66	0.93	0.41	154,192,211,214	0
9	BCL	s	102	66/66	0.93	0.46	171,202,247,248	0
9	BCL	G	102	66/66	0.93	0.40	203,233,249,251	0
9	BCL	A	102	66/66	0.93	0.38	202,230,242,244	0
8	SR	1	103	1/1	0.93	0.06	176,176,176,176	0

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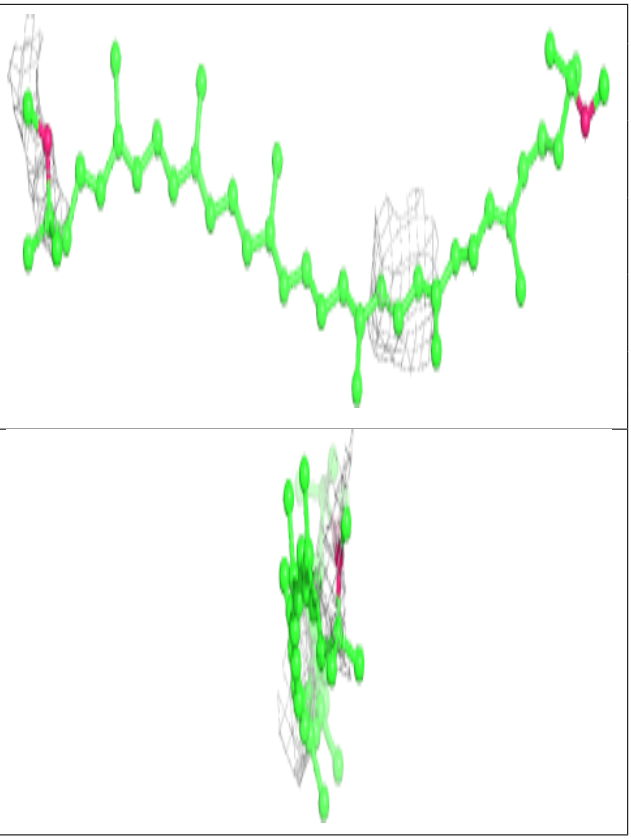
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	HEM	o	503	43/43	0.93	0.42	94,106,122,126	0
9	BCL	U	101	66/66	0.93	0.31	151,179,188,195	0
8	SR	AC	103	1/1	0.94	0.21	265,265,265,265	0
7	HEM	C	503	43/43	0.94	0.39	85,100,116,119	0
9	BCL	x	305	66/66	0.94	0.23	72,82,91,99	0
9	BCL	4	102	66/66	0.94	0.41	138,159,198,209	0
9	BCL	AA	101	66/66	0.94	0.31	177,212,237,244	0
9	BCL	Q	101	66/66	0.94	0.30	165,201,216,224	0
9	BCL	X	102	66/66	0.94	0.29	142,155,182,199	0
8	SR	Y	102	1/1	0.94	0.35	191,191,191,191	0
7	HEM	C	502	43/43	0.94	0.41	97,104,111,113	0
9	BCL	M	401	66/66	0.94	0.35	74,82,88,94	0
9	BCL	p	104	66/66	0.95	0.34	170,202,241,242	0
8	SR	o	505	1/1	0.95	0.16	111,111,111,111	0
9	BCL	5	101	66/66	0.95	0.31	141,165,182,188	0
7	HEM	o	502	43/43	0.96	0.46	125,134,142,145	0
8	SR	A	104	1/1	0.96	0.29	256,256,256,256	0
8	SR	C	505	1/1	0.96	0.12	113,113,113,113	0
8	SR	L	307	1/1	0.97	0.06	205,205,205,205	0
8	SR	j	102	1/1	0.98	0.17	233,233,233,233	0
13	FE	L	309	1/1	0.99	0.13	65,65,65,65	0
13	FE	x	309	1/1	0.99	0.14	65,65,65,65	0

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

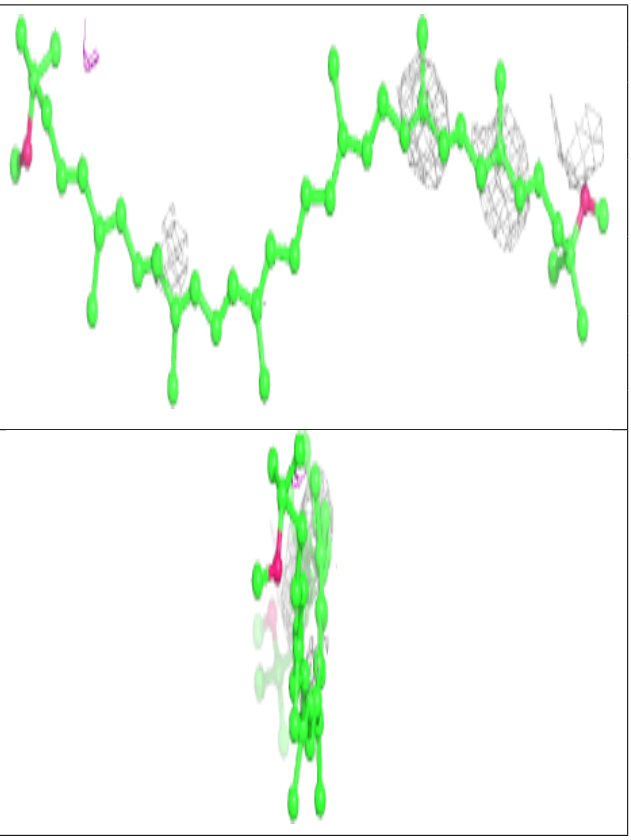
Electron density around CRT J 101:

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



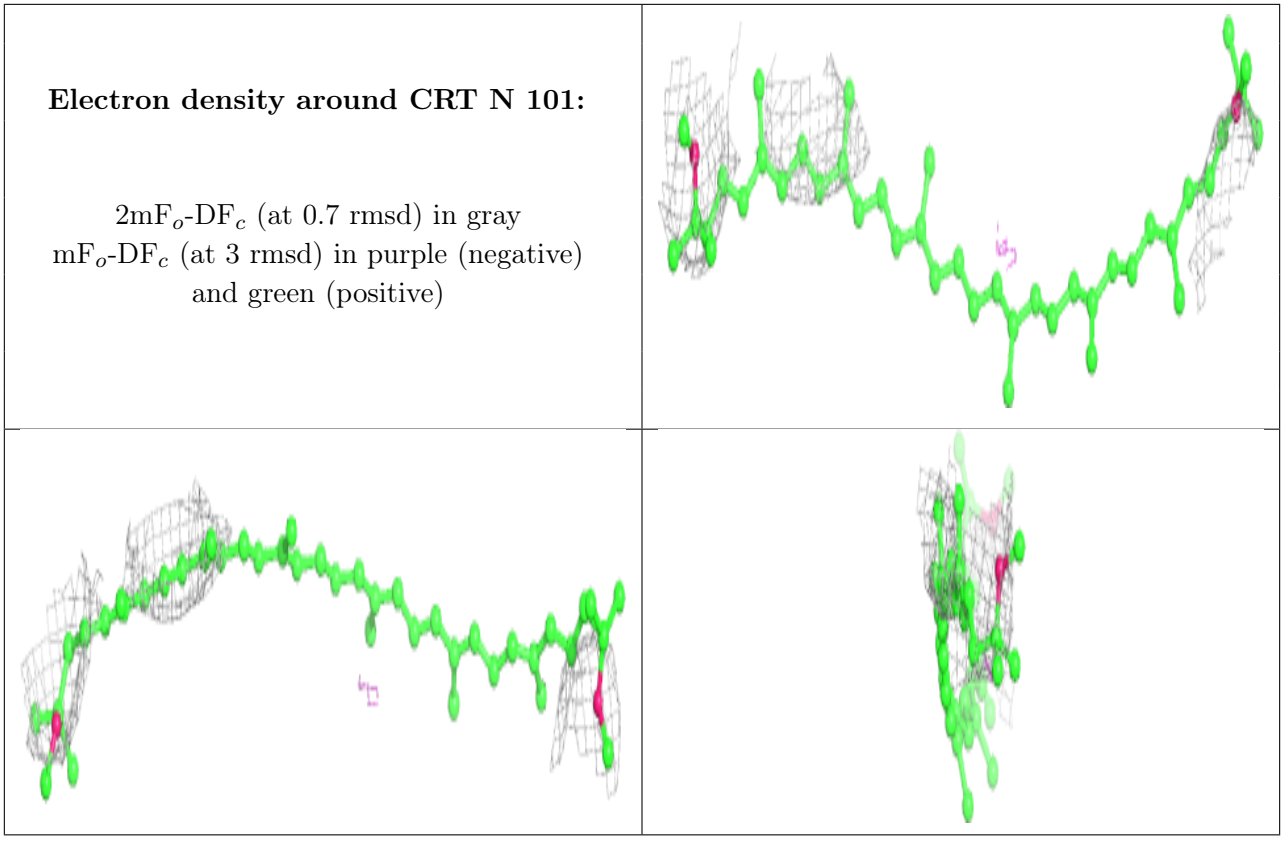
Electron density around CRT c 101:

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



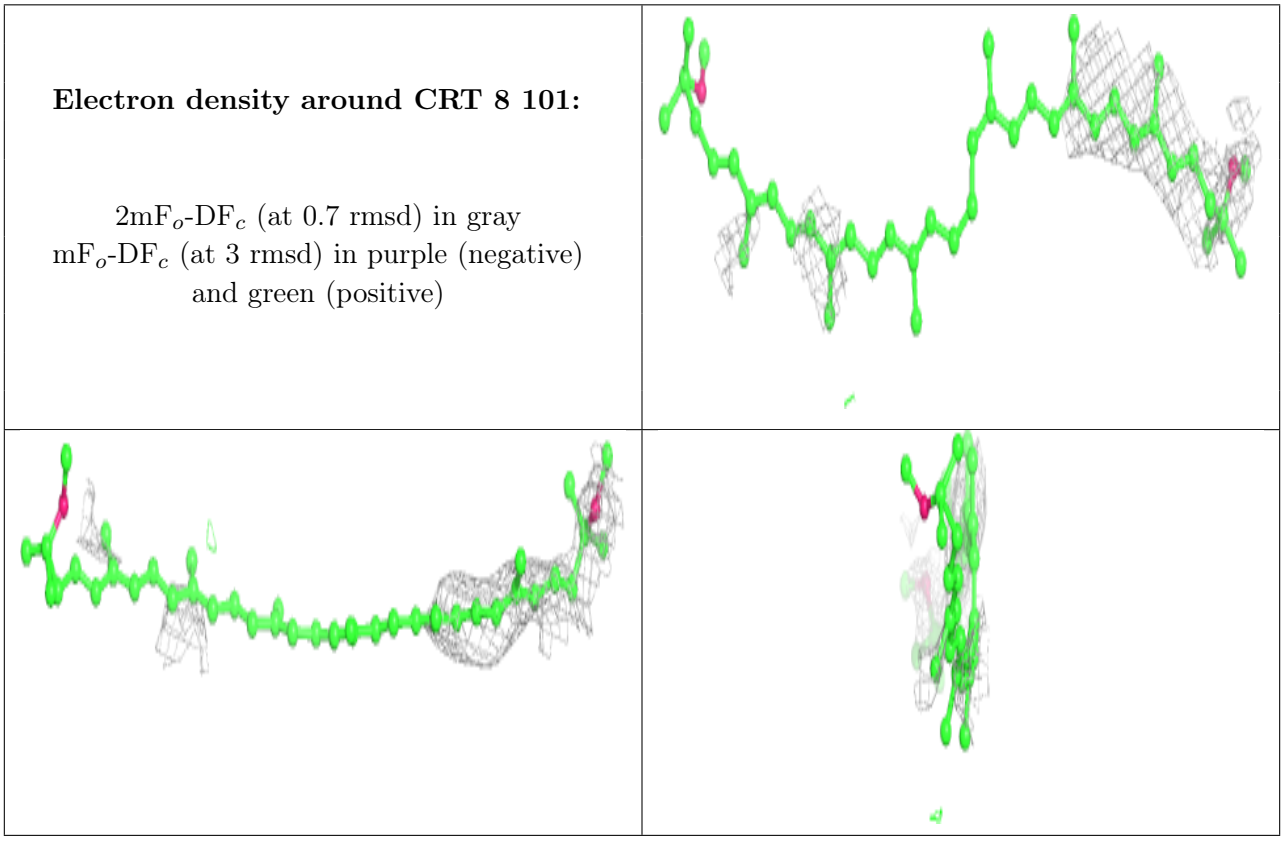
Electron density around CRT N 101:

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



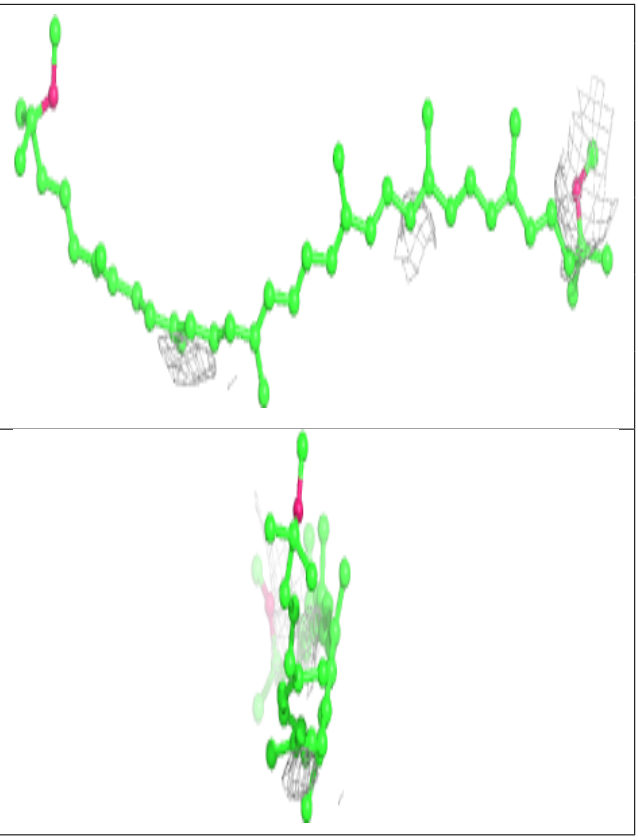
Electron density around CRT 8 101:

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



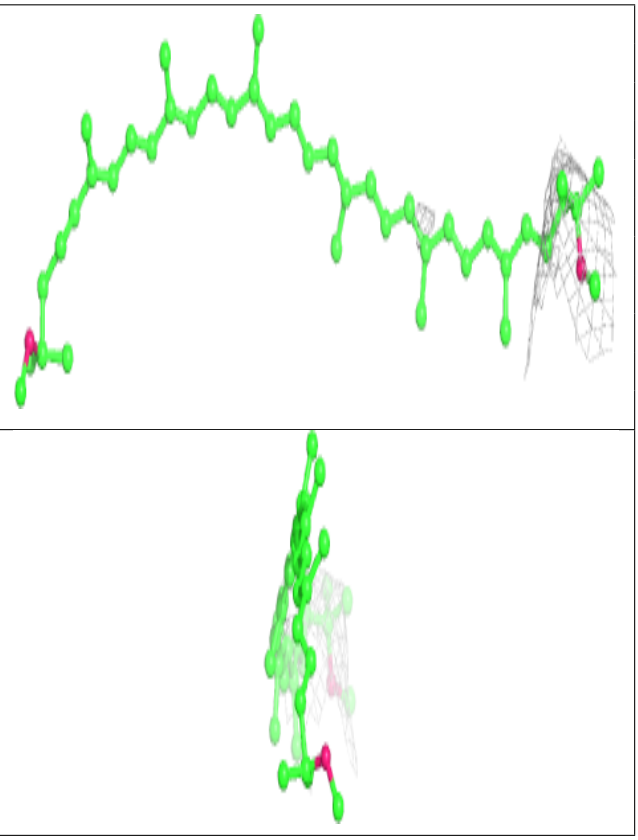
Electron density around CRT n 101:

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



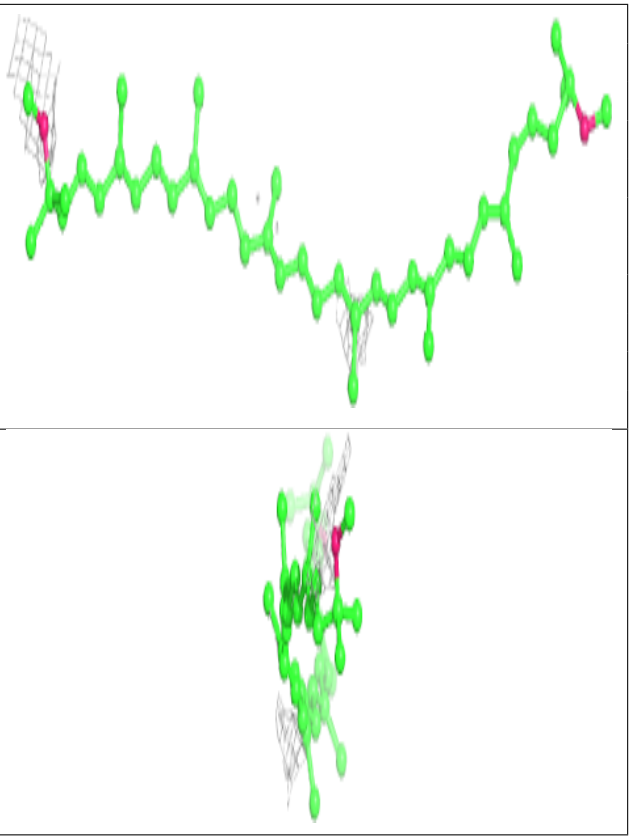
Electron density around CRT A 103:

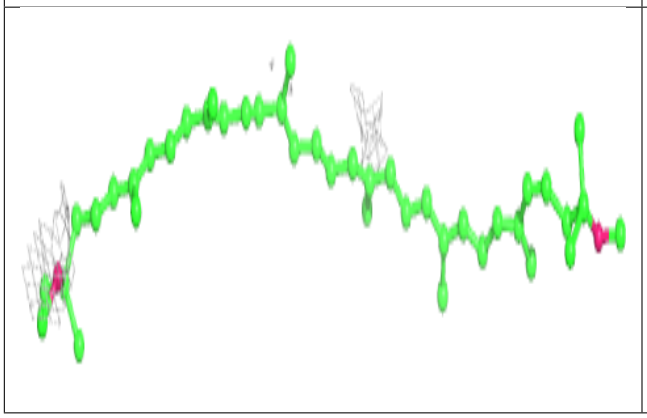
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CRT v 101:

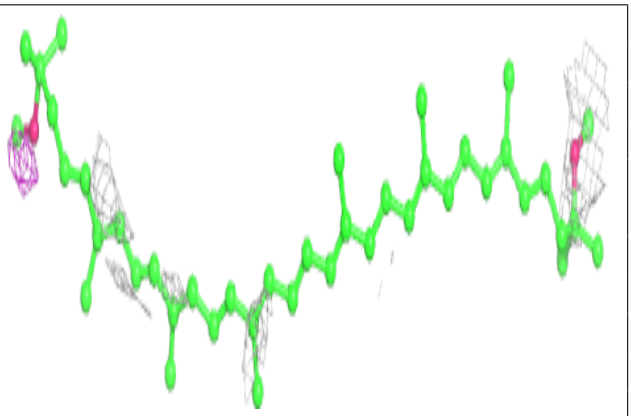
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

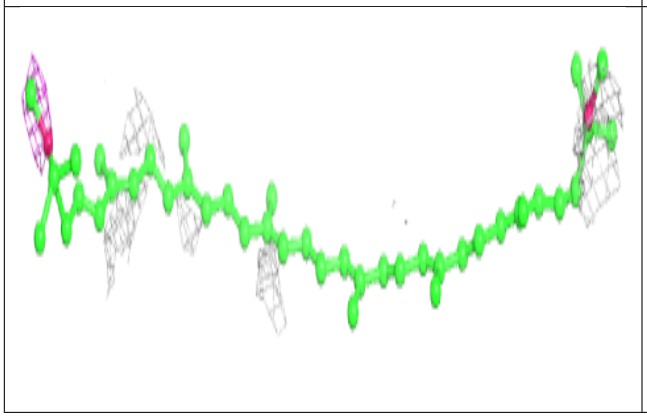




Electron density around CRT p 103:

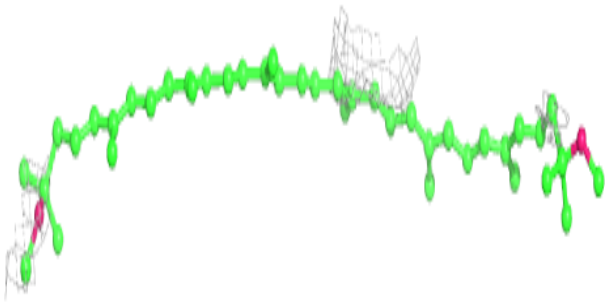
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





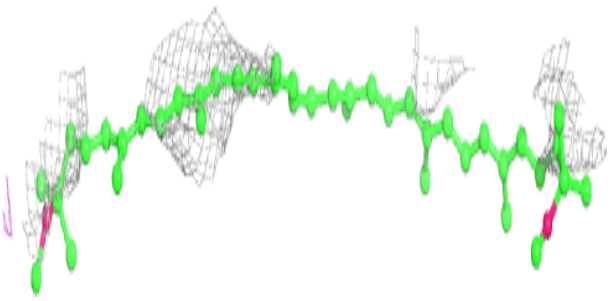
Electron density around CRT AC 101:

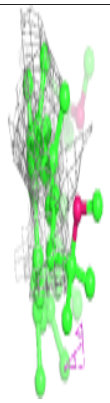
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CRT k 101:

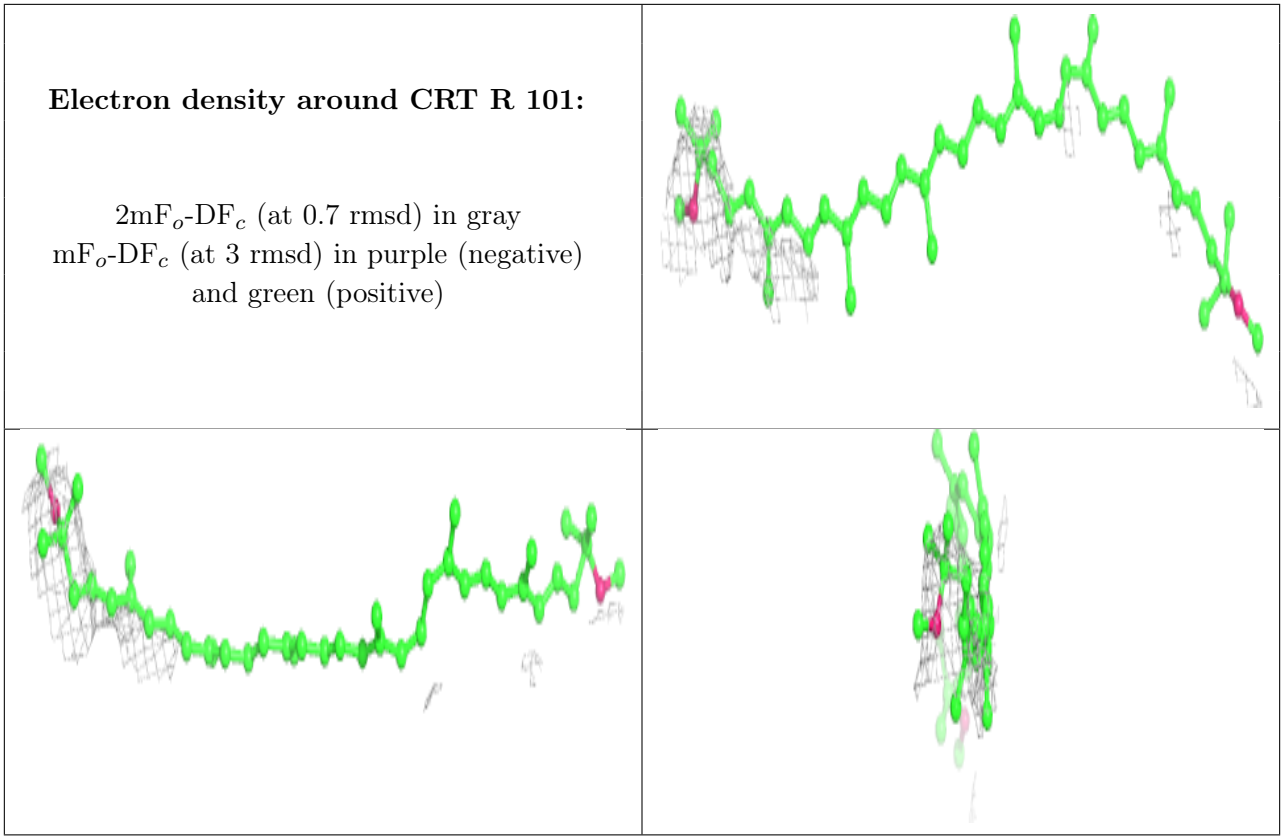
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





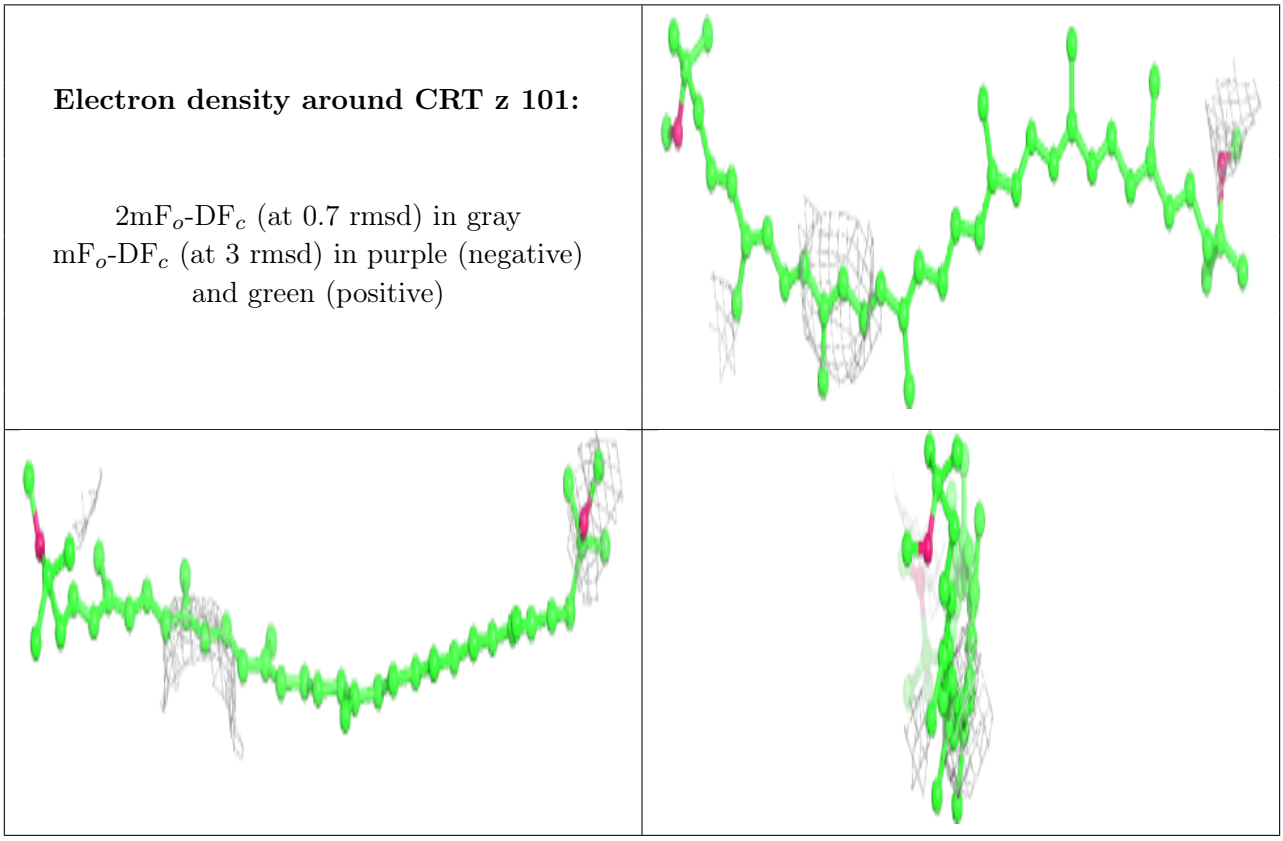
Electron density around CRT R 101:

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



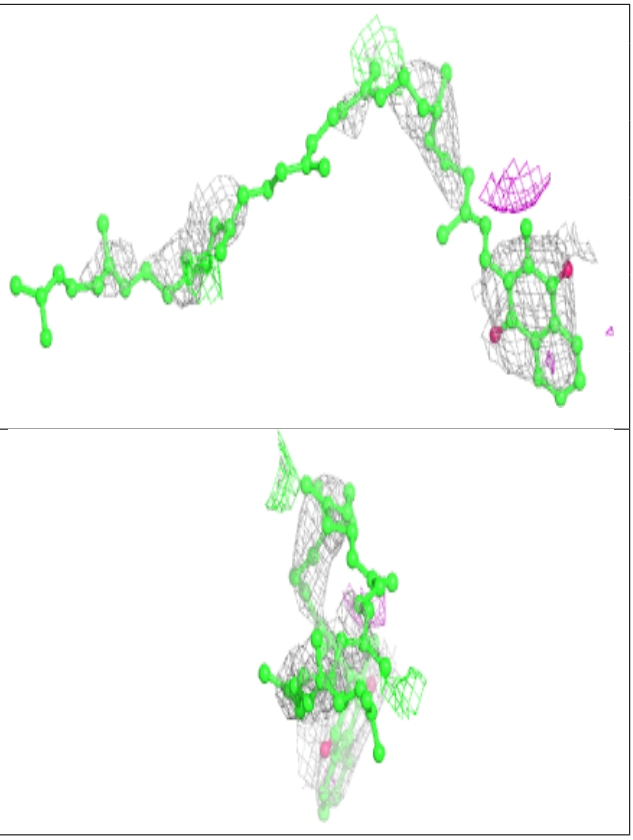
Electron density around CRT z 101:

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



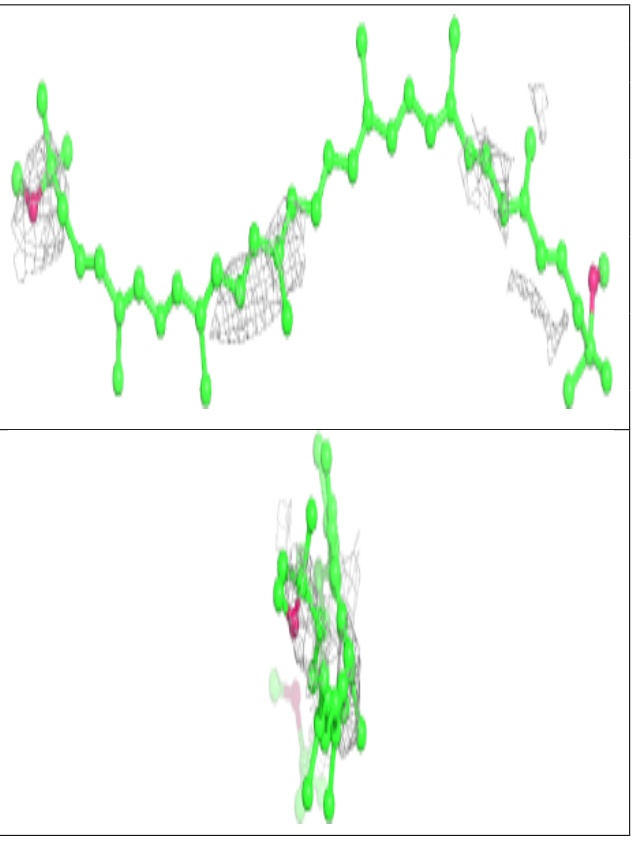
Electron density around MQ8 M 403:

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



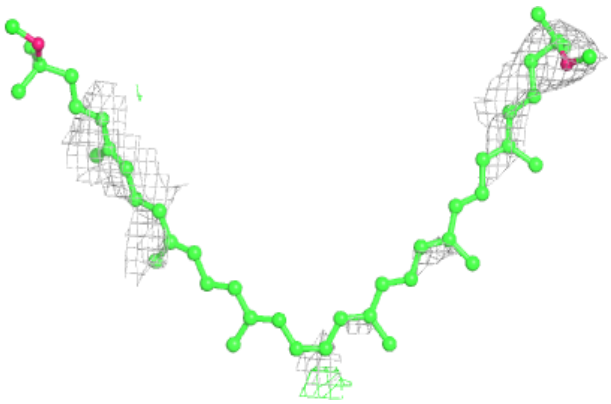
Electron density around CRT i 101:

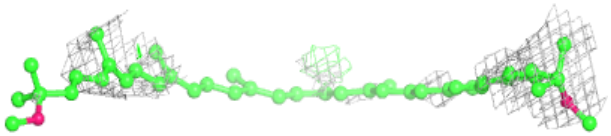
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

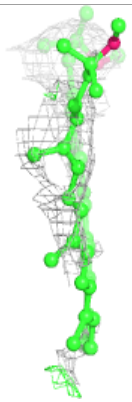


Electron density around CRT M 404:

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

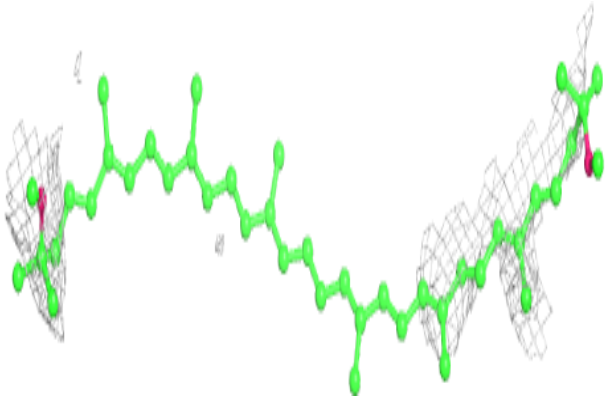


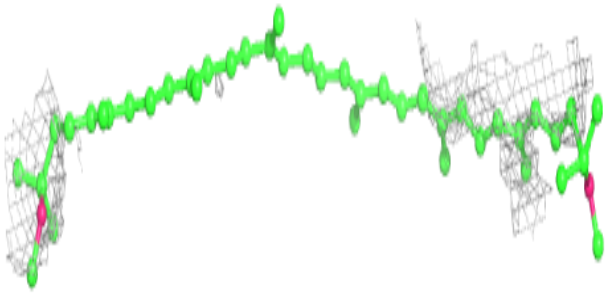


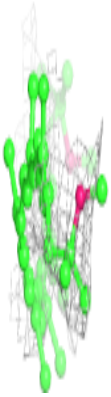


Electron density around CRT E 101:

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

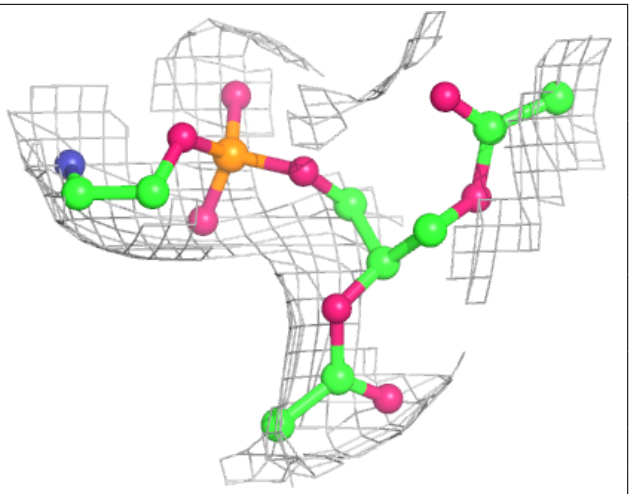


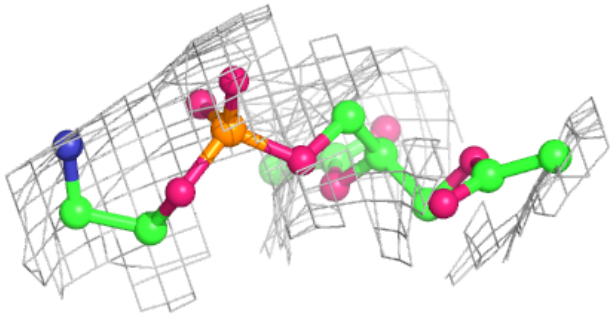


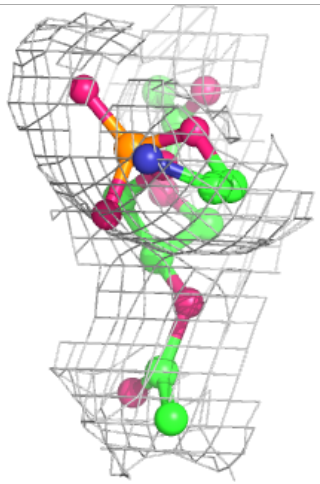


Electron density around PEF H 301:

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

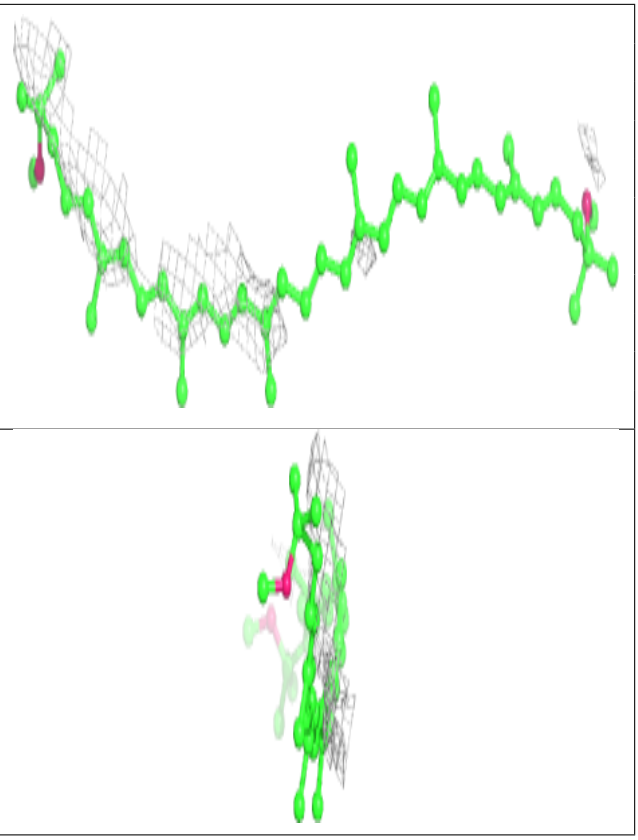






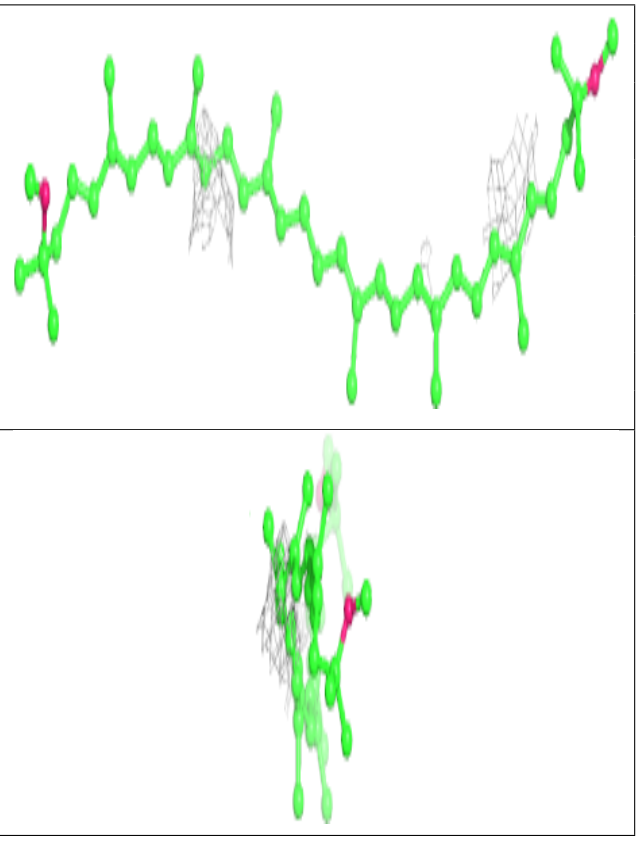
Electron density around CRT G 101:

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



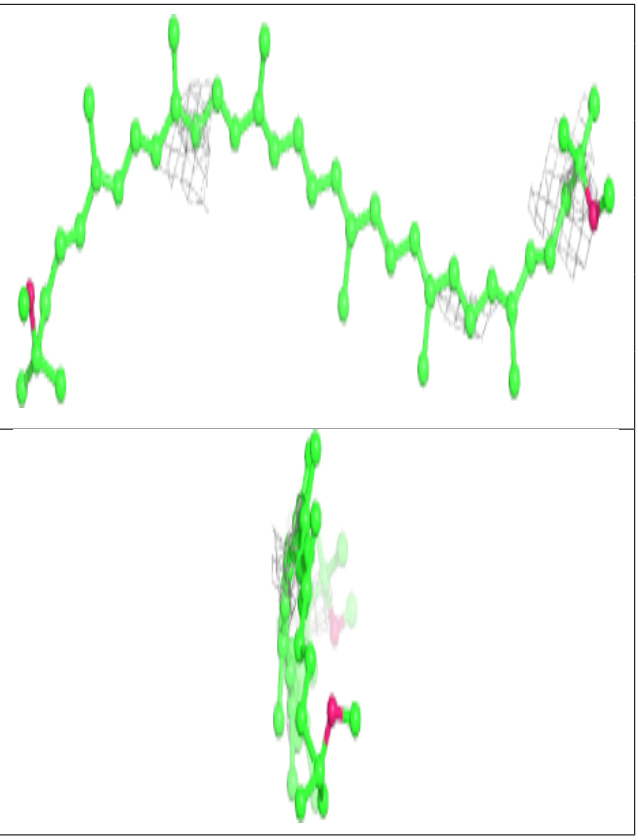
Electron density around CRT AH 102:

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



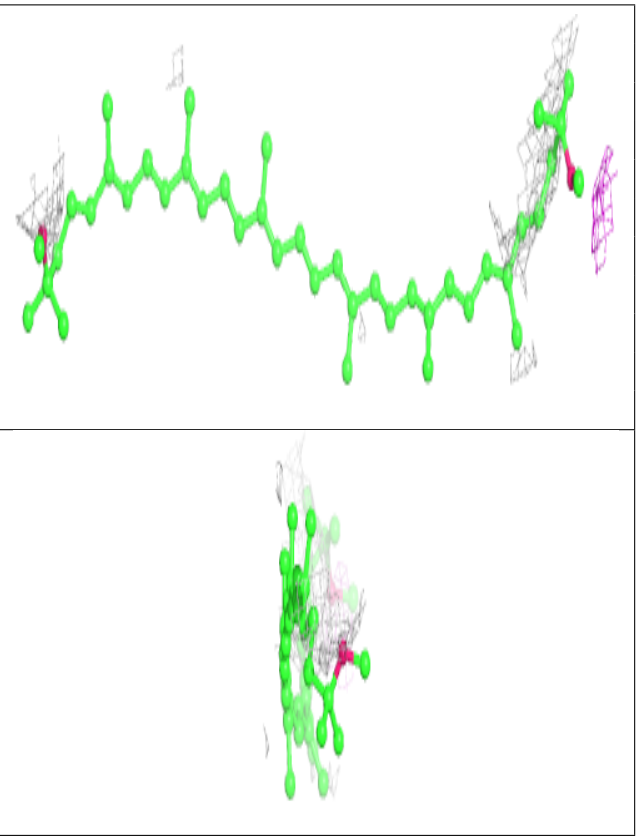
Electron density around CRT 6 101:

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



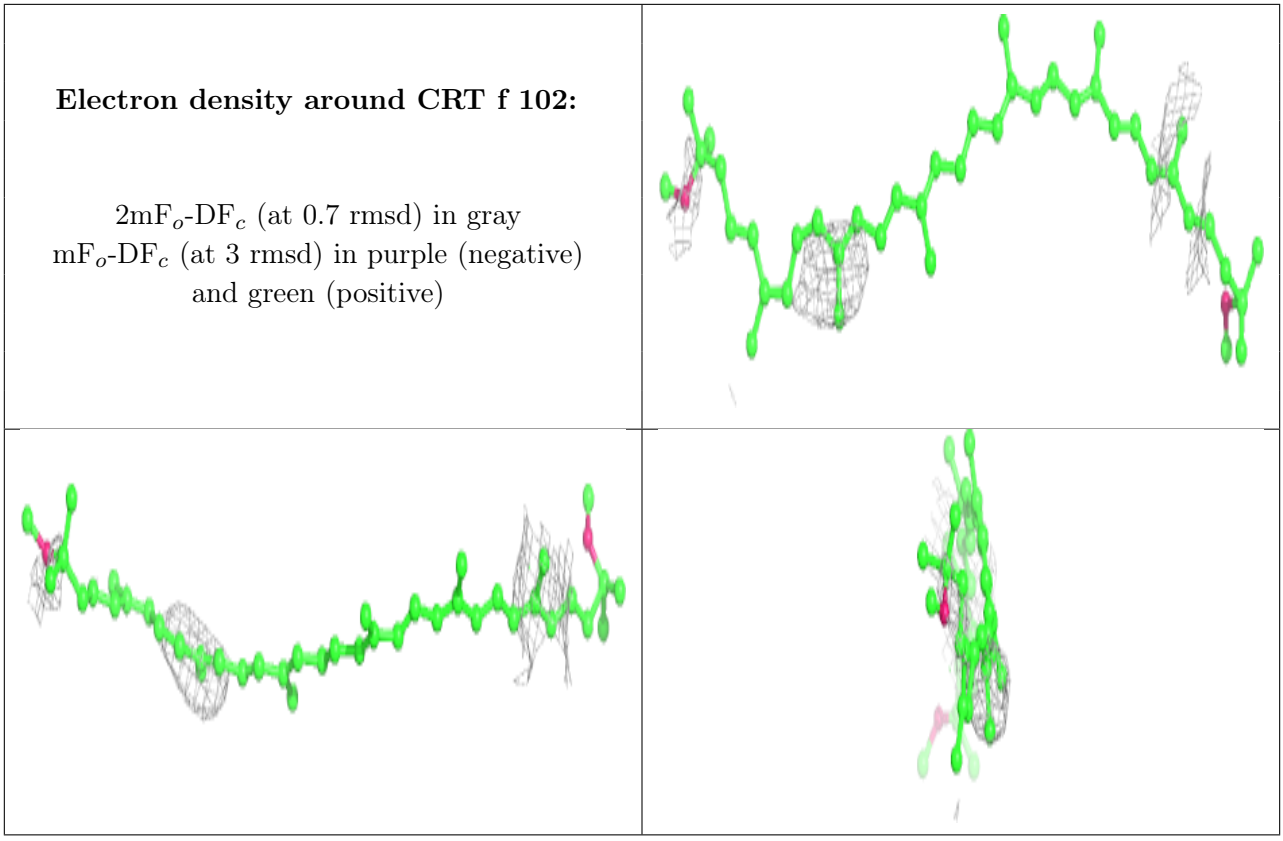
Electron density around CRT s 101:

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



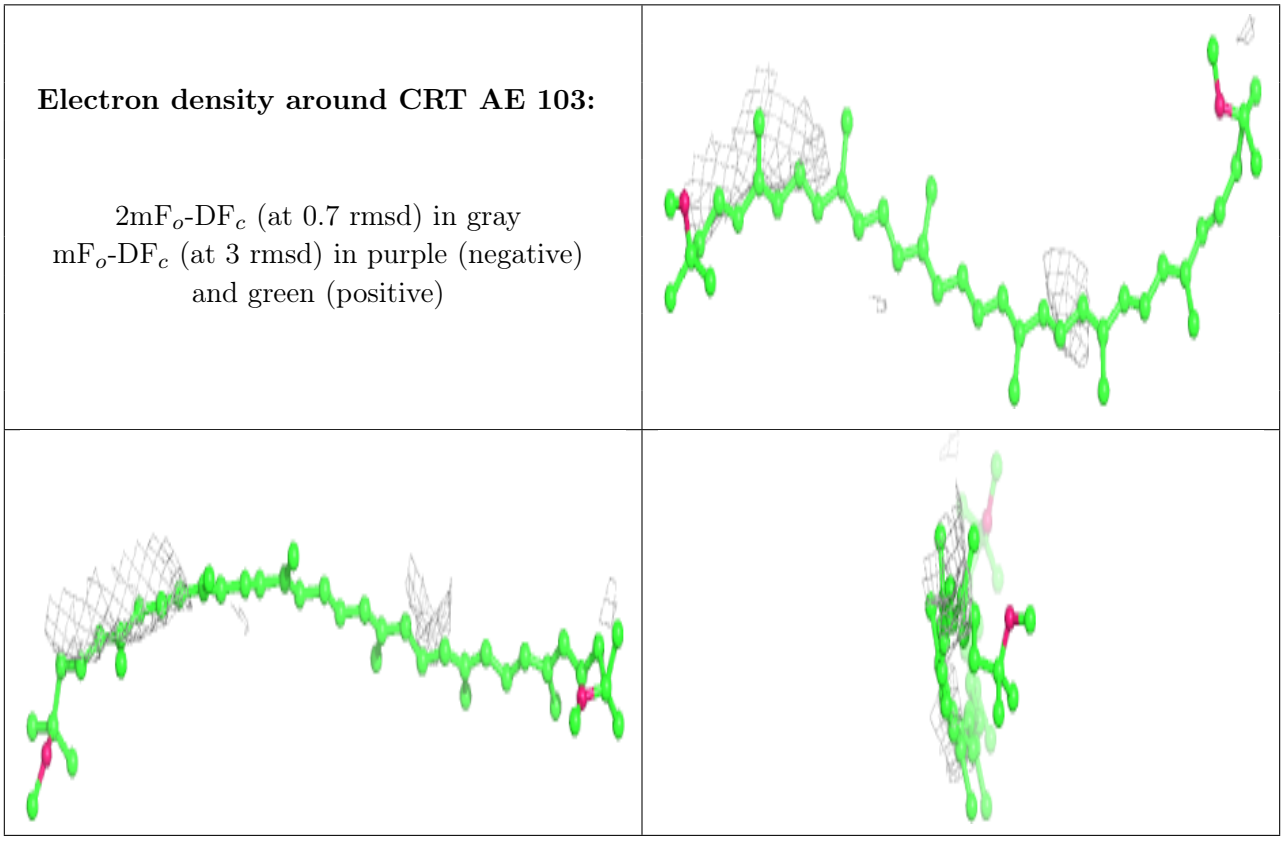
Electron density around CRT f 102:

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



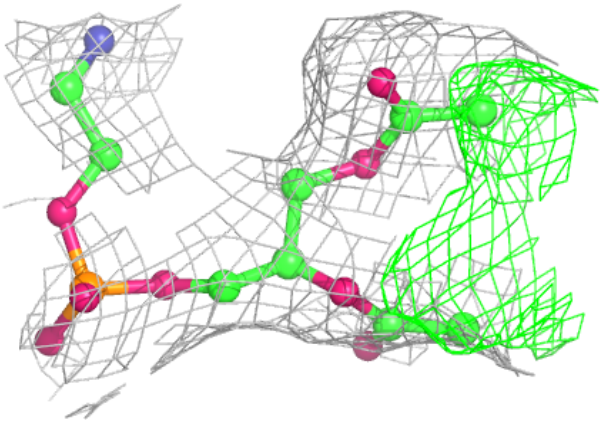
Electron density around CRT AE 103:

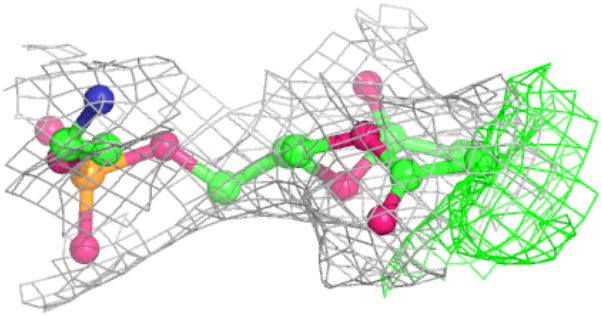
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

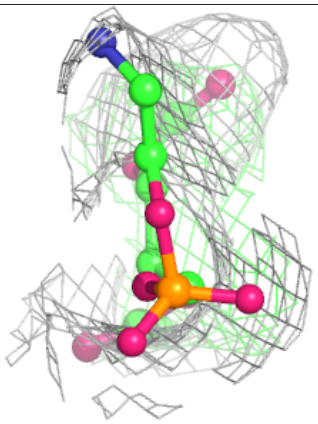


Electron density around PEF A 101:

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

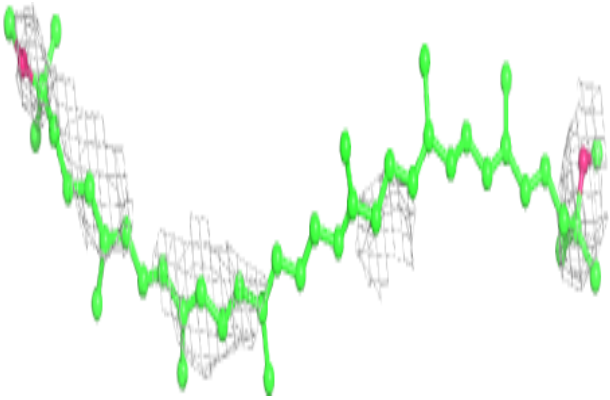


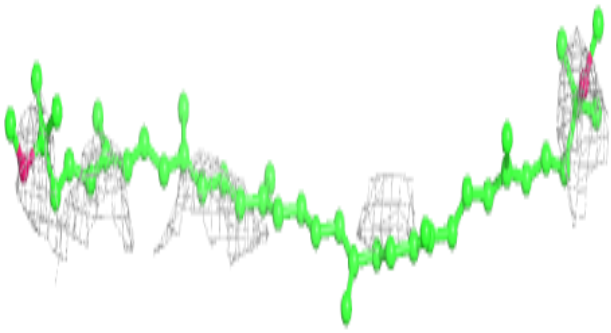


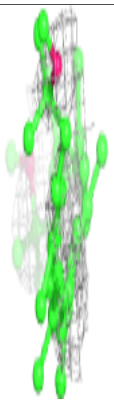


Electron density around CRT P 102:

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

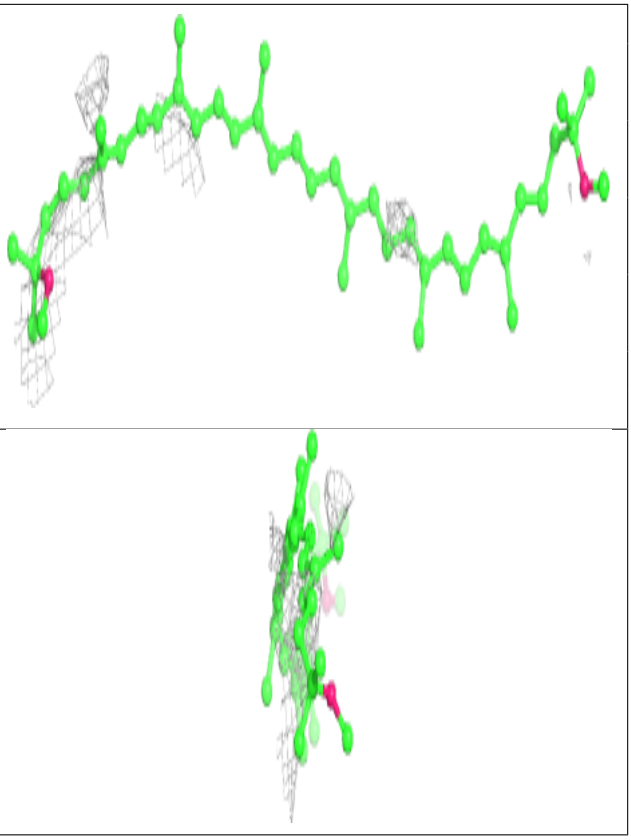


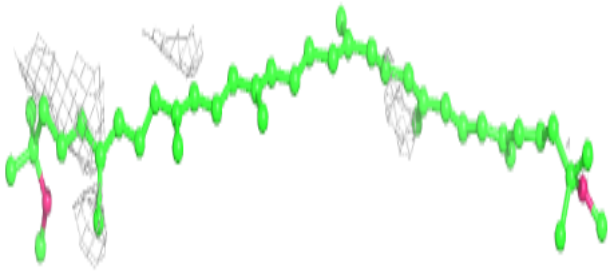




Electron density around CRT e 101:

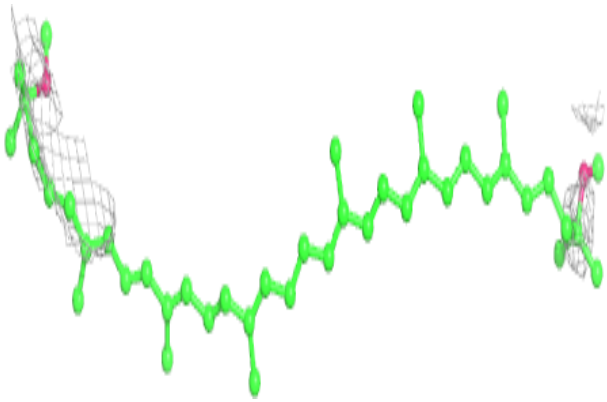
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

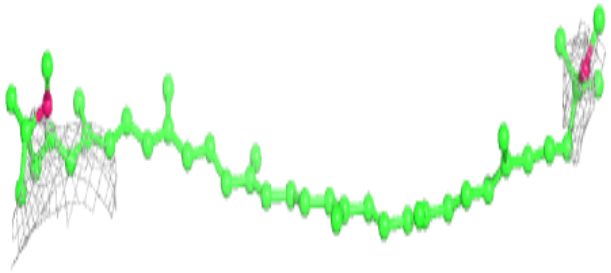


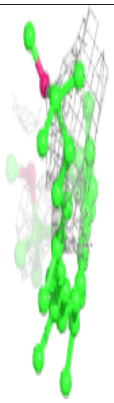


Electron density around CRT T 101:

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

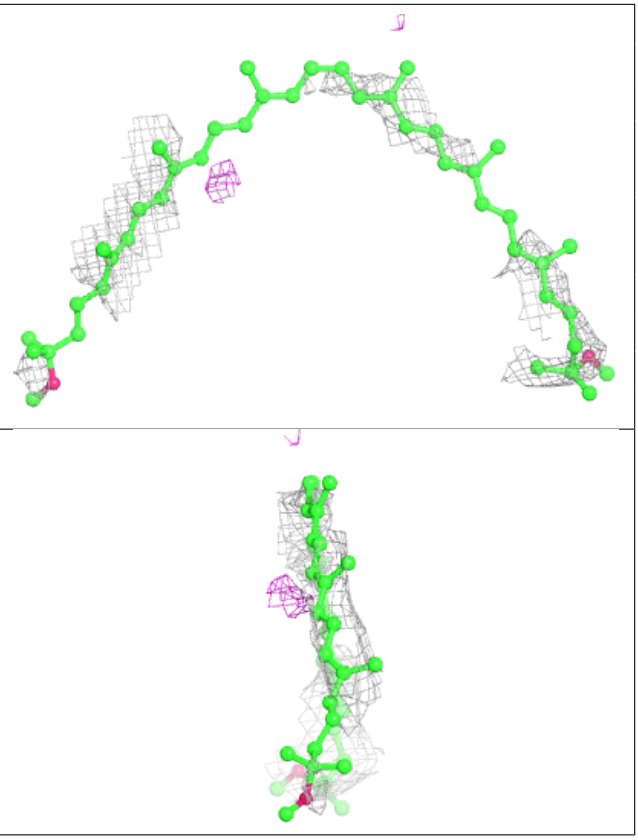






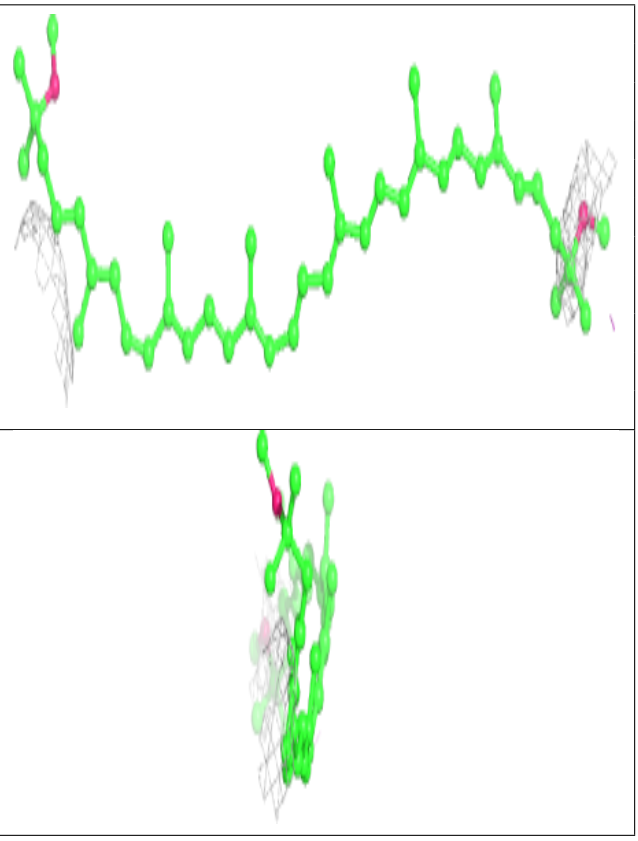
Electron density around CRT y 404:

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



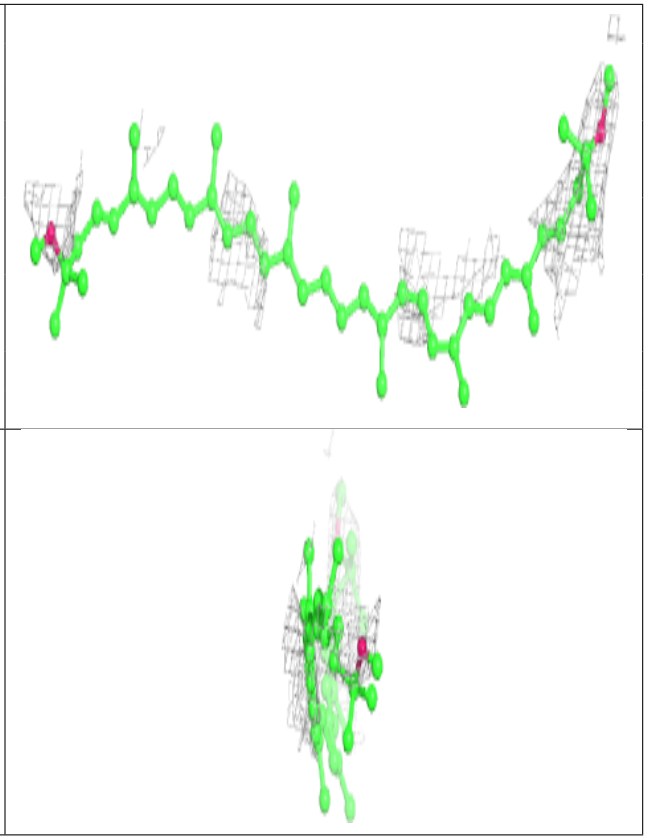
Electron density around CRT AJ 101:

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



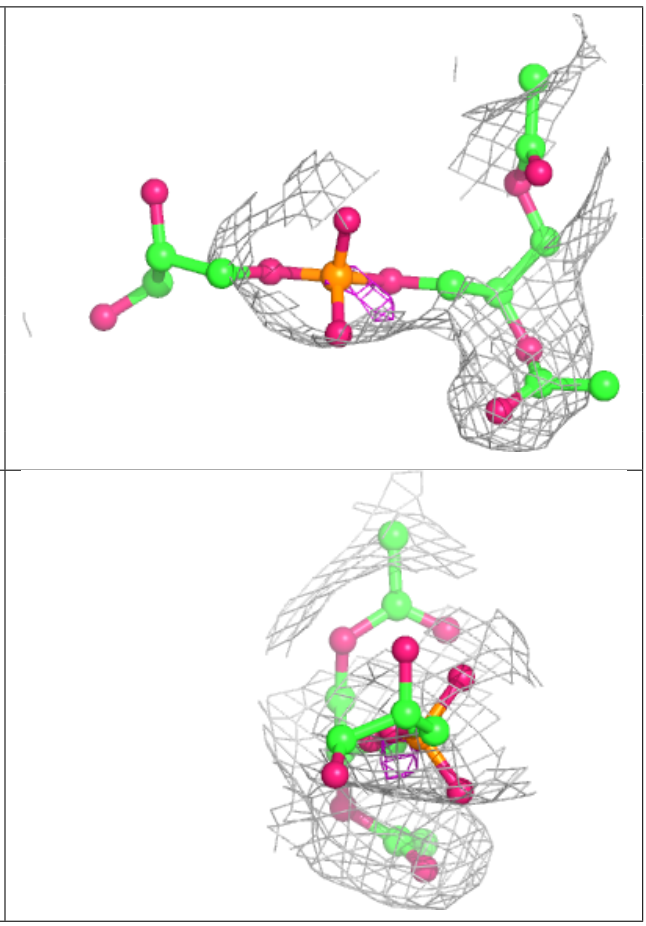
Electron density around CRT AD 102:

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



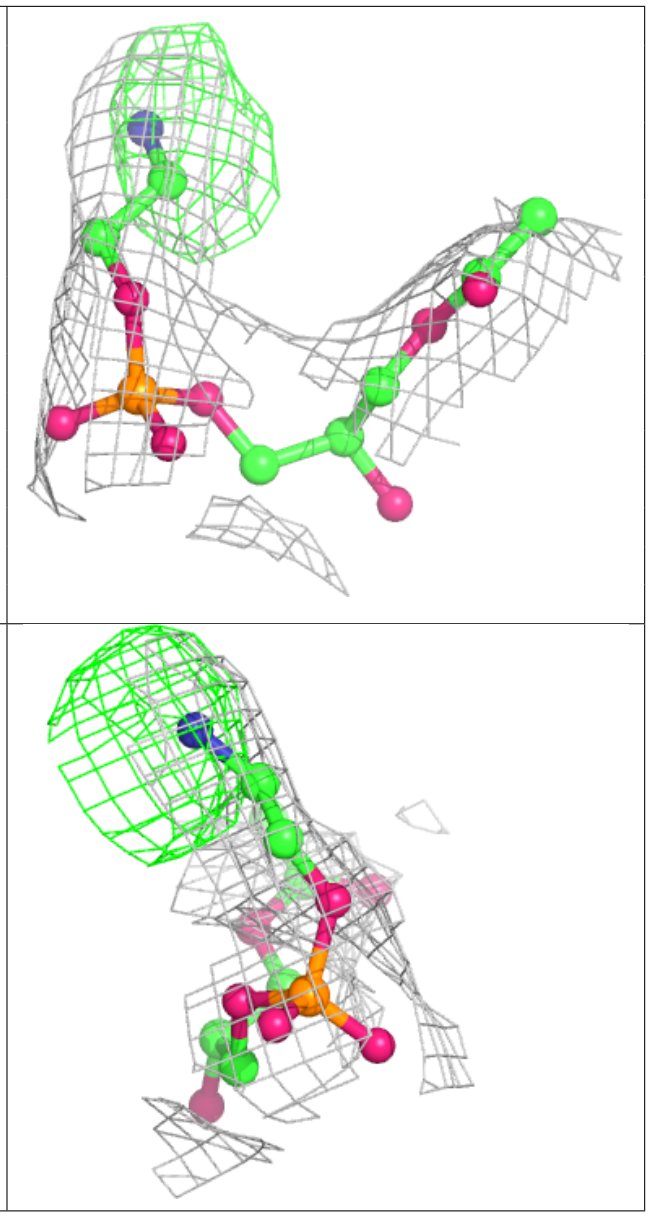
Electron density around PGW AE 101:

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



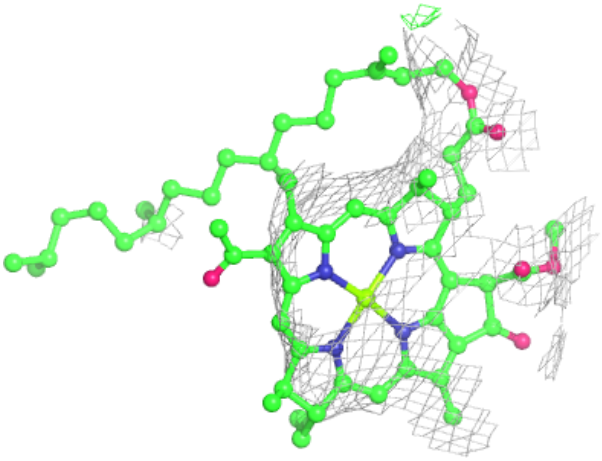
Electron density around PEF p 101:

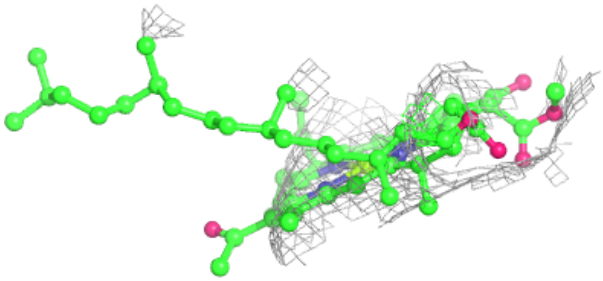
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

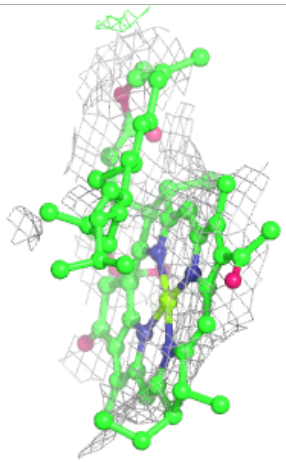


Electron density around BCL AC 102:

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

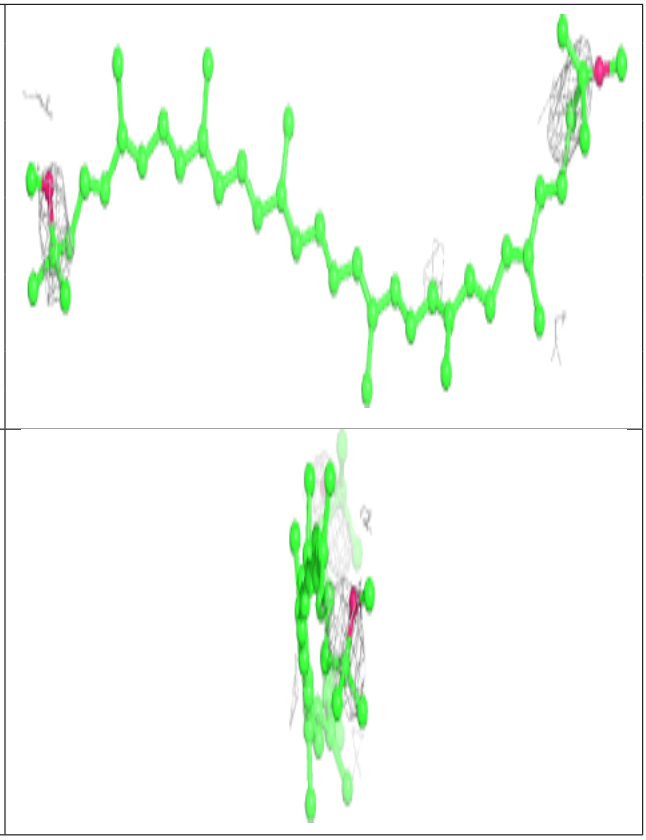






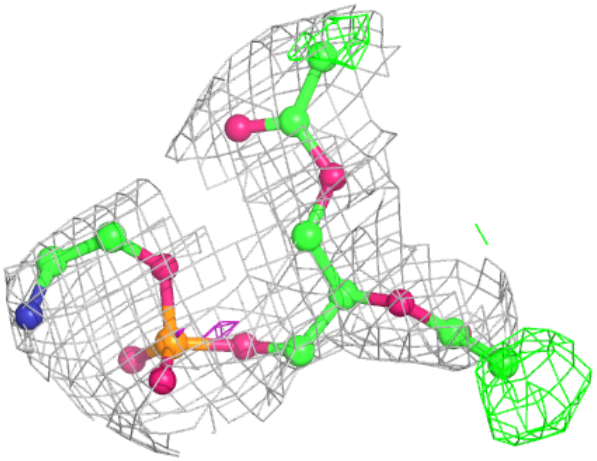
Electron density around CRT U 102:

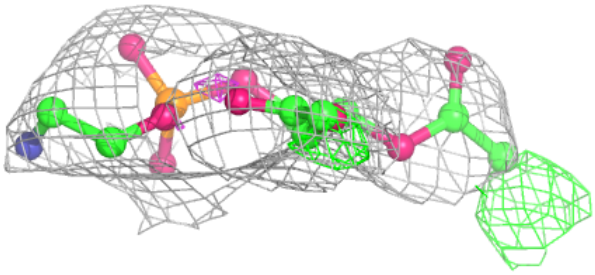
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

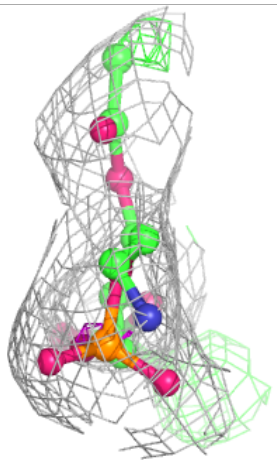


Electron density around PEF m 101:

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

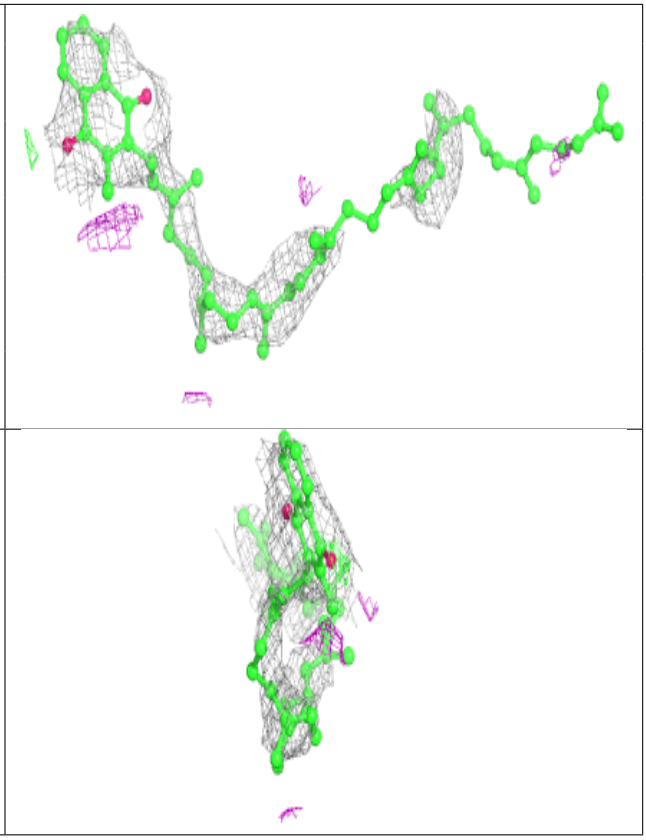






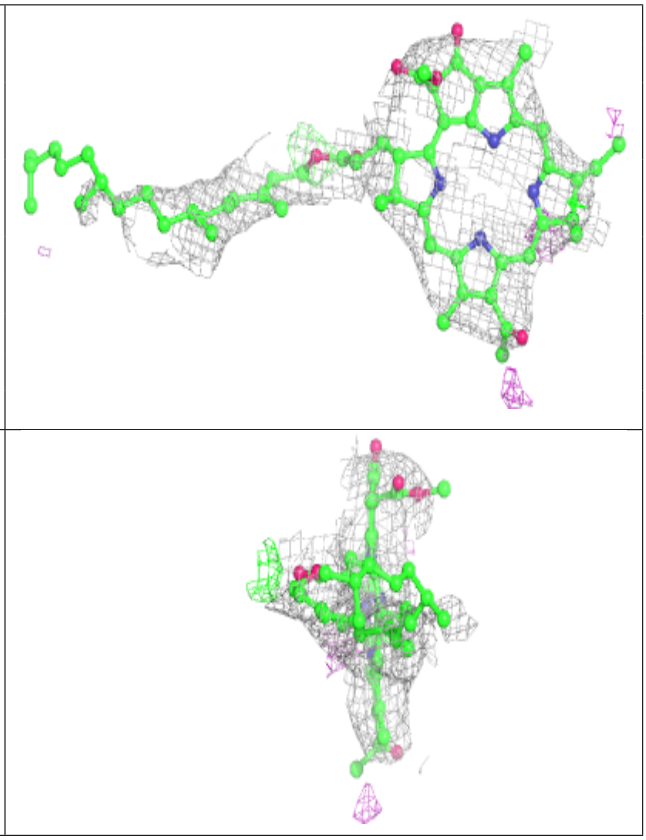
Electron density around MQ8 y 403:

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



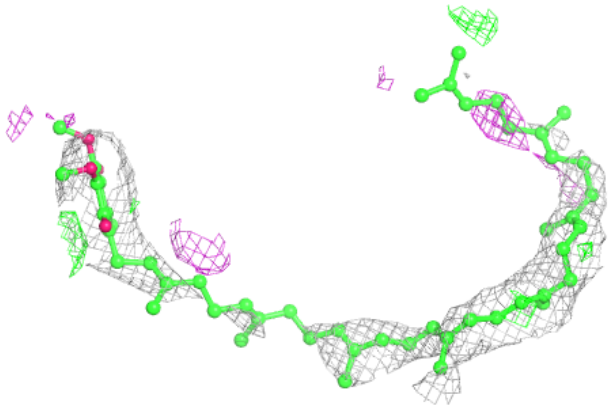
Electron density around BPH y 402:

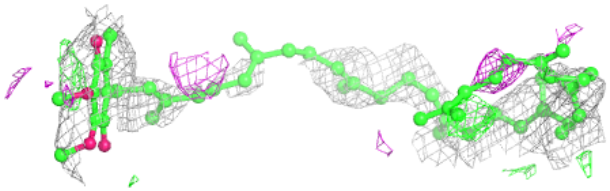
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

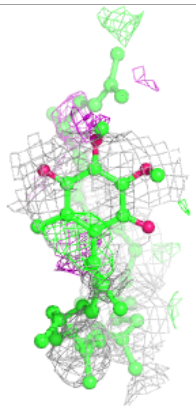


Electron density around UQ8 L 304:

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

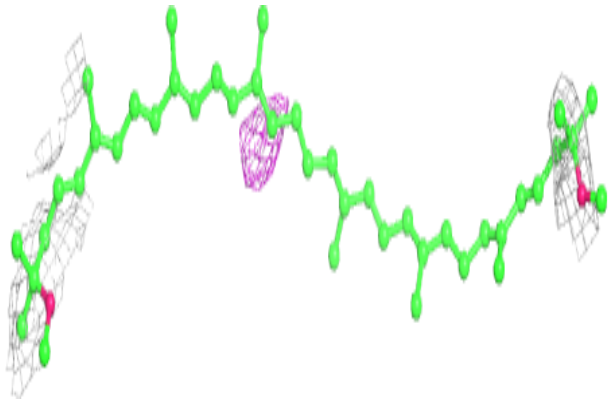


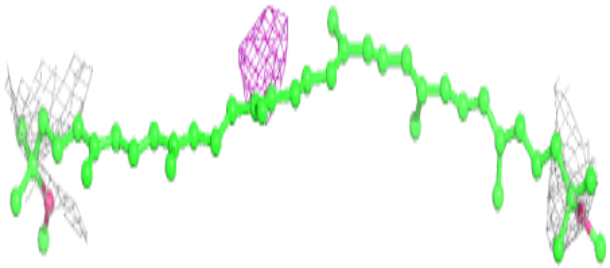




Electron density around CRT AL 101:

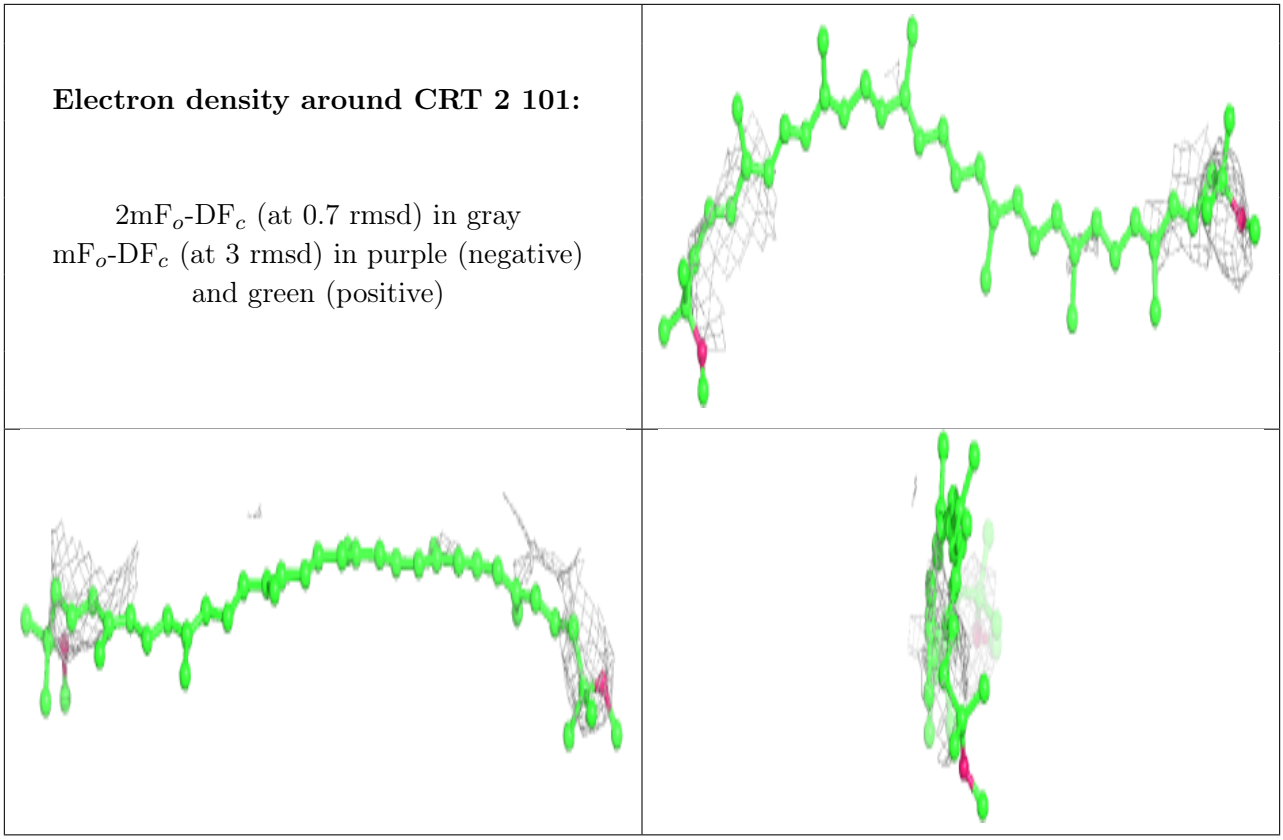
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





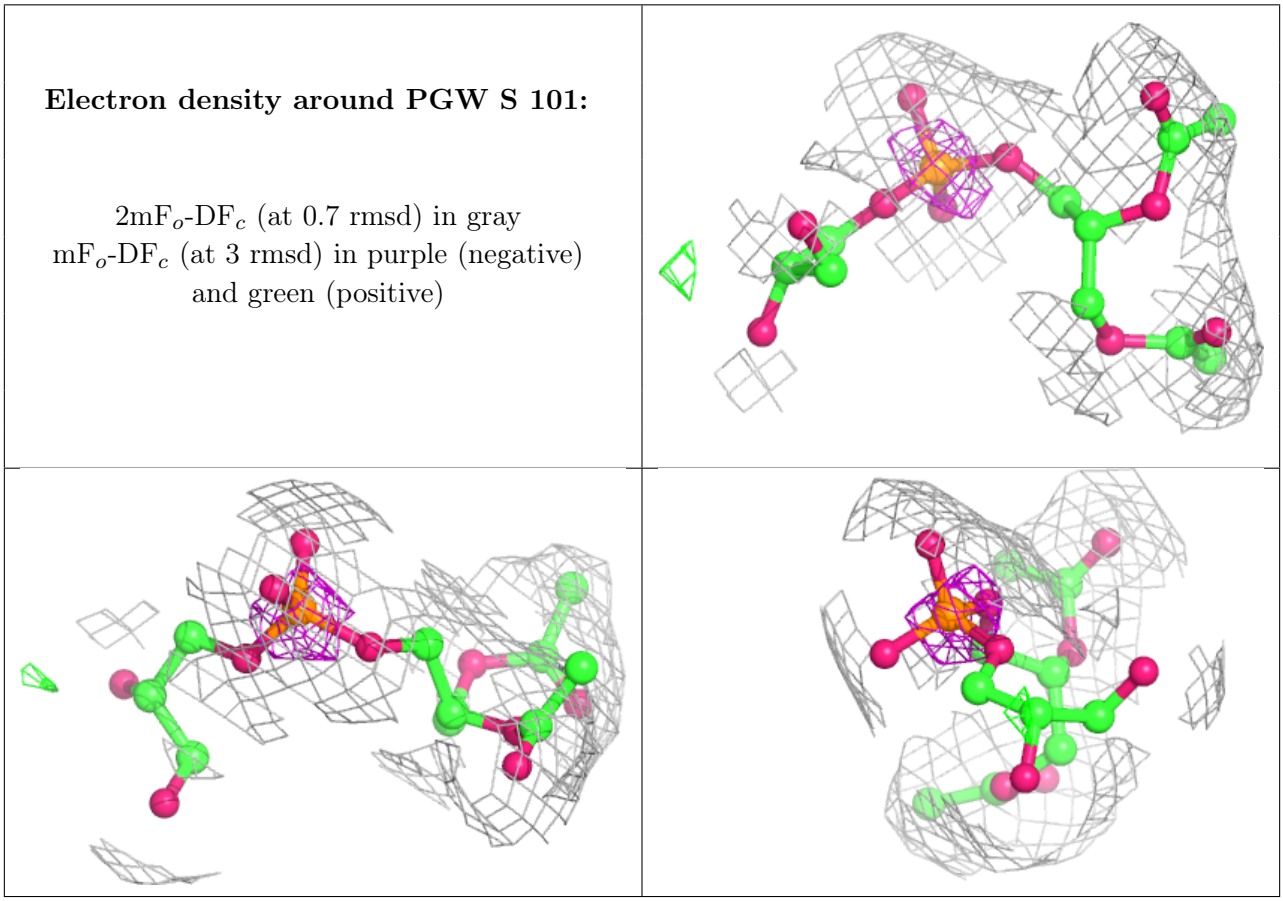
Electron density around CRT 2 101:

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



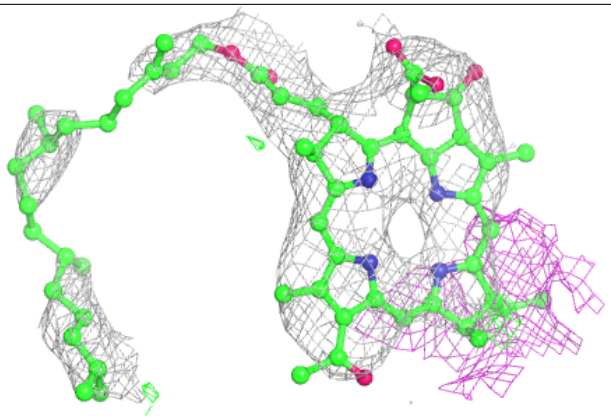
Electron density around PGW S 101:

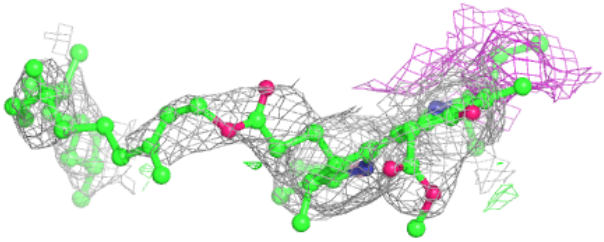
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

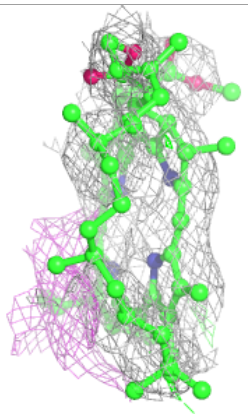


Electron density around BPH x 302:

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

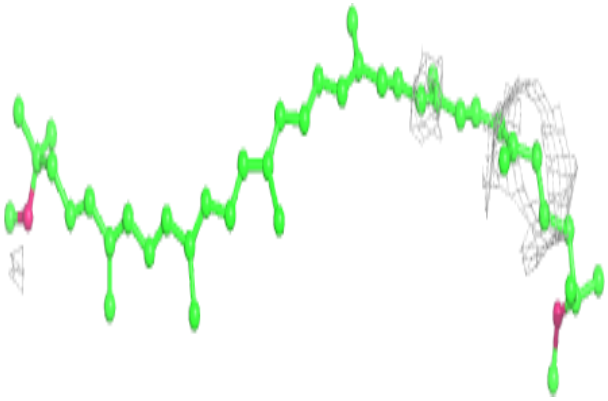


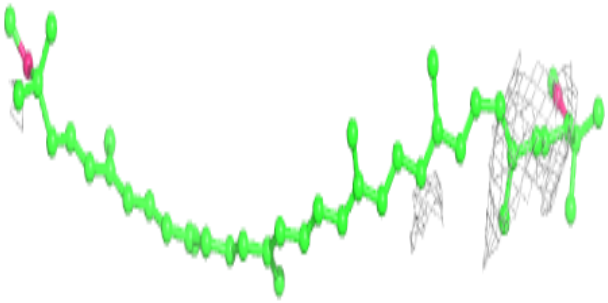




Electron density around CRT 9 102:

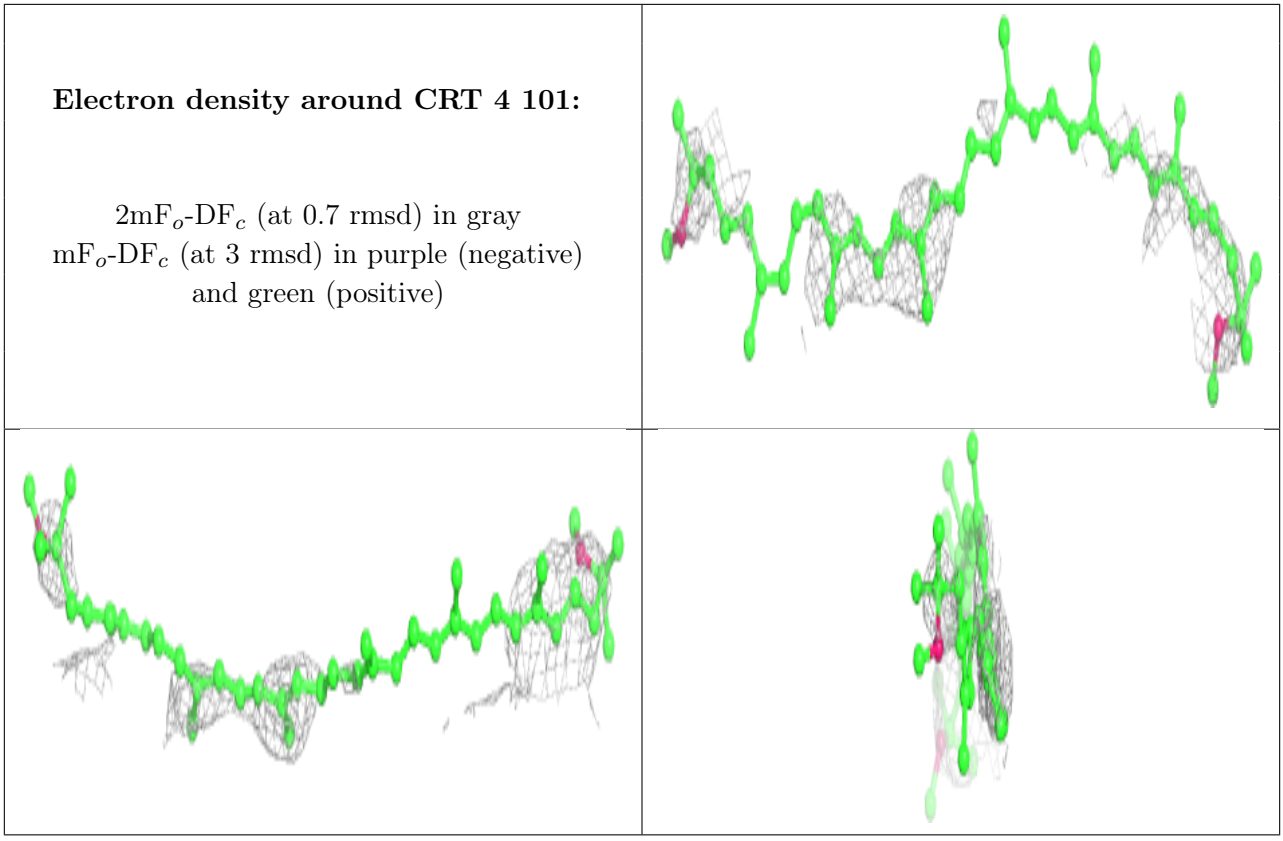
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





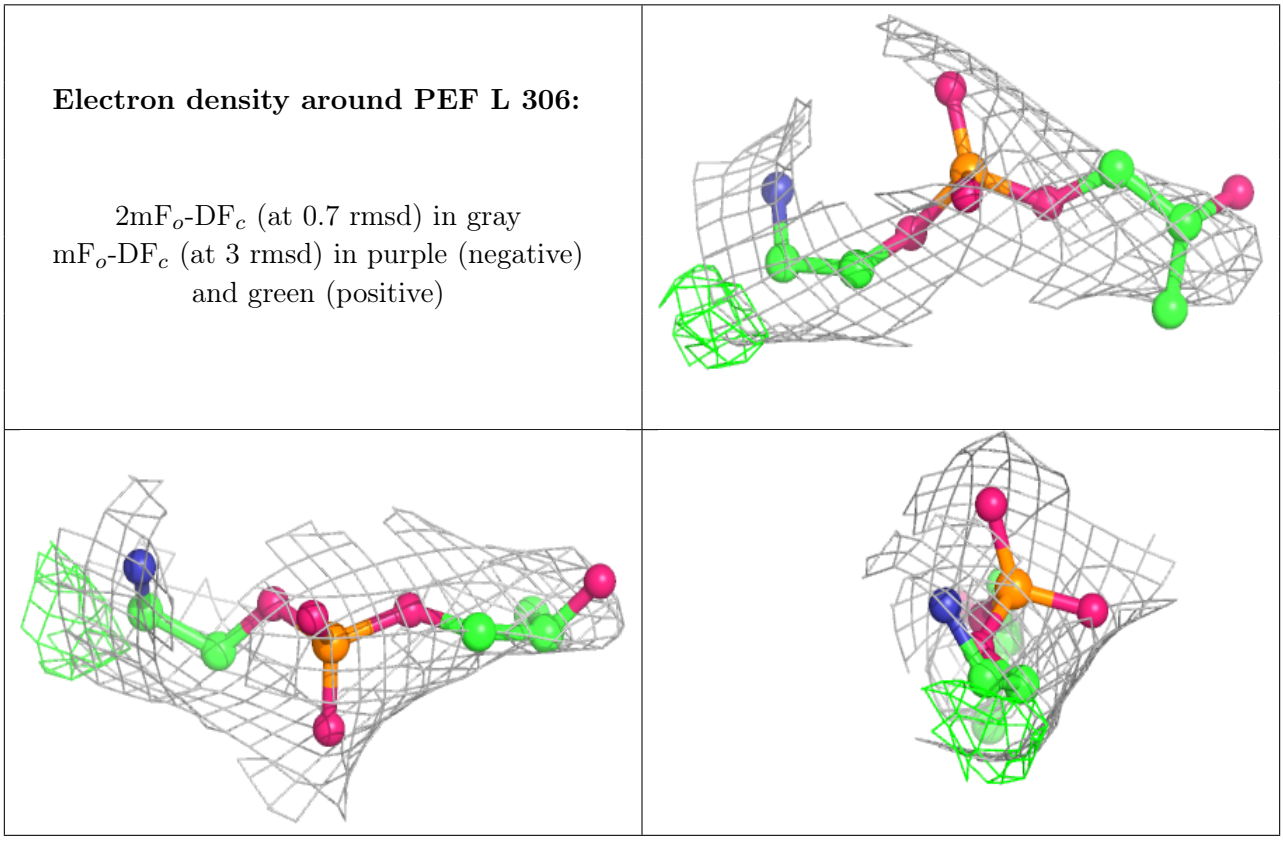
Electron density around CRT 4 101:

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



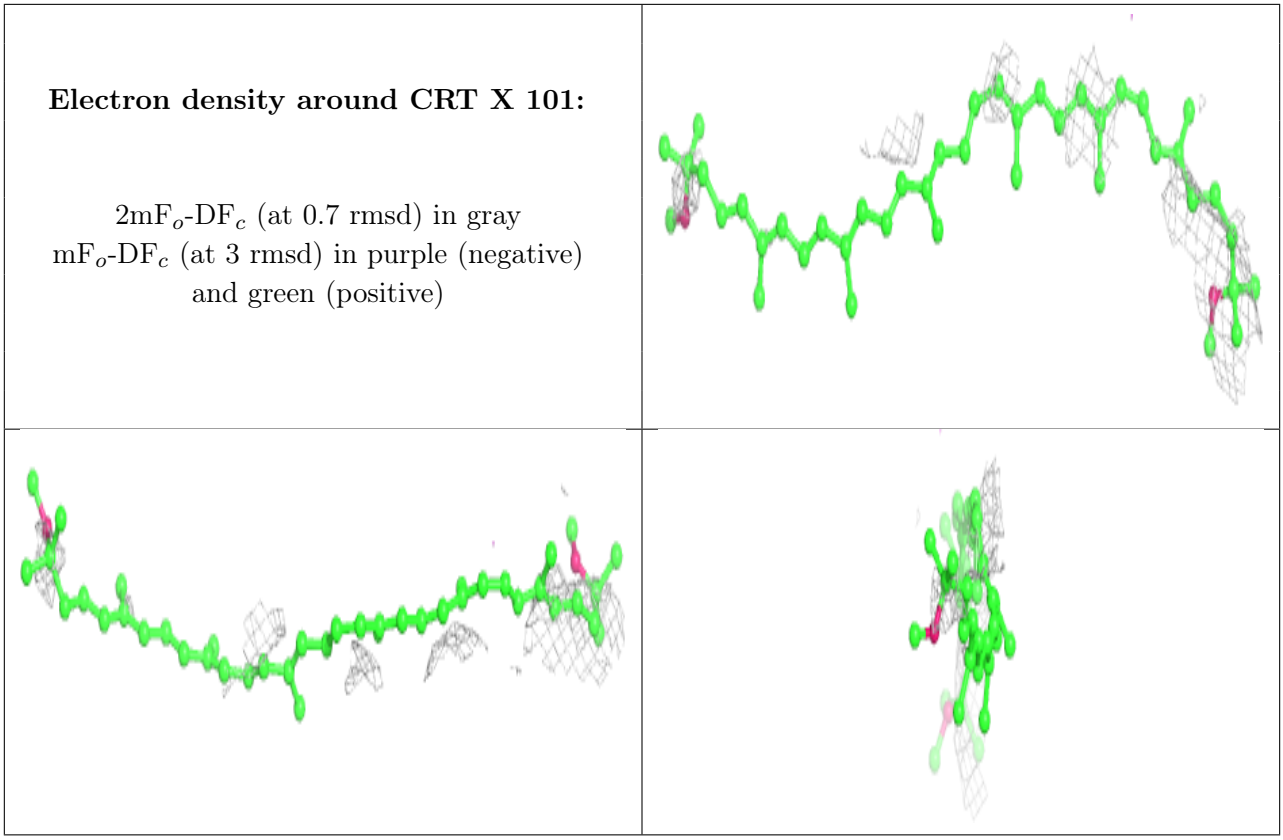
Electron density around PEF L 306:

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



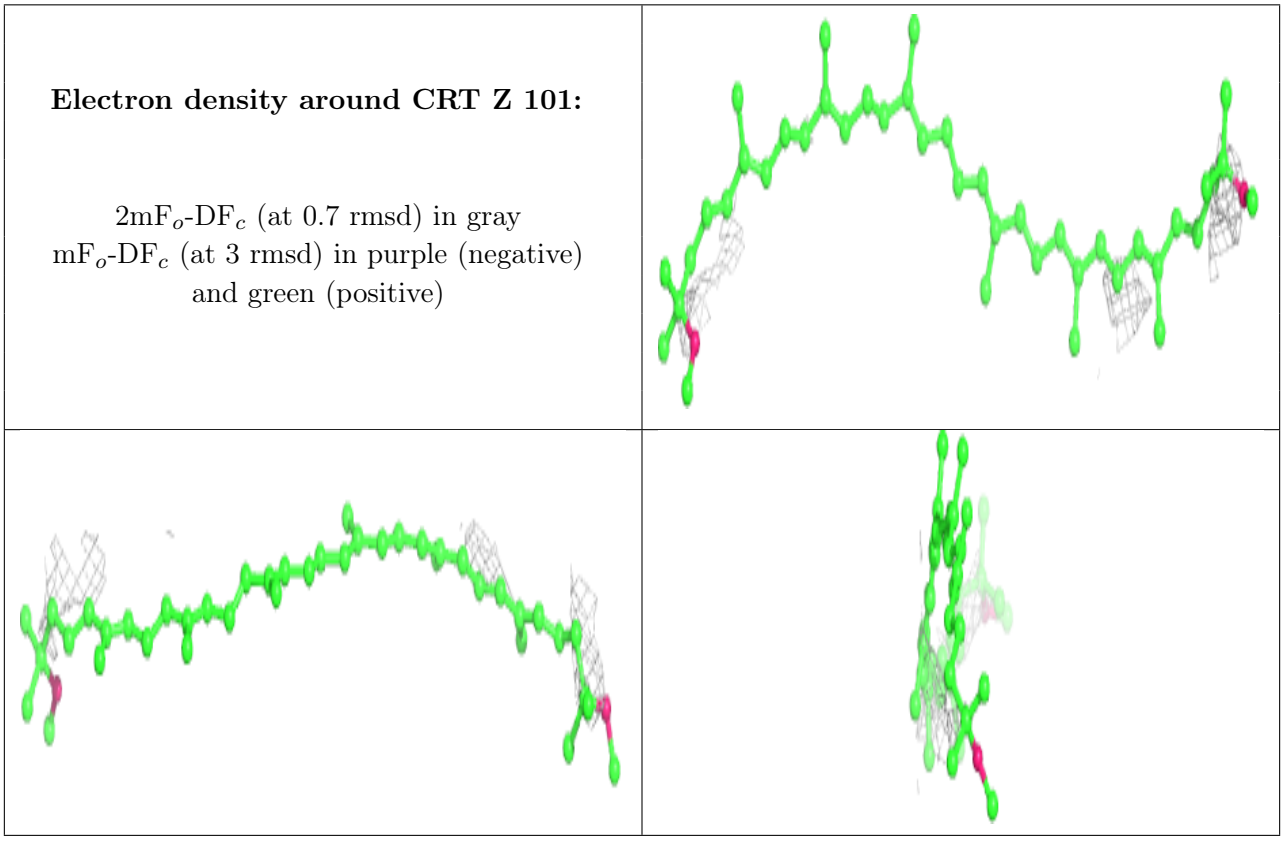
Electron density around CRT X 101:

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



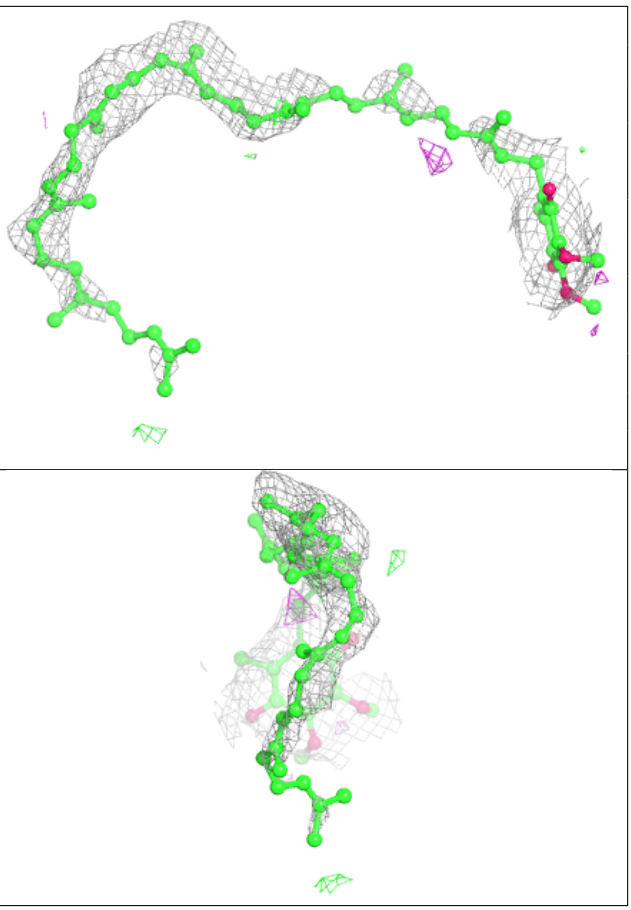
Electron density around CRT Z 101:

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



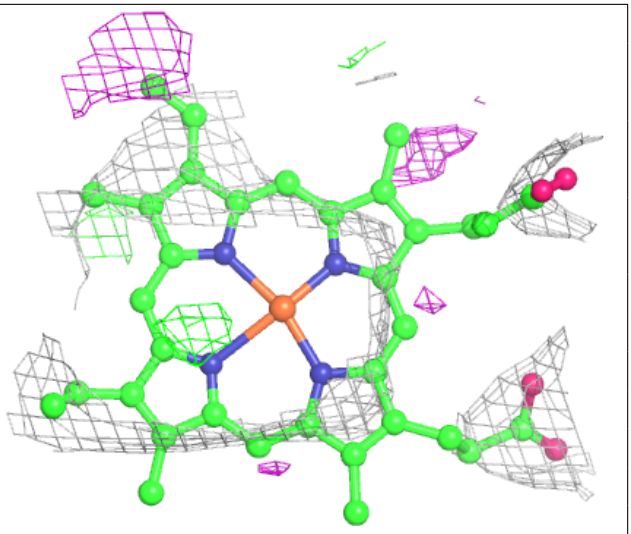
Electron density around UQ8 x 304:

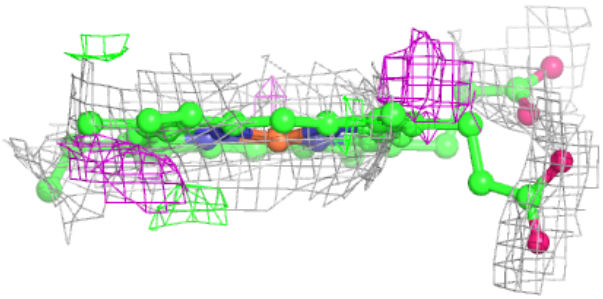
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

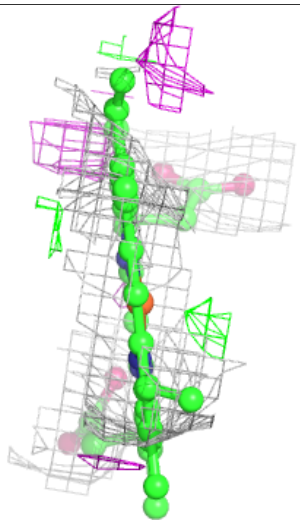


Electron density around HEM o 501:

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

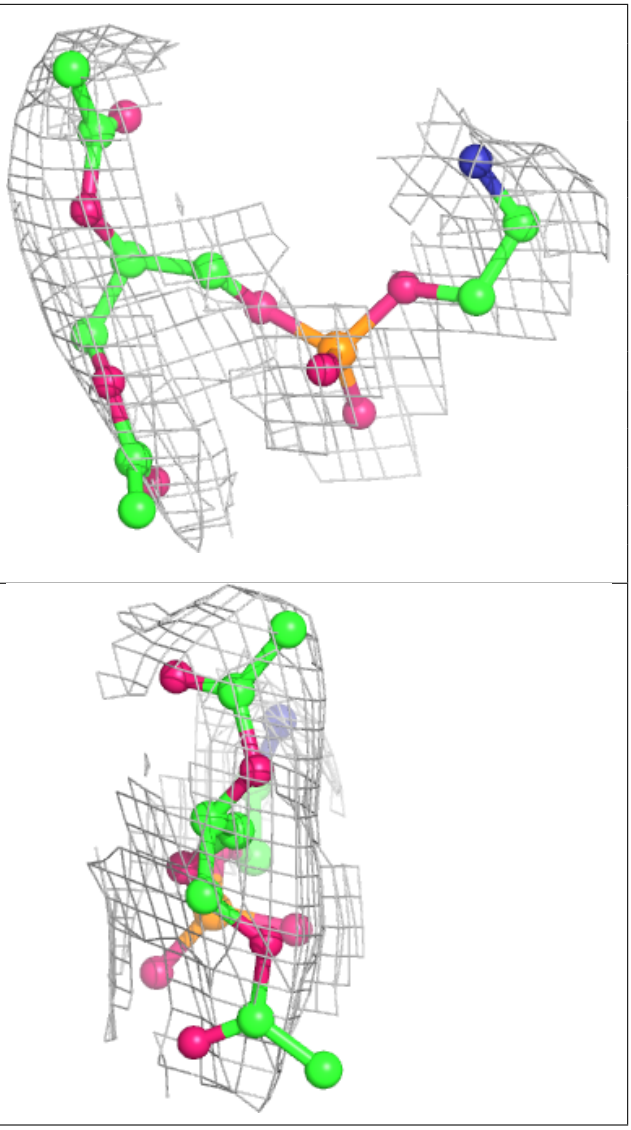






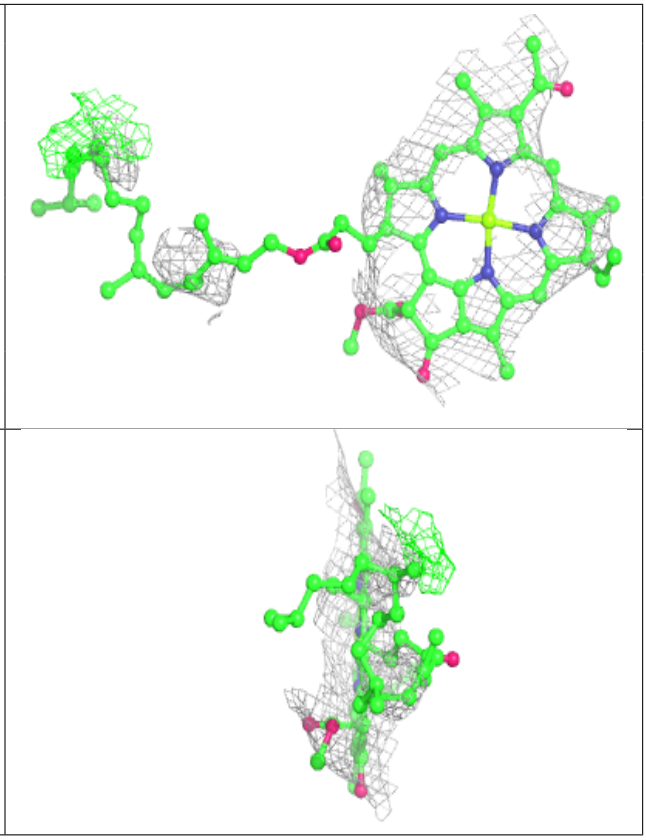
Electron density around PEF y 406:

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



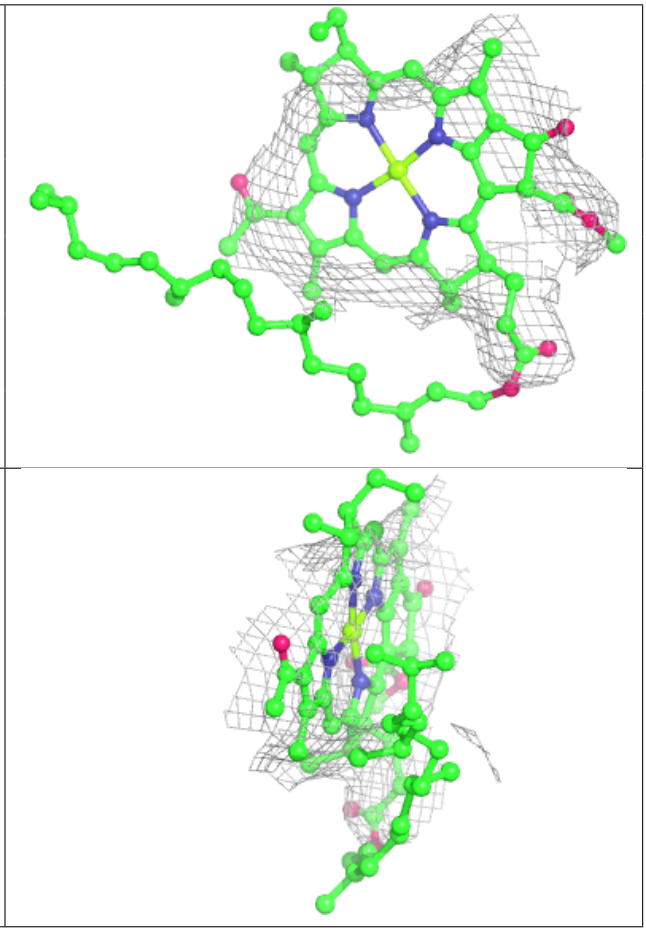
Electron density around BCL j 101:

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



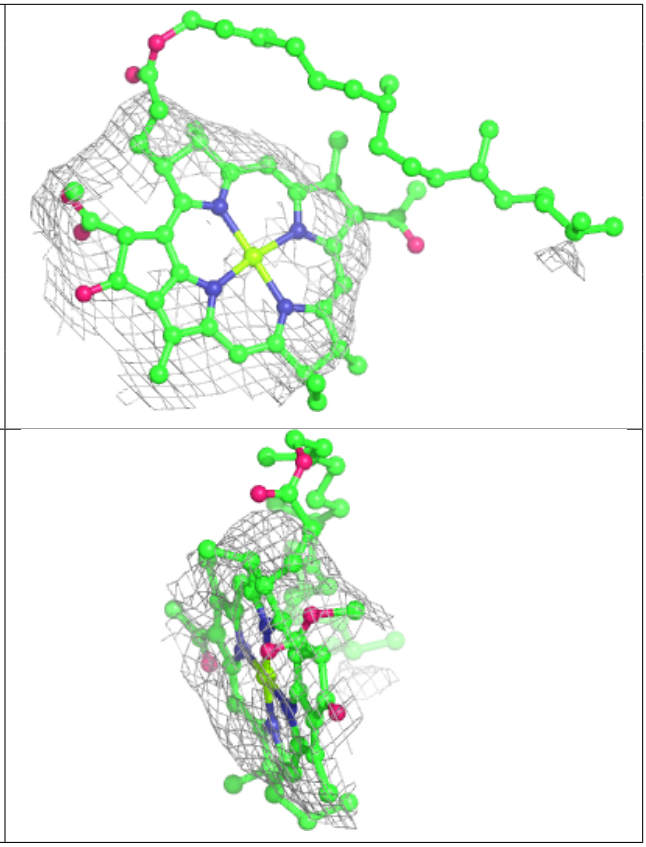
Electron density around BCL 0 101:

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



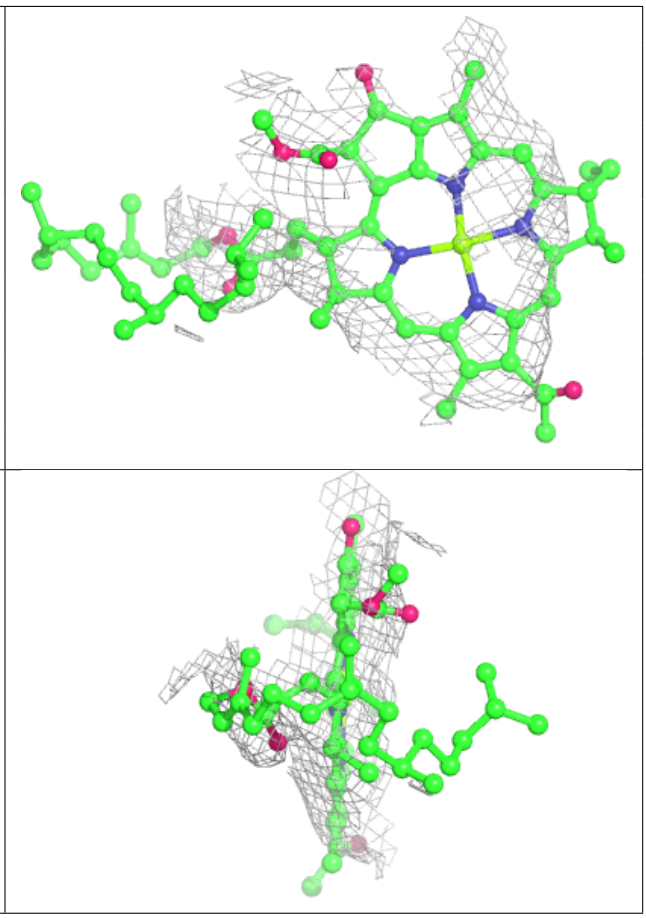
Electron density around BCL AB 101:

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



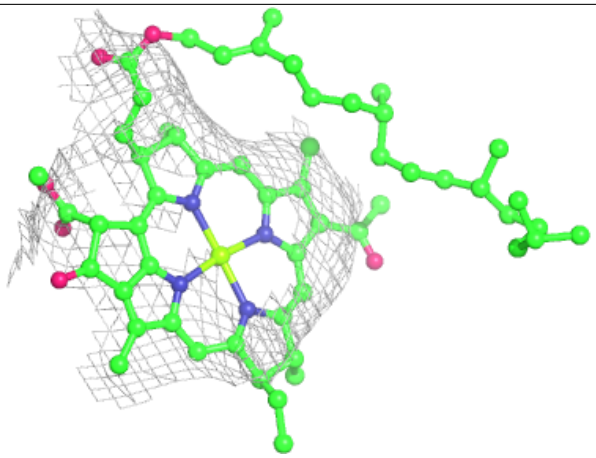
Electron density around BCL AD 101:

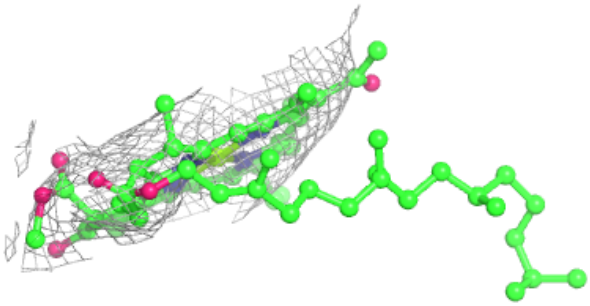
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

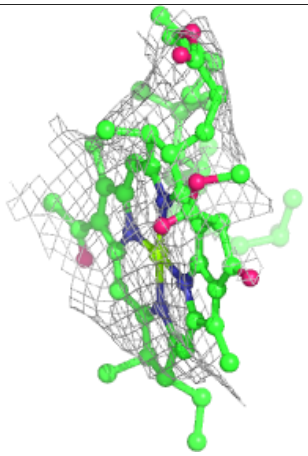


Electron density around BCL O 101:

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

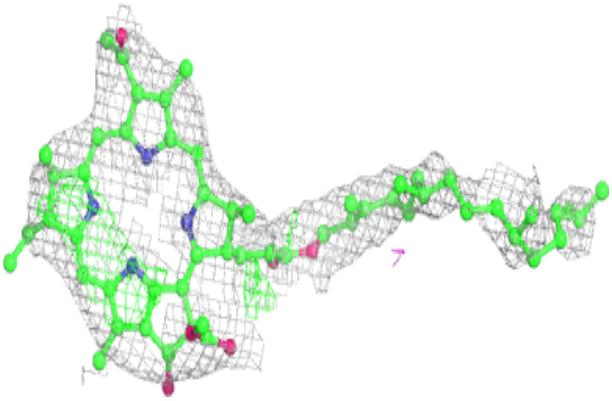


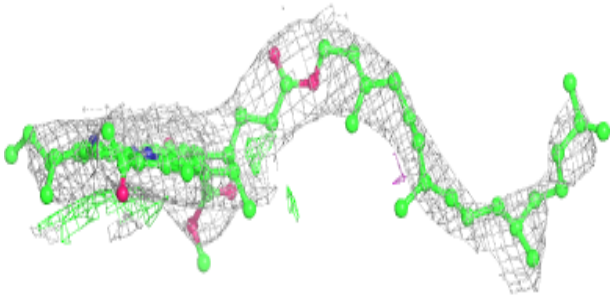


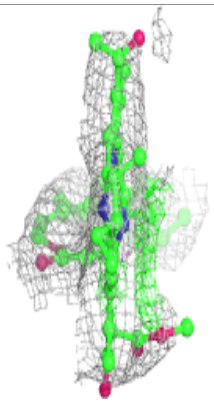


Electron density around BPH M 402:

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

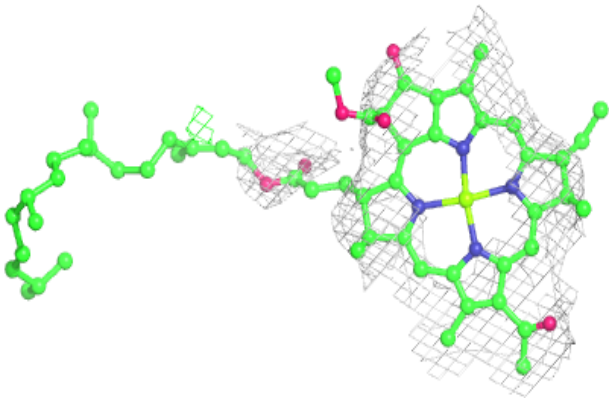


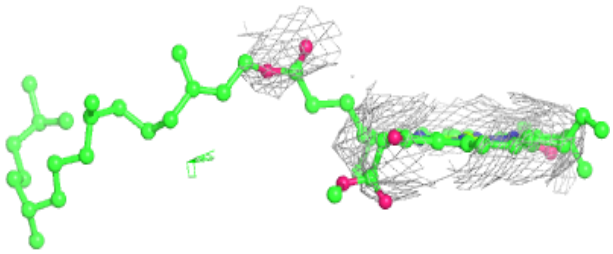


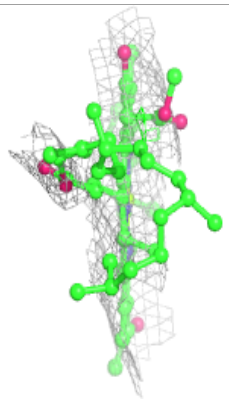


Electron density around BCL m 102:

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

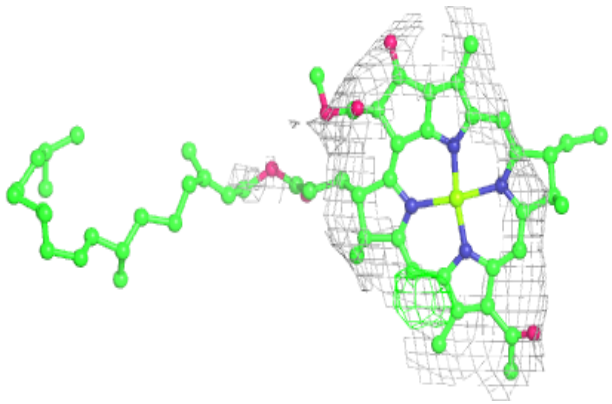


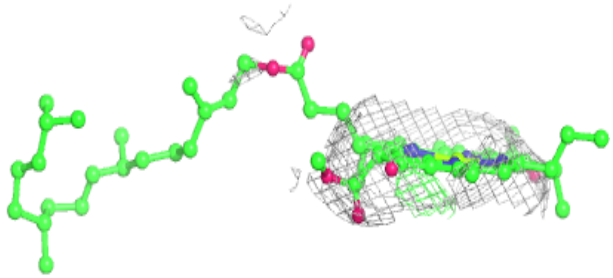


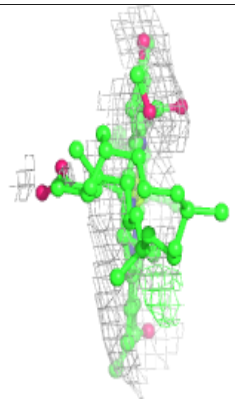


Electron density around BCL K 101:

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

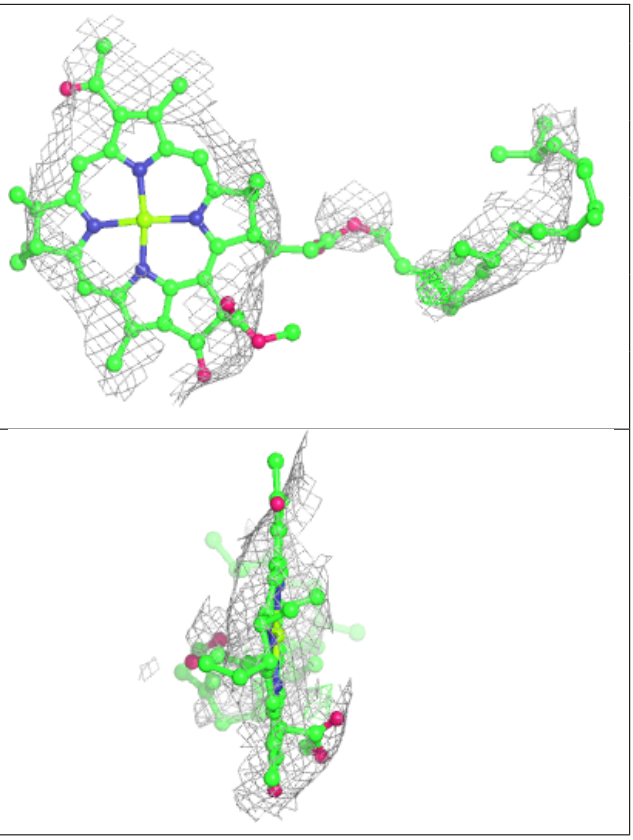






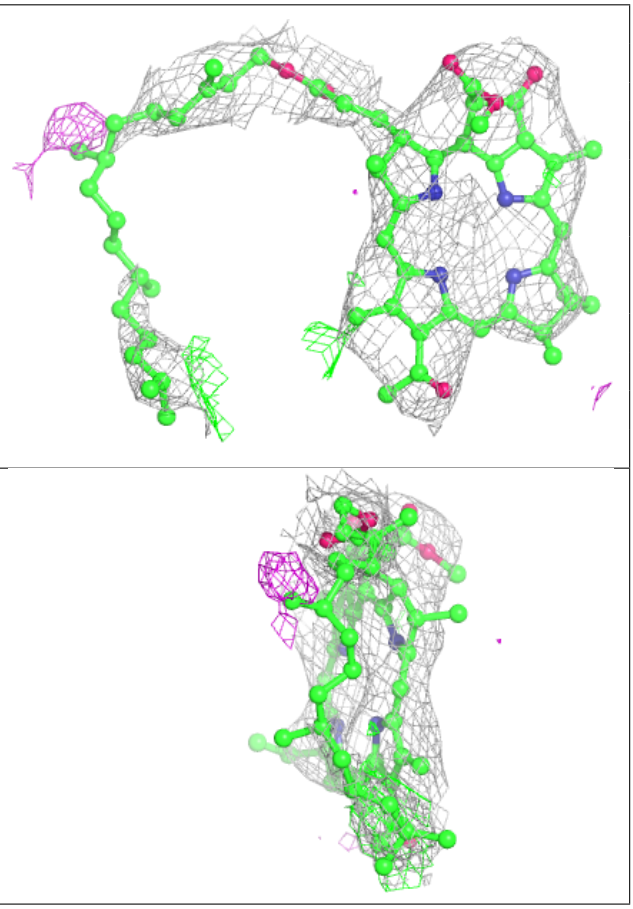
Electron density around BCL l 101:

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



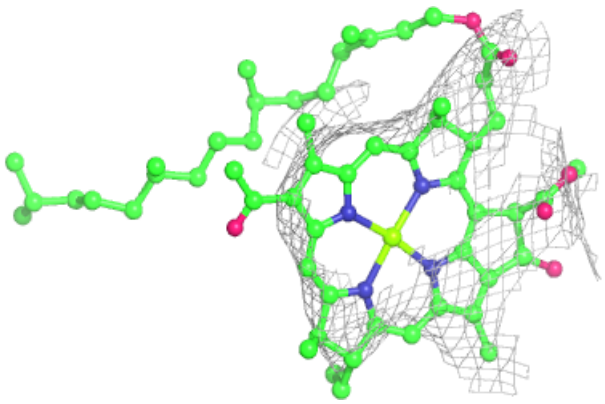
Electron density around BPH L 302:

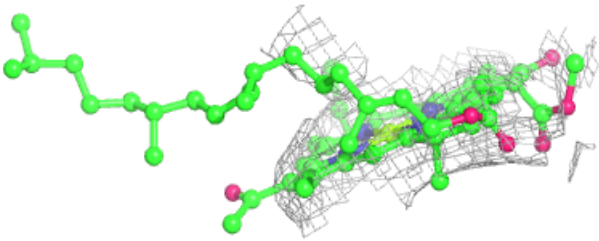
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

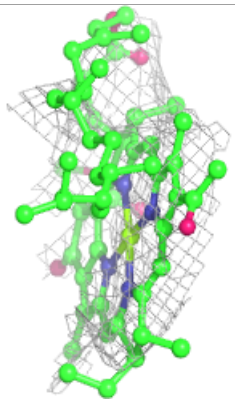


Electron density around BCL AE 104:

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

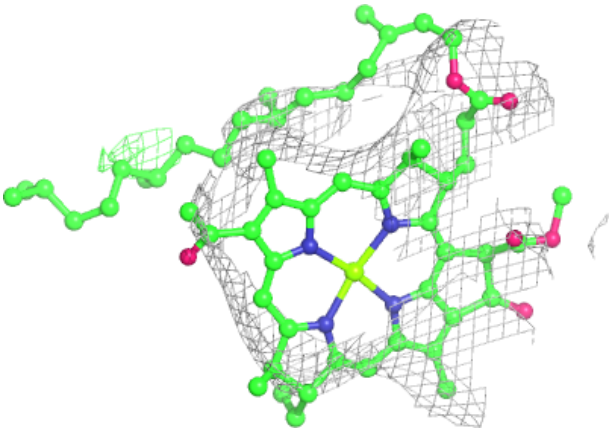


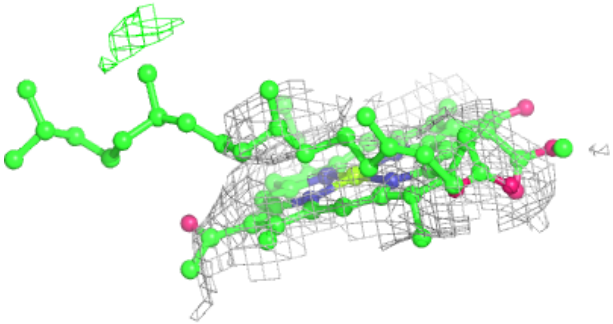


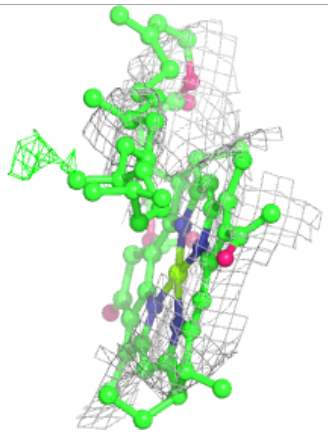


Electron density around BCL AH 103:

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

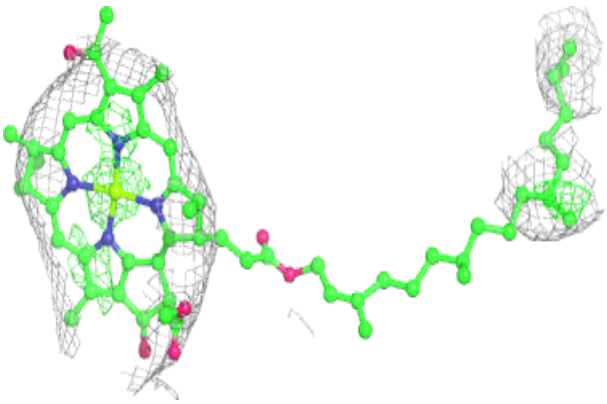


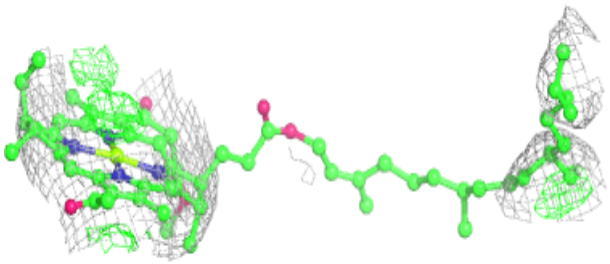


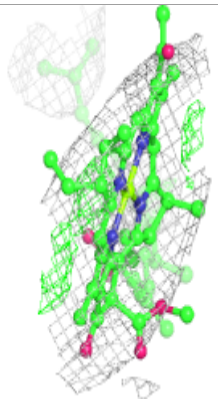


Electron density around BCL d 101:

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

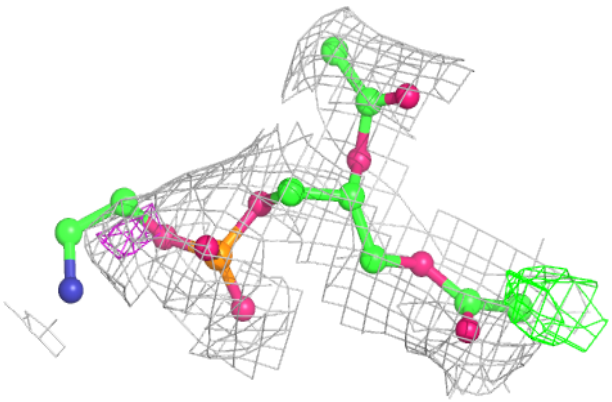


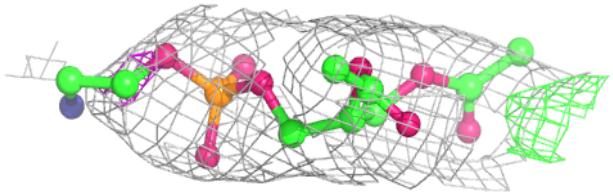


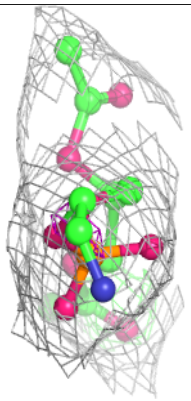


Electron density around PEF t 303:

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

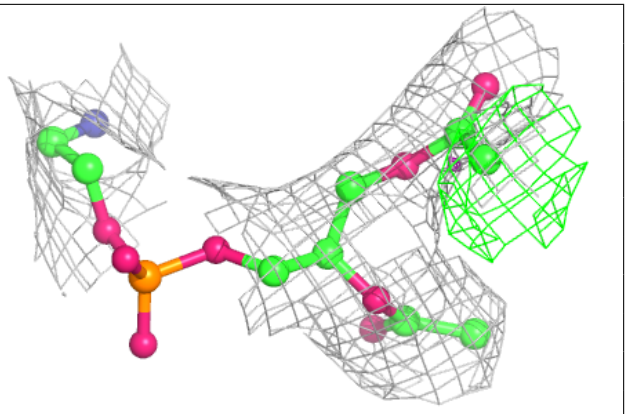


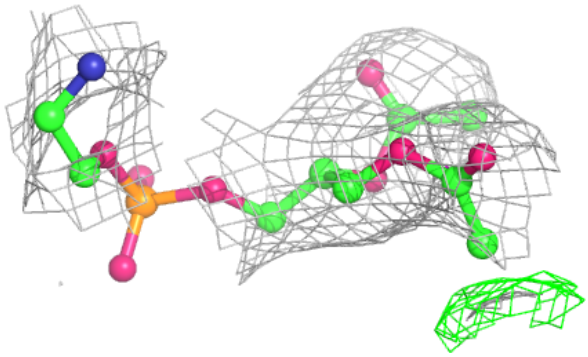


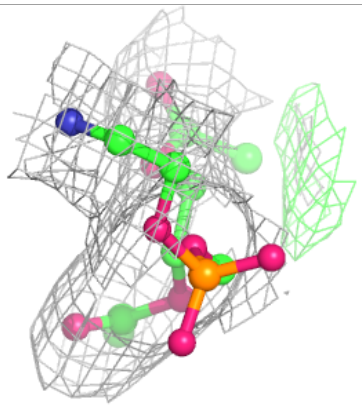


Electron density around PEF y 407:

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

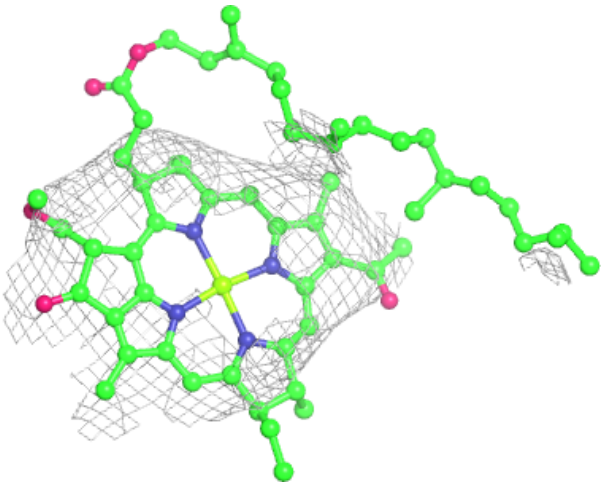


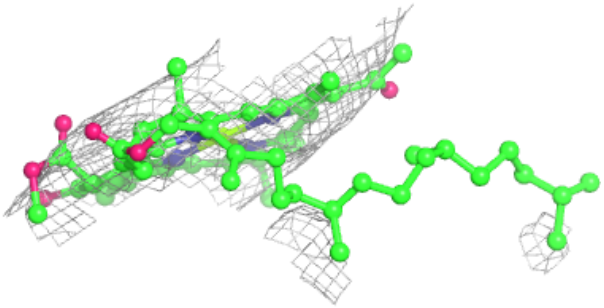


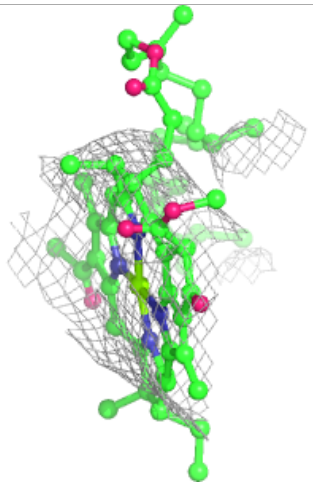


Electron density around BCL z 102:

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

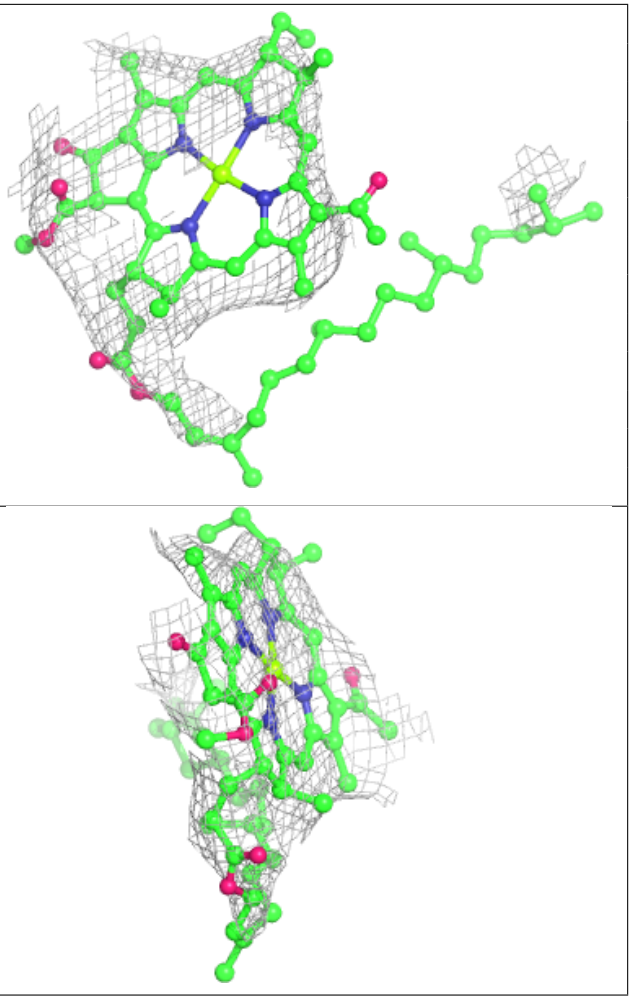






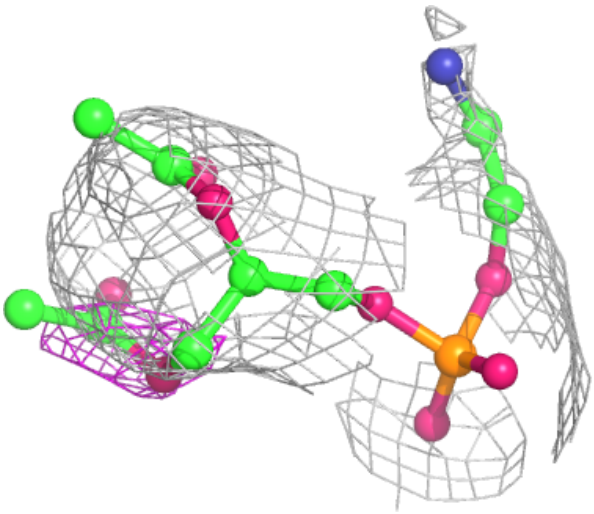
Electron density around BCL V 101:

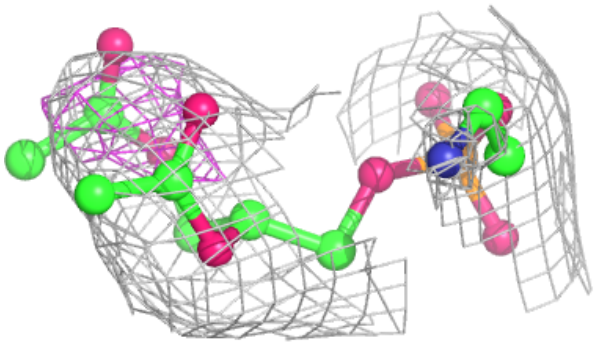
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

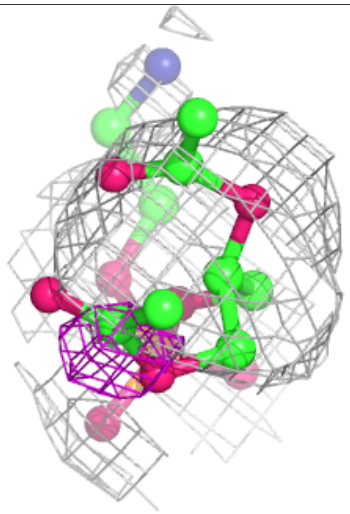


Electron density around PEF M 408:

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

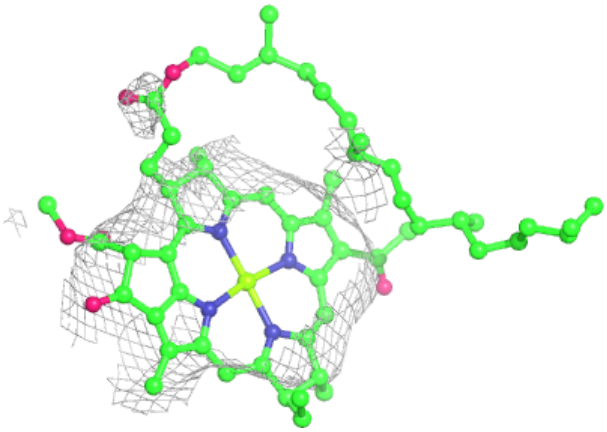


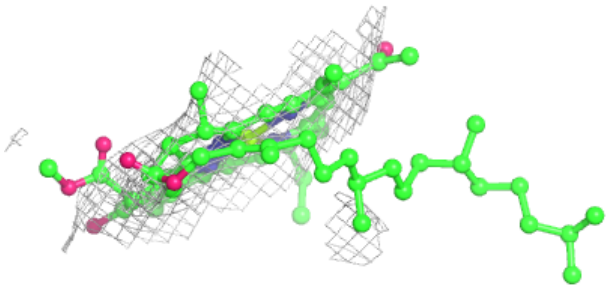


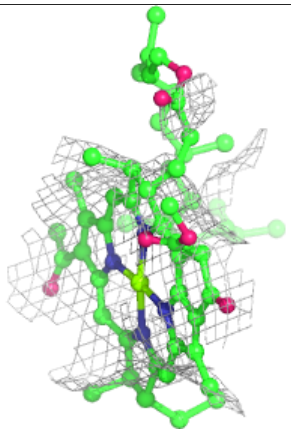


Electron density around BCL c 102:

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

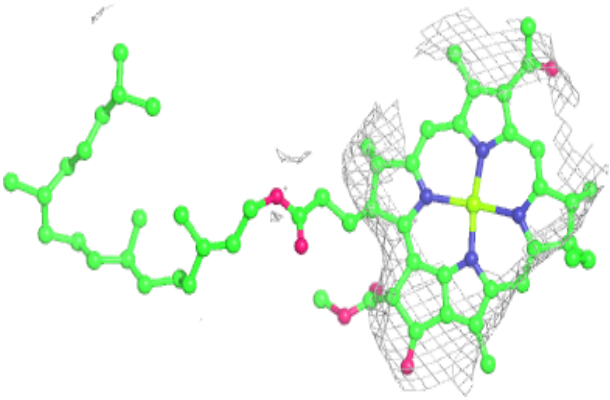


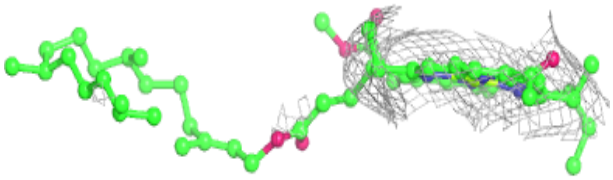


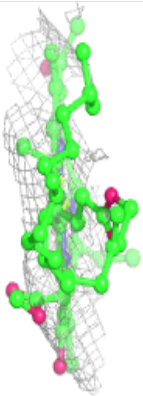


Electron density around BCL 9 103:

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

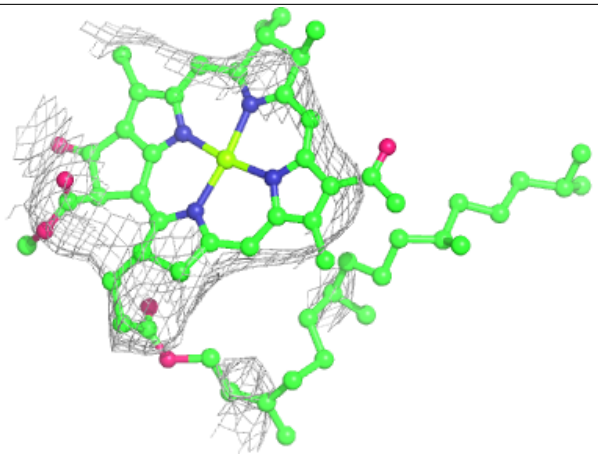


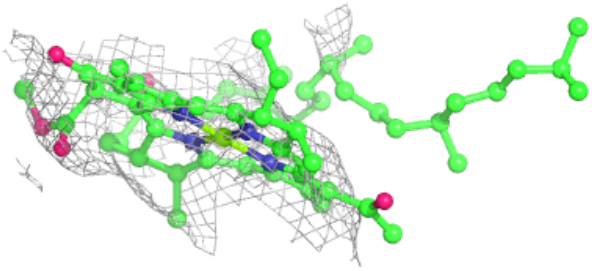


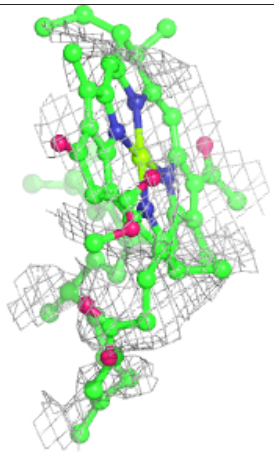


Electron density around BCL 5 102:

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

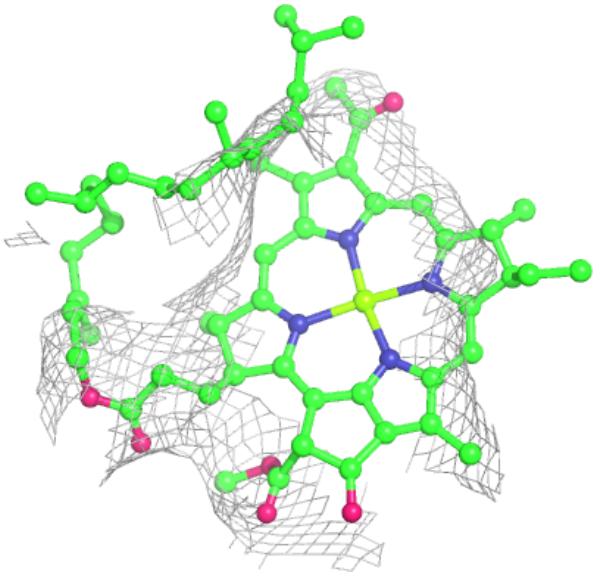


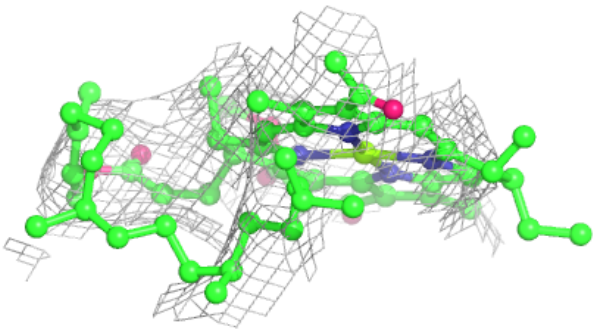


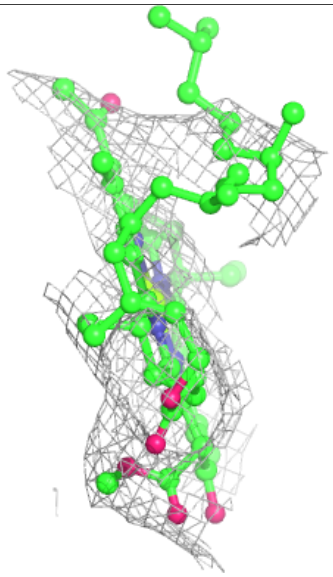


Electron density around BCL 8 102:

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

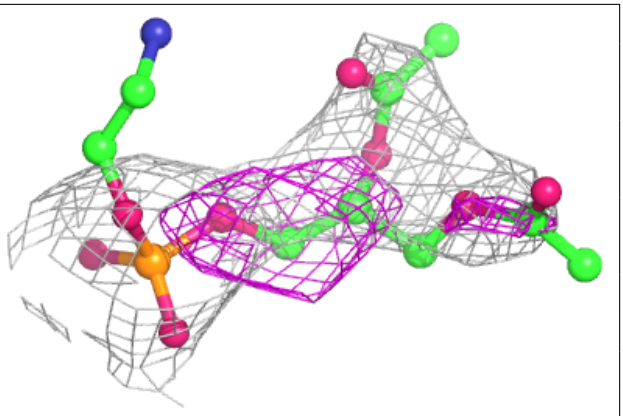


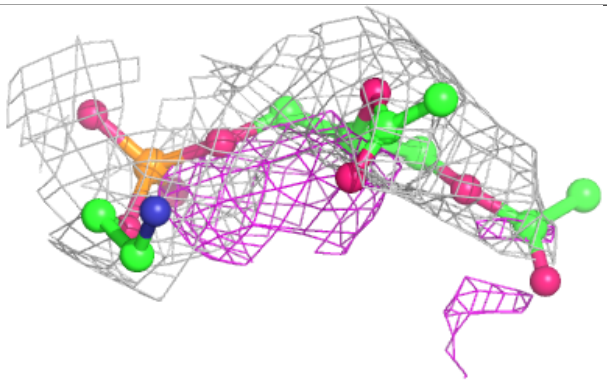


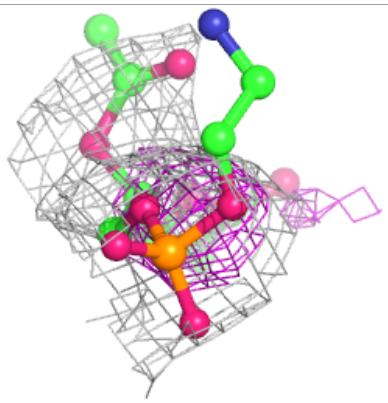


Electron density around PEF y 408:

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

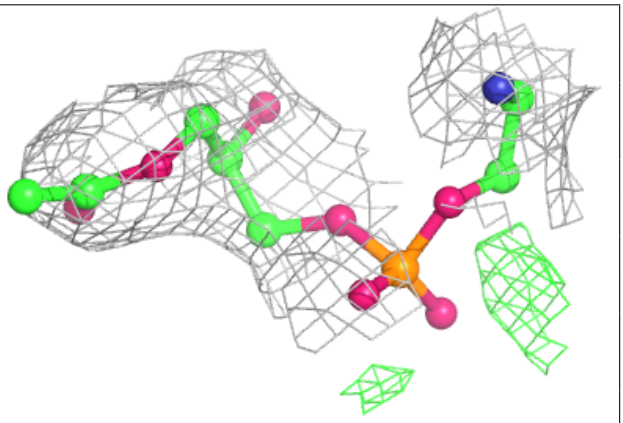


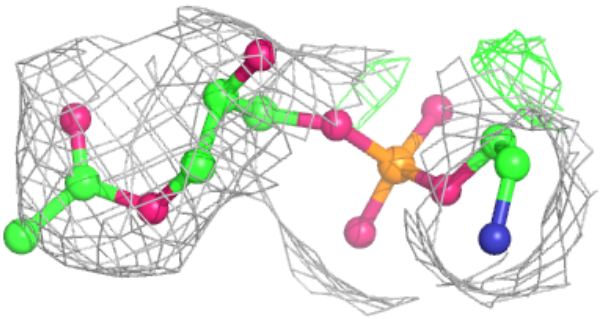


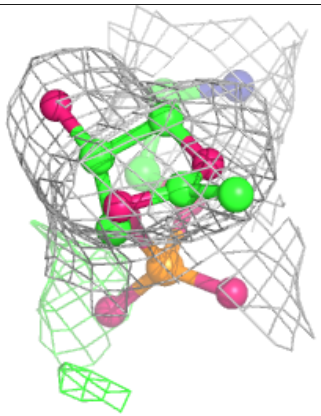


Electron density around PEF M 407:

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

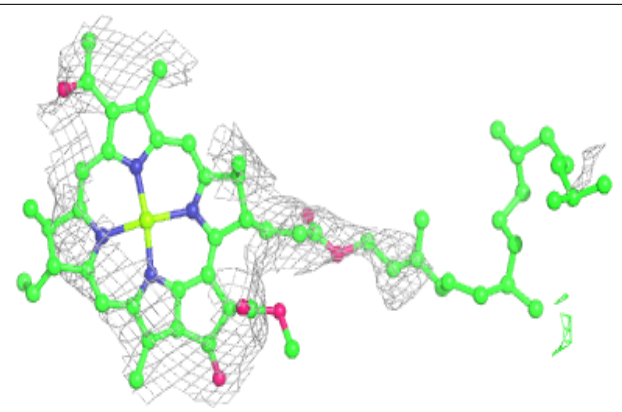


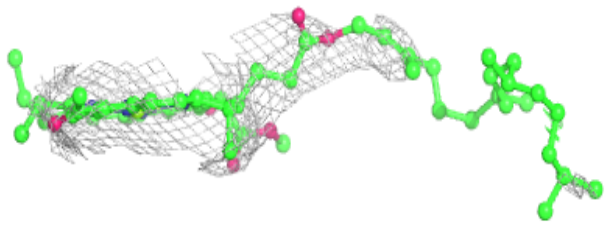


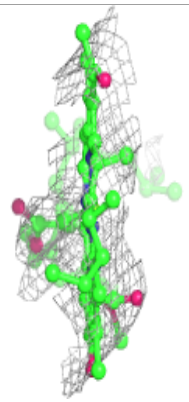


Electron density around BCL 7 101:

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

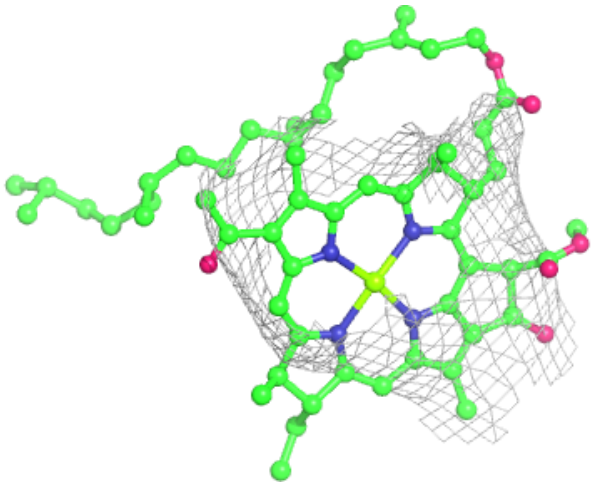


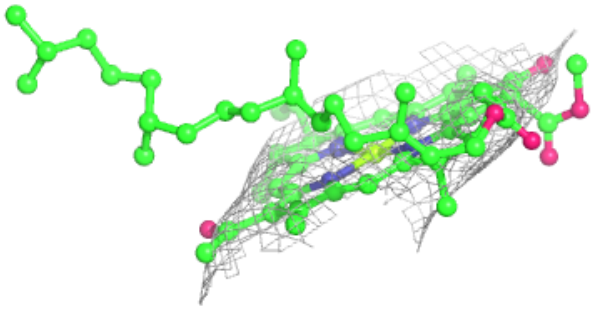


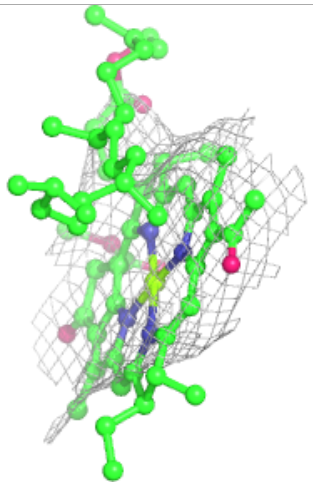


Electron density around BCL N 102:

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

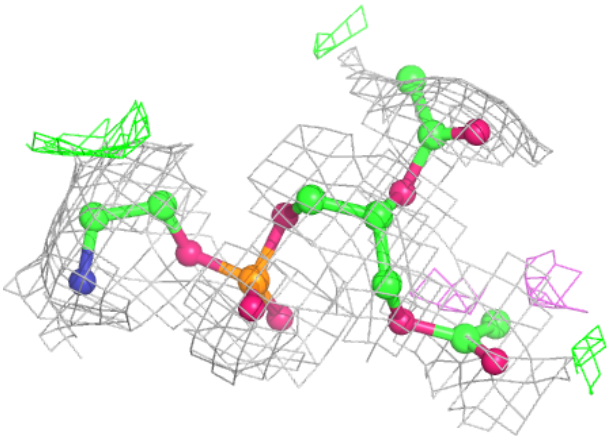


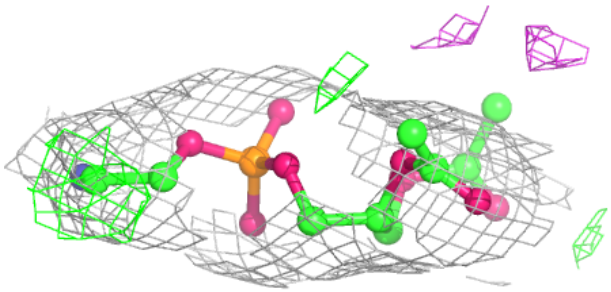


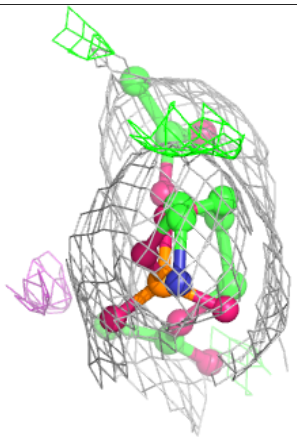


Electron density around PEF H 304:

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

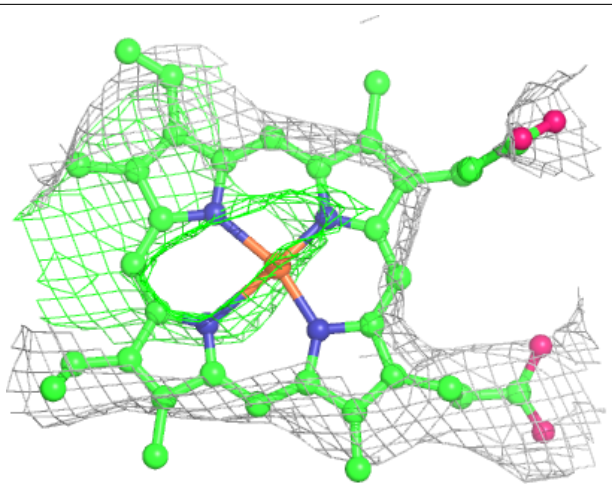


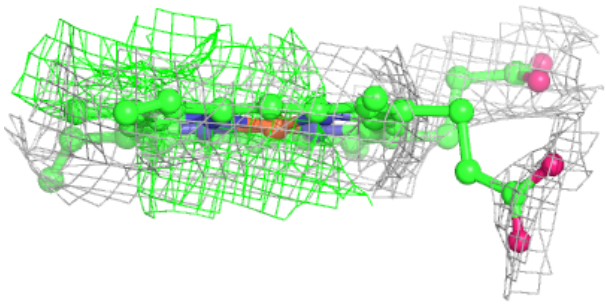


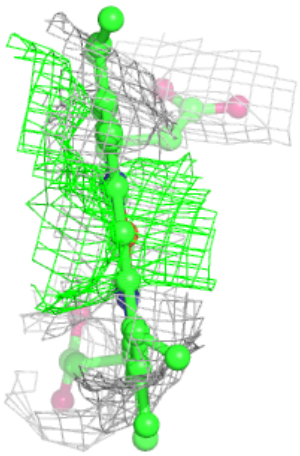


Electron density around HEM C 501:

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

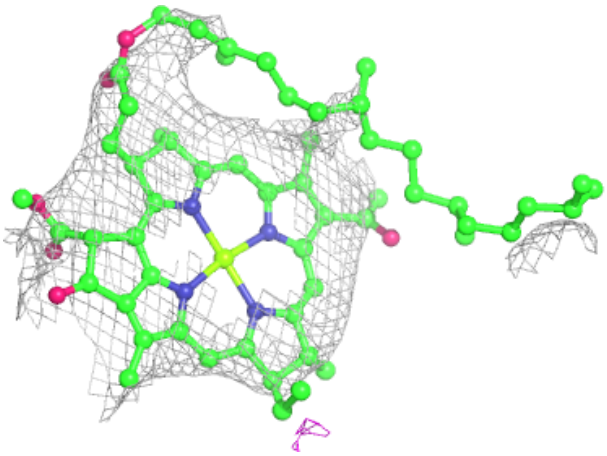


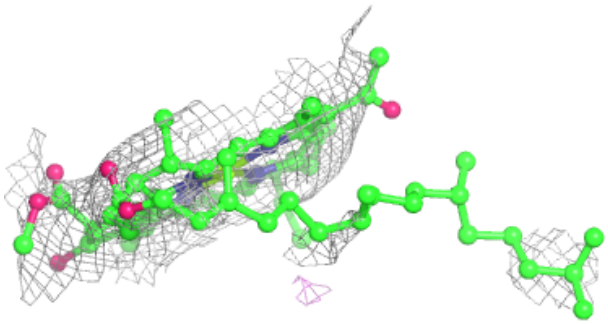


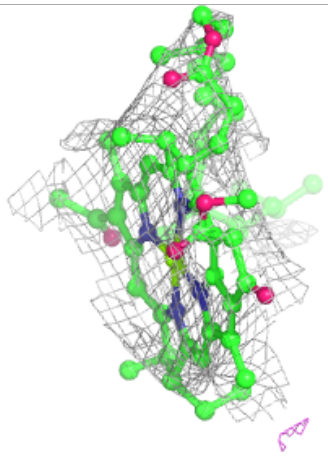


Electron density around BCL T 102:

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

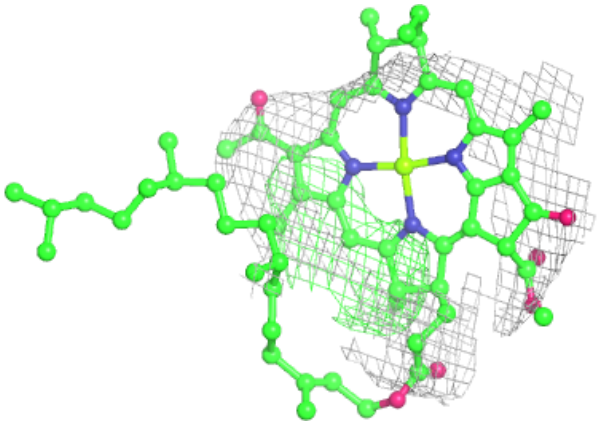


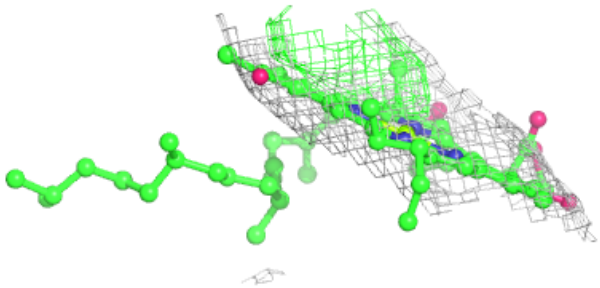


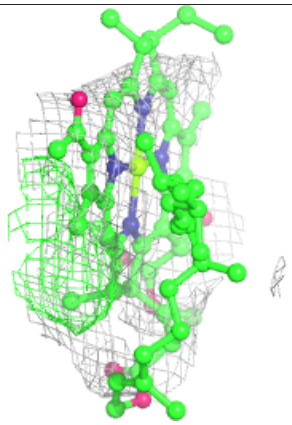


Electron density around BCL D 102:

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

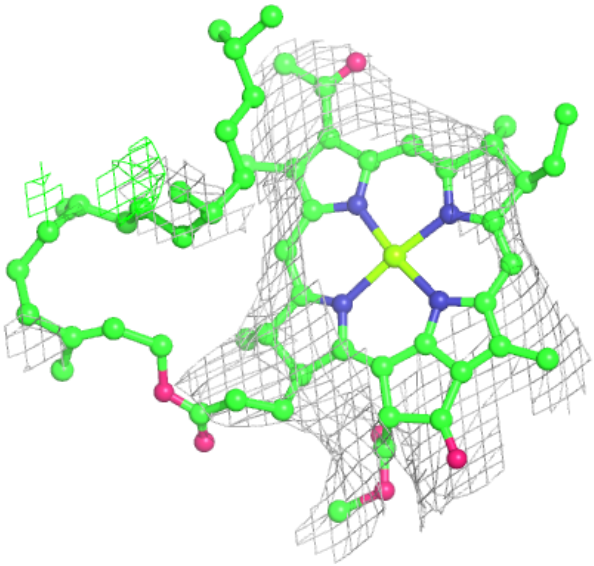


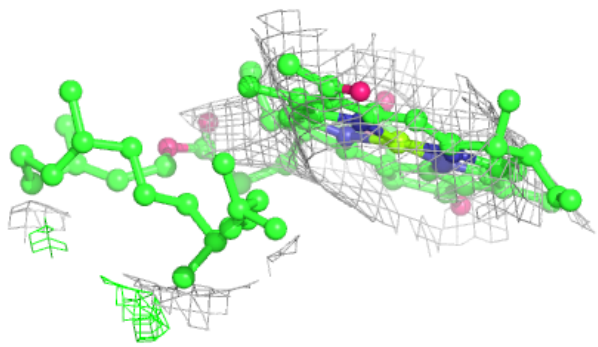


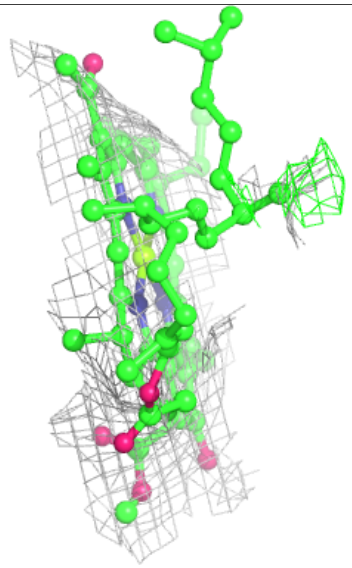


Electron density around BCL m 103:

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

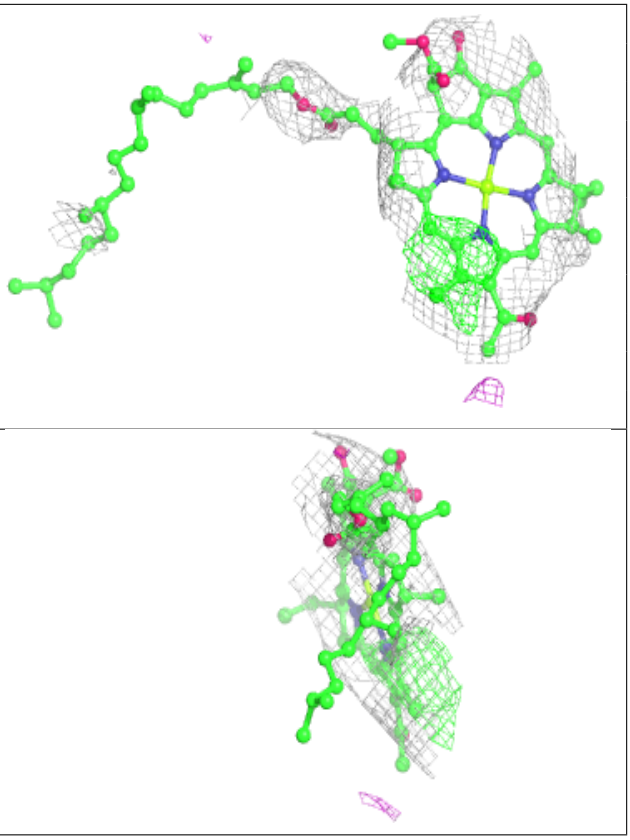






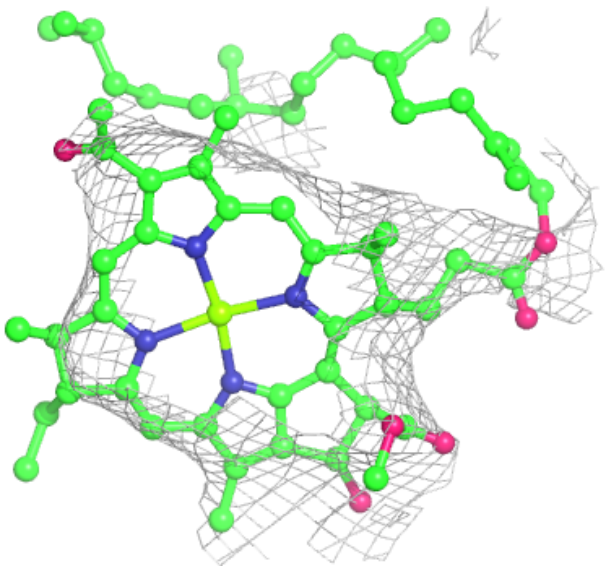
Electron density around BCL u 101:

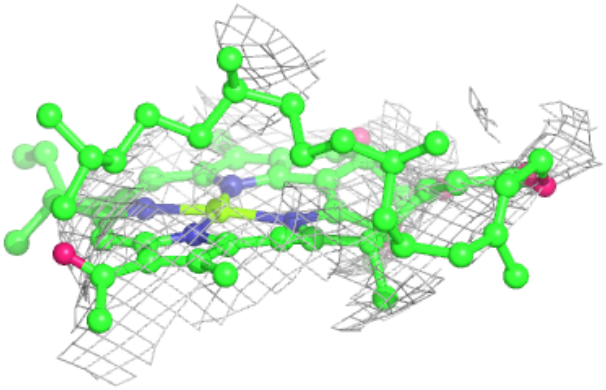
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

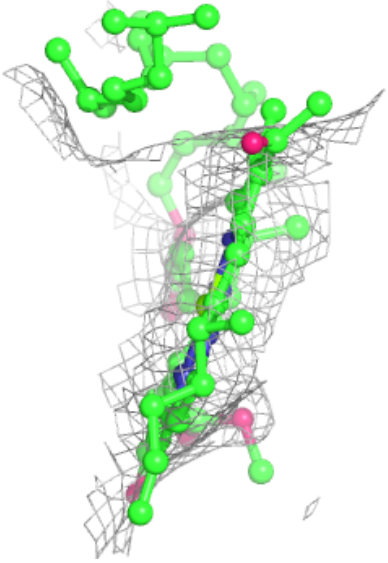


Electron density around BCL k 102:

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

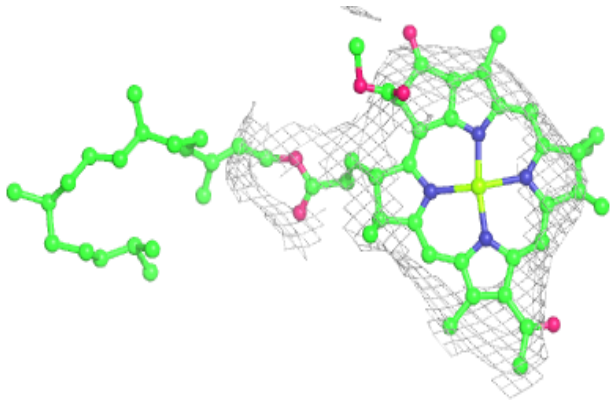


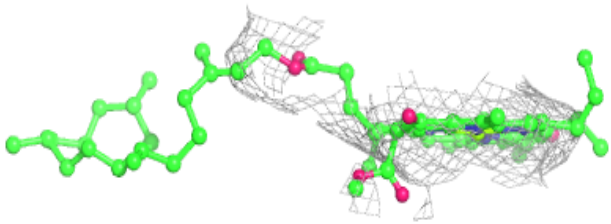


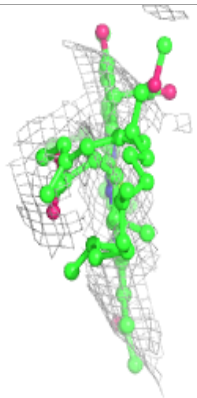


Electron density around BCL AH 101:

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

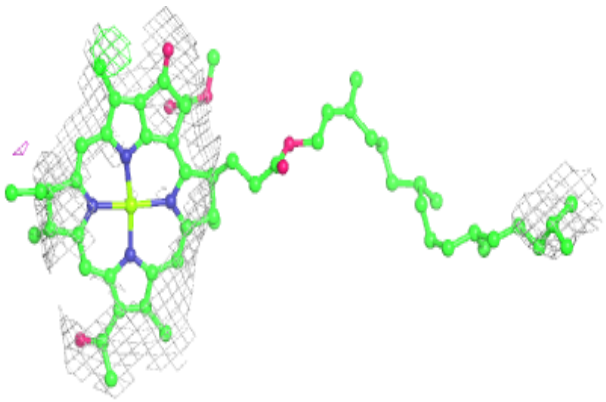


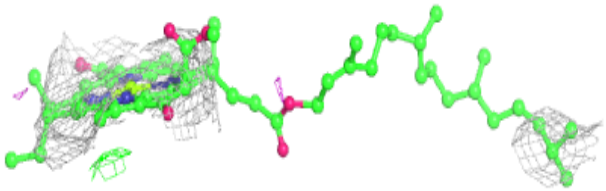


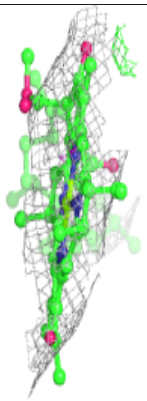


Electron density around BCL p 102:

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

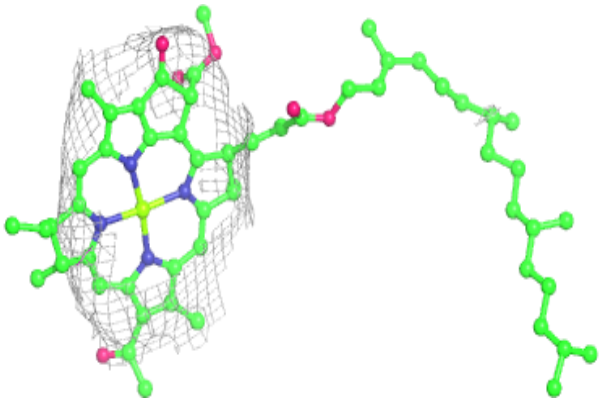


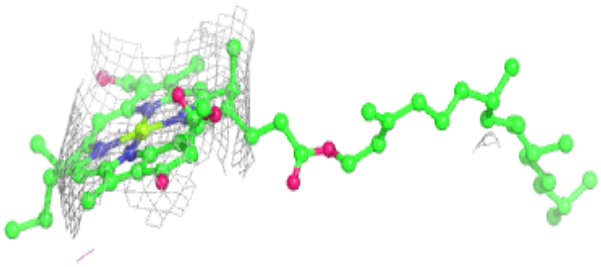


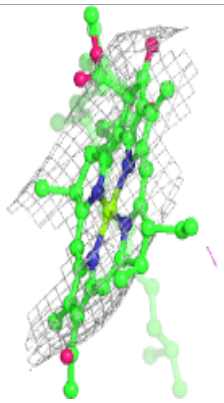


Electron density around BCL I 101:

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

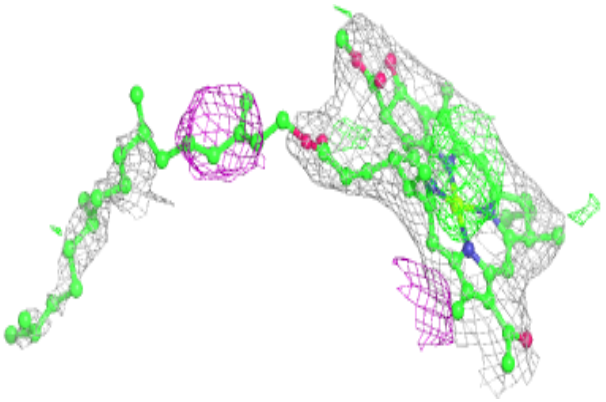


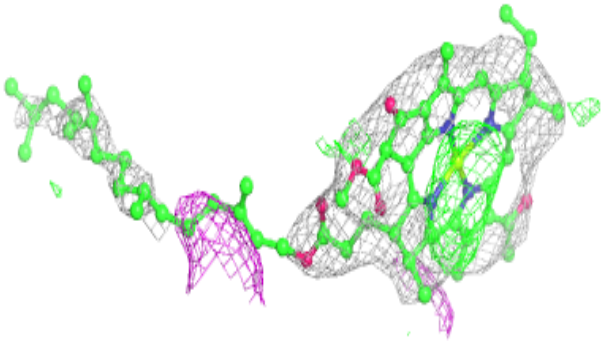


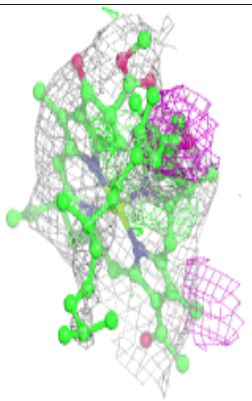


Electron density around BCL x 301:

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

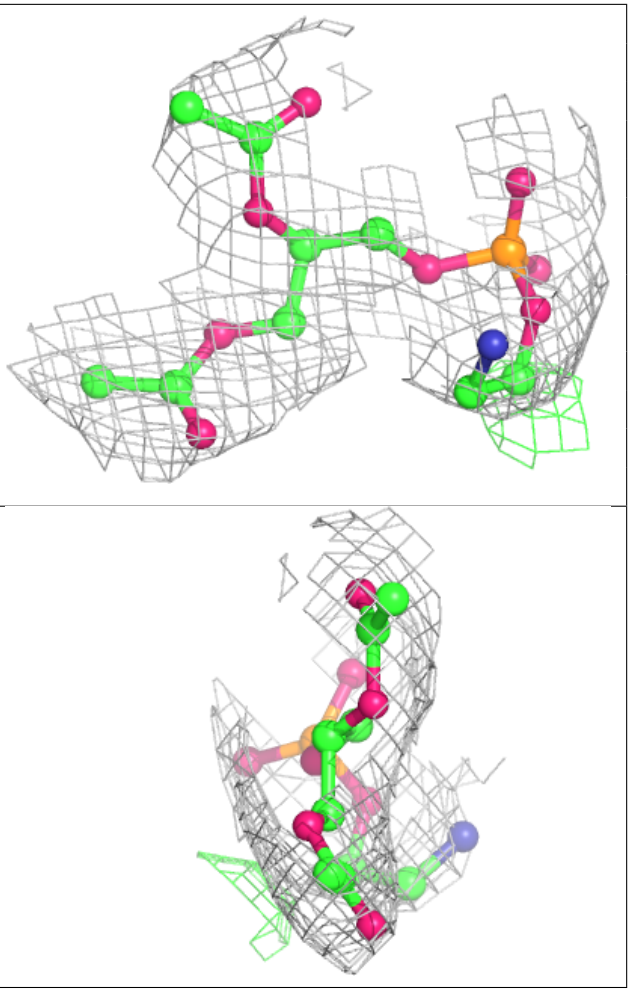






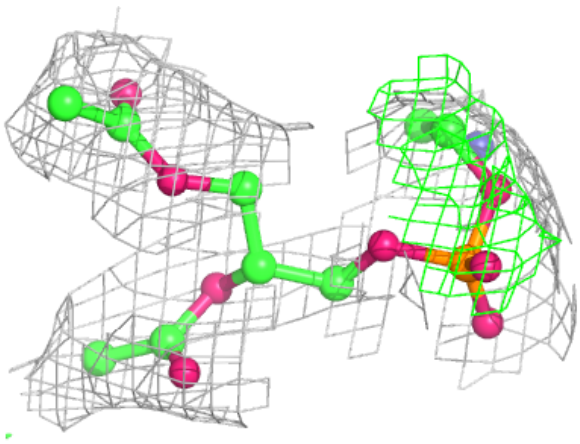
Electron density around PEF t 301:

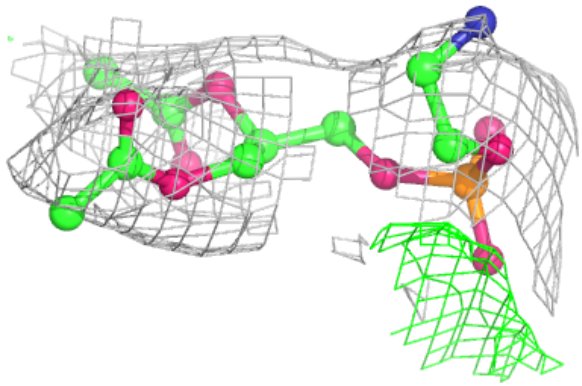
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

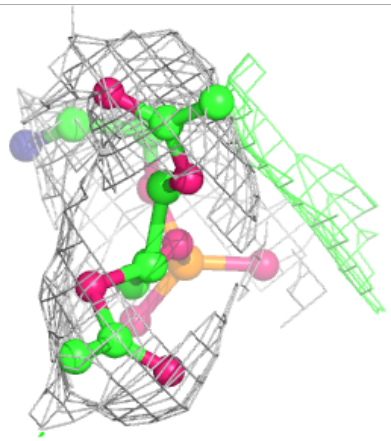


Electron density around PEF M 406:

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

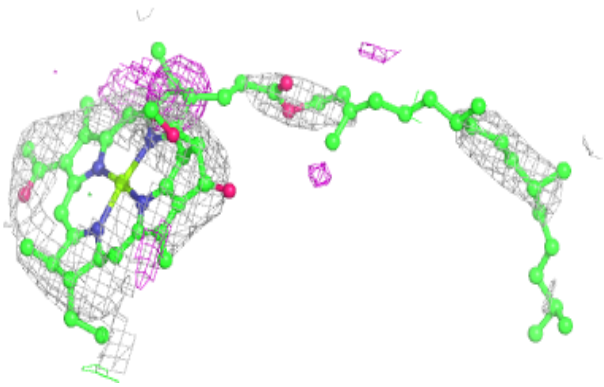


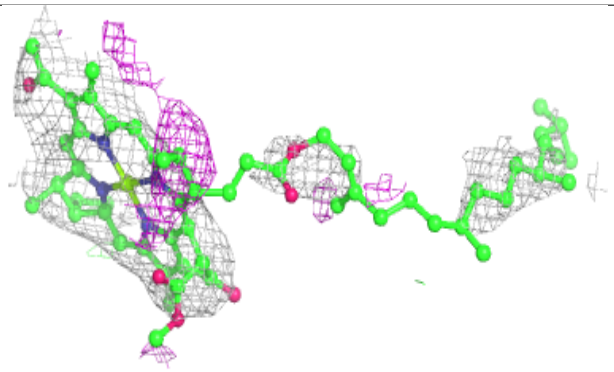


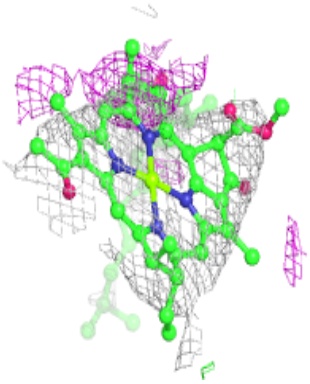


Electron density around BCL y 401:

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

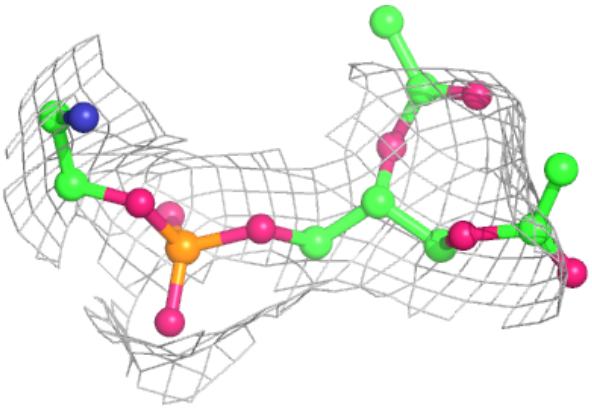


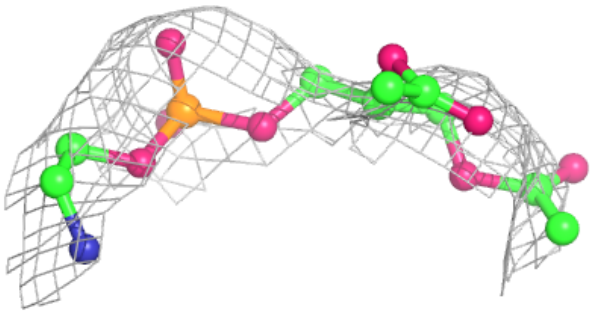


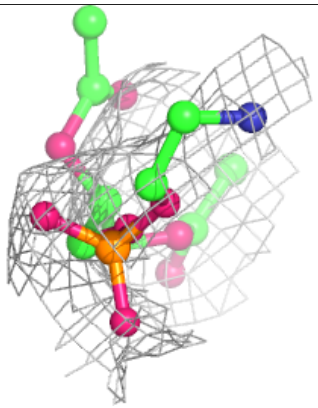


Electron density around PEF H 303:

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

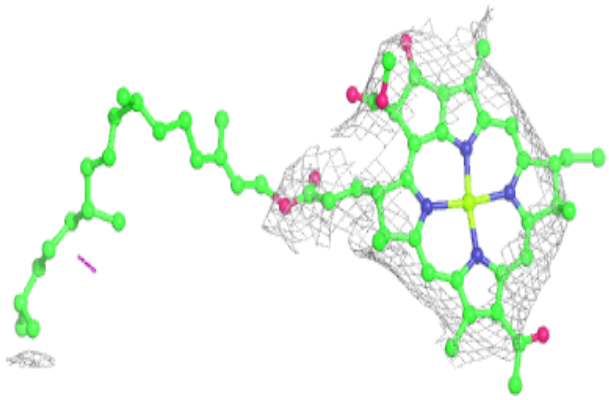


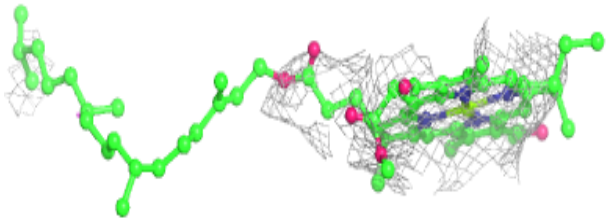


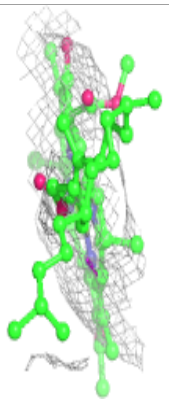


Electron density around BCL AE 102:

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

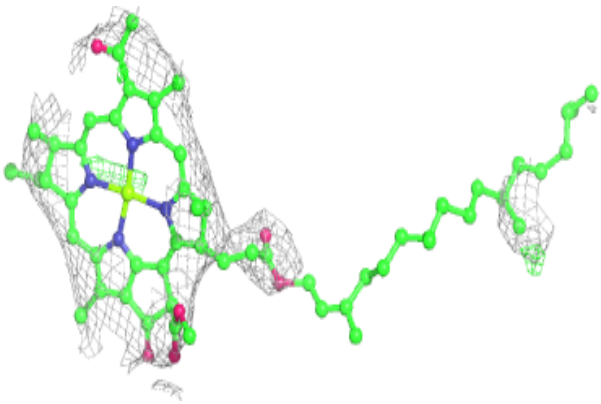


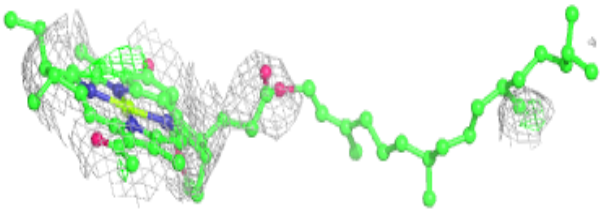


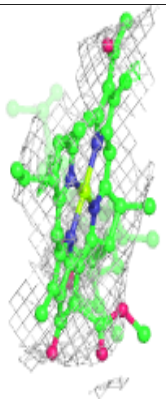


Electron density around BCL 1 101:

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

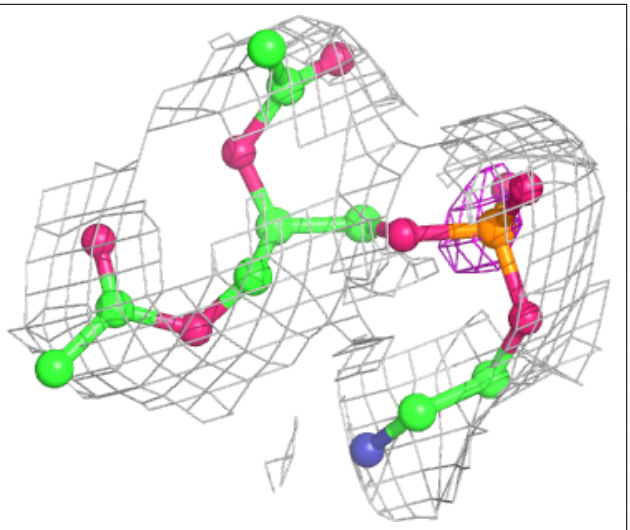


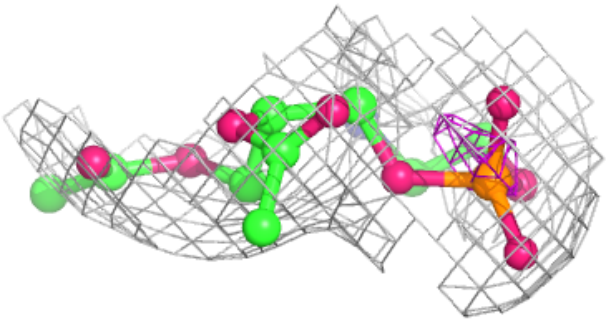


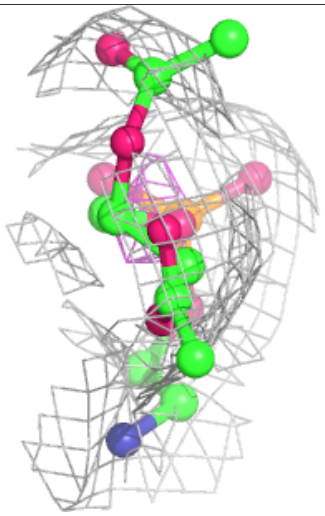


Electron density around PEF x 306:

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

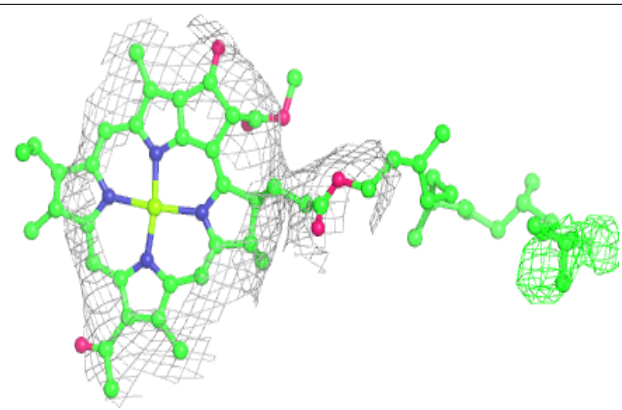


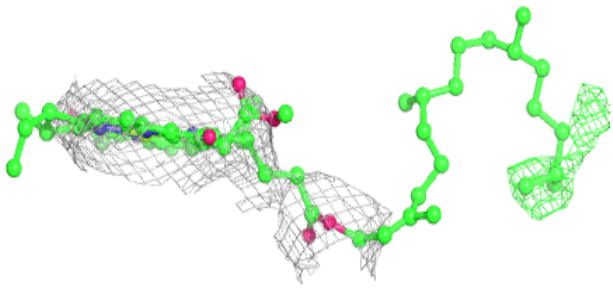


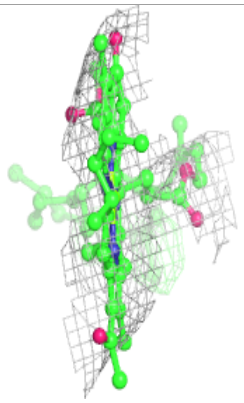


Electron density around BCL P 101:

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

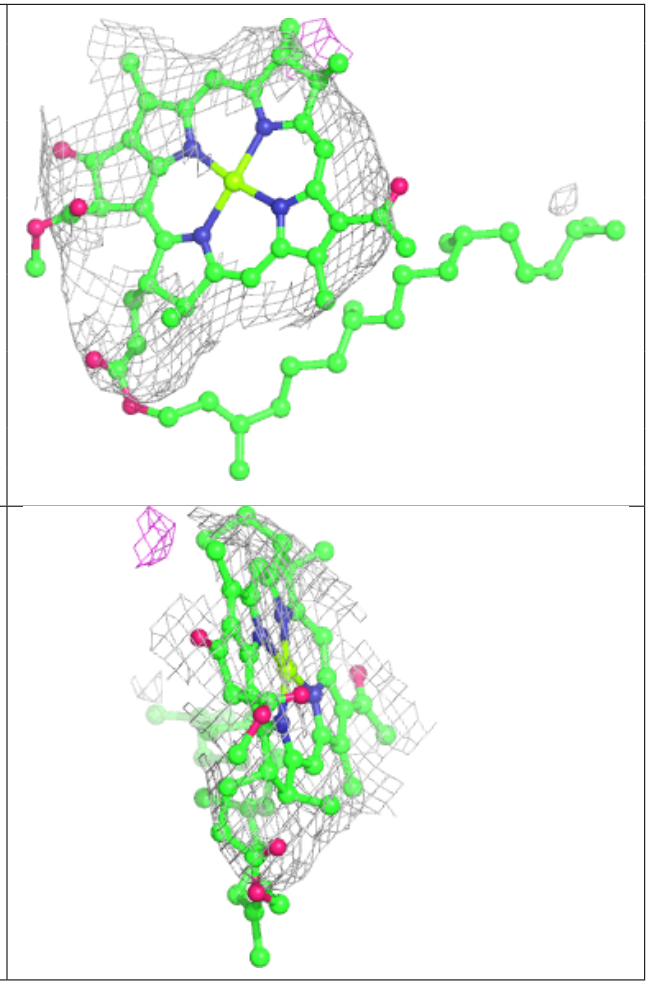






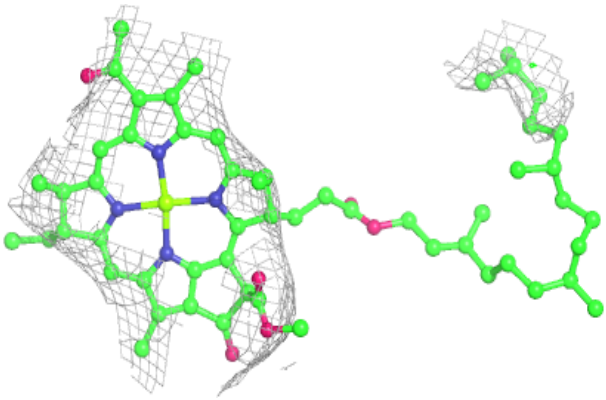
Electron density around BCL R 102:

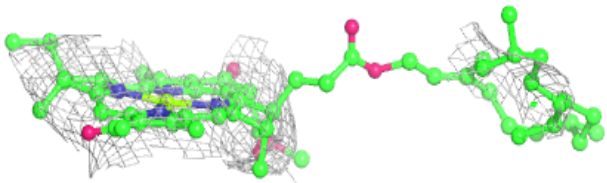
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

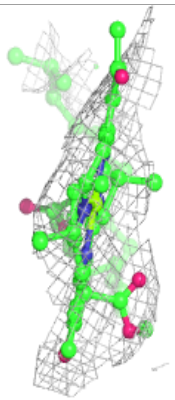


Electron density around BCL f 101:

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

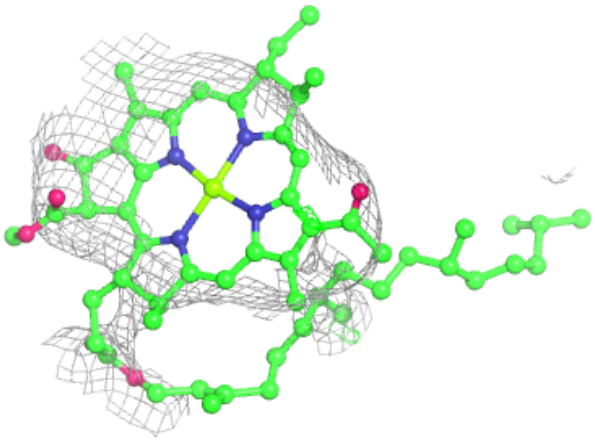


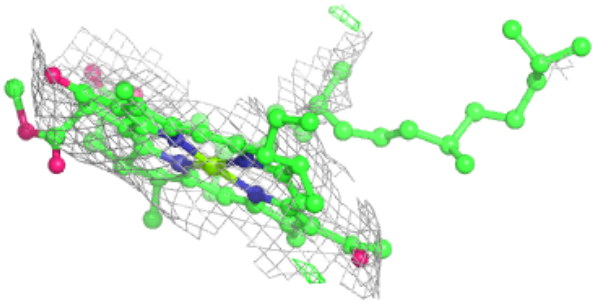


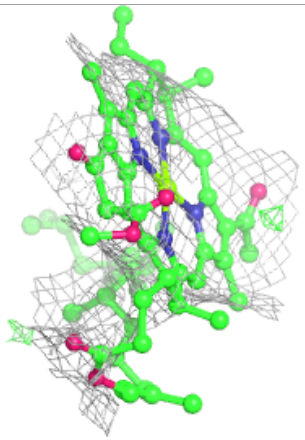


Electron density around BCL g 101:

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

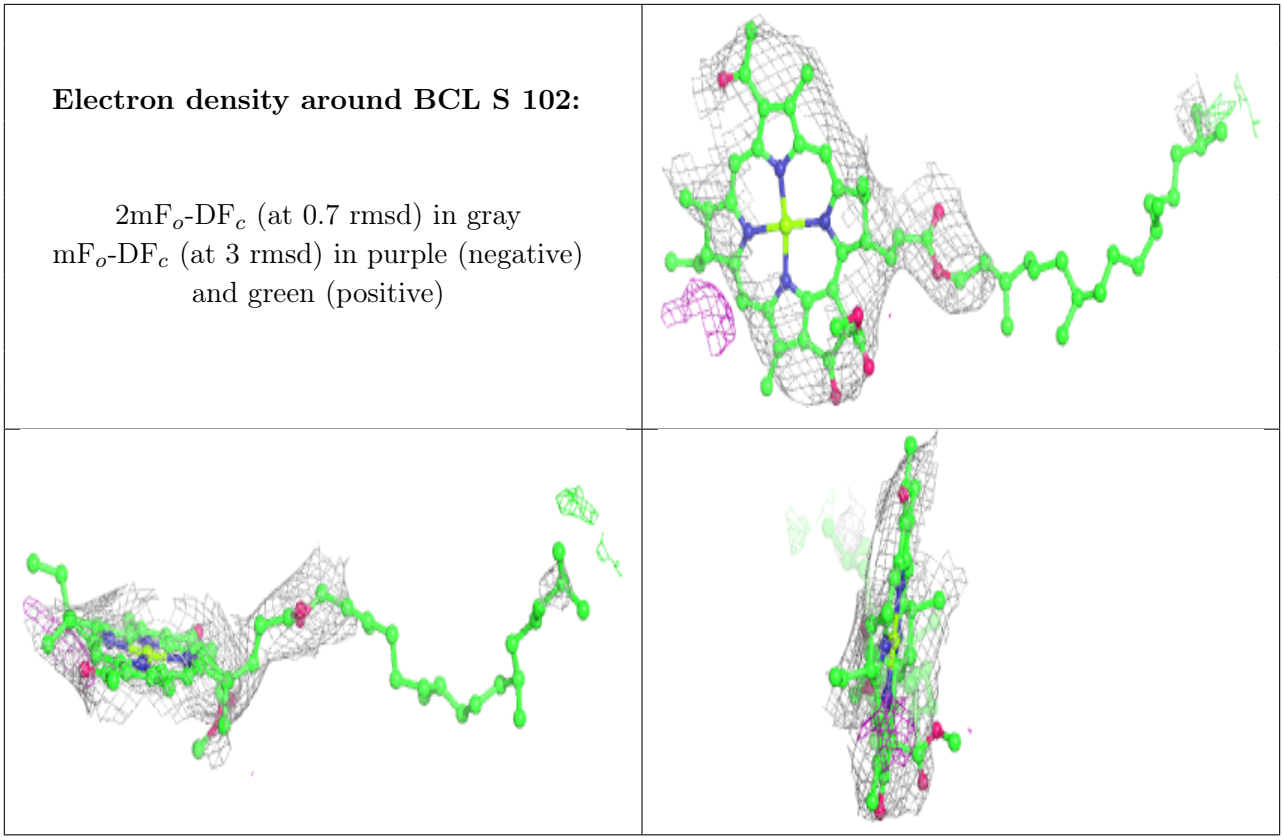






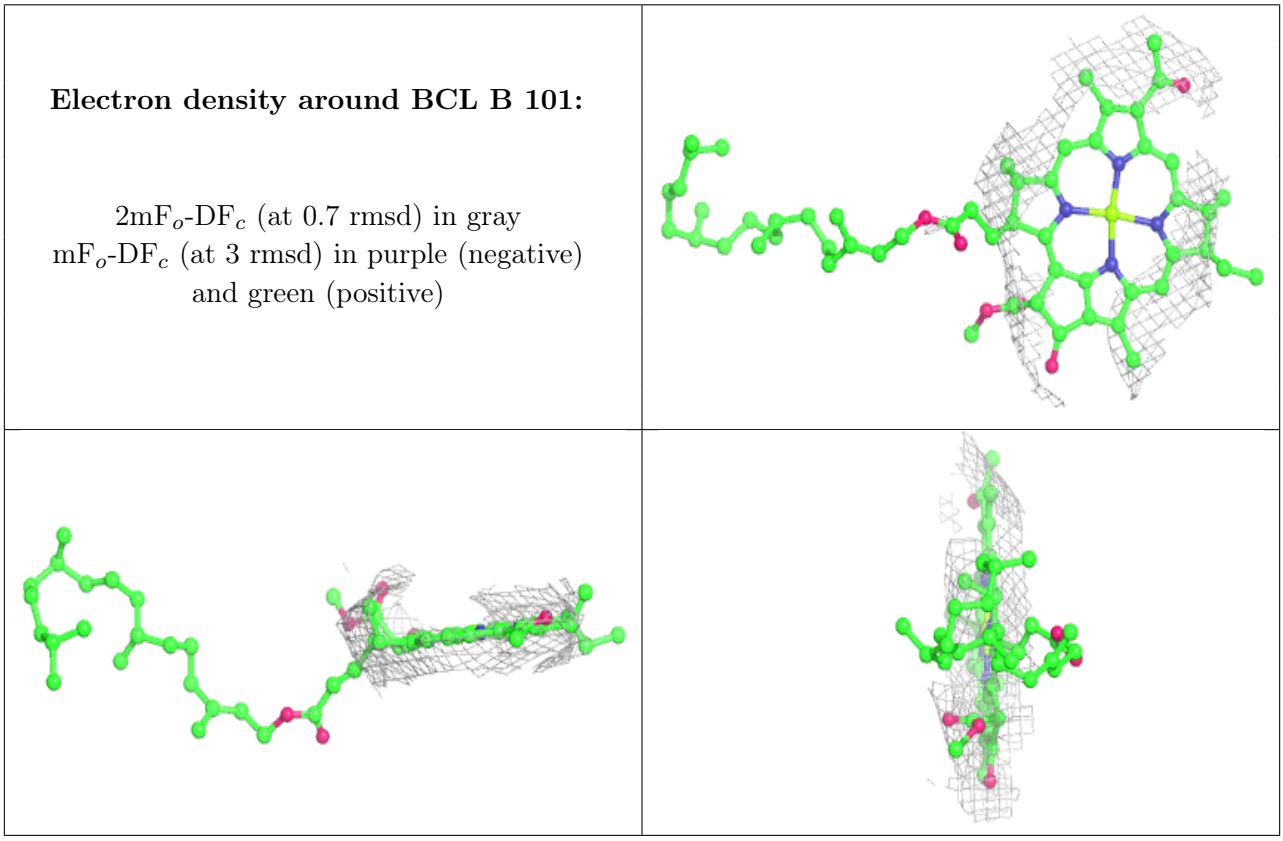
Electron density around BCL S 102:

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



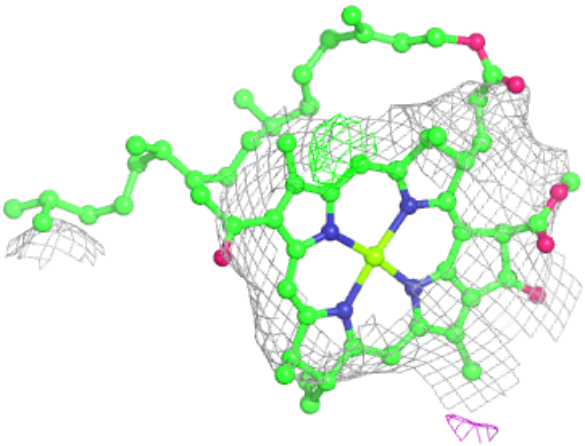
Electron density around BCL B 101:

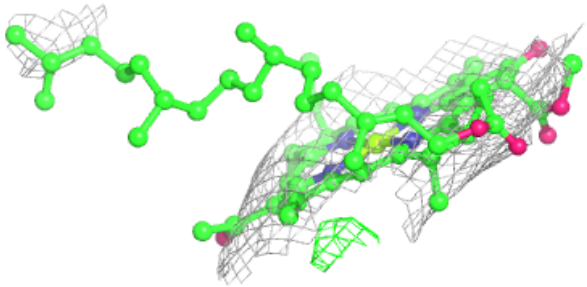
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

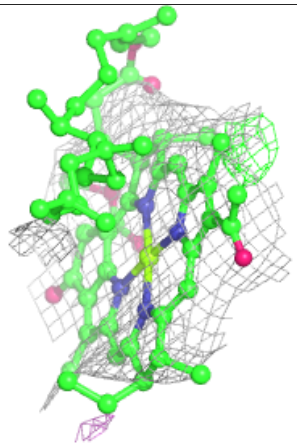


Electron density around BCL J 102:

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

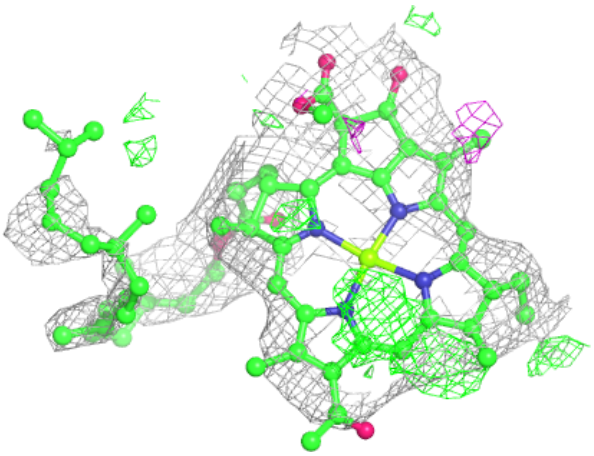


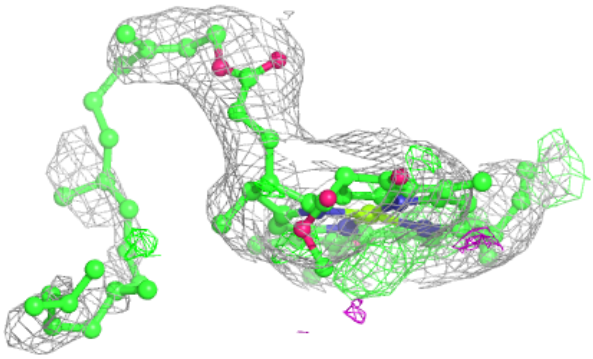


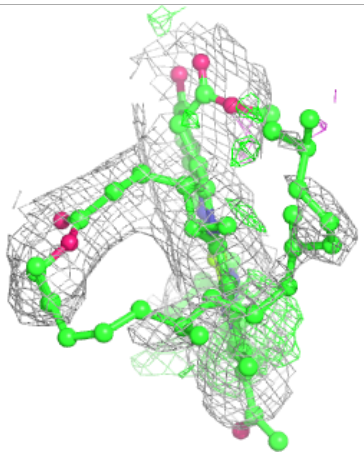


Electron density around BCL L 303:

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

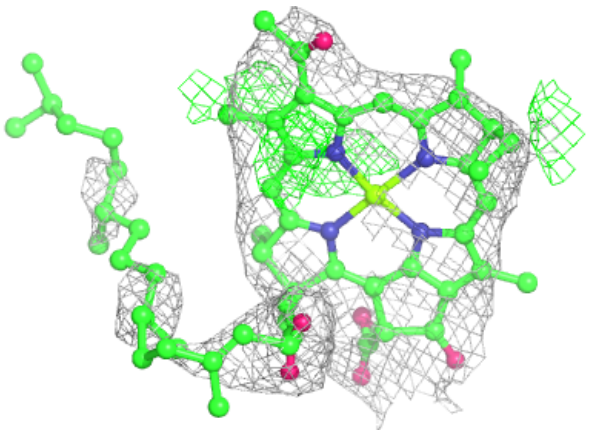


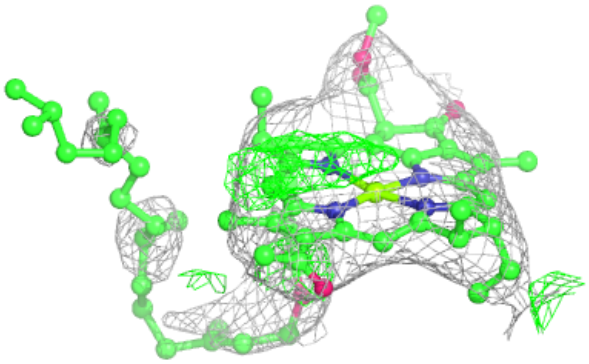




Electron density around BCL L 305:

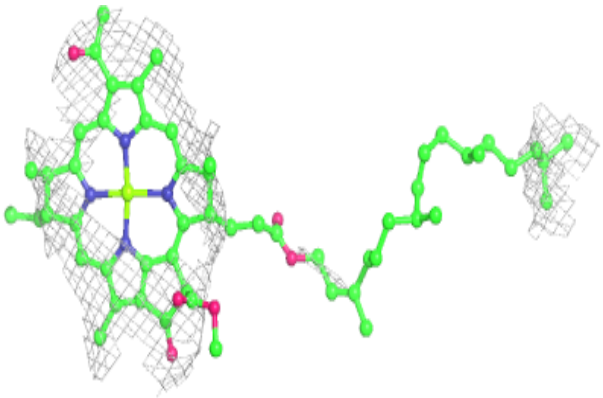
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

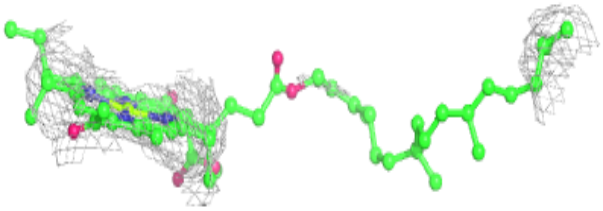


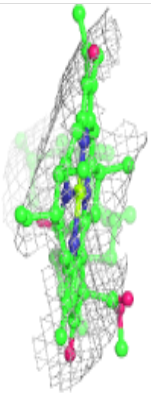


Electron density around BCL D 101:

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

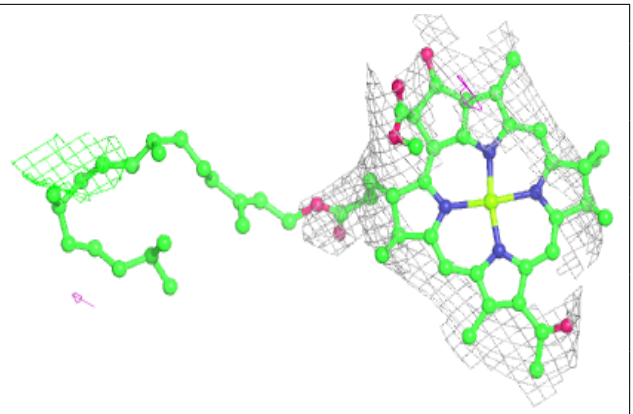


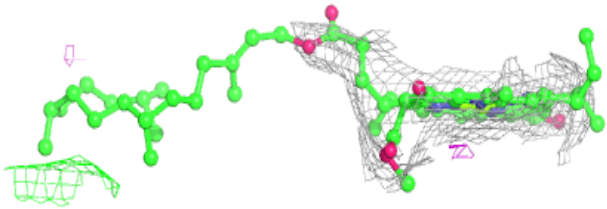


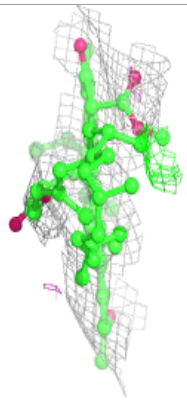


Electron density around BCL AI 101:

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

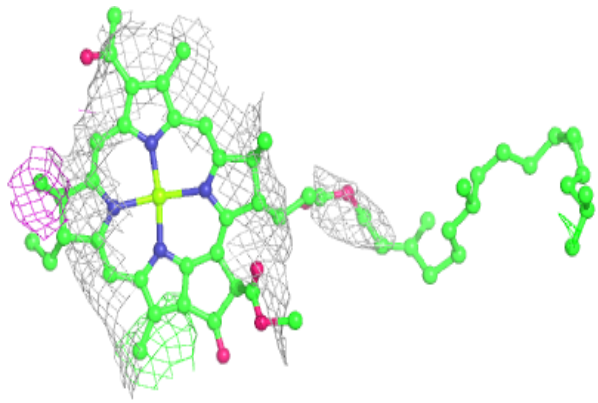


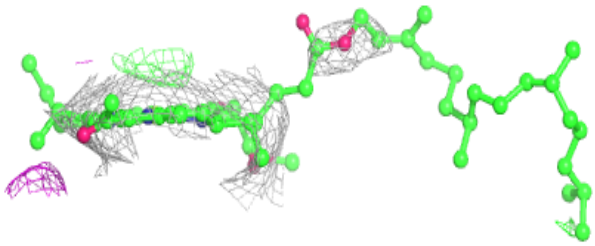


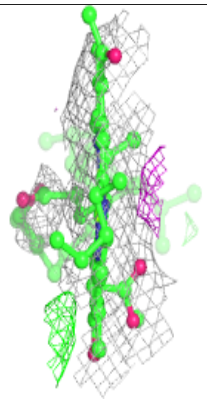


Electron density around BCL AK 101:

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

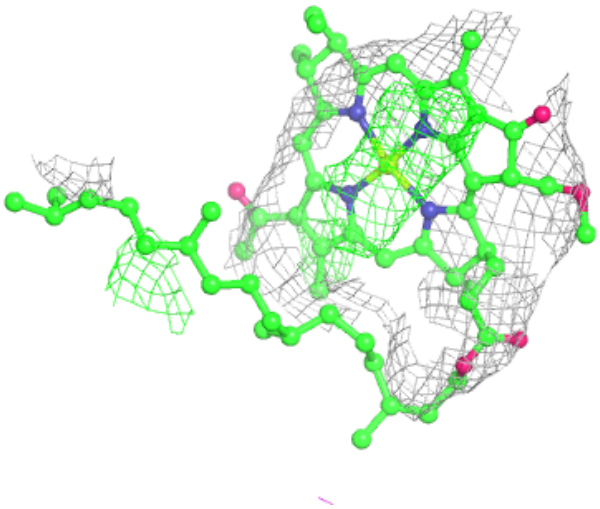


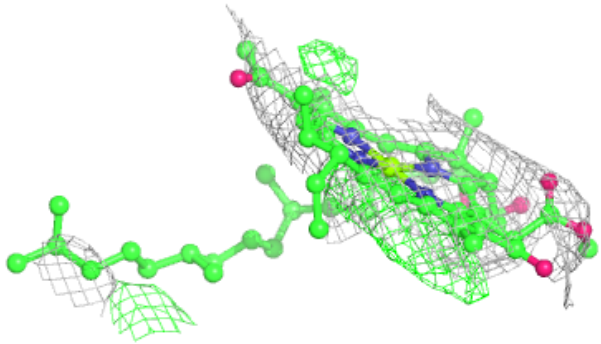


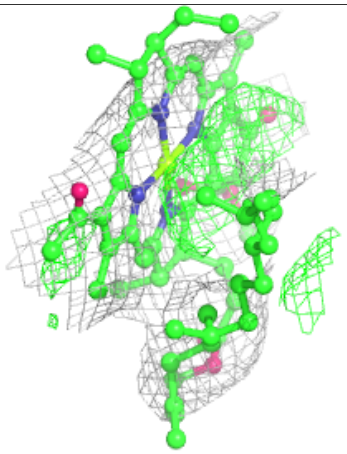


Electron density around BCL AL 102:

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

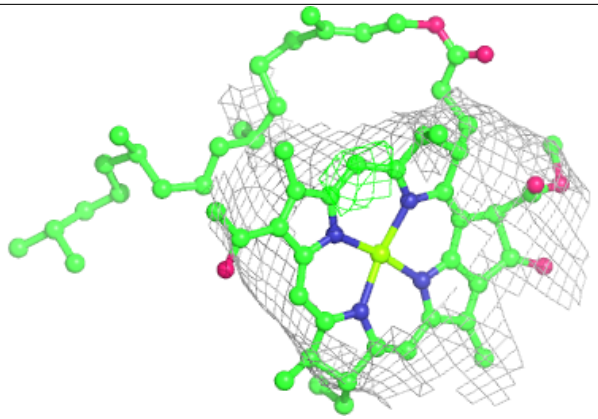


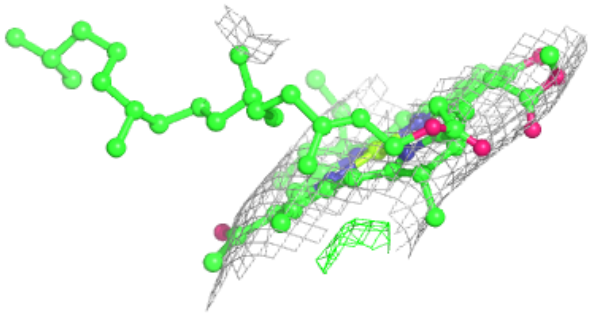


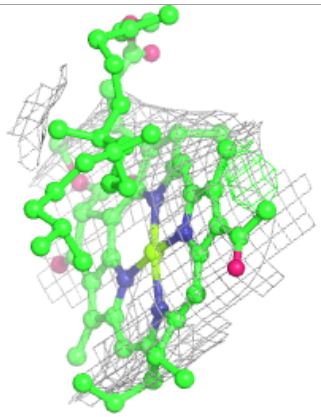


Electron density around BCL v 102:

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

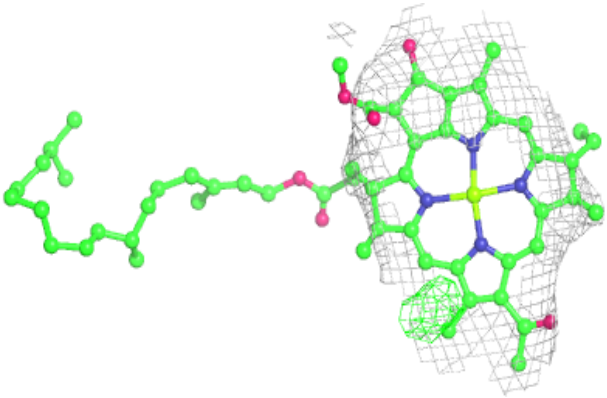


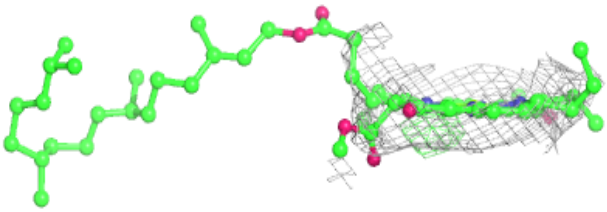


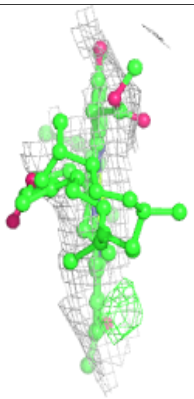


Electron density around BCL w 101:

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

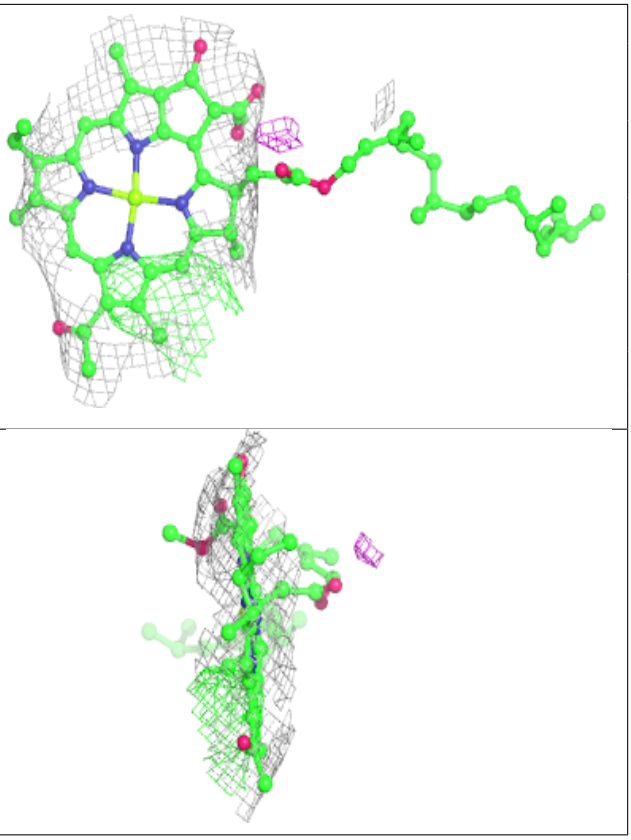


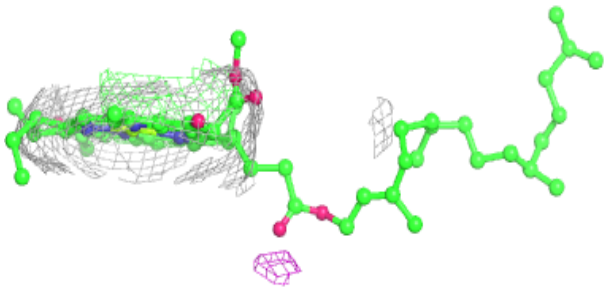




Electron density around BCL F 101:

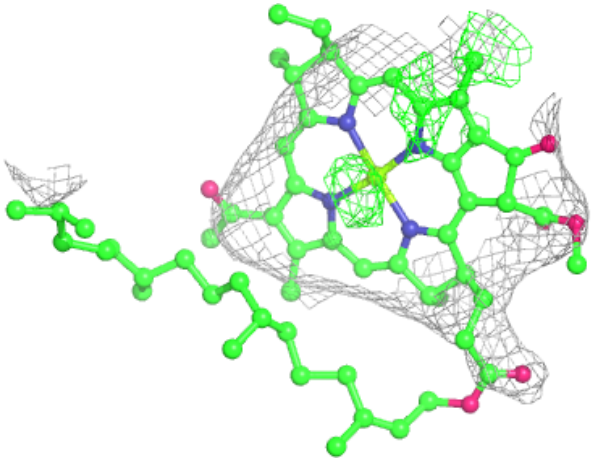
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

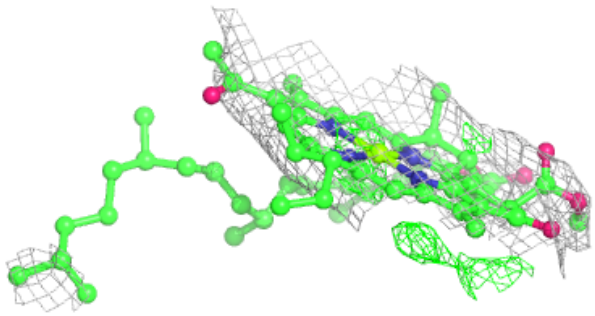


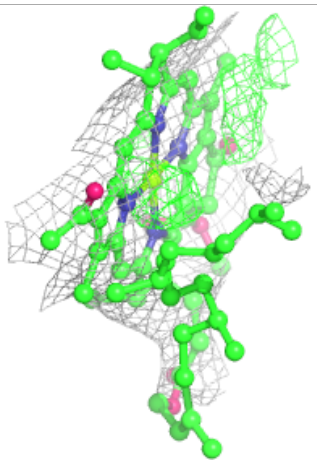


Electron density around BCL e 102:

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

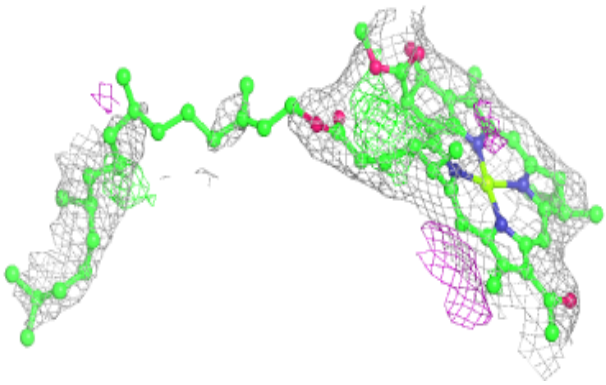


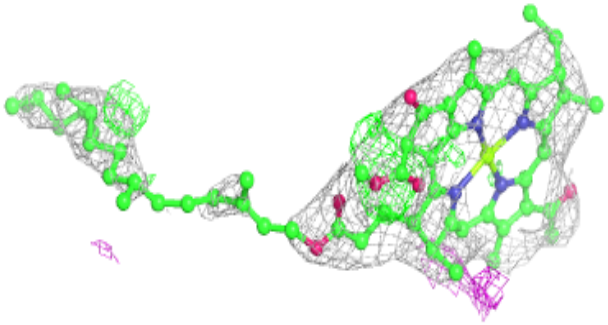


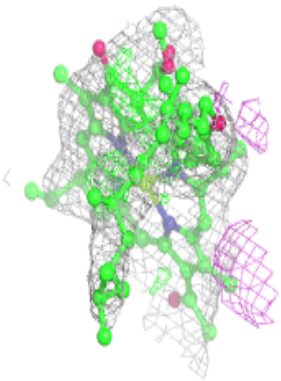


Electron density around BCL L 301:

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

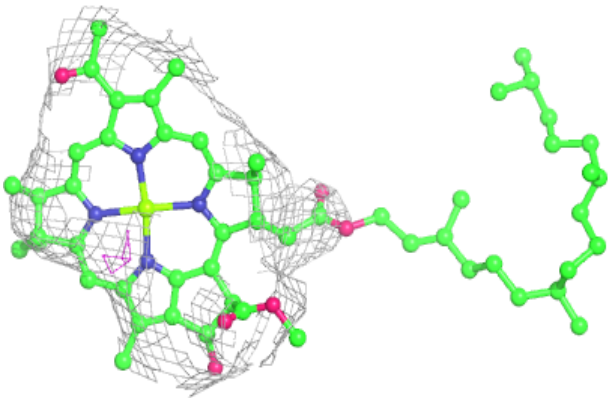


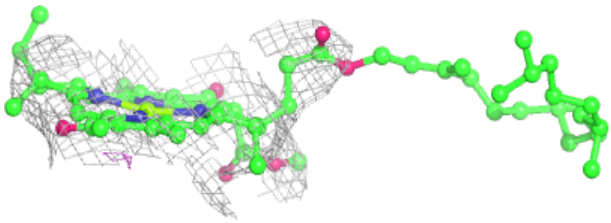


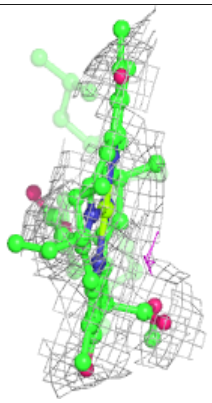


Electron density around BCL 3 101:

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

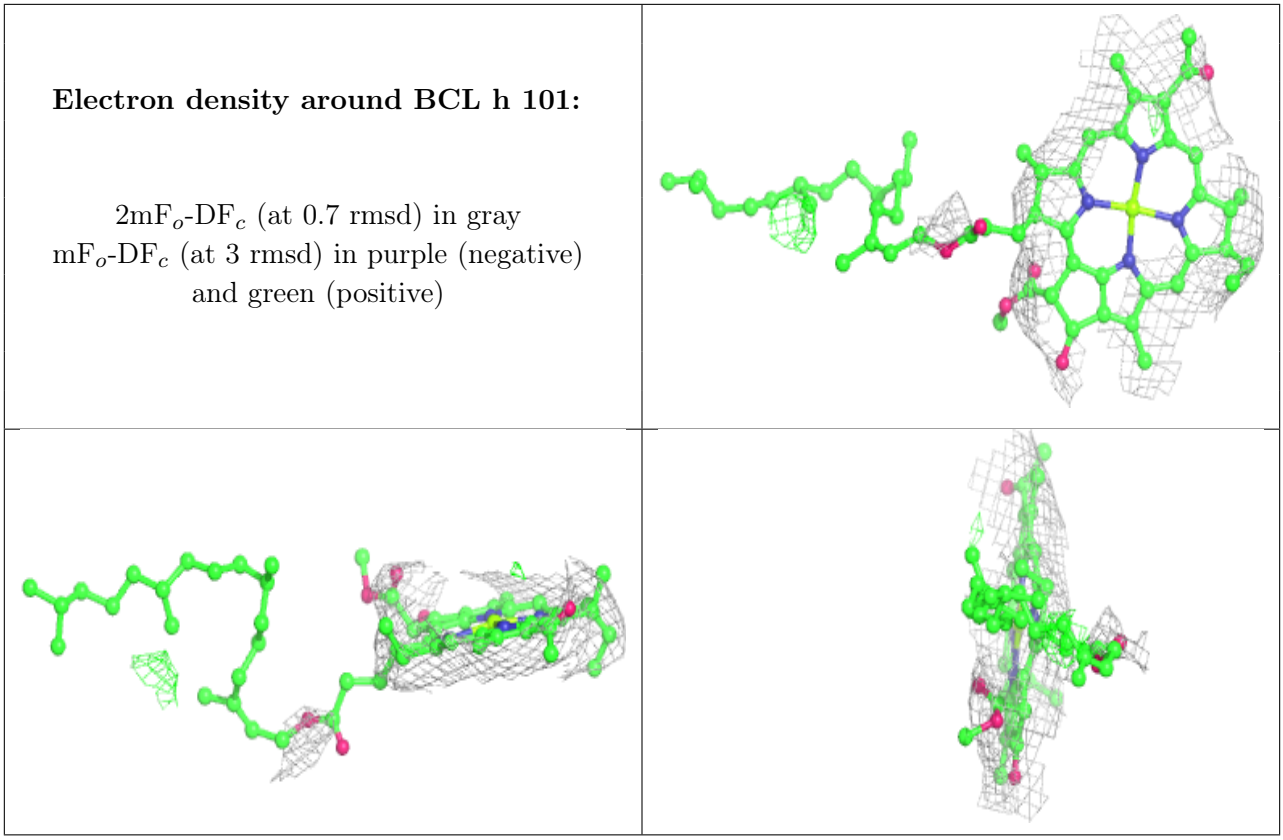






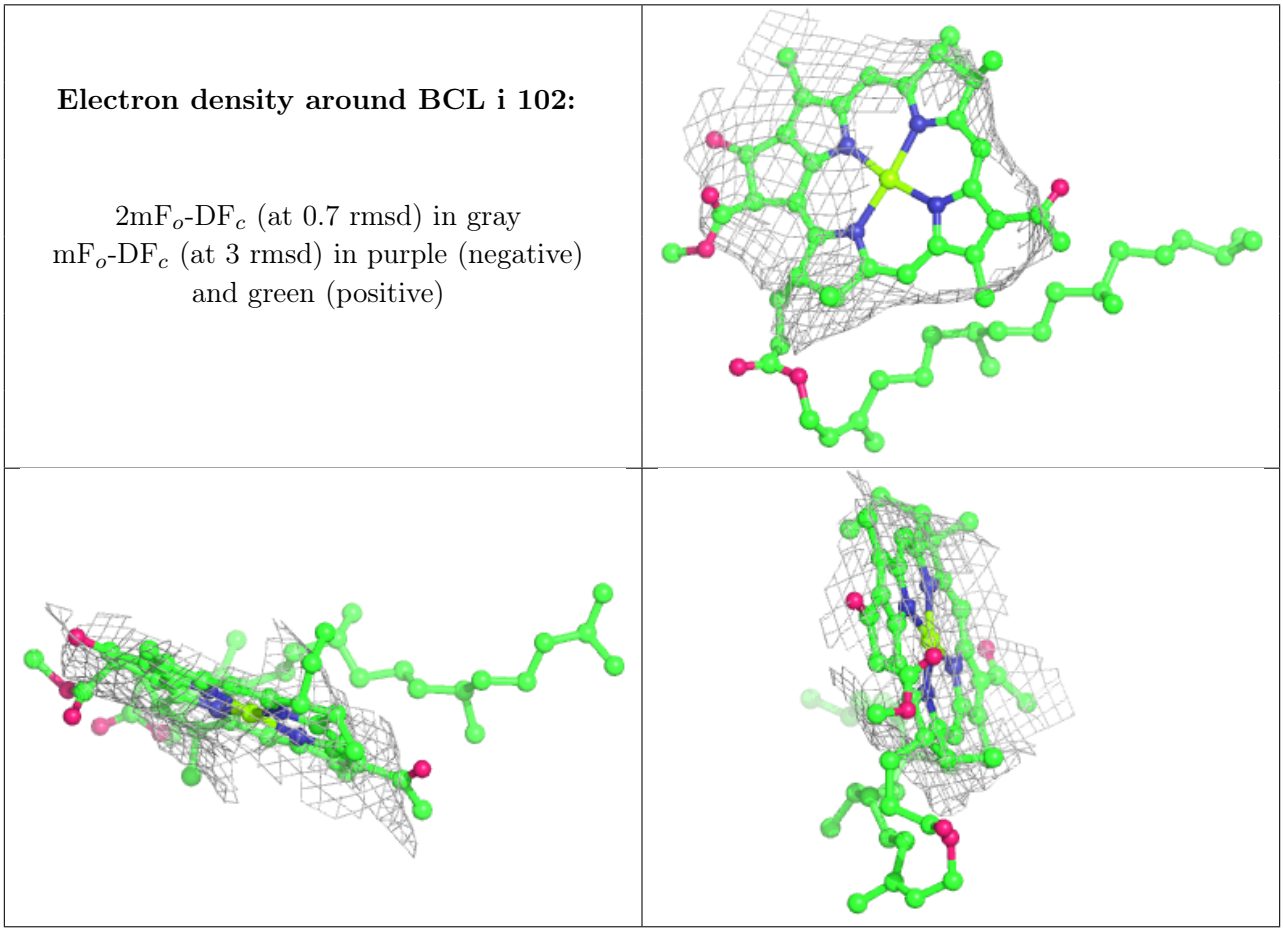
Electron density around BCL h 101:

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



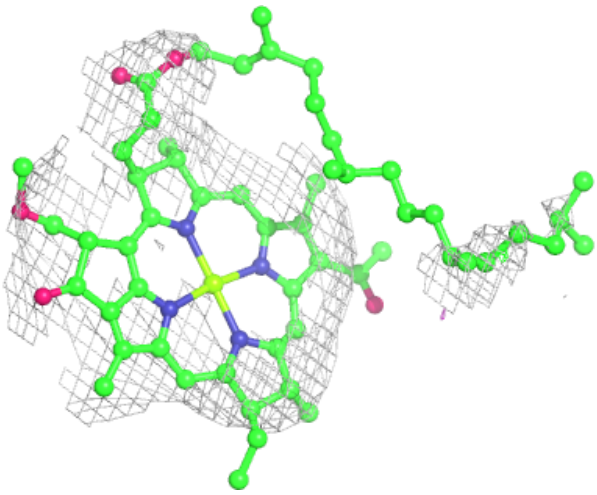
Electron density around BCL i 102:

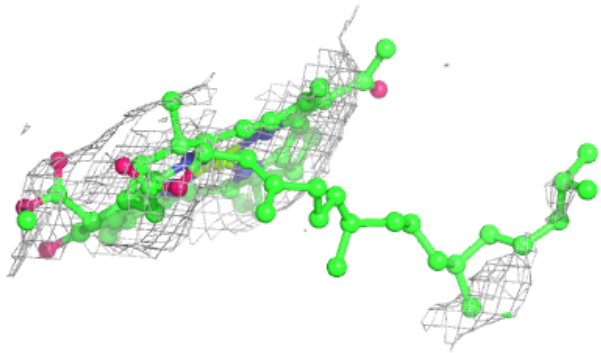
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

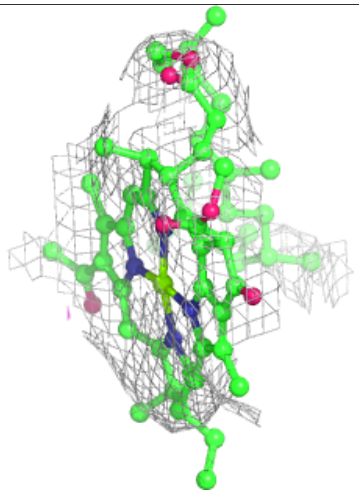


Electron density around BCL AJ 102:

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

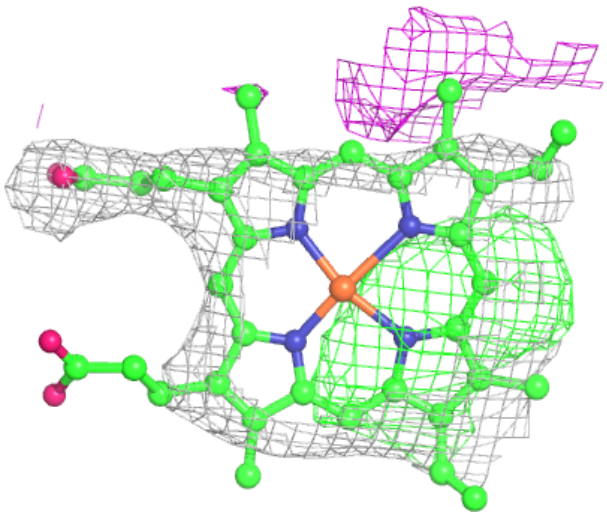


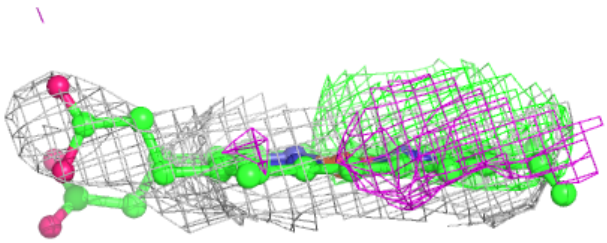


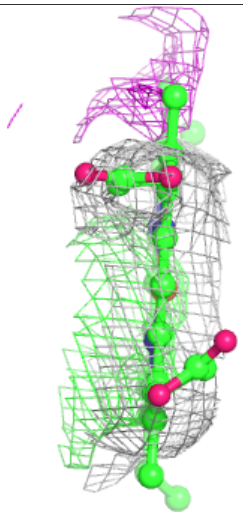


Electron density around HEM o 504:

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

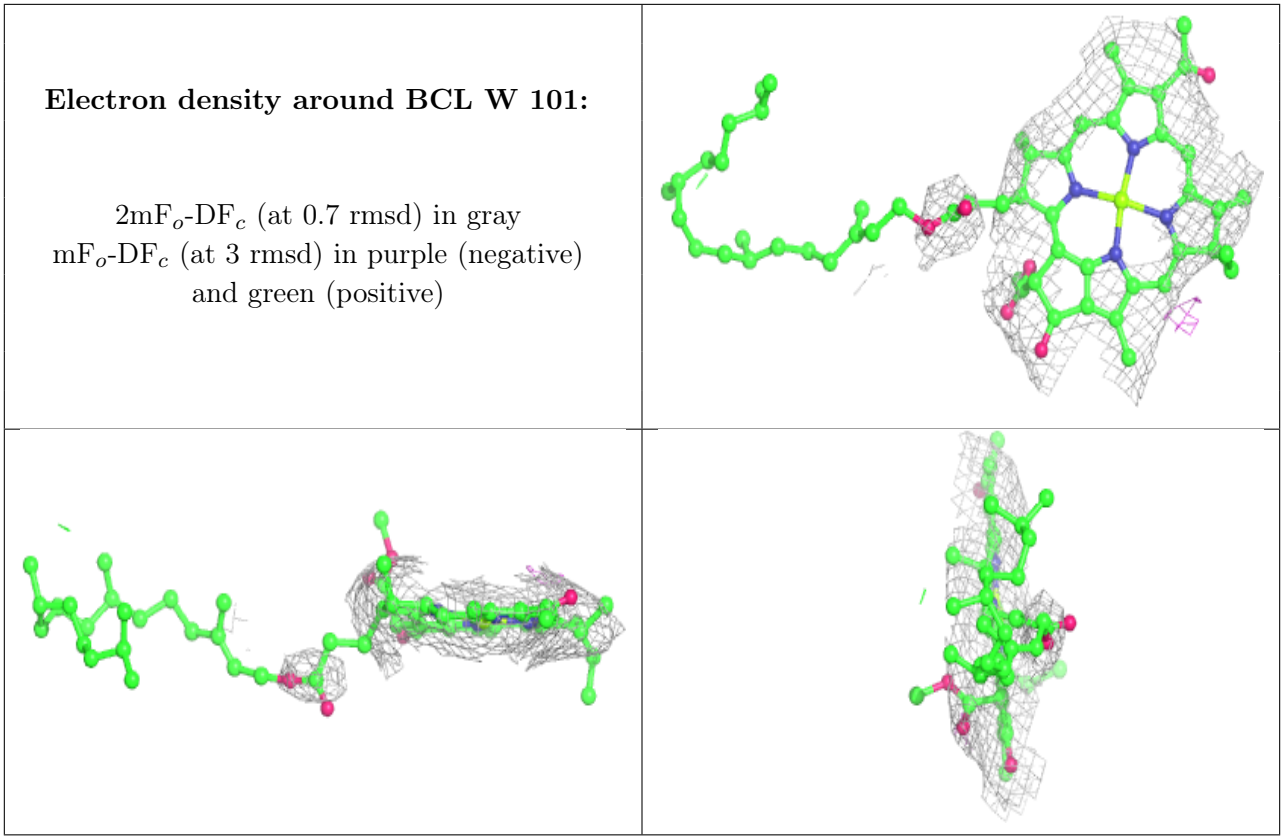






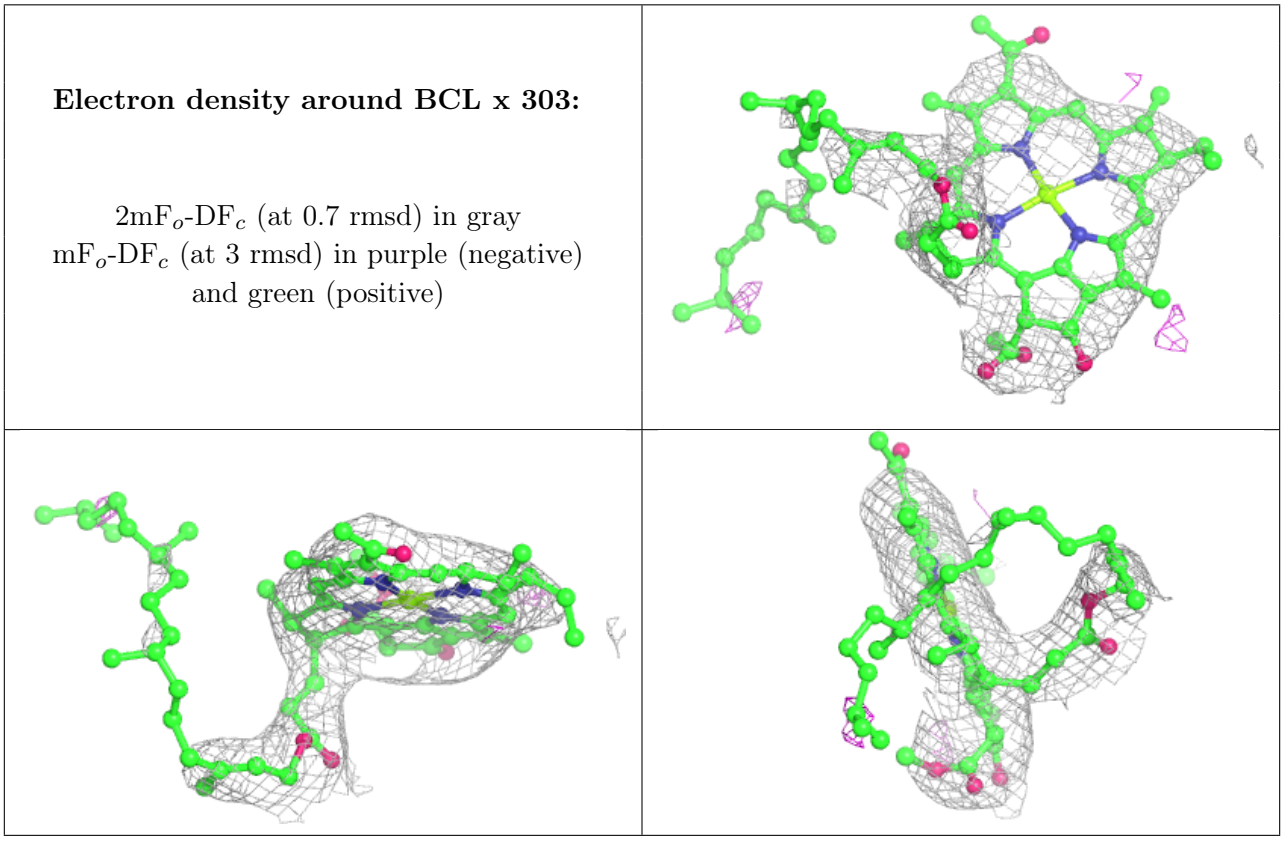
Electron density around BCL W 101:

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



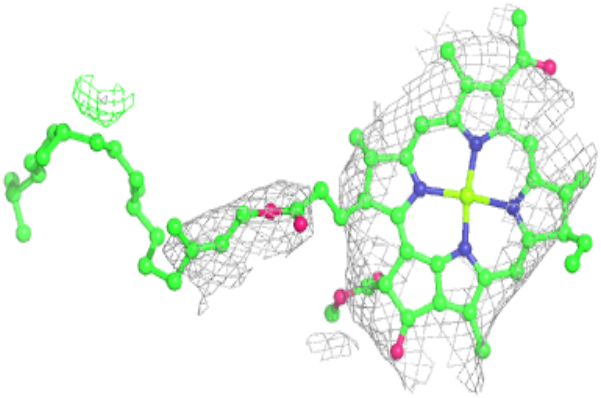
Electron density around BCL x 303:

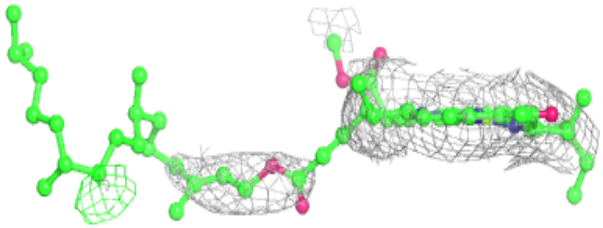
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

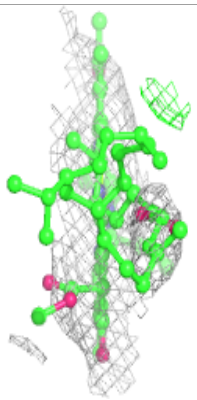


Electron density around BCL Y 101:

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

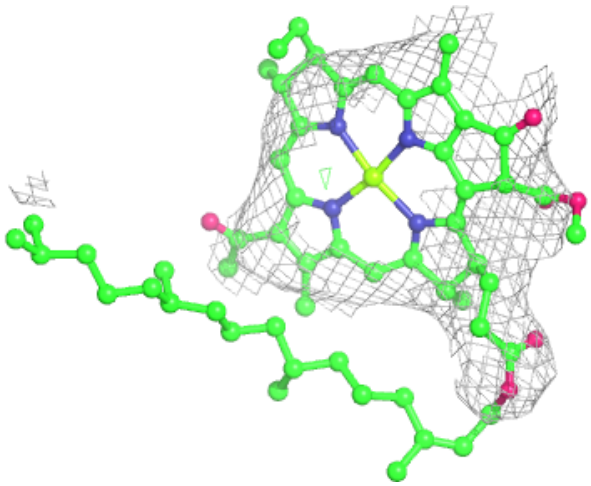


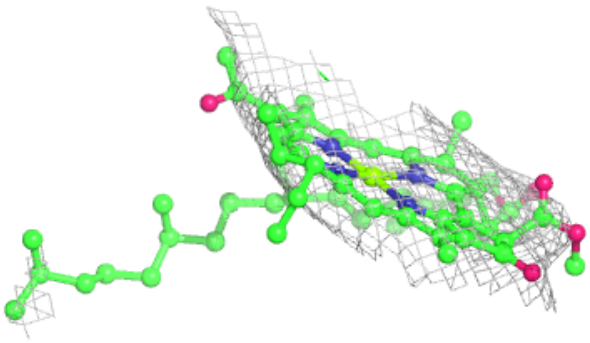


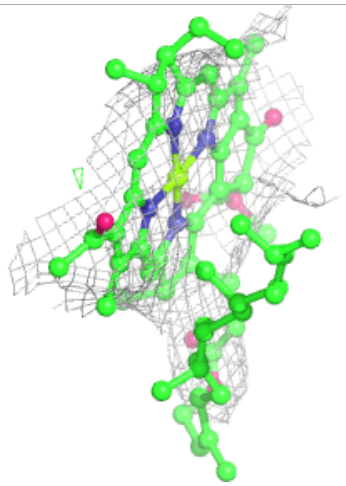


Electron density around BCL Z 102:

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

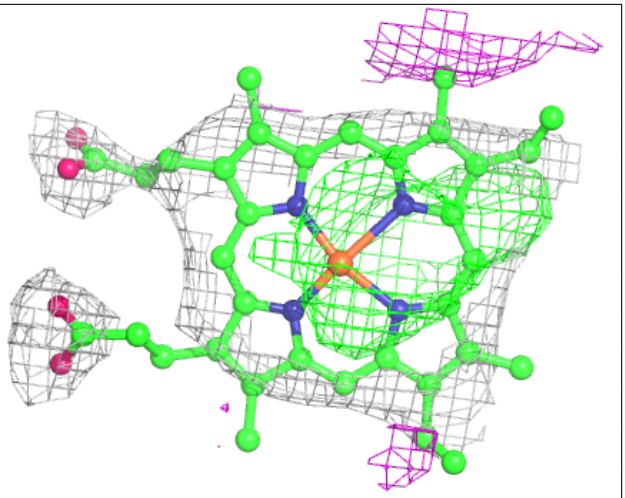


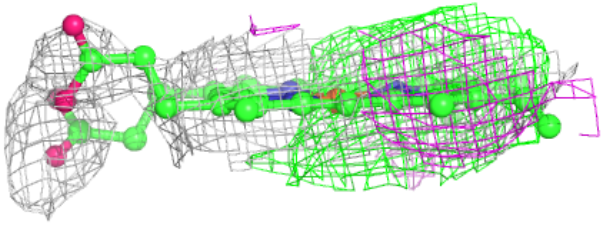


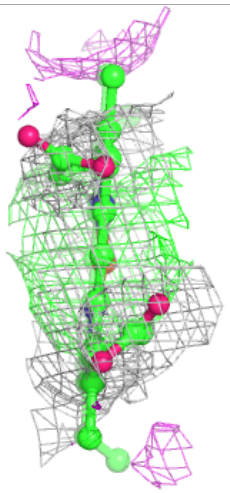


Electron density around HEM C 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

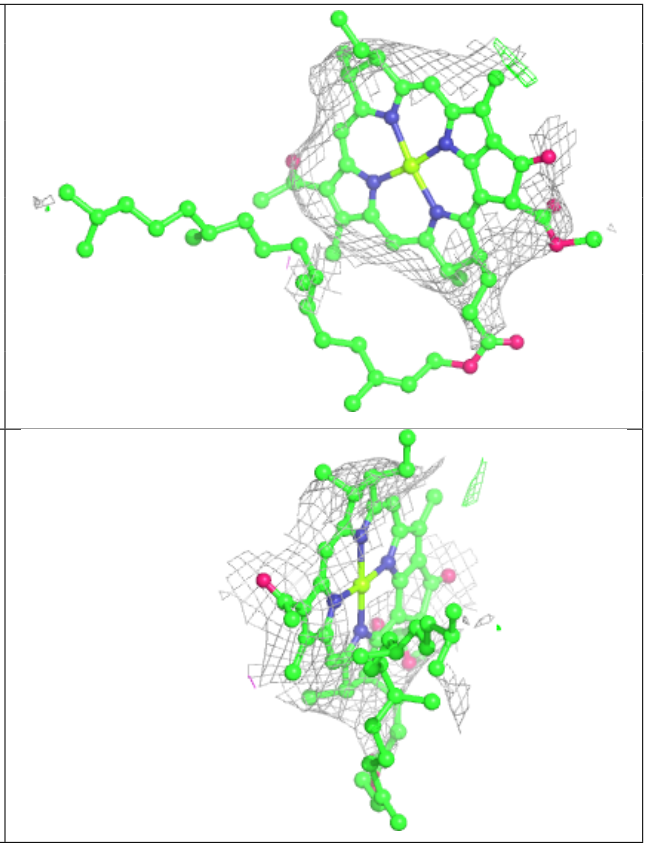






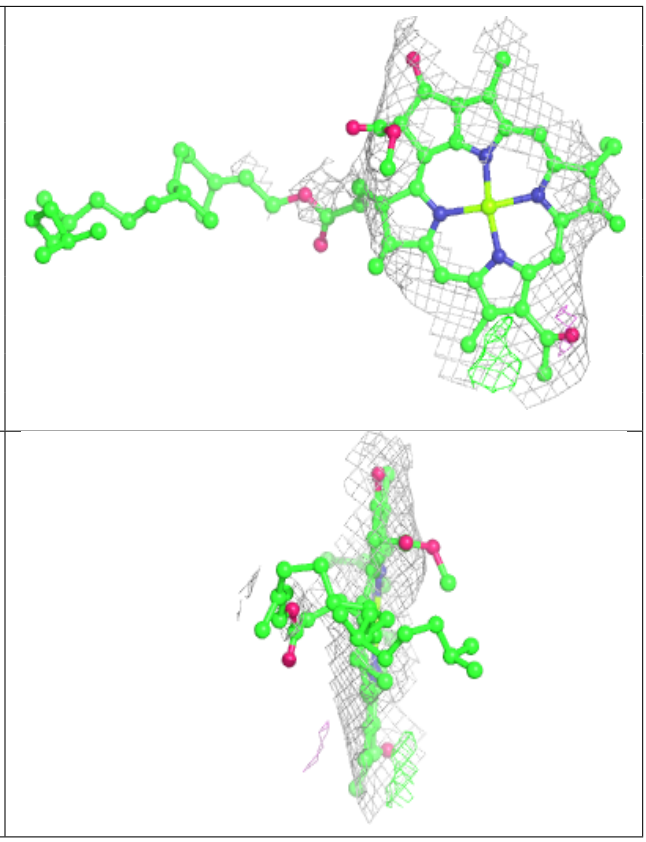
Electron density around BCL 1 102:

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



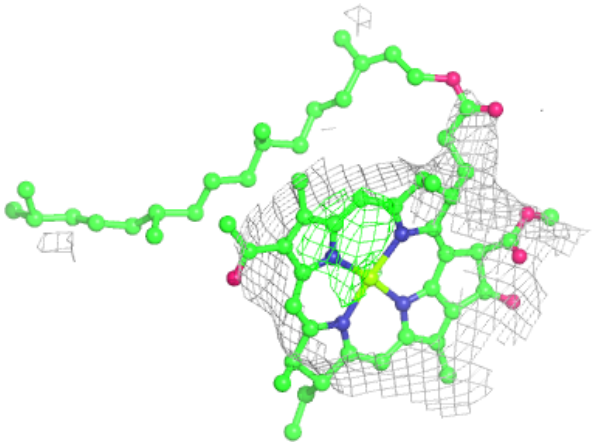
Electron density around BCL r 101:

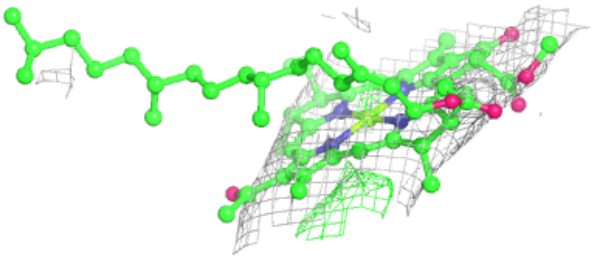
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

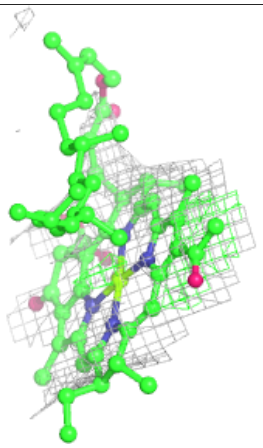


Electron density around BCL s 102:

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

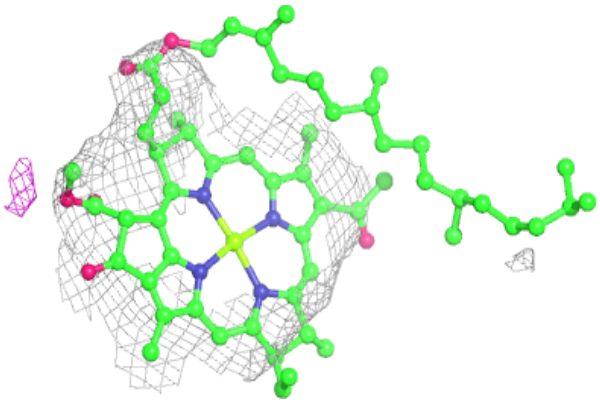


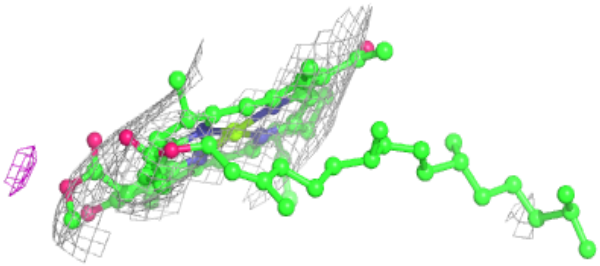


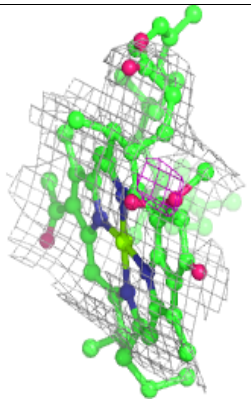


Electron density around BCL G 102:

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

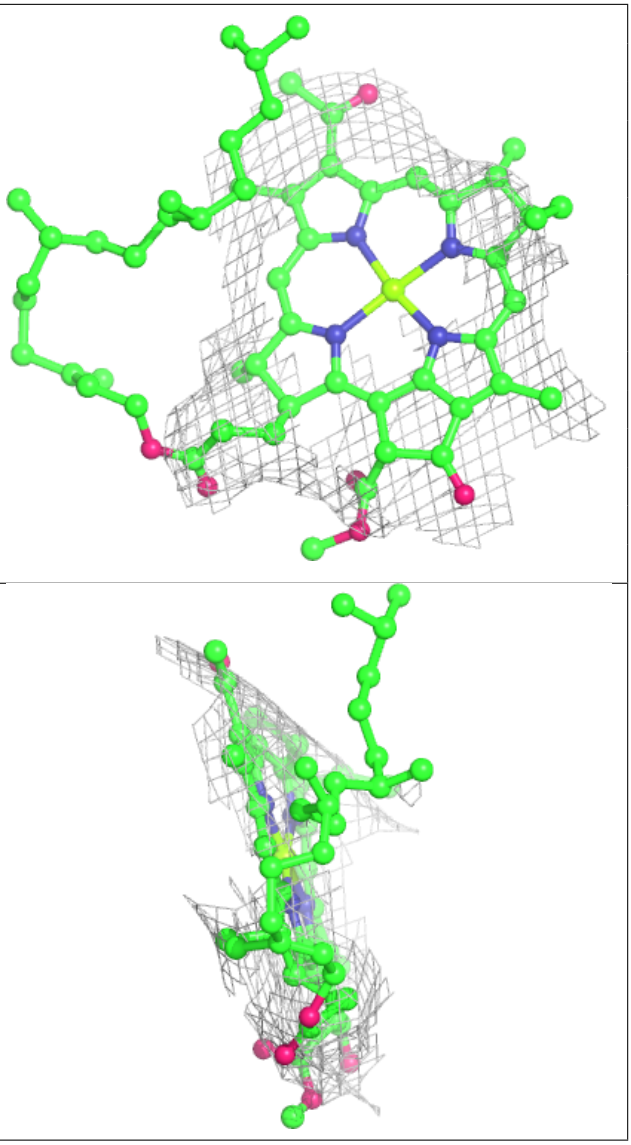






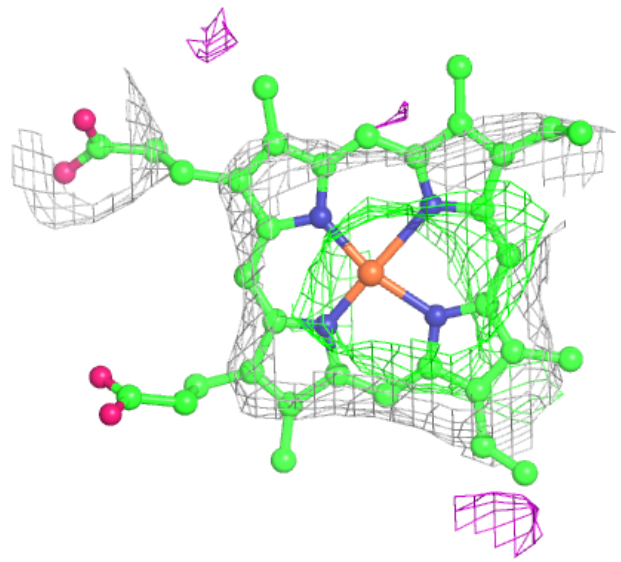
Electron density around BCL A 102:

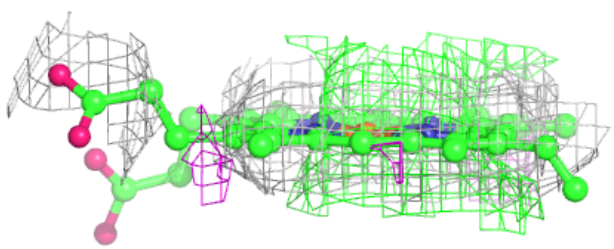
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

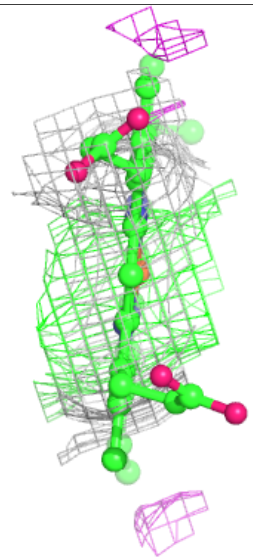


Electron density around HEM o 503:

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

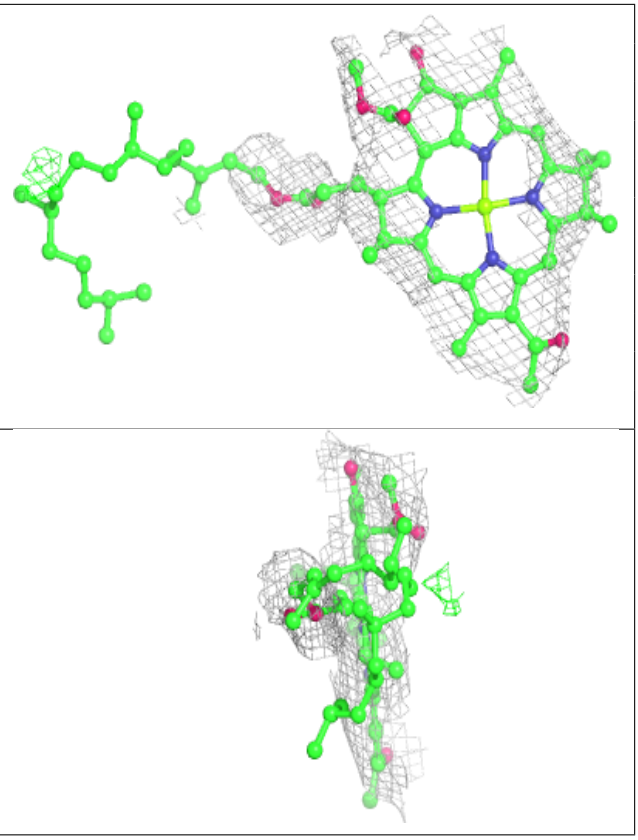






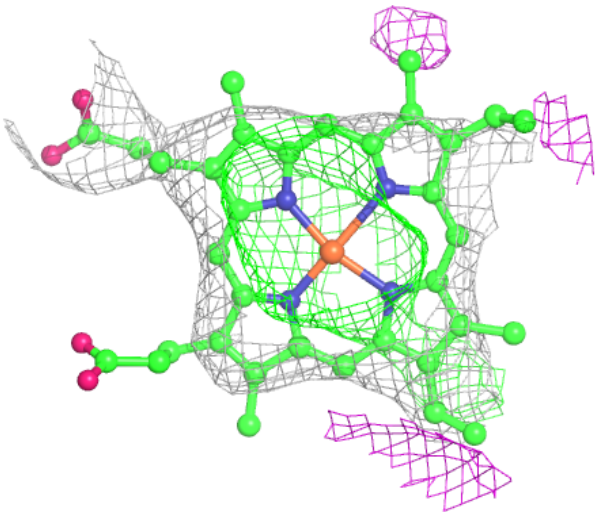
Electron density around BCL U 101:

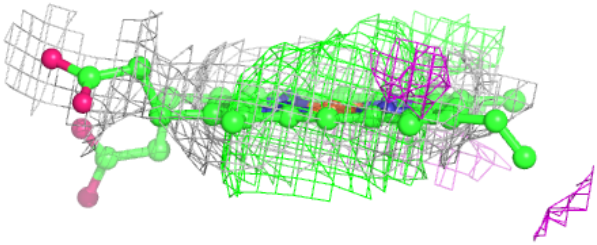
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

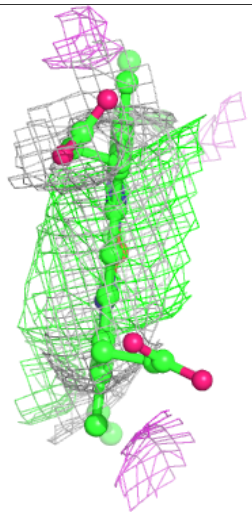


Electron density around HEM C 503:

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

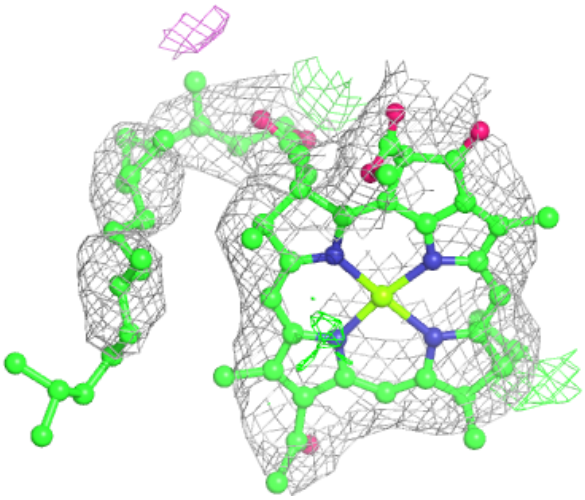


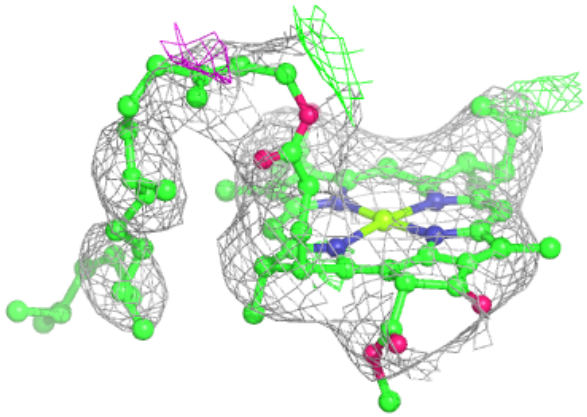


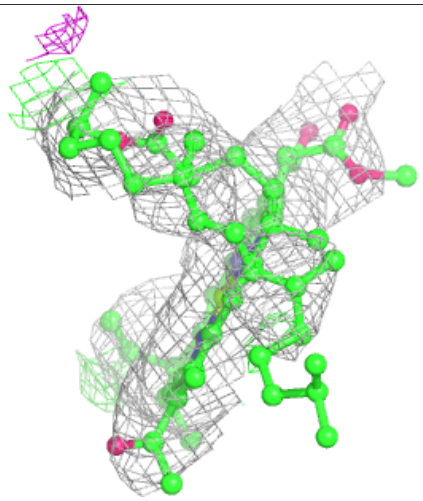


Electron density around BCL x 305:

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

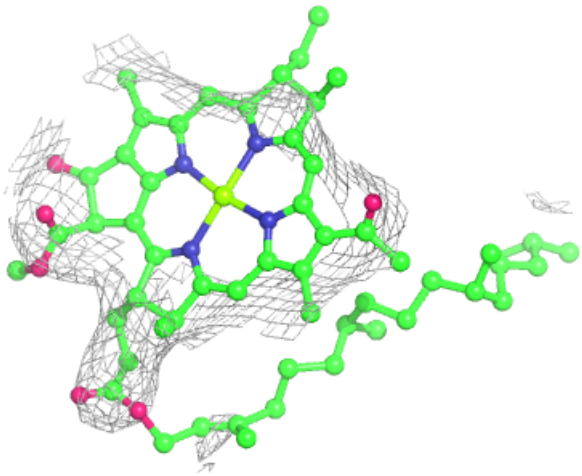


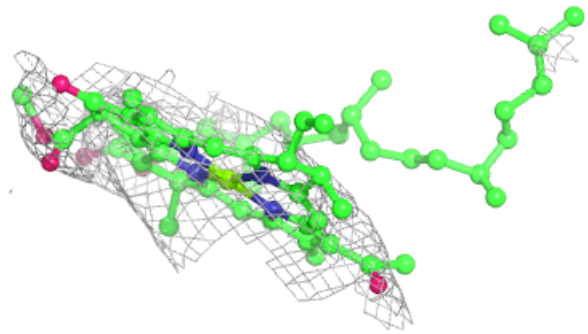


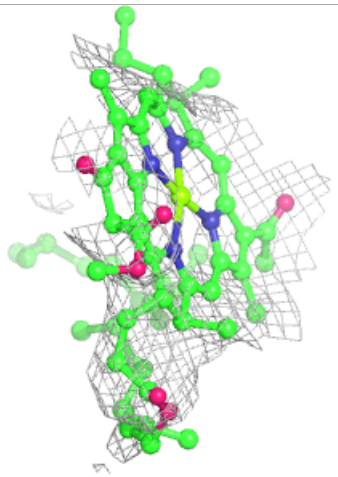


Electron density around BCL 4 102:

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

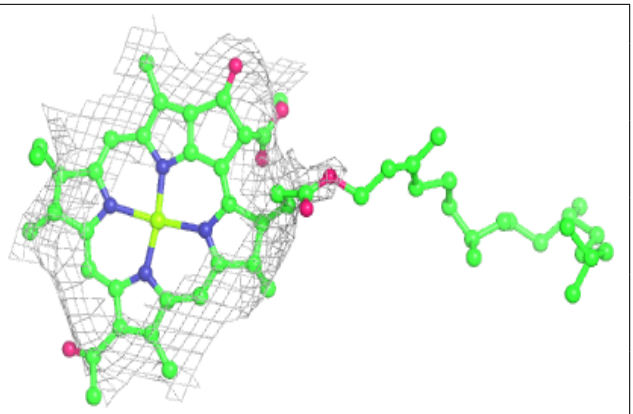


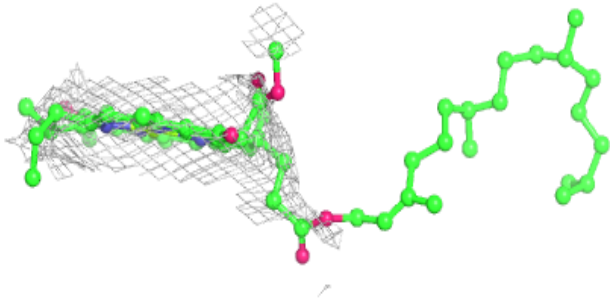


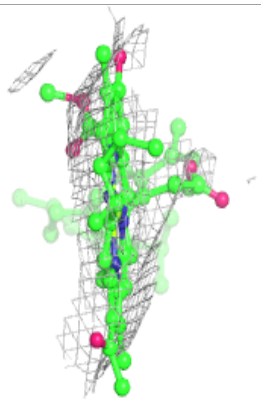


Electron density around BCL AA 101:

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

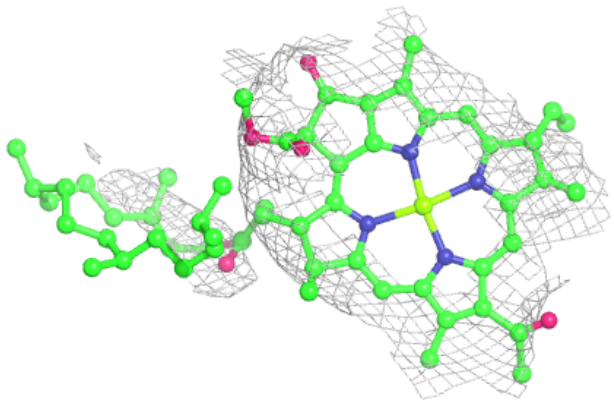


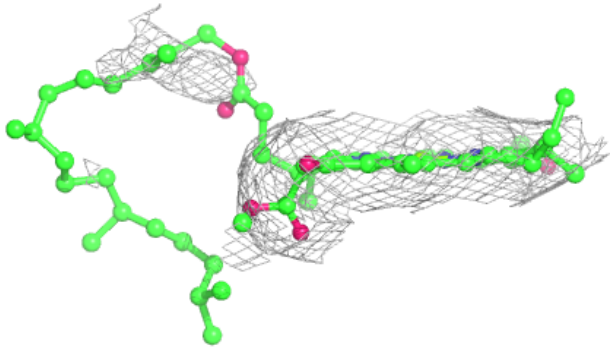


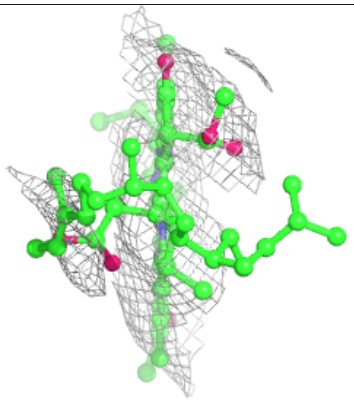


Electron density around BCL Q 101:

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

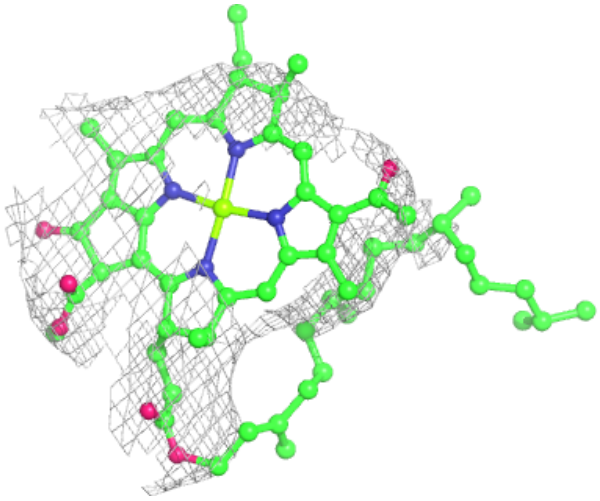


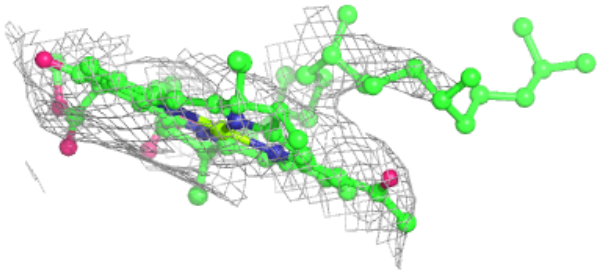


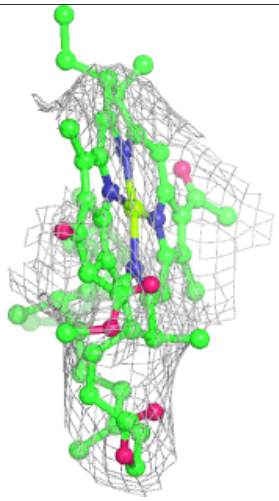


Electron density around BCL X 102:

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

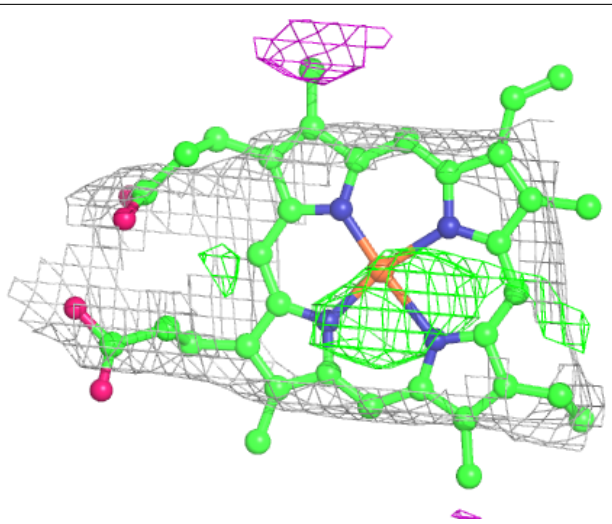


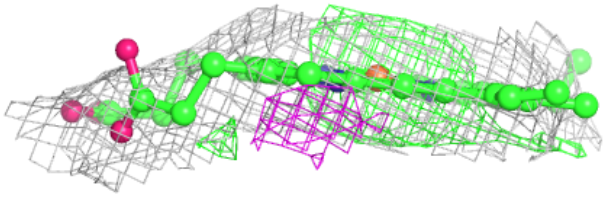


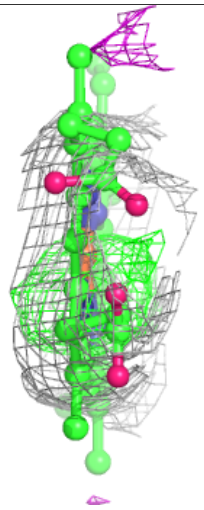


Electron density around HEM C 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

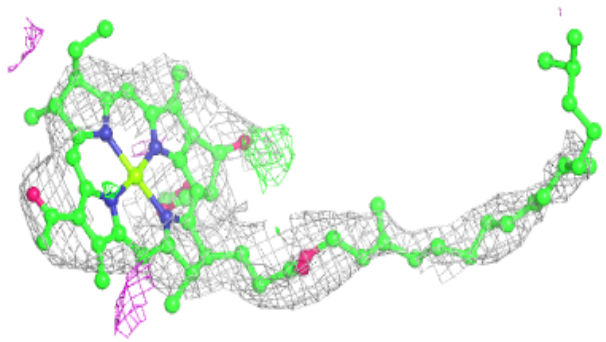


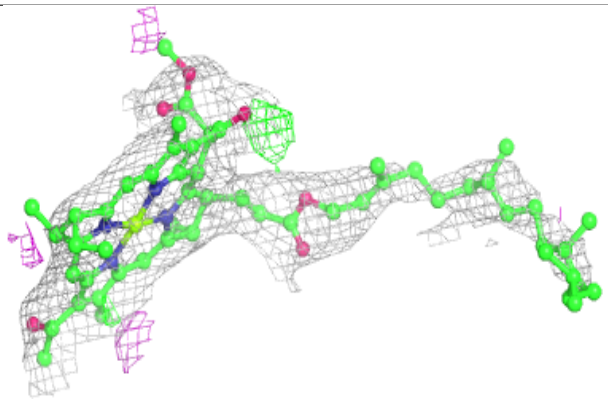


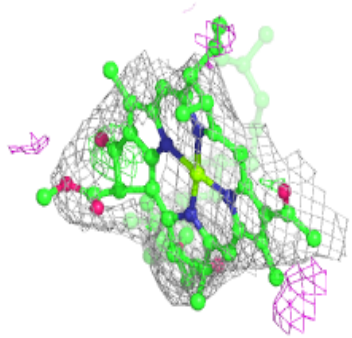


Electron density around BCL M 401:

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

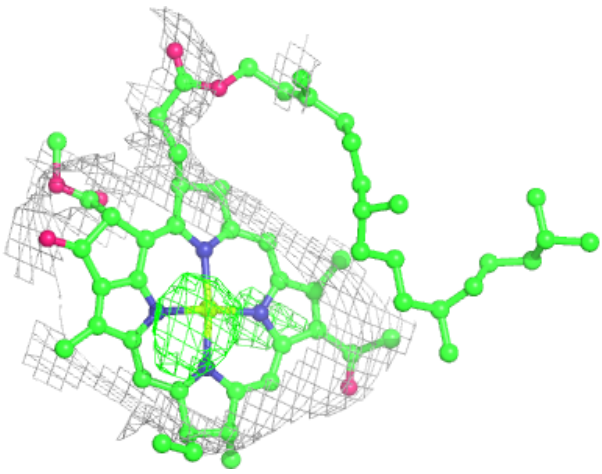


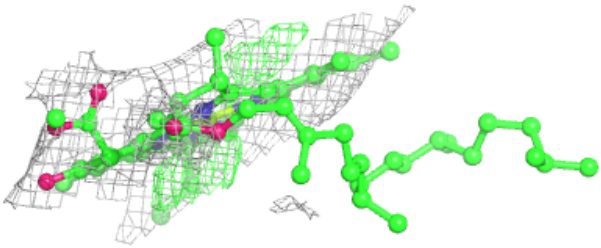


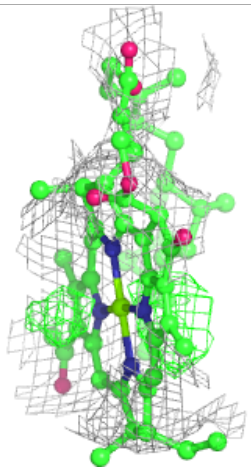


Electron density around BCL p 104:

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

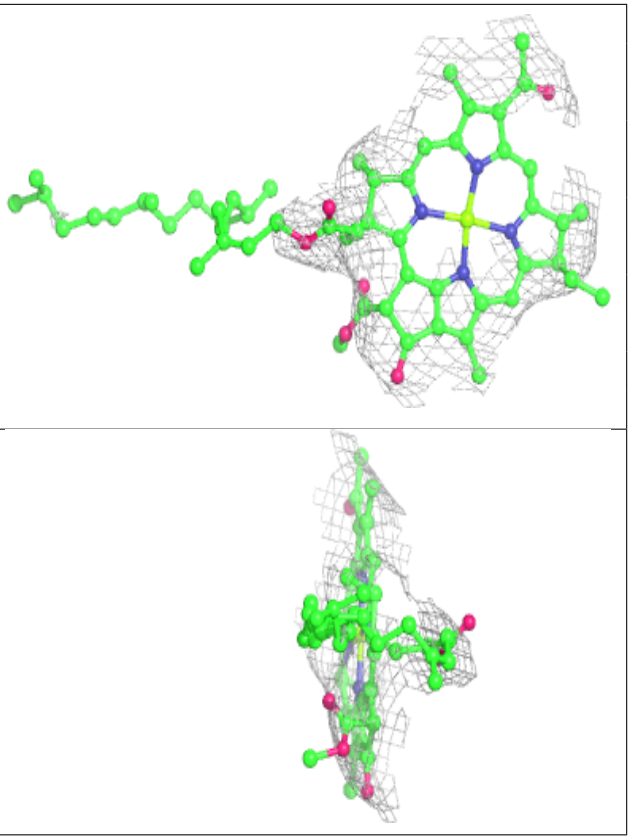


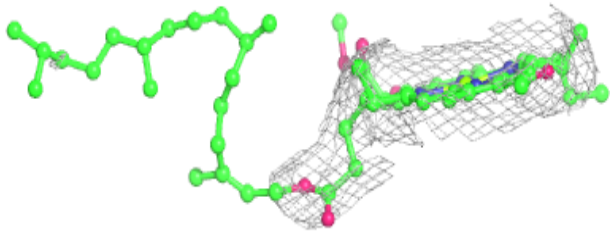




Electron density around BCL 5 101:

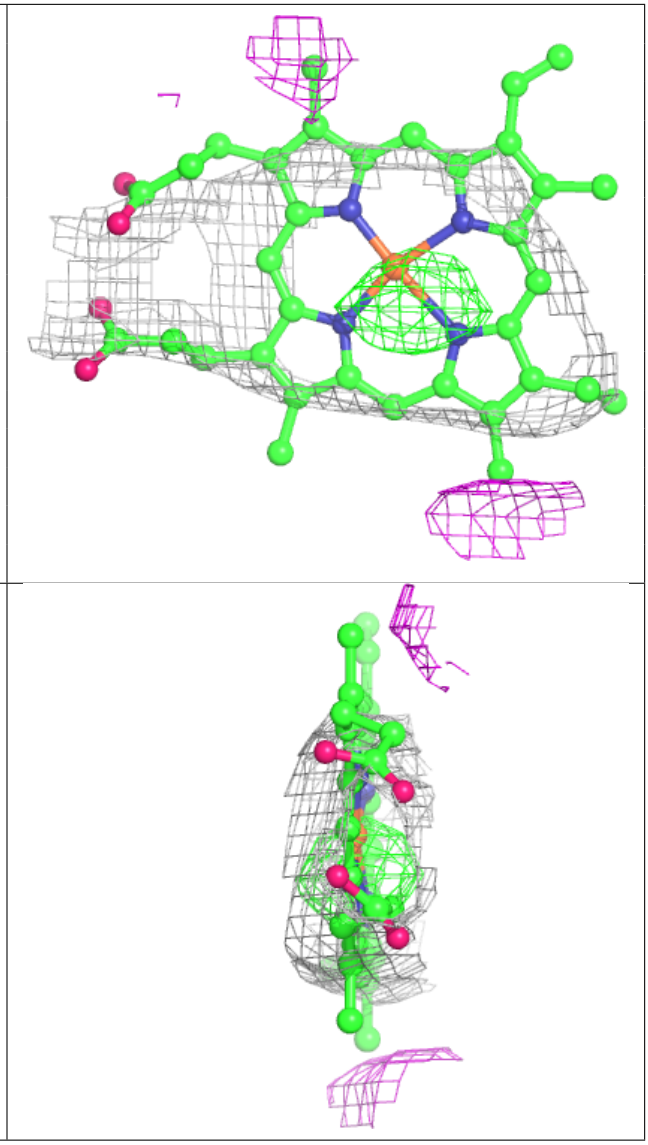
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEM o 502:

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



6.5 Other polymers (i)

There are no such residues in this entry.