wwPDB X-ray Structure Validation Summary Report (i)

Mar 13, 2024 – 08:35 AM EDT

PDB ID	:	4V8K
Title	:	Crystal structure of the LH1-RC complex from Thermochromatium tepidum in P21 form
Authors	:	Niwa, S.; Takeda, K.; Wang-Otomo, Z.-Y.; Miki, K.
Deposited on	:	2013-11-22
Resolution	:	3.01 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:

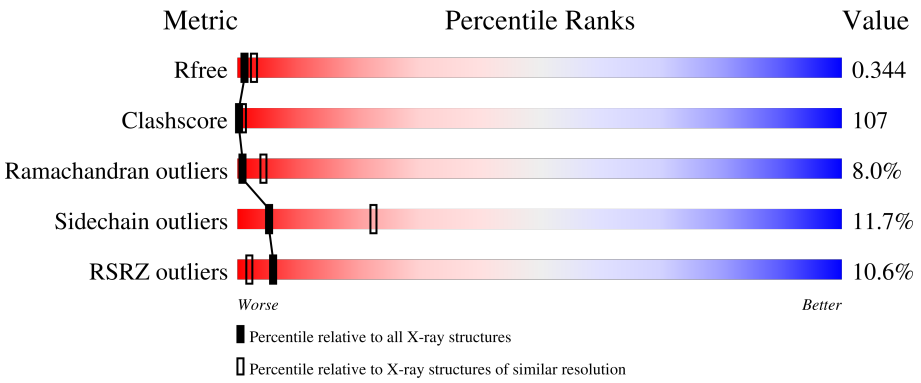
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.01 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	AC	404	5% 14% 50% 13% • 22%
1	BC	404	6% 14% 52% 11% • 22%
2	AL	281	3% 9% 69% 21% •
2	BL	281	6% 10% 75% 14%
3	AM	325	3% 9% 65% 20% • •

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Mol	Chain	Length	Quality of chain
3	BM	325	3% 13% 65% 19%
4	AH	259	6% 18% 69% 12%
4	BH	259	9% 21% 64% 15%
5	A1	61	16% 10% 74% 11% 5%
5	A3	61	10% 20% 64% 8% 7%
5	A5	61	21% 16% 66% 10% 8%
5	A7	61	15% 8% 59% 16% 16%
5	A9	61	21% 20% 72% 7%
5	AA	61	16% 8% 57% 13% 21%
5	AD	61	20% 13% 70% 10% 7%
5	AF	61	10% 31% 49% 16%
5	AI	61	18% 20% 64% 13%
5	AK	61	8% 28% 56% 11% 5%
5	AO	61	16% 13% 66% 18%
5	AQ	61	7% 20% 66% 8% 7%
5	AS	61	10% 18% 67% 10%
5	AU	61	21% 18% 66% 13%
5	AW	61	8% 18% 64% 16%
5	AY	61	13% 15% 67% 16%
5	B1	61	5% 18% 56% 15% 11%
5	B3	61	11% 20% 67% 11%
5	B5	61	33% 23% 54% 5% 16%
5	B7	61	10% 18% 61% 10% 11%
5	B9	61	8% 11% 66% 7% 16%
5	BA	61	15% 15% 64% 10% 10%

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Mol	Chain	Length	Quality of chain
5	BD	61	10% · 64% 7% 26%
5	BF	61	16% 15% 67% 10% 8%
5	BI	61	11% 8% 62% 11% 18%
5	BK	61	21% 25% 61% 13% ·
5	BO	61	16% 16% 74% 7% ·
5	BQ	61	18% 28% 62% 7% ·
5	BS	61	23% 20% 70% 7% ·
5	BU	61	21% 15% 64% 16% 5%
5	BW	61	20% 15% 62% 18% 5%
5	BY	61	5% 13% 56% 20% 11%
6	A0	47	4% 11% 51% 23% 15%
6	A2	47	17% 21% 57% 6% 15%
6	A4	47	6% 17% 53% 15% 15%
6	A6	47	4% 32% 47% 6% 15%
6	A8	47	21% 17% 53% 15% 15%
6	AB	47	13% 21% 51% 13% 15%
6	AE	47	19% 23% 57% · 15%
6	AG	47	2% 9% 60% 17% 15%
6	AJ	47	9% 15% 62% 9% 15%
6	AN	47	4% 13% 60% 13% 15%
6	AP	47	9% 9% 66% 11% 15%
6	AR	47	21% 21% 53% 11% 15%
6	AT	47	6% 17% 51% 17% 15%
6	AV	47	15% 21% 53% 11% 15%
6	AX	47	9% 9% 72% · 15%

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Mol	Chain	Length	Quality of chain
6	AZ	47	15% 17% 57% 9% 15%
6	B0	47	17% 11% 64% 11% 15%
6	B2	47	15% 64% 6% 15%
6	B4	47	9% 26% 47% 13% 15%
6	B6	47	21% 28% 51% 6% 15%
6	B8	47	9% 17% 53% 15% 15%
6	BB	47	17% 19% 49% 17% 15%
6	BE	47	13% 17% 60% 9% 15%
6	BG	47	15% 15% 66% 15%
6	BJ	47	13% 11% 68% 6% 15%
6	BN	47	9% 17% 62% 6% 15%
6	BP	47	11% 9% 70% 6% 15%
6	BR	47	9% 28% 45% 13% 15%
6	BT	47	6% 13% 62% 11% 15%
6	BV	47	4% 26% 55% 15%
6	BX	47	2% 21% 55% 9% 15%
6	BZ	47	9% 26% 53% 6% 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	BL	304	-	-	-	X
14	CRT	A0	101	-	-	X	X
14	CRT	A1	103	-	-	X	X
14	CRT	A2	102	-	-	X	X
14	CRT	A5	103	-	-	X	X
14	CRT	A7	102	-	-	X	X
14	CRT	AA	102	-	-	X	X
14	CRT	AB	102	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CRT	AG	102	-	-	-	X
14	CRT	AJ	102	-	-	X	X
14	CRT	AN	102	-	-	-	X
14	CRT	AP	102	-	-	X	X
14	CRT	AR	102	-	-	-	X
14	CRT	AS	104	-	-	X	X
14	CRT	AT	102	-	-	-	X
14	CRT	AW	102	-	-	X	X
14	CRT	AX	102	-	-	X	X
14	CRT	B0	101	-	-	X	X
14	CRT	B1	103	-	-	X	X
14	CRT	B2	102	-	-	X	X
14	CRT	B5	103	-	-	X	X
14	CRT	B7	102	-	-	X	X
14	CRT	BA	102	-	-	X	X
14	CRT	BB	102	-	-	X	X
14	CRT	BF	103	-	-	-	X
14	CRT	BG	102	-	-	-	X
14	CRT	BM	406	-	-	-	X
14	CRT	BN	102	-	-	-	X
14	CRT	BO	103	-	-	-	X
14	CRT	BP	102	-	-	X	X
14	CRT	BS	103	-	-	-	X
14	CRT	BU	103	-	-	X	X
14	CRT	BV	102	-	-	X	X
14	CRT	BW	103	-	-	X	X
15	PEF	AM	407	-	X	-	X
15	PEF	AM	409	-	-	-	X
15	PEF	AS	101	-	-	X	X
15	PEF	BM	407	-	-	-	X
15	PEF	BQ	101	-	-	-	X
8	CA	AO	101	-	-	-	X
9	BCL	A0	102	-	-	X	-
9	BCL	A1	102	-	-	X	-
9	BCL	A2	101	-	-	X	-
9	BCL	A3	103	-	-	X	-
9	BCL	A3	104	-	-	X	-
9	BCL	A5	102	-	-	X	-
9	BCL	A6	101	-	-	X	-
9	BCL	A7	103	-	-	X	-
9	BCL	A8	101	-	-	X	-
9	BCL	A9	102	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BCL	AA	101	-	-	X	-
9	BCL	AB	101	-	-	X	-
9	BCL	AD	102	-	-	X	-
9	BCL	AE	101	-	-	X	-
9	BCL	AF	102	-	-	X	-
9	BCL	AG	101	-	-	X	-
9	BCL	AI	102	-	-	X	-
9	BCL	AJ	101	-	-	X	-
9	BCL	AK	102	-	-	X	-
9	BCL	AL	301	-	-	X	-
9	BCL	AL	303	-	-	X	-
9	BCL	AM	402	-	-	X	-
9	BCL	AN	101	-	-	X	-
9	BCL	AO	102	-	-	X	-
9	BCL	AP	101	-	-	X	-
9	BCL	AQ	102	-	-	X	-
9	BCL	AR	101	-	-	X	-
9	BCL	AS	103	-	-	X	-
9	BCL	AT	101	-	-	X	-
9	BCL	AU	102	-	-	X	-
9	BCL	AV	102	-	-	X	-
9	BCL	AW	101	-	-	X	-
9	BCL	AX	101	-	-	X	-
9	BCL	AY	102	-	-	X	-
9	BCL	AZ	101	-	-	X	-
9	BCL	B0	102	-	-	X	-
9	BCL	B1	102	-	-	X	-
9	BCL	B2	101	-	-	X	-
9	BCL	B3	102	-	-	X	-
9	BCL	B4	101	-	-	X	-
9	BCL	B5	102	-	-	X	-
9	BCL	B6	101	-	-	X	-
9	BCL	B7	103	-	-	X	-
9	BCL	B8	101	-	-	X	-
9	BCL	B9	102	-	-	X	X
9	BCL	BA	101	-	-	X	X
9	BCL	BB	101	-	-	X	-
9	BCL	BD	102	-	-	X	-
9	BCL	BE	101	-	-	X	-
9	BCL	BF	102	-	-	X	-
9	BCL	BG	101	-	-	X	-
9	BCL	BI	102	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BCL	BJ	101	-	-	X	-
9	BCL	BK	102	-	-	X	X
9	BCL	BL	301	-	-	X	-
9	BCL	BM	402	-	-	X	-
9	BCL	BN	101	-	-	X	-
9	BCL	BO	102	-	-	X	-
9	BCL	BP	101	-	-	X	-
9	BCL	BQ	103	-	-	X	-
9	BCL	BQ	104	-	-	X	-
9	BCL	BS	102	-	-	X	-
9	BCL	BU	102	-	-	X	-
9	BCL	BV	101	-	-	X	X
9	BCL	BW	102	-	-	X	-
9	BCL	BX	101	-	-	X	-
9	BCL	BY	102	-	-	X	-
9	BCL	BZ	101	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 50862 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	AC	317	2458	1551	430	460	17	0	0	0
1	BC	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	AL	280	2231	1501	359	361	10	0	0	0
2	BL	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	AM	319	2551	1713	417	410	11	0	0	0
3	BM	319	2551	1713	417	410	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	AH	258	1982	1275	339	363	5	0	0	0
4	BH	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	AA	48	392	265	62	64	1	0	0	0
5	AD	57	447	295	74	77	1	0	0	0
5	AF	59	462	304	76	80	2	0	0	0
5	AI	59	462	304	76	80	2	0	0	0
5	AK	58	455	300	75	78	2	0	0	0
5	AO	59	462	304	76	80	2	0	0	0
5	AQ	57	447	295	74	77	1	0	0	0
5	AS	59	462	304	76	80	2	0	0	0
5	AU	60	473	313	77	81	2	0	0	0
5	AW	60	473	313	77	81	2	0	0	0
5	AY	60	473	313	77	81	2	0	0	0
5	A1	58	455	300	75	78	2	0	0	0
5	A3	57	447	295	74	77	1	0	0	0
5	A5	56	444	294	73	75	2	0	0	0
5	A7	51	417	279	67	69	2	0	0	0
5	A9	60	473	313	77	81	2	0	0	0
5	BA	55	448	299	72	75	2	0	0	0
5	BD	45	370	250	59	60	1	0	0	0
5	BF	56	444	294	73	75	2	0	0	0
5	BI	50	409	274	66	68	1	0	0	0
5	BK	60	473	313	77	81	2	0	0	0
5	BO	59	462	304	76	80	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	BQ	59	467	310	76	79	2	0	0	0
			Total	C	N	O	S			
5	BS	59	462	304	76	80	2	0	0	0
			Total	C	N	O	S			
5	BU	58	462	307	75	78	2	0	0	0
			Total	C	N	O	S			
5	BW	58	455	300	75	78	2	0	0	0
			Total	C	N	O	S			
5	BY	54	426	284	69	72	1	0	0	0
			Total	C	N	O	S			
5	B1	54	426	284	69	72	1	0	0	0
			Total	C	N	O	S			
5	B3	60	473	313	77	81	2	0	0	0
			Total	C	N	O	S			
5	B5	51	417	279	67	69	2	0	0	0
			Total	C	N	O	S			
5	B7	54	426	284	69	72	1	0	0	0
			Total	C	N	O	S			
5	B9	51	417	279	67	69	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	AB	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AE	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AG	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	AN	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AP	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AR	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AT	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AV	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	AX	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	AZ	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	A2	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	A4	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	A6	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	A8	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	A0	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BB	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BE	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BG	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BJ	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BN	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BP	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BR	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BT	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BV	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BX	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	BZ	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	B2	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	B4	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	B6	40	337	228	52	55	2	0	0	0

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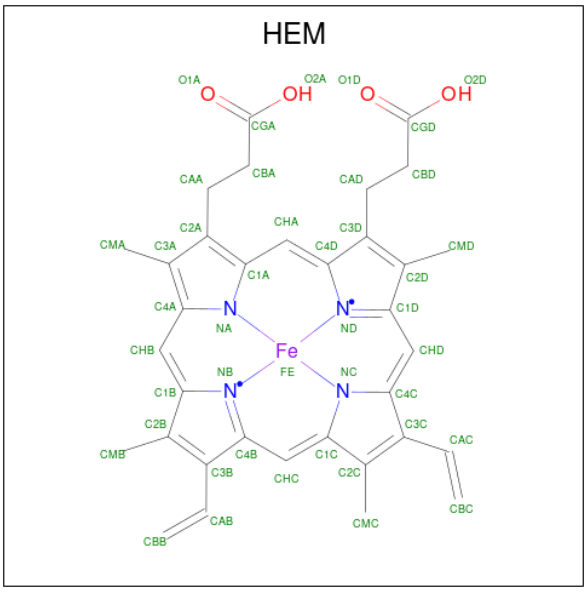
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	B8	40	337	228	52	55	2	0	0	0
			Total	C	N	O	S			
6	B0	40	337	228	52	55	2	0	0	0

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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
8	AC	1	1	1	0	0
8	AA	1	1	1	0	0
8	AD	1	1	1	0	0
8	AF	1	1	1	0	0
8	AI	1	1	1	0	0
8	AK	1	1	1	0	0
8	AO	1	1	1	0	0
8	AQ	1	1	1	0	0
8	AS	1	1	1	0	0
8	AU	1	1	1	0	0
8	AV	1	1	1	0	0
8	AY	1	1	1	0	0
8	A1	1	1	1	0	0
8	A3	1	1	1	0	0
8	A5	1	1	1	0	0
8	A7	1	1	1	0	0
8	A9	1	1	1	0	0
8	BC	1	1	1	0	0
8	BA	1	1	1	0	0
8	BD	1	1	1	0	0
8	BF	1	1	1	0	0
8	BI	1	1	1	0	0

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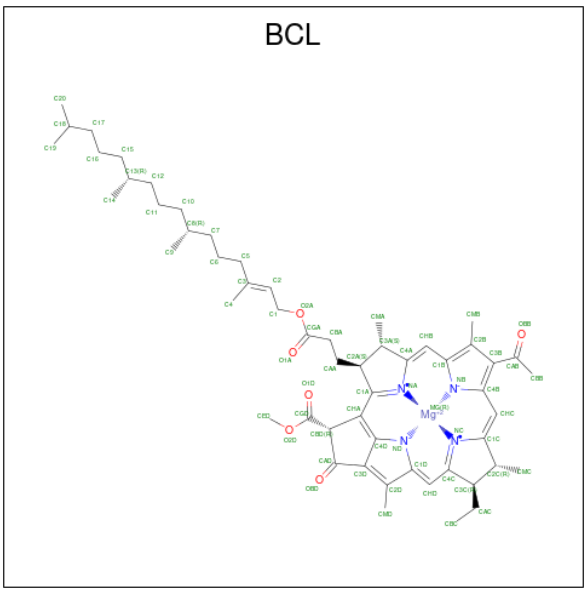
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	BK	1	Total Ca 1 1	0	0
8	BO	1	Total Ca 1 1	0	0
8	BQ	1	Total Ca 1 1	0	0
8	BS	1	Total Ca 1 1	0	0
8	BU	1	Total Ca 1 1	0	0
8	BW	1	Total Ca 1 1	0	0
8	BY	1	Total Ca 1 1	0	0
8	B1	1	Total Ca 1 1	0	0
8	B3	1	Total Ca 1 1	0	0
8	B5	1	Total Ca 1 1	0	0
8	B7	1	Total Ca 1 1	0	0
8	B9	1	Total Ca 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	AL	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AL	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AM	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AM	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AA	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AB	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AD	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AE	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AF	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AG	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AI	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AJ	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AK	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AN	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AO	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AP	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AQ	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AR	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AS	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AT	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AU	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
9	AV	1	66	55	1	4	6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
9	AW	1	66	55	1	4	6	0	0
9	AX	1	66	55	1	4	6	0	0
9	AY	1	66	55	1	4	6	0	0
9	AZ	1	66	55	1	4	6	0	0
9	A1	1	66	55	1	4	6	0	0
9	A2	1	66	55	1	4	6	0	0
9	A3	1	66	55	1	4	6	0	0
9	A3	1	66	55	1	4	6	0	0
9	A5	1	66	55	1	4	6	0	0
9	A6	1	66	55	1	4	6	0	0
9	A7	1	66	55	1	4	6	0	0
9	A8	1	66	55	1	4	6	0	0
9	A9	1	66	55	1	4	6	0	0
9	A0	1	66	55	1	4	6	0	0
9	BL	1	66	55	1	4	6	0	0
9	BL	1	66	55	1	4	6	0	0
9	BM	1	66	55	1	4	6	0	0
9	BM	1	66	55	1	4	6	0	0
9	BA	1	66	55	1	4	6	0	0
9	BB	1	66	55	1	4	6	0	0
9	BD	1	66	55	1	4	6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
9	BE	1	66	55	1	4	6	0	0
9	BF	1	66	55	1	4	6	0	0
9	BG	1	66	55	1	4	6	0	0
9	BI	1	66	55	1	4	6	0	0
9	BJ	1	66	55	1	4	6	0	0
9	BK	1	66	55	1	4	6	0	0
9	BN	1	66	55	1	4	6	0	0
9	BO	1	66	55	1	4	6	0	0
9	BP	1	66	55	1	4	6	0	0
9	BQ	1	66	55	1	4	6	0	0
9	BQ	1	66	55	1	4	6	0	0
9	BS	1	66	55	1	4	6	0	0
9	BT	1	66	55	1	4	6	0	0
9	BU	1	66	55	1	4	6	0	0
9	BV	1	66	55	1	4	6	0	0
9	BW	1	66	55	1	4	6	0	0
9	BX	1	66	55	1	4	6	0	0
9	BY	1	66	55	1	4	6	0	0
9	BZ	1	66	55	1	4	6	0	0
9	B1	1	66	55	1	4	6	0	0
9	B2	1	66	55	1	4	6	0	0

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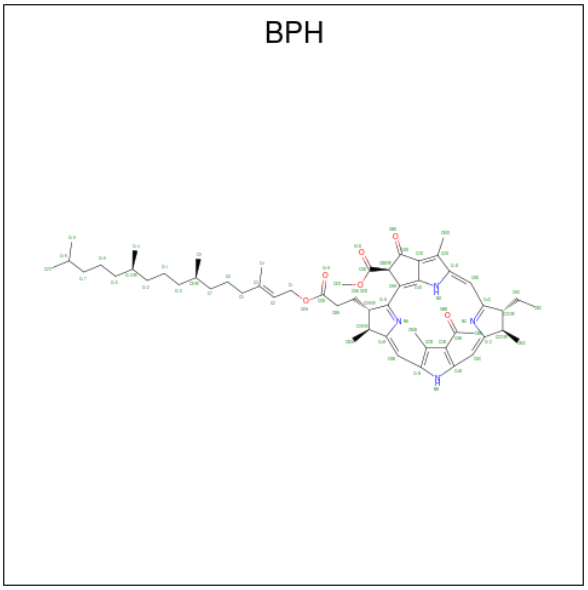
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
9	B3	1	66	55	1	4	6	0	0
9	B4	1	66	55	1	4	6	0	0
9	B5	1	66	55	1	4	6	0	0
9	B6	1	66	55	1	4	6	0	0
9	B7	1	66	55	1	4	6	0	0
9	B8	1	66	55	1	4	6	0	0
9	B9	1	66	55	1	4	6	0	0
9	B0	1	66	55	1	4	6	0	0

- 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	AL	1	65	55	4	6	0	0
10	AM	1	65	55	4	6	0	0
10	BL	1	65	55	4	6	0	0

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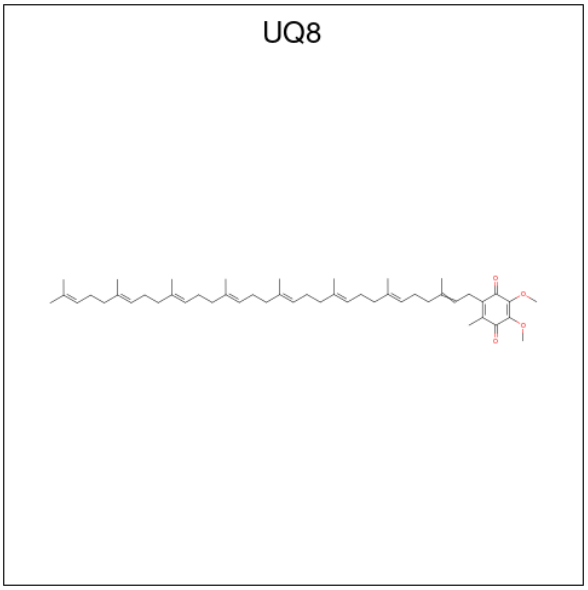
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	BM	1	65	55	4	6	0	0

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

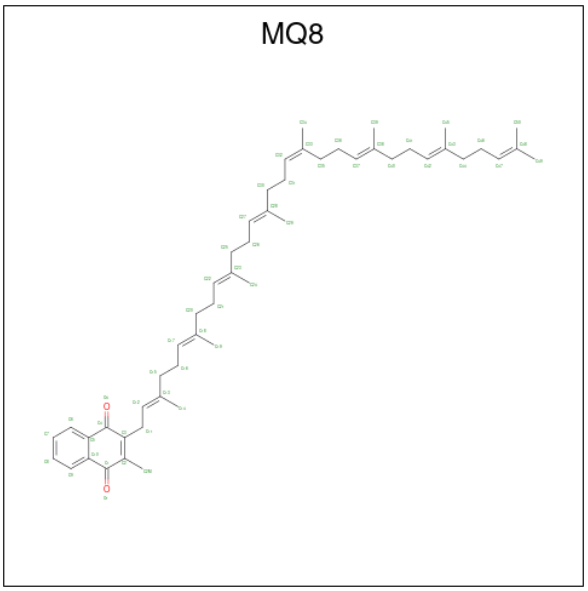


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	AL	1	53	49	4	0	0
11	BL	1	53	49	4	0	0

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

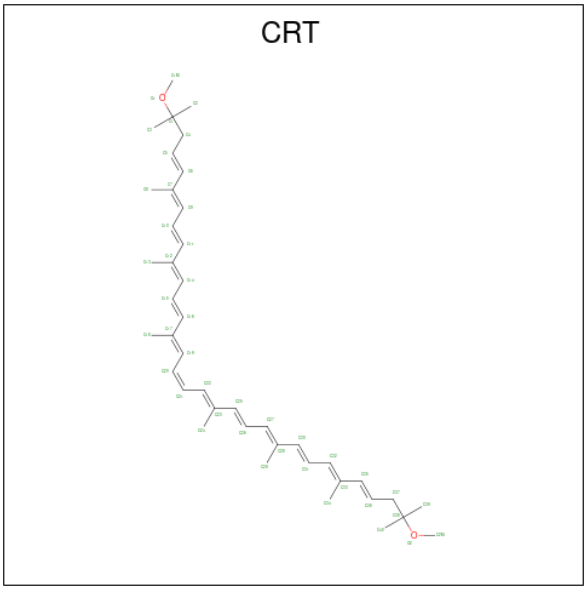
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
12	AM	1	1	1	0	0
12	BM	1	1	1	0	0

- Molecule 13 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	AM	1	53	51	2	0	0
			Total	C	O		
13	BM	1	53	51	2	0	0

- Molecule 14 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	AM	1	44	42	2	0	0
			Total	C	O		
14	AA	1	44	42	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	AB	1	44	42	2	0	0
14	AG	1	44	42	2	0	0
14	AJ	1	44	42	2	0	0
14	AN	1	44	42	2	0	0
14	AP	1	44	42	2	0	0
14	AR	1	44	42	2	0	0
14	AS	1	44	42	2	0	0
14	AT	1	44	42	2	0	0
14	AW	1	44	42	2	0	0
14	AX	1	44	42	2	0	0
14	A1	1	44	42	2	0	0
14	A2	1	44	42	2	0	0
14	A5	1	44	42	2	0	0
14	A7	1	44	42	2	0	0
14	A0	1	44	42	2	0	0
14	BM	1	44	42	2	0	0
14	BA	1	44	42	2	0	0
14	BB	1	44	42	2	0	0
14	BF	1	44	42	2	0	0
14	BG	1	44	42	2	0	0
14	BN	1	44	42	2	0	0

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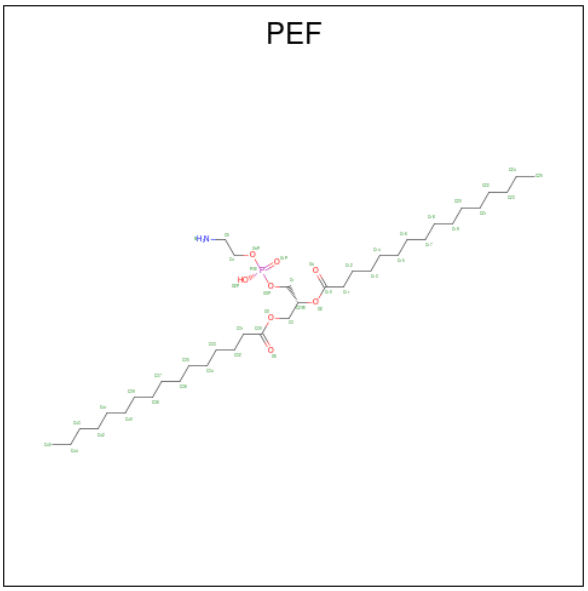
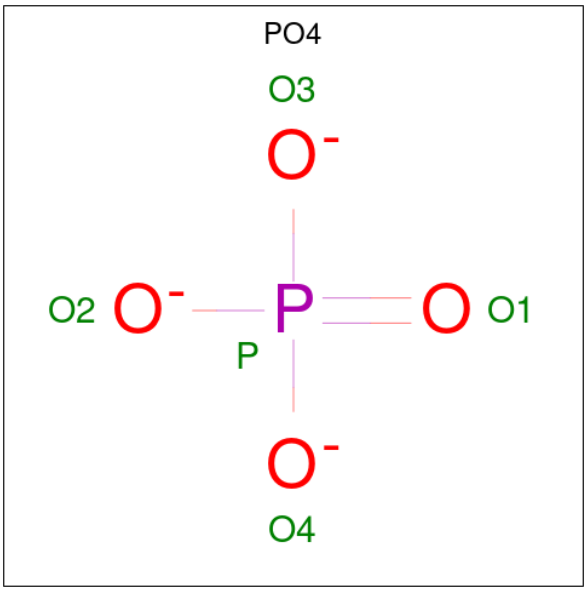
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
14	BO	1	44	42	2	0	0
14	BP	1	44	42	2	0	0
14	BS	1	44	42	2	0	0
14	BU	1	44	42	2	0	0
14	BV	1	44	42	2	0	0
14	BW	1	44	42	2	0	0
14	B1	1	44	42	2	0	0
14	B2	1	44	42	2	0	0
14	B5	1	44	42	2	0	0
14	B7	1	44	42	2	0	0
14	B0	1	44	42	2	0	0

- Molecule 15 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
15	AM	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
15	AM	1	14	6	1	6	1	0	0
			Total	C	N	O	P		
15	AM	1	47	37	1	8	1	0	0
			Total	C	N	O	P		
15	AH	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
15	AS	1	47	37	1	8	1	0	0
			Total	C	N	O	P		
15	BM	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
15	BQ	1	47	37	1	8	1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
16	AM	1	5	4	1	0	0
			Total	O	P		
16	AH	1	5	4	1	0	0
			Total	O	P		
16	A3	1	5	4	1	0	0
			Total	O	P		
16	BH	1	5	4	1	0	0

- Molecule 17 is water.

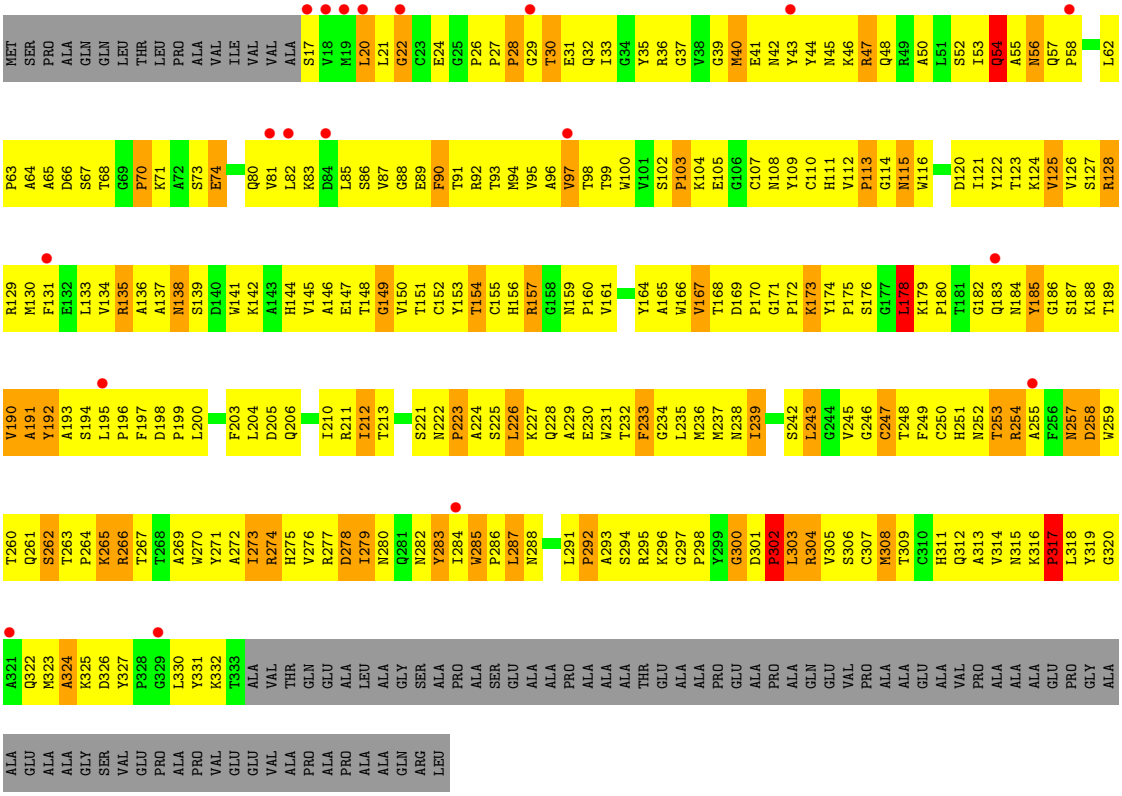
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
17	AC	1	1	1	0	0
			Total	O		
17	AL	3	3	3	0	0
			Total	O		
17	AM	3	3	3	0	0
			Total	O		
17	AH	2	2	2	0	0
			Total	O		
17	AA	1	1	1	0	0
			Total	O		
17	AI	1	1	1	0	0
			Total	O		
17	AW	1	1	1	0	0
			Total	O		
17	BC	1	1	1	0	0
			Total	O		
17	BL	3	3	3	0	0
			Total	O		
17	BM	3	3	3	0	0
			Total	O		
17	BH	1	1	1	0	0
			Total	O		
17	B1	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.

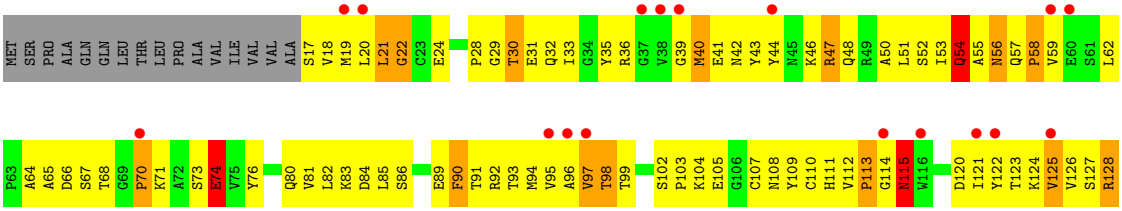
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

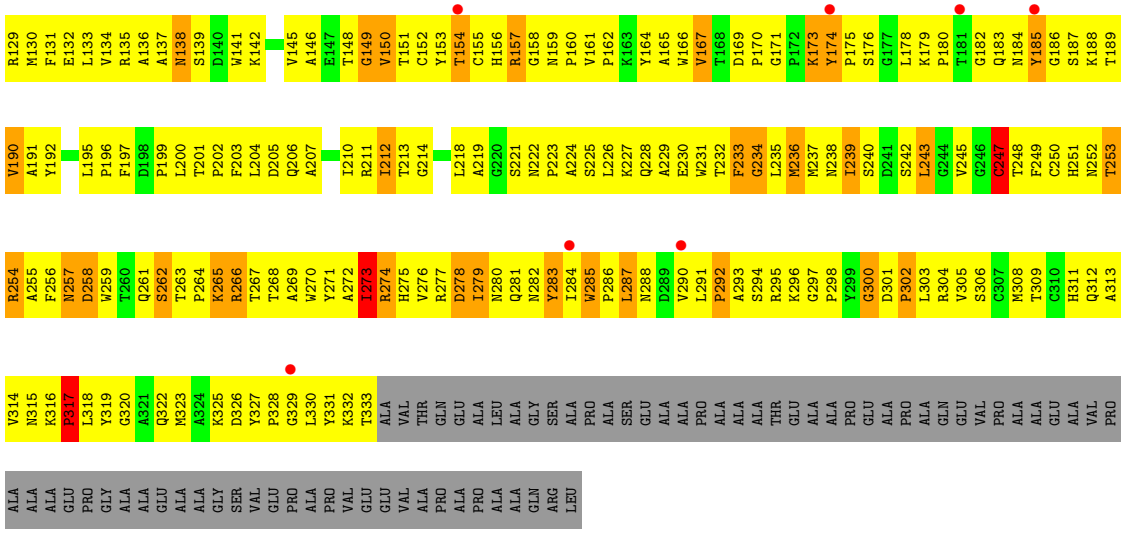
Chain AC:



• Molecule 1: Photosynthetic reaction center cytochrome c subunit

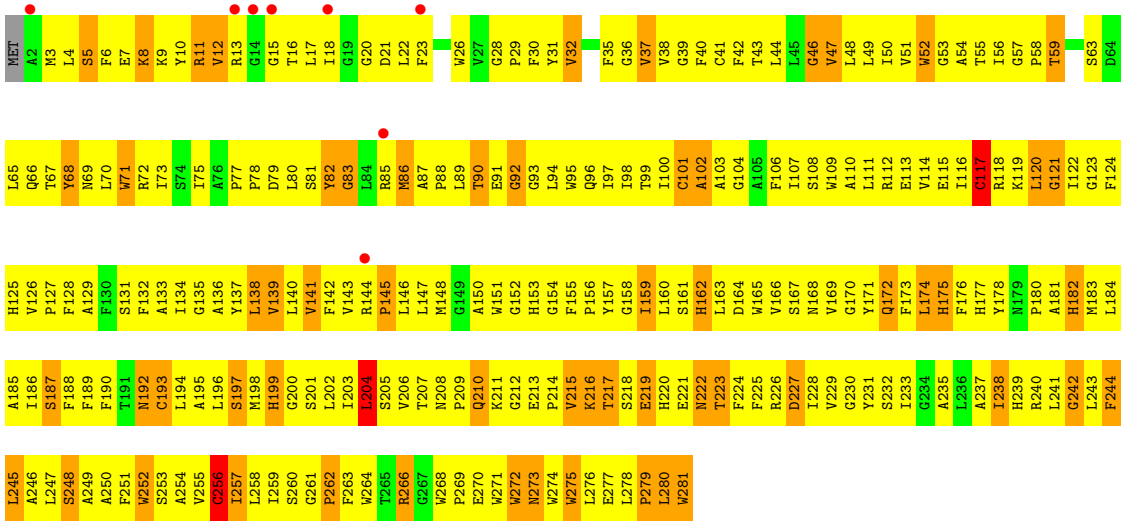
Chain BC:





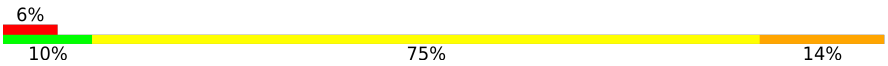
- Molecule 2: Photosynthetic reaction center L subunit

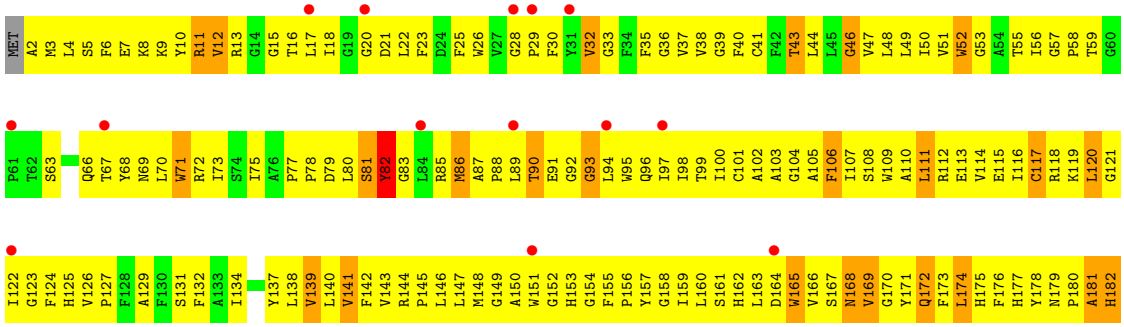
Chain AL:

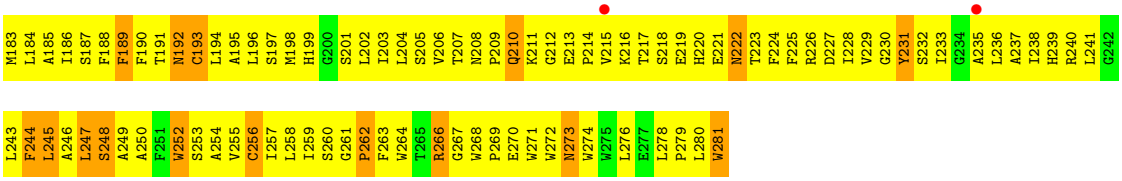


- Molecule 2: Photosynthetic reaction center L subunit

Chain BL:

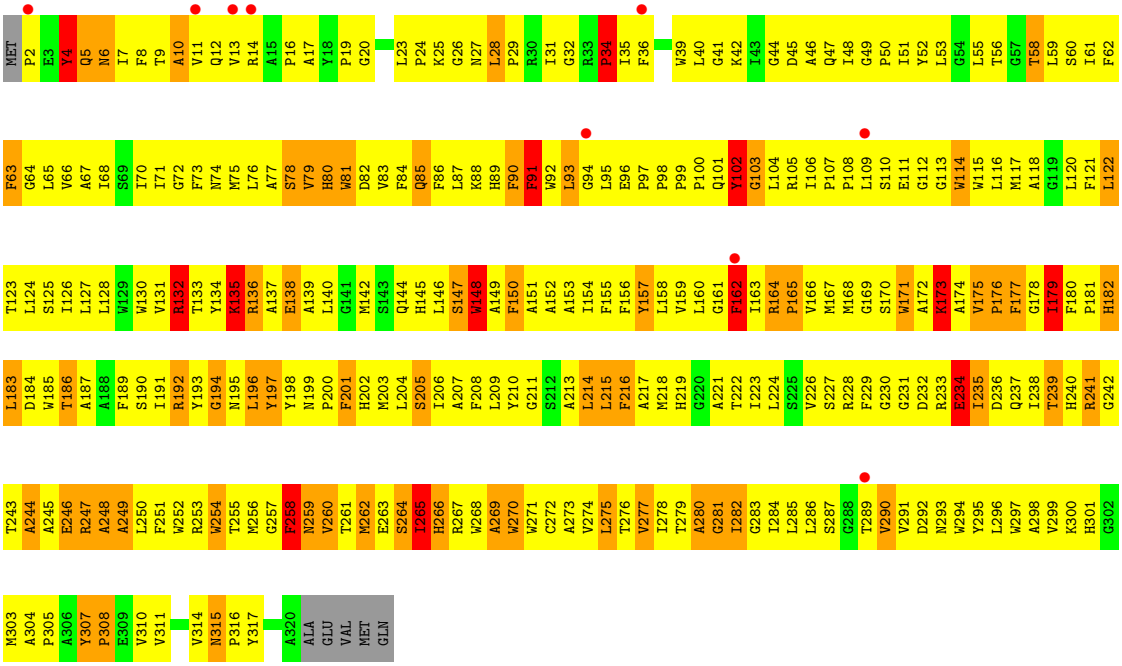






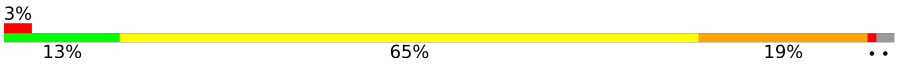
• Molecule 3: Photosynthetic reaction center M subunit

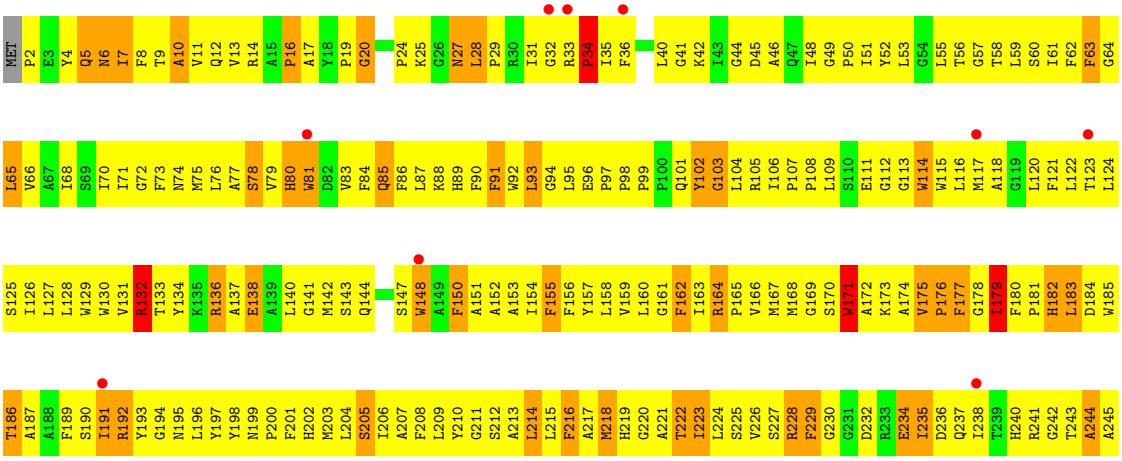
Chain AM:



• Molecule 3: Photosynthetic reaction center M subunit

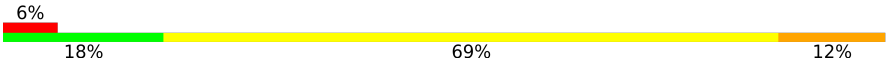
Chain BM:

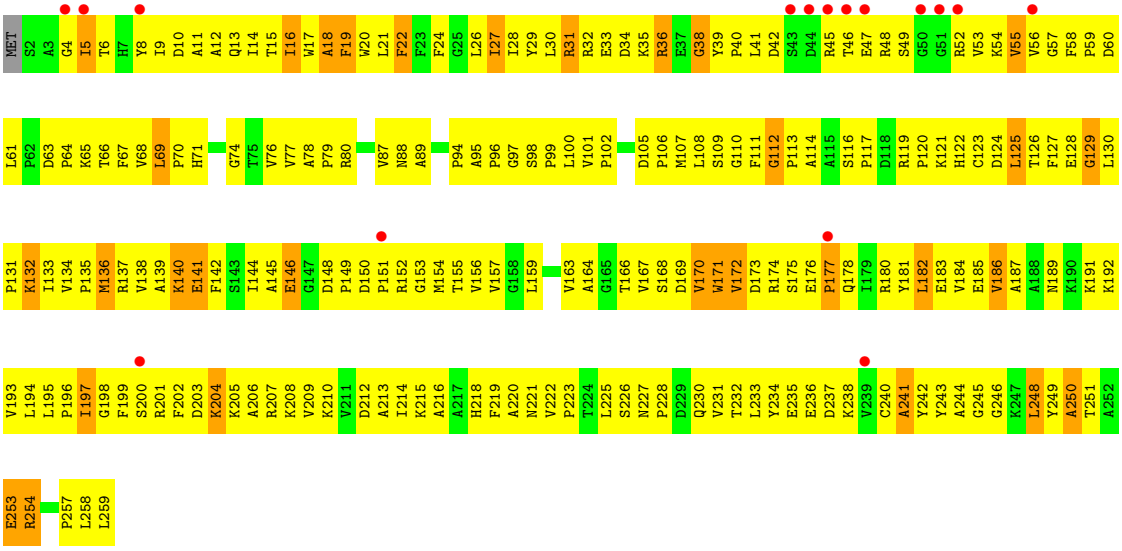




• Molecule 4: Photosynthetic reaction center H subunit

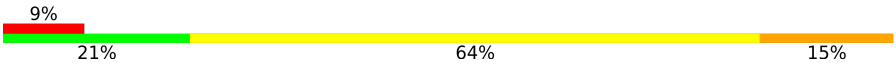
Chain AH:

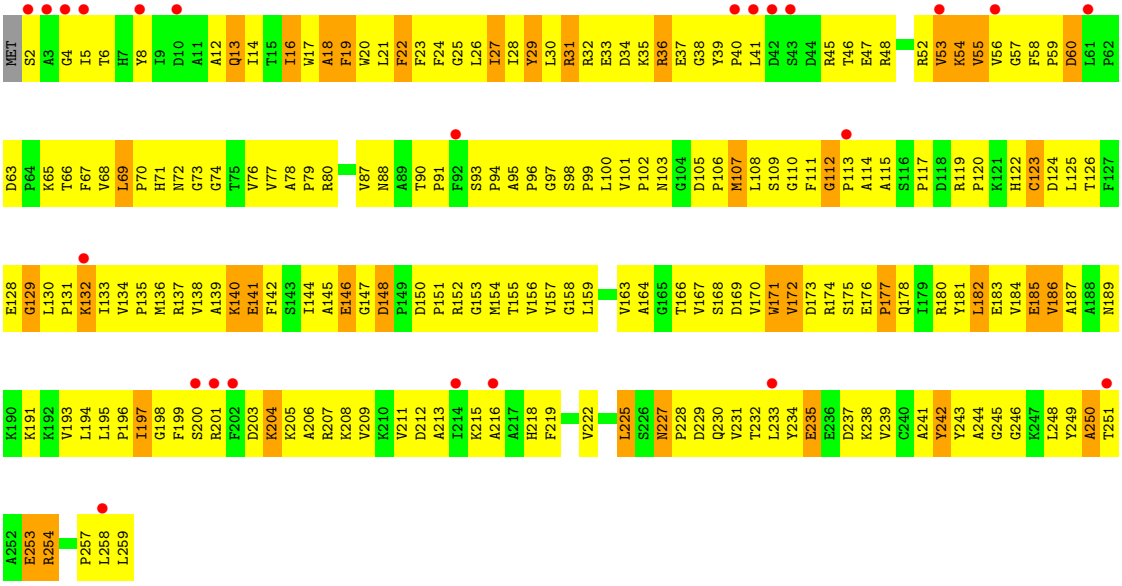




• Molecule 4: Photosynthetic reaction center H subunit

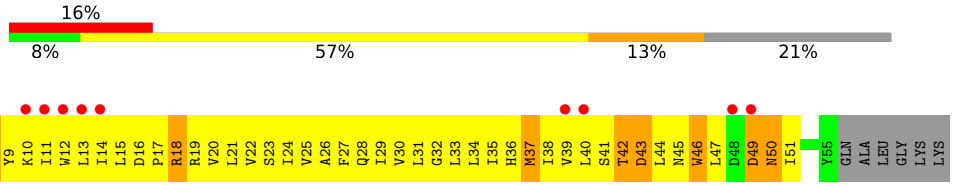
Chain BH:





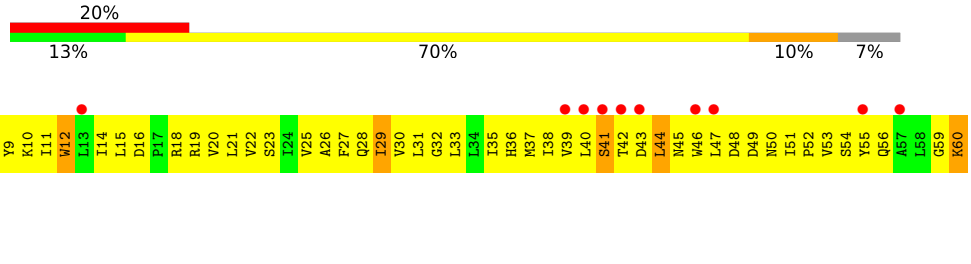
• Molecule 5: LH1 alpha polypeptide

Chain AA:



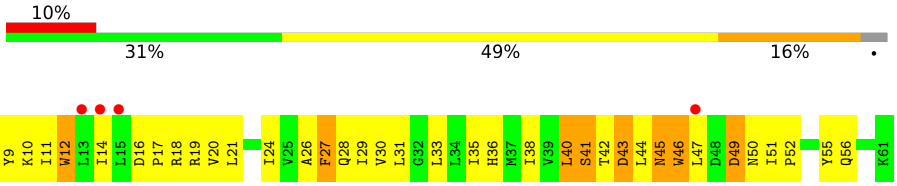
• Molecule 5: LH1 alpha polypeptide

Chain AD:



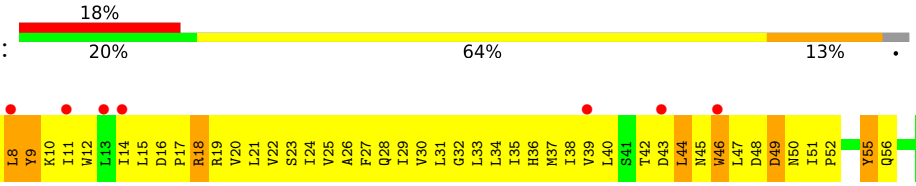
• Molecule 5: LH1 alpha polypeptide

Chain AF:



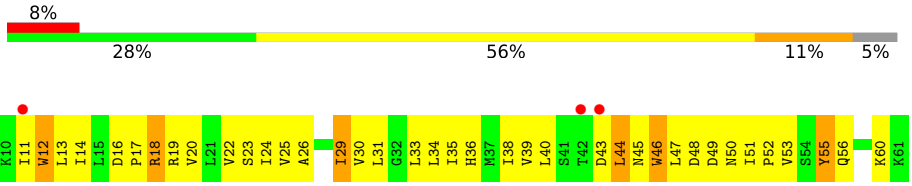
• Molecule 5: LH1 alpha polypeptide

Chain AI:



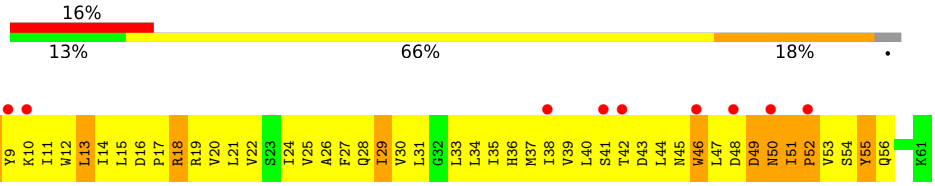
• Molecule 5: LH1 alpha polypeptide

Chain AK:



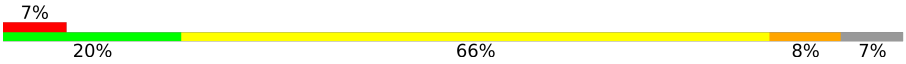
• Molecule 5: LH1 alpha polypeptide

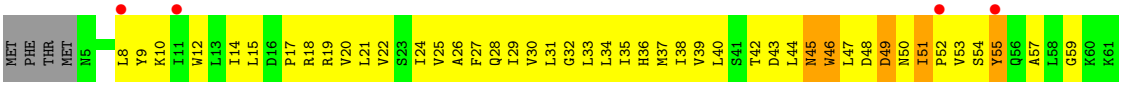
Chain AO:



• Molecule 5: LH1 alpha polypeptide

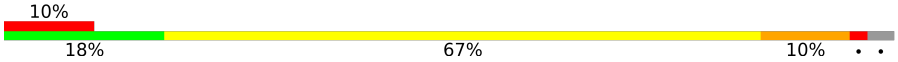
Chain AQ:





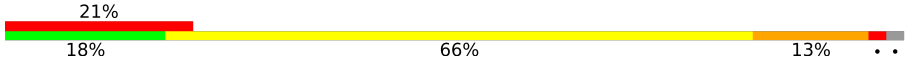
• Molecule 5: LH1 alpha polypeptide

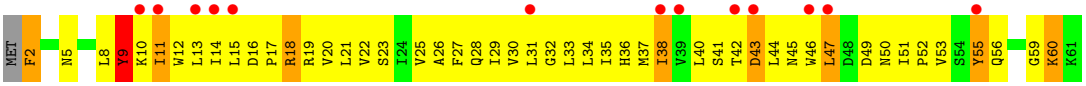
Chain AS:



• Molecule 5: LH1 alpha polypeptide

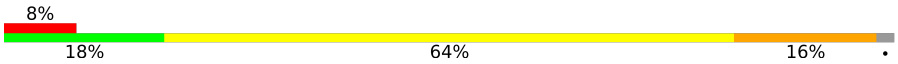
Chain AU:

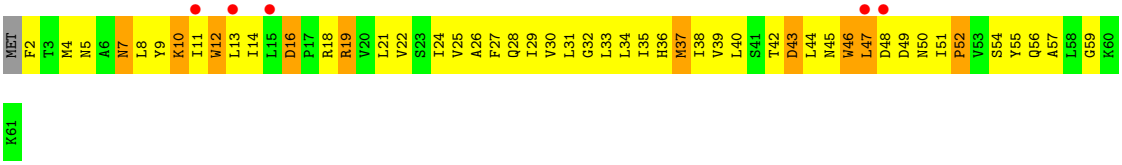




• Molecule 5: LH1 alpha polypeptide

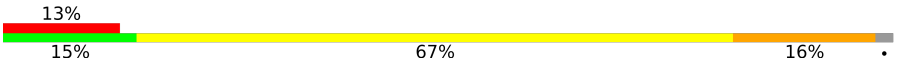
Chain AW:

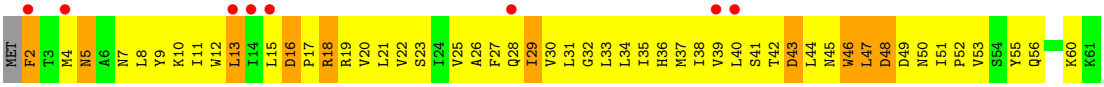




• Molecule 5: LH1 alpha polypeptide

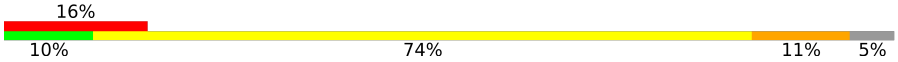
Chain AY:

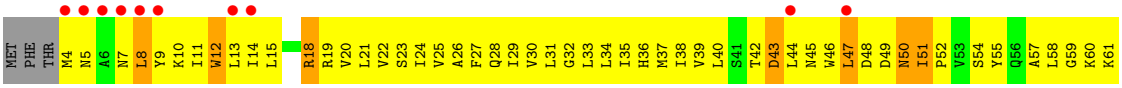




• Molecule 5: LH1 alpha polypeptide

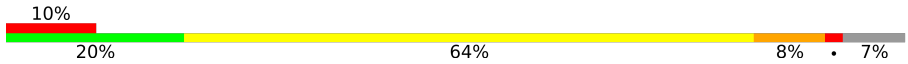
Chain A1:

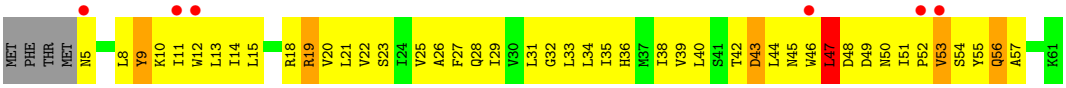




• Molecule 5: LH1 alpha polypeptide

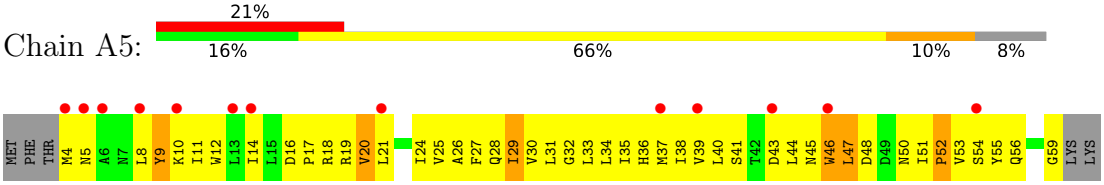
Chain A3:





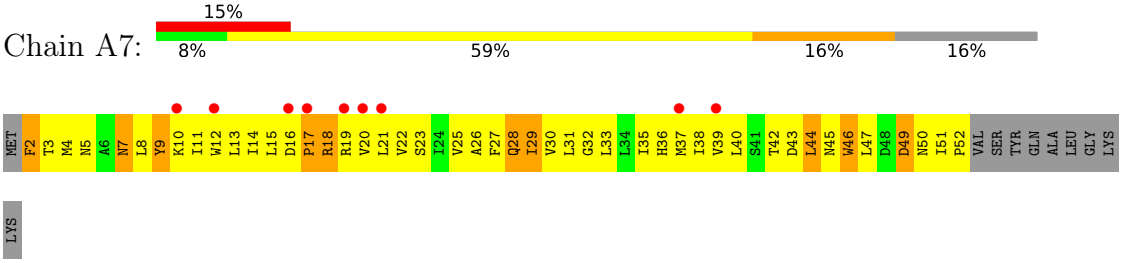
• Molecule 5: LH1 alpha polypeptide

Chain A5:



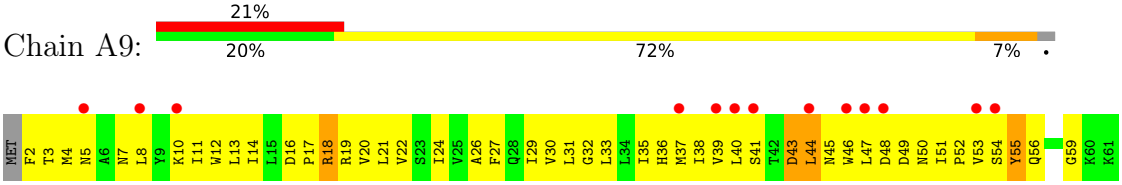
• Molecule 5: LH1 alpha polypeptide

Chain A7:



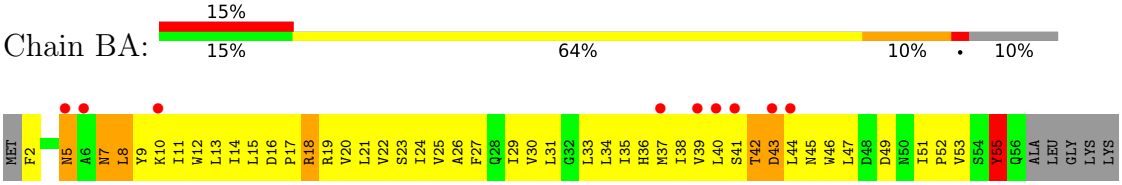
• Molecule 5: LH1 alpha polypeptide

Chain A9:



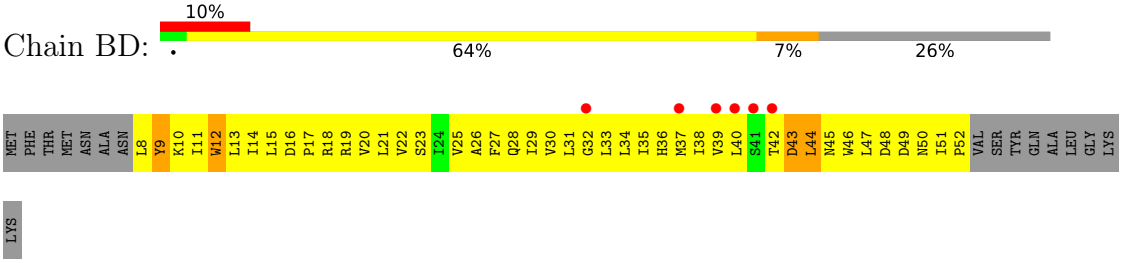
• Molecule 5: LH1 alpha polypeptide

Chain BA:



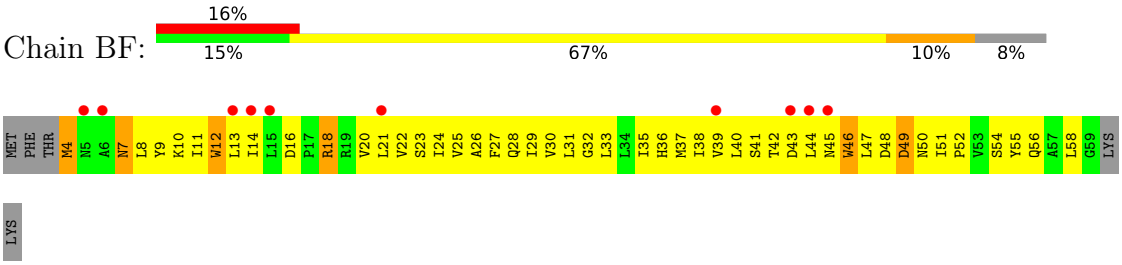
• Molecule 5: LH1 alpha polypeptide

Chain BD:



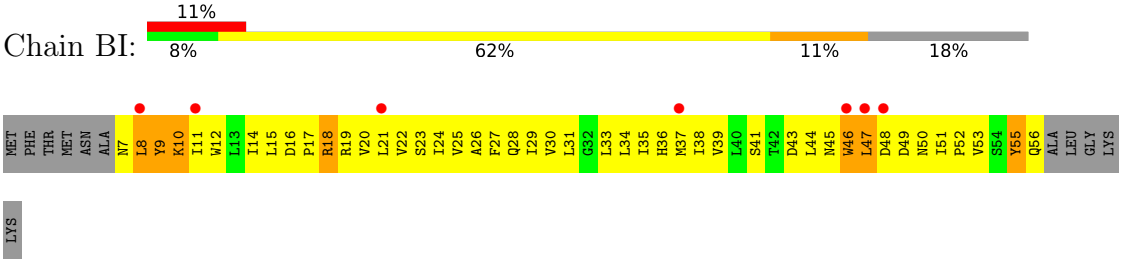
• Molecule 5: LH1 alpha polypeptide

Chain BF:



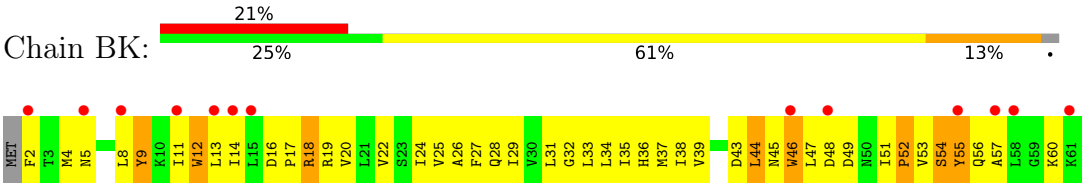
• Molecule 5: LH1 alpha polypeptide

Chain BI:



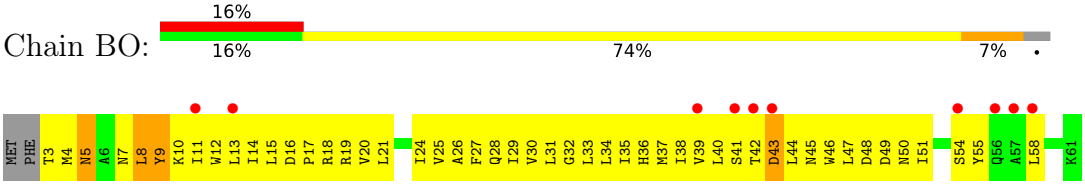
• Molecule 5: LH1 alpha polypeptide

Chain BK:



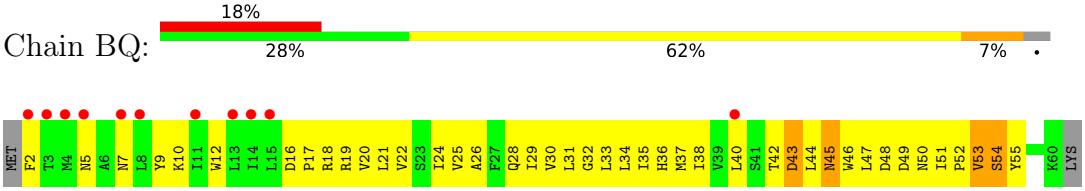
• Molecule 5: LH1 alpha polypeptide

Chain BO:



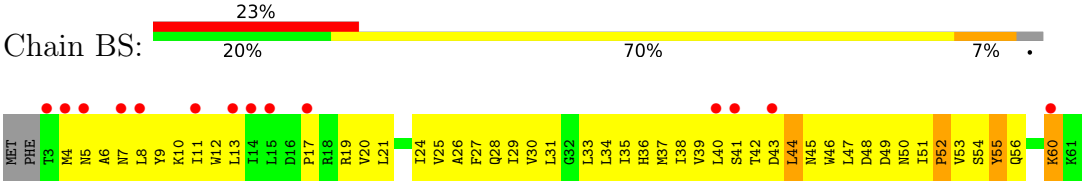
• Molecule 5: LH1 alpha polypeptide

Chain BQ:



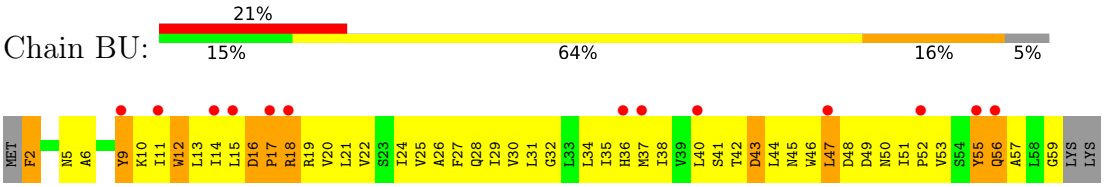
• Molecule 5: LH1 alpha polypeptide

Chain BS:



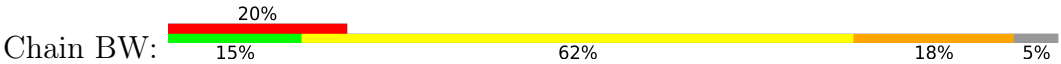
• Molecule 5: LH1 alpha polypeptide

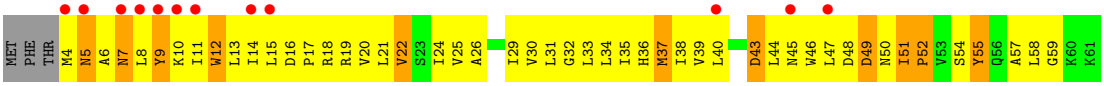
Chain BU:



• Molecule 5: LH1 alpha polypeptide

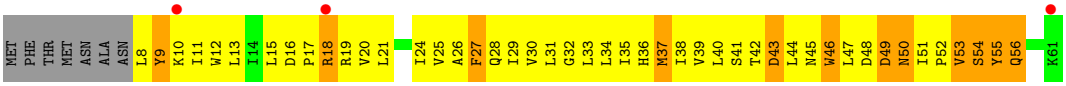
Chain BW:





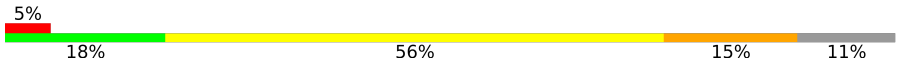
• Molecule 5: LH1 alpha polypeptide

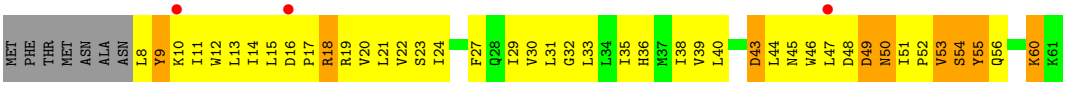
Chain BY:



• Molecule 5: LH1 alpha polypeptide

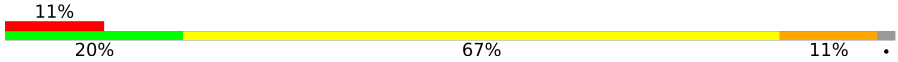
Chain B1:

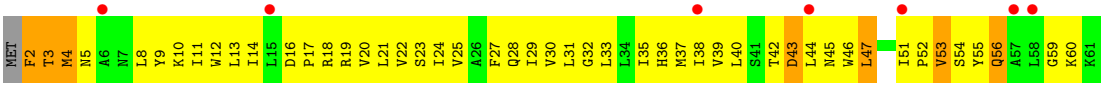




• Molecule 5: LH1 alpha polypeptide

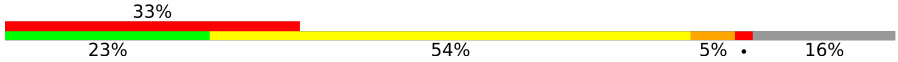
Chain B3:

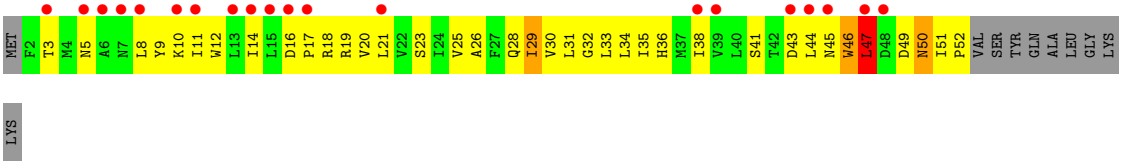




• Molecule 5: LH1 alpha polypeptide

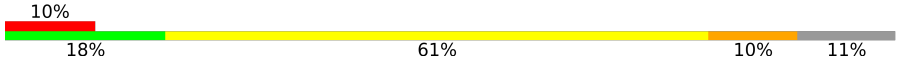
Chain B5:

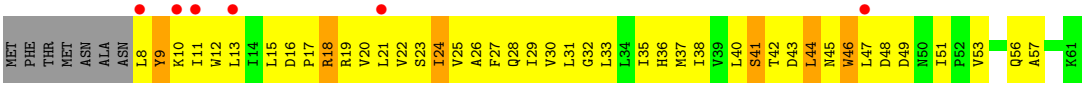




• Molecule 5: LH1 alpha polypeptide

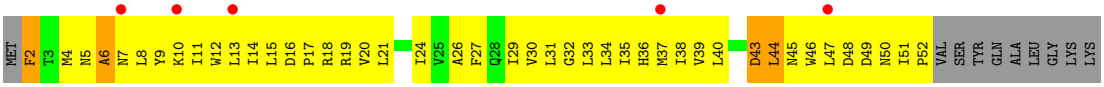
Chain B7:





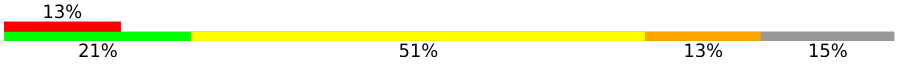
• Molecule 5: LH1 alpha polypeptide

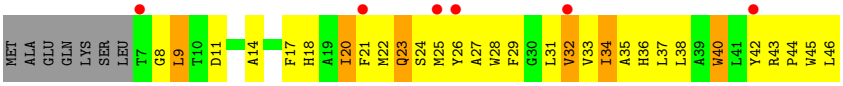
Chain B9:



• Molecule 6: LH1 beta polypeptide

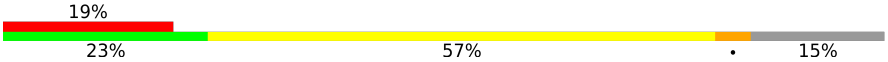
Chain AB:

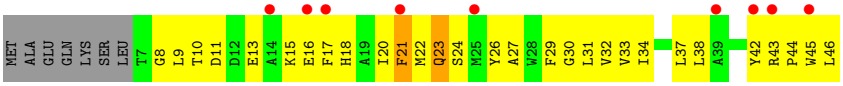




• Molecule 6: LH1 beta polypeptide

Chain AE:



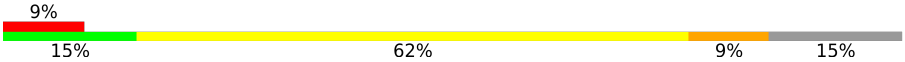


• Molecule 6: LH1 beta polypeptide

Chain AG:

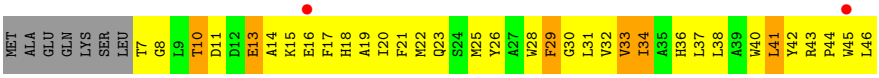
• Molecule 6: LH1 beta polypeptide

Chain AJ:



• Molecule 6: LH1 beta polypeptide

Chain AN:

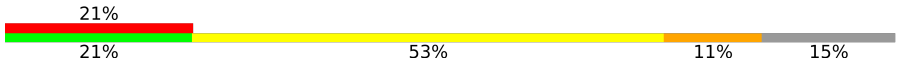


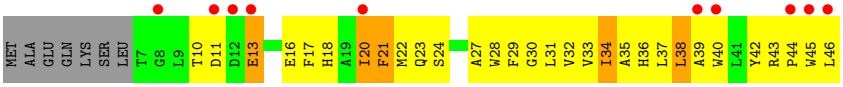
• Molecule 6: LH1 beta polypeptide

Chain AP:

• Molecule 6: LH1 beta polypeptide

Chain AR:



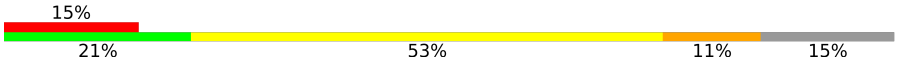


- Molecule 6: LH1 beta polypeptide

Chain AT:

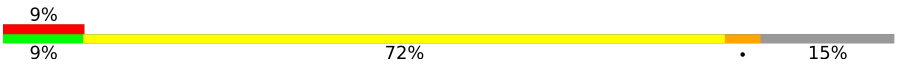
- Molecule 6: LH1 beta polypeptide

Chain AV:



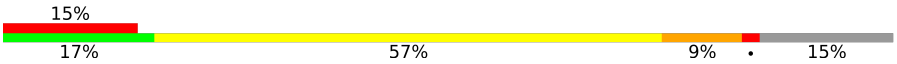
- Molecule 6: LH1 beta polypeptide

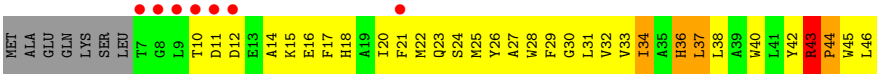
Chain AX:



- Molecule 6: LH1 beta polypeptide

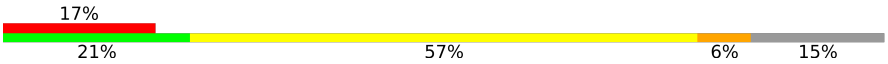
Chain AZ:





- Molecule 6: LH1 beta polypeptide

Chain A2:

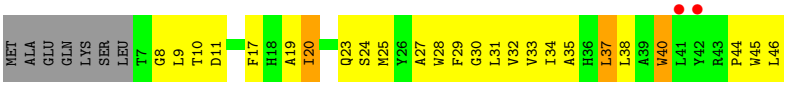


- Molecule 6: LH1 beta polypeptide

Chain A4:

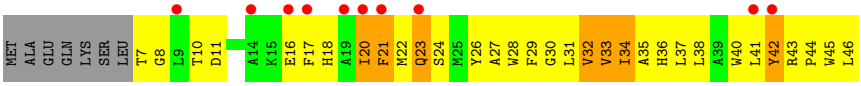
- Molecule 6: LH1 beta polypeptide

Chain A6:



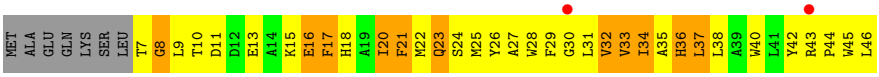
- Molecule 6: LH1 beta polypeptide

Chain A8:



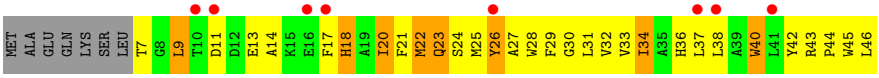
- Molecule 6: LH1 beta polypeptide

Chain A0:



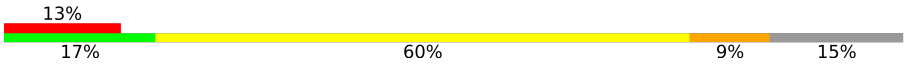
- Molecule 6: LH1 beta polypeptide

Chain BB:



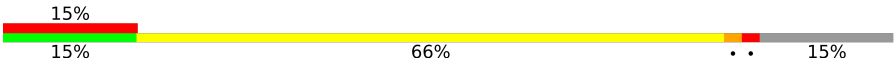
- Molecule 6: LH1 beta polypeptide

Chain BE:



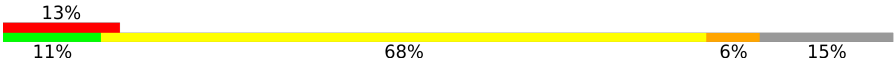
- Molecule 6: LH1 beta polypeptide

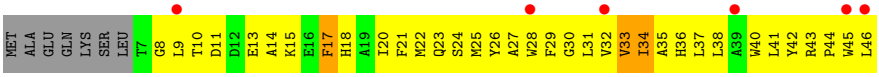
Chain BG:



- Molecule 6: LH1 beta polypeptide

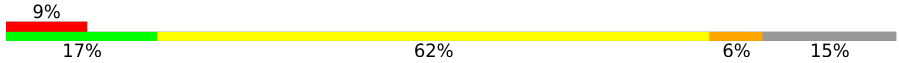
Chain BJ:

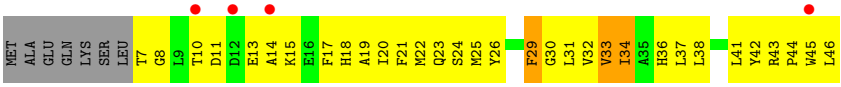




- Molecule 6: LH1 beta polypeptide

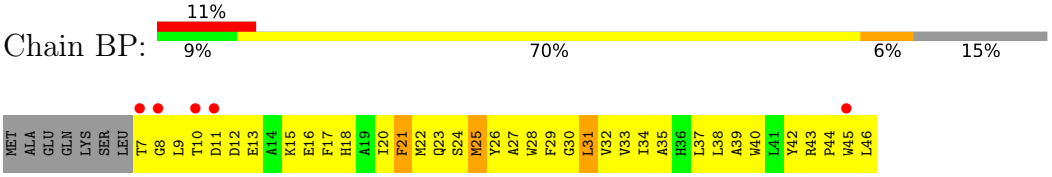
Chain BN:





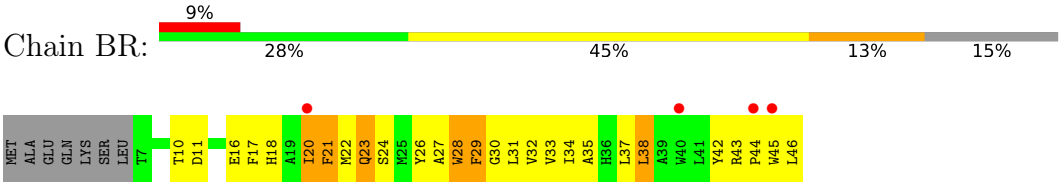
- Molecule 6: LH1 beta polypeptide

Chain BP:



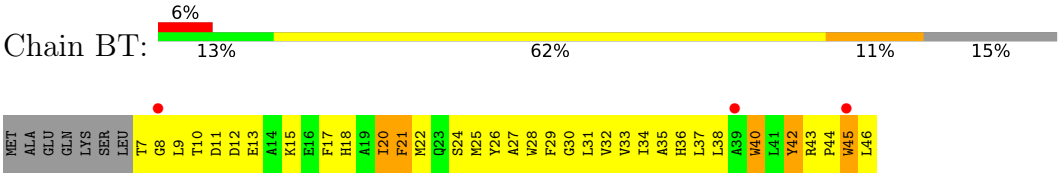
- Molecule 6: LH1 beta polypeptide

Chain BR:



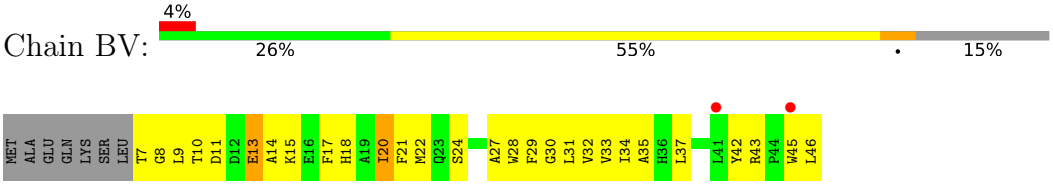
- Molecule 6: LH1 beta polypeptide

Chain BT:



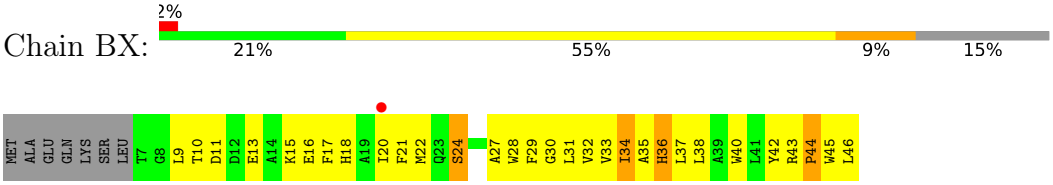
- Molecule 6: LH1 beta polypeptide

Chain BV:



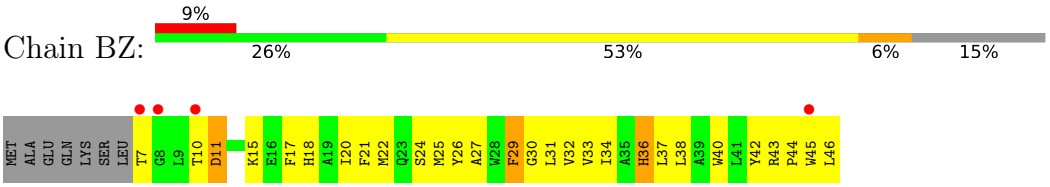
- Molecule 6: LH1 beta polypeptide

Chain BX:



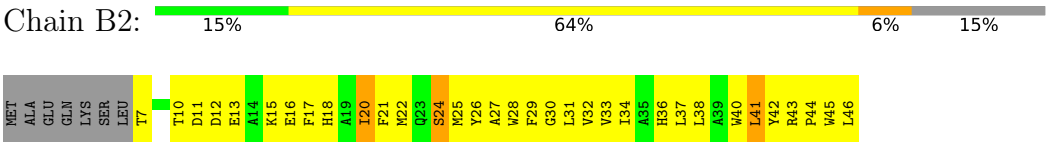
- Molecule 6: LH1 beta polypeptide

Chain BZ:



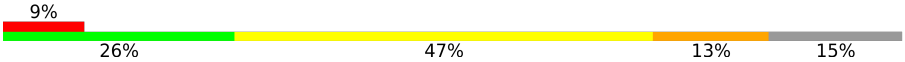
- Molecule 6: LH1 beta polypeptide

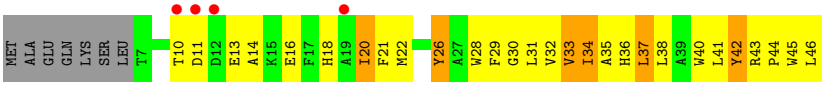
Chain B2:



• Molecule 6: LH1 beta polypeptide

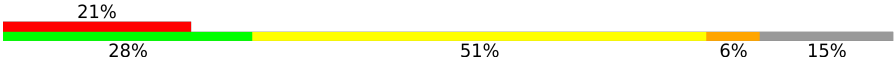
Chain B4:





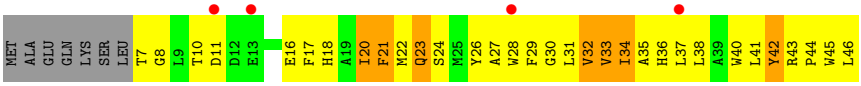
• Molecule 6: LH1 beta polypeptide

Chain B6:



• Molecule 6: LH1 beta polypeptide

Chain B8:



• Molecule 6: LH1 beta polypeptide

Chain B0:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	167.16Å 145.43Å 210.53Å 90.00° 108.50° 90.00°	Depositor
Resolution (Å)	43.79 – 3.01 43.79 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.79-3.01) 69.3 (43.79-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.335 , 0.356 0.343 , 0.344	Depositor DCC
R_{free} test set	8241 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , -34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	50862	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% 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: BCL, PEF, UQ8, MQ8, BPH, CRT, PO4, HEM, CA, 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	AC	0.61	0/2528	0.81	2/3451 (0.1%)
1	BC	0.59	1/2528 (0.0%)	0.79	1/3451 (0.0%)
2	AL	0.39	0/2318	0.63	0/3167
2	BL	0.36	0/2318	0.60	0/3167
3	AM	0.37	0/2651	0.63	0/3628
3	BM	0.36	0/2651	0.61	0/3628
4	AH	0.34	0/2037	0.57	0/2776
4	BH	0.33	0/2037	0.58	0/2776
5	A1	0.38	0/464	0.70	0/634
5	A3	0.30	0/456	0.64	0/624
5	A5	0.34	0/453	0.66	0/620
5	A7	0.30	0/426	0.61	0/583
5	A9	0.33	0/483	0.67	0/660
5	AA	0.31	0/401	0.57	0/550
5	AD	0.30	0/456	0.58	0/624
5	AF	0.30	0/471	0.62	0/644
5	AI	0.39	0/471	0.67	0/644
5	AK	0.28	0/464	0.57	0/634
5	AO	0.45	0/471	0.80	0/644
5	AQ	0.30	0/456	0.62	0/624
5	AS	0.32	0/471	0.65	0/644
5	AU	0.34	0/483	0.64	0/660
5	AW	0.34	0/483	0.61	0/660
5	AY	0.34	0/483	0.70	0/660
5	B1	0.32	0/435	0.58	0/595
5	B3	0.33	0/483	0.60	0/660
5	B5	0.32	0/426	0.68	0/583
5	B7	0.31	0/435	0.57	0/595
5	B9	0.35	0/426	0.65	0/583
5	BA	0.31	0/458	0.61	0/627
5	BD	0.41	0/378	0.67	0/518
5	BF	0.37	0/453	0.64	0/620

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	BI	0.33	0/418	0.61	0/573
5	BK	0.29	0/483	0.56	0/660
5	BO	0.37	0/471	0.71	0/644
5	BQ	0.29	0/477	0.58	0/653
5	BS	0.29	0/471	0.58	0/644
5	BU	0.42	1/472 (0.2%)	0.62	1/646 (0.2%)
5	BW	0.34	0/464	0.60	0/634
5	BY	0.31	0/435	0.58	0/595
6	A0	0.46	0/350	0.58	0/476
6	A2	0.33	0/350	0.52	0/476
6	A4	0.43	0/350	0.61	0/476
6	A6	0.34	0/350	0.57	0/476
6	A8	0.47	0/350	0.61	0/476
6	AB	0.40	0/350	0.53	0/476
6	AE	0.40	0/350	0.51	0/476
6	AG	0.46	0/350	0.59	0/476
6	AJ	0.45	0/350	0.57	0/476
6	AN	0.43	0/350	0.54	0/476
6	AP	0.41	0/350	0.56	0/476
6	AR	0.37	0/350	0.53	0/476
6	AT	0.35	0/350	0.52	0/476
6	AV	0.40	0/350	0.65	0/476
6	AX	0.39	0/350	0.56	0/476
6	AZ	0.52	1/350 (0.3%)	0.68	1/476 (0.2%)
6	B0	0.44	0/350	0.62	0/476
6	B2	0.40	0/350	0.59	0/476
6	B4	0.42	0/350	0.64	0/476
6	B6	0.33	0/350	0.55	0/476
6	B8	0.47	0/350	0.61	0/476
6	BB	0.43	0/350	0.59	0/476
6	BE	0.37	0/350	0.56	0/476
6	BG	0.49	0/350	0.76	1/476 (0.2%)
6	BJ	0.42	0/350	0.57	0/476
6	BN	0.45	0/350	0.60	0/476
6	BP	0.42	0/350	0.57	0/476
6	BR	0.38	0/350	0.57	0/476
6	BT	0.42	0/350	0.63	0/476
6	BV	0.37	0/350	0.71	0/476
6	BX	0.36	0/350	0.60	0/476
6	BZ	0.40	0/350	0.53	0/476
All	All	0.40	3/44845 (0.0%)	0.64	6/61215 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	BU	17	PRO	N-CD	5.25	1.55	1.47
6	AZ	44	PRO	N-CD	5.16	1.55	1.47
1	BC	247	CYS	CB-SG	-5.11	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	AZ	43	ARG	C-N-CD	5.83	140.64	128.40
1	AC	178	LEU	N-CA-C	5.77	126.58	111.00
5	BU	16	ASP	C-N-CD	5.61	140.17	128.40
6	BG	21	PHE	CB-CG-CD2	-5.49	116.95	120.80
1	BC	186	GLY	N-CA-C	-5.10	100.35	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AC	2458	0	2377	475	0
1	BC	2458	0	2377	488	0
2	AL	2231	0	2192	644	0
2	BL	2231	0	2192	563	0
3	AM	2551	0	2526	741	0
3	BM	2551	0	2526	662	0
4	AH	1982	0	1981	399	0
4	BH	1982	0	1981	373	0
5	A1	455	0	460	165	0
5	A3	447	0	451	135	0
5	A5	444	0	456	138	0
5	A7	417	0	441	159	0
5	A9	473	0	476	126	0
5	AA	392	0	412	138	0
5	AD	447	0	451	124	0
5	AF	462	0	467	153	0
5	AI	462	0	467	147	0
5	AK	455	0	460	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AO	462	0	467	153	0
5	AQ	447	0	451	118	0
5	AS	462	0	467	187	0
5	AU	473	0	476	150	0
5	AW	473	0	476	184	0
5	AY	473	0	476	165	0
5	B1	426	0	434	137	0
5	B3	473	0	476	134	0
5	B5	417	0	441	92	0
5	B7	426	0	434	133	0
5	B9	417	0	441	137	0
5	BA	448	0	462	154	0
5	BD	370	0	399	134	0
5	BF	444	0	456	146	0
5	BI	409	0	426	108	0
5	BK	473	0	476	102	0
5	BO	462	0	467	145	0
5	BQ	467	0	474	121	0
5	BS	462	0	467	111	0
5	BU	462	0	472	174	0
5	BW	455	0	460	159	0
5	BY	426	0	434	149	0
6	A0	337	0	323	111	0
6	A2	337	0	323	106	0
6	A4	337	0	323	82	0
6	A6	337	0	323	57	0
6	A8	337	0	323	105	0
6	AB	337	0	321	89	0
6	AE	337	0	323	69	0
6	AG	337	0	323	89	0
6	AJ	337	0	323	94	0
6	AN	337	0	323	86	0
6	AP	337	0	323	105	0
6	AR	337	0	323	73	0
6	AT	337	0	323	79	0
6	AV	337	0	323	98	0
6	AX	337	0	323	82	0
6	AZ	337	0	323	99	0
6	B0	337	0	323	123	0
6	B2	337	0	323	132	0
6	B4	337	0	323	70	0
6	B6	337	0	323	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B8	337	0	323	71	0
6	BB	337	0	323	97	0
6	BE	337	0	323	72	0
6	BG	337	0	323	78	0
6	BJ	337	0	323	91	0
6	BN	337	0	323	66	0
6	BP	337	0	323	91	0
6	BR	337	0	323	68	0
6	BT	337	0	323	64	0
6	BV	337	0	323	107	0
6	BX	337	0	323	71	0
6	BZ	337	0	323	80	0
7	AC	172	0	120	35	0
7	BC	172	0	120	33	0
8	A1	1	0	0	0	0
8	A3	1	0	0	0	0
8	A5	1	0	0	0	0
8	A7	1	0	0	0	0
8	A9	1	0	0	0	0
8	AA	1	0	0	0	0
8	AC	1	0	0	0	0
8	AD	1	0	0	0	0
8	AF	1	0	0	0	0
8	AI	1	0	0	0	0
8	AK	1	0	0	0	0
8	AO	1	0	0	0	0
8	AQ	1	0	0	0	0
8	AS	1	0	0	0	0
8	AU	1	0	0	0	0
8	AV	1	0	0	0	0
8	AY	1	0	0	0	0
8	B1	1	0	0	0	0
8	B3	1	0	0	0	0
8	B5	1	0	0	0	0
8	B7	1	0	0	0	0
8	B9	1	0	0	0	0
8	BA	1	0	0	0	0
8	BC	1	0	0	0	0
8	BD	1	0	0	0	0
8	BF	1	0	0	0	0
8	BI	1	0	0	0	0
8	BK	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BO	1	0	0	0	0
8	BQ	1	0	0	0	0
8	BS	1	0	0	0	0
8	BU	1	0	0	0	0
8	BW	1	0	0	0	0
8	BY	1	0	0	0	0
9	A0	66	0	72	71	0
9	A1	66	0	74	55	0
9	A2	66	0	74	31	0
9	A3	132	0	148	69	0
9	A5	66	0	74	40	0
9	A6	66	0	74	31	0
9	A7	66	0	74	51	0
9	A8	66	0	74	46	0
9	A9	66	0	74	35	0
9	AA	66	0	74	41	0
9	AB	66	0	74	33	0
9	AD	66	0	74	29	0
9	AE	66	0	74	32	0
9	AF	66	0	74	38	0
9	AG	66	0	74	37	0
9	AI	66	0	74	41	0
9	AJ	66	0	74	44	0
9	AK	66	0	74	67	0
9	AL	132	0	148	62	0
9	AM	132	0	148	48	0
9	AN	66	0	74	57	0
9	AO	66	0	74	50	0
9	AP	66	0	74	41	0
9	AQ	66	0	74	26	0
9	AR	66	0	74	34	0
9	AS	66	0	74	32	0
9	AT	66	0	74	25	0
9	AU	66	0	73	46	0
9	AV	66	0	74	28	0
9	AW	66	0	72	40	0
9	AX	66	0	74	36	0
9	AY	66	0	74	47	0
9	AZ	66	0	72	41	0
9	B0	66	0	74	54	0
9	B1	66	0	74	40	0
9	B2	66	0	74	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B3	66	0	74	51	0
9	B4	66	0	74	24	0
9	B5	66	0	74	25	0
9	B6	66	0	74	26	0
9	B7	66	0	74	41	0
9	B8	66	0	74	37	0
9	B9	66	0	74	35	0
9	BA	66	0	74	37	0
9	BB	66	0	74	51	0
9	BD	66	0	74	38	0
9	BE	66	0	74	48	0
9	BF	66	0	74	41	0
9	BG	66	0	74	44	0
9	BI	66	0	74	50	0
9	BJ	66	0	74	30	0
9	BK	66	0	74	32	0
9	BL	132	0	148	48	0
9	BM	132	0	148	50	0
9	BN	66	0	74	31	0
9	BO	66	0	74	50	0
9	BP	66	0	74	40	0
9	BQ	132	0	148	53	0
9	BS	66	0	74	25	0
9	BT	66	0	74	19	0
9	BU	66	0	74	41	0
9	BV	66	0	74	25	0
9	BW	66	0	74	44	0
9	BX	66	0	74	37	0
9	BY	66	0	74	37	0
9	BZ	66	0	74	30	0
10	AL	65	0	76	17	0
10	AM	65	0	76	14	0
10	BL	65	0	76	11	0
10	BM	65	0	76	9	0
11	AL	53	0	74	8	0
11	BL	53	0	74	12	0
12	AM	1	0	0	0	0
12	BM	1	0	0	0	0
13	AM	53	0	72	9	0
13	BM	53	0	72	9	0
14	A0	44	0	60	27	0
14	A1	44	0	60	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A2	44	0	60	51	0
14	A5	44	0	60	29	0
14	A7	44	0	60	45	0
14	AA	44	0	60	24	0
14	AB	44	0	60	45	0
14	AG	44	0	60	11	0
14	AJ	44	0	60	21	0
14	AM	44	0	60	13	0
14	AN	44	0	60	14	0
14	AP	44	0	60	24	0
14	AR	44	0	60	20	0
14	AS	44	0	60	77	0
14	AT	44	0	60	17	0
14	AW	44	0	60	32	0
14	AX	44	0	60	46	0
14	B0	44	0	60	42	0
14	B1	44	0	60	40	0
14	B2	44	0	60	75	0
14	B5	44	0	60	21	0
14	B7	44	0	60	39	0
14	BA	44	0	60	26	0
14	BB	44	0	60	27	0
14	BF	44	0	60	19	0
14	BG	44	0	60	14	0
14	BM	44	0	60	8	0
14	BN	44	0	60	15	0
14	BO	44	0	60	14	0
14	BP	44	0	60	28	0
14	BS	44	0	60	11	0
14	BU	44	0	60	61	0
14	BV	44	0	60	59	0
14	BW	44	0	60	21	0
15	AH	19	0	11	8	0
15	AM	80	0	92	23	0
15	AS	47	0	73	37	0
15	BM	19	0	11	2	0
15	BQ	47	0	73	12	0
16	A3	5	0	0	0	0
16	AH	5	0	0	1	0
16	AM	5	0	0	0	0
16	BH	5	0	0	1	0
17	AA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	AC	1	0	0	0	0
17	AH	2	0	0	0	0
17	AI	1	0	0	0	0
17	AL	3	0	0	2	0
17	AM	3	0	0	2	0
17	AW	1	0	0	1	0
17	B1	1	0	0	0	0
17	BC	1	0	0	0	0
17	BH	1	0	0	0	0
17	BL	3	0	0	3	0
17	BM	3	0	0	0	0
All	All	50862	0	51516	10984	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 107.

The worst 5 of 10984 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A7:102:CRT:C22	14:A7:102:CRT:C21	1.82	1.56
14:AS:104:CRT:C9	6:AV:20:ILE:HD12	1.38	1.54
5:AS:30:VAL:HG22	15:AS:101:PEF:C41	1.47	1.44
5:AS:30:VAL:CG2	15:AS:101:PEF:H412	1.46	1.43
9:AW:101:BCL:O2A	9:AW:101:BCL:C1	1.65	1.42

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AC	315/404 (78%)	195 (62%)	75 (24%)	45 (14%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BC	315/404 (78%)	192 (61%)	87 (28%)	36 (11%)	0	2
2	AL	278/281 (99%)	137 (49%)	97 (35%)	44 (16%)	0	1
2	BL	278/281 (99%)	149 (54%)	97 (35%)	32 (12%)	0	2
3	AM	317/325 (98%)	162 (51%)	94 (30%)	61 (19%)	0	0
3	BM	317/325 (98%)	188 (59%)	85 (27%)	44 (14%)	0	1
4	AH	256/259 (99%)	162 (63%)	73 (28%)	21 (8%)	1	4
4	BH	256/259 (99%)	166 (65%)	66 (26%)	24 (9%)	0	3
5	A1	56/61 (92%)	43 (77%)	9 (16%)	4 (7%)	1	5
5	A3	55/61 (90%)	45 (82%)	7 (13%)	3 (6%)	2	10
5	A5	54/61 (88%)	42 (78%)	10 (18%)	2 (4%)	3	19
5	A7	49/61 (80%)	35 (71%)	11 (22%)	3 (6%)	1	8
5	A9	58/61 (95%)	47 (81%)	10 (17%)	1 (2%)	9	39
5	AA	46/61 (75%)	33 (72%)	11 (24%)	2 (4%)	2	15
5	AD	55/61 (90%)	40 (73%)	12 (22%)	3 (6%)	2	10
5	AF	57/61 (93%)	41 (72%)	13 (23%)	3 (5%)	2	11
5	AI	57/61 (93%)	47 (82%)	6 (10%)	4 (7%)	1	6
5	AK	56/61 (92%)	44 (79%)	10 (18%)	2 (4%)	3	19
5	AO	57/61 (93%)	46 (81%)	6 (10%)	5 (9%)	1	3
5	AQ	55/61 (90%)	36 (66%)	17 (31%)	2 (4%)	3	19
5	AS	57/61 (93%)	46 (81%)	7 (12%)	4 (7%)	1	6
5	AU	58/61 (95%)	43 (74%)	11 (19%)	4 (7%)	1	6
5	AW	58/61 (95%)	45 (78%)	8 (14%)	5 (9%)	1	3
5	AY	58/61 (95%)	43 (74%)	11 (19%)	4 (7%)	1	6
5	B1	52/61 (85%)	34 (65%)	11 (21%)	7 (14%)	0	1
5	B3	58/61 (95%)	38 (66%)	16 (28%)	4 (7%)	1	6
5	B5	49/61 (80%)	35 (71%)	10 (20%)	4 (8%)	1	4
5	B7	52/61 (85%)	40 (77%)	10 (19%)	2 (4%)	3	18
5	B9	49/61 (80%)	33 (67%)	14 (29%)	2 (4%)	3	16
5	BA	53/61 (87%)	29 (55%)	20 (38%)	4 (8%)	1	5
5	BD	43/61 (70%)	32 (74%)	8 (19%)	3 (7%)	1	6
5	BF	54/61 (88%)	42 (78%)	11 (20%)	1 (2%)	8	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BI	48/61 (79%)	32 (67%)	13 (27%)	3 (6%)	1	7
5	BK	58/61 (95%)	43 (74%)	12 (21%)	3 (5%)	2	12
5	BO	57/61 (93%)	46 (81%)	11 (19%)	0	100	100
5	BQ	57/61 (93%)	41 (72%)	14 (25%)	2 (4%)	3	20
5	BS	57/61 (93%)	45 (79%)	9 (16%)	3 (5%)	2	11
5	BU	56/61 (92%)	43 (77%)	12 (21%)	1 (2%)	8	37
5	BW	56/61 (92%)	38 (68%)	14 (25%)	4 (7%)	1	5
5	BY	52/61 (85%)	30 (58%)	16 (31%)	6 (12%)	0	2
6	A0	38/47 (81%)	30 (79%)	7 (18%)	1 (3%)	5	27
6	A2	38/47 (81%)	29 (76%)	8 (21%)	1 (3%)	5	27
6	A4	38/47 (81%)	31 (82%)	6 (16%)	1 (3%)	5	27
6	A6	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	A8	38/47 (81%)	27 (71%)	10 (26%)	1 (3%)	5	27
6	AB	38/47 (81%)	33 (87%)	5 (13%)	0	100	100
6	AE	38/47 (81%)	33 (87%)	5 (13%)	0	100	100
6	AG	38/47 (81%)	32 (84%)	5 (13%)	1 (3%)	5	27
6	AJ	38/47 (81%)	29 (76%)	9 (24%)	0	100	100
6	AN	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	AP	38/47 (81%)	28 (74%)	10 (26%)	0	100	100
6	AR	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
6	AT	38/47 (81%)	30 (79%)	5 (13%)	3 (8%)	1	4
6	AV	38/47 (81%)	35 (92%)	2 (5%)	1 (3%)	5	27
6	AX	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	AZ	38/47 (81%)	29 (76%)	9 (24%)	0	100	100
6	B0	38/47 (81%)	30 (79%)	8 (21%)	0	100	100
6	B2	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
6	B4	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	B6	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	B8	38/47 (81%)	27 (71%)	10 (26%)	1 (3%)	5	27
6	BB	38/47 (81%)	33 (87%)	5 (13%)	0	100	100
6	BE	38/47 (81%)	32 (84%)	6 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BG	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	BJ	38/47 (81%)	29 (76%)	9 (24%)	0	100	100
6	BN	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	BP	38/47 (81%)	25 (66%)	12 (32%)	1 (3%)	5	27
6	BR	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
6	BT	38/47 (81%)	30 (79%)	5 (13%)	3 (8%)	1	4
6	BV	38/47 (81%)	36 (95%)	2 (5%)	0	100	100
6	BX	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	BZ	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
All	All	5285/5994 (88%)	3628 (69%)	1236 (23%)	421 (8%)	1	4

5 of 421 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AC	64	ALA
1	AC	70	PRO
1	AC	97	VAL
1	AC	138	ASN
1	AC	154	THR

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	AC	265/317 (84%)	239 (90%)	26 (10%)	8	30
1	BC	265/317 (84%)	238 (90%)	27 (10%)	7	28
2	AL	228/229 (100%)	199 (87%)	29 (13%)	4	19
2	BL	228/229 (100%)	206 (90%)	22 (10%)	8	32
3	AM	256/261 (98%)	217 (85%)	39 (15%)	3	14
3	BM	256/261 (98%)	219 (86%)	37 (14%)	3	15
4	AH	210/211 (100%)	194 (92%)	16 (8%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BH	210/211 (100%)	189 (90%)	21 (10%)	7	29
5	A1	48/56 (86%)	45 (94%)	3 (6%)	18	51
5	A3	47/56 (84%)	41 (87%)	6 (13%)	4	19
5	A5	48/56 (86%)	44 (92%)	4 (8%)	11	39
5	A7	48/56 (86%)	40 (83%)	8 (17%)	2	11
5	A9	50/56 (89%)	46 (92%)	4 (8%)	12	40
5	AA	44/56 (79%)	38 (86%)	6 (14%)	3	17
5	AD	47/56 (84%)	44 (94%)	3 (6%)	17	51
5	AF	49/56 (88%)	42 (86%)	7 (14%)	3	15
5	AI	49/56 (88%)	45 (92%)	4 (8%)	11	39
5	AK	48/56 (86%)	42 (88%)	6 (12%)	4	20
5	AO	49/56 (88%)	43 (88%)	6 (12%)	5	21
5	AQ	47/56 (84%)	43 (92%)	4 (8%)	10	38
5	AS	49/56 (88%)	44 (90%)	5 (10%)	7	28
5	AU	50/56 (89%)	43 (86%)	7 (14%)	3	16
5	AW	50/56 (89%)	45 (90%)	5 (10%)	7	29
5	AY	50/56 (89%)	43 (86%)	7 (14%)	3	16
5	B1	45/56 (80%)	43 (96%)	2 (4%)	28	65
5	B3	50/56 (89%)	46 (92%)	4 (8%)	12	40
5	B5	48/56 (86%)	45 (94%)	3 (6%)	18	51
5	B7	45/56 (80%)	41 (91%)	4 (9%)	9	35
5	B9	48/56 (86%)	46 (96%)	2 (4%)	30	66
5	BA	50/56 (89%)	45 (90%)	5 (10%)	7	29
5	BD	43/56 (77%)	42 (98%)	1 (2%)	50	80
5	BF	48/56 (86%)	43 (90%)	5 (10%)	7	27
5	BI	46/56 (82%)	40 (87%)	6 (13%)	4	19
5	BK	50/56 (89%)	44 (88%)	6 (12%)	5	22
5	BO	49/56 (88%)	45 (92%)	4 (8%)	11	39
5	BQ	50/56 (89%)	46 (92%)	4 (8%)	12	40
5	BS	49/56 (88%)	46 (94%)	3 (6%)	18	53
5	BU	50/56 (89%)	43 (86%)	7 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	BW	48/56 (86%)	41 (85%)	7 (15%)	3	15
5	BY	45/56 (80%)	39 (87%)	6 (13%)	4	17
6	A0	33/39 (85%)	23 (70%)	10 (30%)	0	1
6	A2	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	A4	33/39 (85%)	26 (79%)	7 (21%)	1	5
6	A6	33/39 (85%)	30 (91%)	3 (9%)	9	34
6	A8	33/39 (85%)	26 (79%)	7 (21%)	1	5
6	AB	33/39 (85%)	27 (82%)	6 (18%)	1	9
6	AE	33/39 (85%)	31 (94%)	2 (6%)	18	53
6	AG	33/39 (85%)	25 (76%)	8 (24%)	0	3
6	AJ	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	AN	33/39 (85%)	27 (82%)	6 (18%)	1	9
6	AP	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	AR	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	AT	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	AV	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	AX	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	AZ	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	B0	33/39 (85%)	27 (82%)	6 (18%)	1	9
6	B2	33/39 (85%)	30 (91%)	3 (9%)	9	34
6	B4	33/39 (85%)	27 (82%)	6 (18%)	1	9
6	B6	33/39 (85%)	30 (91%)	3 (9%)	9	34
6	B8	33/39 (85%)	25 (76%)	8 (24%)	0	3
6	BB	33/39 (85%)	24 (73%)	9 (27%)	0	2
6	BE	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	BG	33/39 (85%)	30 (91%)	3 (9%)	9	34
6	BJ	33/39 (85%)	30 (91%)	3 (9%)	9	34
6	BN	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	BP	33/39 (85%)	31 (94%)	2 (6%)	18	53
6	BR	33/39 (85%)	27 (82%)	6 (18%)	1	9
6	BT	33/39 (85%)	30 (91%)	3 (9%)	9	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BV	33/39 (85%)	31 (94%)	2 (6%)	18	53
6	BX	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	BZ	33/39 (85%)	30 (91%)	3 (9%)	9	34
All	All	4511/5076 (89%)	3985 (88%)	526 (12%)	5	22

5 of 526 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	BV	13	GLU
5	BY	9	TYR
5	BU	56	GLN
6	B0	17	PHE
5	AU	9	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
5	A9	7	ASN
6	B8	23	GLN
2	BL	192	ASN
6	B6	23	GLN
5	BO	7	ASN

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 169 ligands modelled in this entry, 36 are monoatomic - leaving 133 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	$\#\|Z\| > 2$
14	CRT	AR	102	-	41,43,43	1.42	7 (17%)	50,54,54	1.78	15 (30%)
9	BCL	AO	102	-	64,74,74	1.55	13 (20%)	78,115,115	2.28	24 (30%)
9	BCL	B4	101	-	64,74,74	1.75	18 (28%)	78,115,115	2.44	26 (33%)
9	BCL	BW	102	-	64,74,74	1.63	12 (18%)	78,115,115	2.35	25 (32%)
9	BCL	AM	401	-	64,74,74	1.43	8 (12%)	78,115,115	2.30	24 (30%)
14	CRT	AN	102	-	41,43,43	1.45	8 (19%)	50,54,54	1.70	17 (34%)
14	CRT	A5	103	-	41,43,43	1.45	7 (17%)	50,54,54	1.64	17 (34%)
9	BCL	BA	101	-	64,74,74	1.57	13 (20%)	78,115,115	2.27	23 (29%)
14	CRT	AA	102	-	41,43,43	1.59	4 (9%)	50,54,54	1.49	12 (24%)
15	PEF	AM	409	-	46,46,46	2.18	7 (15%)	49,51,51	1.30	6 (12%)
9	BCL	AR	101	-	64,74,74	1.70	15 (23%)	78,115,115	2.36	24 (30%)
9	BCL	BX	101	-	64,74,74	1.86	17 (26%)	78,115,115	2.44	23 (29%)
9	BCL	AY	102	-	64,74,74	1.84	13 (20%)	78,115,115	2.45	27 (34%)
9	BCL	AI	102	-	64,74,74	1.66	12 (18%)	78,115,115	2.30	22 (28%)
9	BCL	AF	102	-	64,74,74	1.64	13 (20%)	78,115,115	2.28	23 (29%)
14	CRT	BA	102	-	41,43,43	1.59	4 (9%)	50,54,54	1.46	12 (24%)
9	BCL	BI	102	-	64,74,74	1.73	15 (23%)	78,115,115	2.35	21 (26%)
9	BCL	B5	102	-	64,74,74	1.69	10 (15%)	78,115,115	2.31	23 (29%)
14	CRT	B5	103	-	41,43,43	1.55	5 (12%)	50,54,54	1.54	14 (28%)
11	UQ8	BL	304	-	53,53,53	1.47	3 (5%)	64,67,67	1.68	15 (23%)
9	BCL	A8	101	-	64,74,74	1.97	18 (28%)	78,115,115	3.11	28 (35%)
9	BCL	A3	104	-	64,74,74	1.71	14 (21%)	78,115,115	3.24	26 (33%)
9	BCL	B6	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.37	28 (35%)
9	BCL	BQ	103	-	64,74,74	1.69	15 (23%)	78,115,115	2.24	19 (24%)
7	HEM	BC	501	1	41,50,50	1.98	13 (31%)	45,82,82	1.70	9 (20%)
9	BCL	B1	102	-	64,74,74	1.51	13 (20%)	78,115,115	2.29	19 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	BCL	AJ	101	-	64,74,74	1.64	13 (20%)	78,115,115	2.40	23 (29%)
16	PO4	AM	410	-	4,4,4	1.68	0	6,6,6	0.43	0
9	BCL	AE	101	-	64,74,74	1.81	14 (21%)	78,115,115	2.49	26 (33%)
9	BCL	AT	101	-	64,74,74	1.85	15 (23%)	78,115,115	2.31	25 (32%)
9	BCL	BD	102	-	64,74,74	2.03	17 (26%)	78,115,115	2.40	25 (32%)
7	HEM	AC	502	1	41,50,50	1.86	12 (29%)	45,82,82	1.65	9 (20%)
9	BCL	BE	101	-	64,74,74	2.04	17 (26%)	78,115,115	2.16	20 (25%)
14	CRT	AJ	102	-	41,43,43	1.58	7 (17%)	50,54,54	1.63	16 (32%)
14	CRT	BU	103	-	41,43,43	1.62	9 (21%)	50,54,54	2.25	16 (32%)
9	BCL	BY	102	-	64,74,74	1.59	14 (21%)	78,115,115	2.33	21 (26%)
14	CRT	BW	103	-	41,43,43	1.64	7 (17%)	50,54,54	1.60	15 (30%)
9	BCL	AB	101	-	64,74,74	1.69	14 (21%)	78,115,115	2.43	24 (30%)
9	BCL	BF	102	-	64,74,74	2.03	13 (20%)	78,115,115	2.44	24 (30%)
9	BCL	BZ	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.33	26 (33%)
9	BCL	AK	102	-	64,74,74	1.57	14 (21%)	78,115,115	2.38	24 (30%)
14	CRT	BP	102	-	41,43,43	1.80	8 (19%)	50,54,54	1.58	14 (28%)
9	BCL	AD	102	-	64,74,74	1.64	11 (17%)	78,115,115	2.36	24 (30%)
9	BCL	BK	102	-	64,74,74	1.61	13 (20%)	78,115,115	2.29	23 (29%)
9	BCL	A7	103	-	64,74,74	2.12	15 (23%)	78,115,115	2.55	25 (32%)
9	BCL	A2	101	-	64,74,74	1.64	13 (20%)	78,115,115	2.71	22 (28%)
14	CRT	BN	102	-	41,43,43	1.63	9 (21%)	50,54,54	1.62	14 (28%)
9	BCL	AW	101	-	64,74,74	1.83	13 (20%)	78,115,115	3.78	27 (34%)
10	BPH	BM	403	-	51,70,70	0.92	2 (3%)	52,101,101	1.26	6 (11%)
9	BCL	AL	303	-	64,74,74	1.44	10 (15%)	78,115,115	2.34	22 (28%)
7	HEM	AC	504	1	41,50,50	1.85	9 (21%)	45,82,82	1.71	9 (20%)
14	CRT	A0	101	-	41,43,43	1.60	7 (17%)	50,54,54	1.93	13 (26%)
14	CRT	BF	103	-	41,43,43	1.57	8 (19%)	50,54,54	1.77	16 (32%)
7	HEM	BC	503	1	41,50,50	1.92	11 (26%)	45,82,82	1.66	9 (20%)
9	BCL	A5	102	-	64,74,74	1.89	16 (25%)	78,115,115	2.85	25 (32%)
9	BCL	A9	102	-	64,74,74	1.68	16 (25%)	78,115,115	3.03	27 (34%)
14	CRT	BS	103	-	41,43,43	1.53	5 (12%)	50,54,54	1.52	13 (26%)
9	BCL	BG	101	-	64,74,74	1.82	12 (18%)	78,115,115	2.41	24 (30%)
9	BCL	BJ	101	-	64,74,74	1.86	17 (26%)	78,115,115	2.21	25 (32%)
14	CRT	AW	102	-	41,43,43	1.66	9 (21%)	50,54,54	1.65	18 (36%)
9	BCL	B7	103	-	64,74,74	1.71	13 (20%)	78,115,115	2.40	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CRT	B0	101	-	41,43,43	2.14	10 (24%)	50,54,54	1.85	14 (28%)
9	BCL	BS	102	-	64,74,74	1.44	11 (17%)	78,115,115	2.41	22 (28%)
14	CRT	AT	102	-	41,43,43	1.61	7 (17%)	50,54,54	1.54	12 (24%)
13	MQ8	BM	405	-	54,54,54	1.18	5 (9%)	66,69,69	1.40	11 (16%)
15	PEF	AS	101	-	46,46,46	2.18	7 (15%)	49,51,51	1.38	6 (12%)
9	BCL	AL	301	-	64,74,74	1.62	14 (21%)	78,115,115	2.24	24 (30%)
9	BCL	B8	101	-	64,74,74	1.74	14 (21%)	78,115,115	2.60	28 (35%)
9	BCL	B2	101	-	64,74,74	1.76	14 (21%)	78,115,115	2.36	26 (33%)
9	BCL	B3	102	-	64,74,74	1.49	9 (14%)	78,115,115	2.32	22 (28%)
9	BCL	AV	102	-	64,74,74	1.84	16 (25%)	78,115,115	2.23	27 (34%)
10	BPH	AL	302	-	51,70,70	0.92	2 (3%)	52,101,101	1.25	6 (11%)
9	BCL	A0	102	-	64,74,74	2.07	14 (21%)	78,115,115	3.46	26 (33%)
15	PEF	BQ	101	-	46,46,46	2.17	7 (15%)	49,51,51	1.37	6 (12%)
9	BCL	BO	102	-	64,74,74	1.59	12 (18%)	78,115,115	2.36	23 (29%)
15	PEF	BM	407	-	18,18,46	3.11	7 (38%)	21,23,51	1.96	5 (23%)
9	BCL	BP	101	-	64,74,74	1.96	17 (26%)	78,115,115	2.51	26 (33%)
9	BCL	A3	103	-	64,74,74	1.87	13 (20%)	78,115,115	2.33	23 (29%)
9	BCL	B9	102	-	64,74,74	1.66	12 (18%)	78,115,115	2.40	23 (29%)
14	CRT	BM	406	-	41,43,43	1.56	7 (17%)	50,54,54	1.53	11 (22%)
9	BCL	AX	101	-	64,74,74	2.22	14 (21%)	78,115,115	2.95	24 (30%)
9	BCL	BT	101	-	64,74,74	1.79	16 (25%)	78,115,115	2.30	27 (34%)
16	PO4	AH	302	-	4,4,4	1.63	0	6,6,6	0.41	0
9	BCL	B0	102	-	64,74,74	1.56	13 (20%)	78,115,115	2.40	27 (34%)
14	CRT	AX	102	-	41,43,43	1.91	9 (21%)	50,54,54	2.00	11 (22%)
9	BCL	AM	402	-	64,74,74	1.45	10 (15%)	78,115,115	2.38	23 (29%)
7	HEM	BC	502	1	41,50,50	1.83	11 (26%)	45,82,82	1.71	10 (22%)
10	BPH	AM	403	-	51,70,70	0.92	4 (7%)	52,101,101	1.11	5 (9%)
13	MQ8	AM	405	-	54,54,54	1.13	3 (5%)	66,69,69	1.54	13 (19%)
16	PO4	BH	301	-	4,4,4	1.62	0	6,6,6	0.40	0
9	BCL	BQ	104	-	64,74,74	1.82	14 (21%)	78,115,115	2.27	23 (29%)
14	CRT	AS	104	-	41,43,43	1.57	5 (12%)	50,54,54	1.83	15 (30%)
9	BCL	BM	402	-	64,74,74	1.56	10 (15%)	78,115,115	2.49	22 (28%)
14	CRT	AP	102	-	41,43,43	1.70	8 (19%)	50,54,54	1.61	15 (30%)
14	CRT	AG	102	-	41,43,43	1.48	8 (19%)	50,54,54	1.58	17 (34%)
14	CRT	BG	102	-	41,43,43	1.52	6 (14%)	50,54,54	1.61	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	BCL	BL	301	-	64,74,74	1.64	14 (21%)	78,115,115	2.23	23 (29%)
14	CRT	A1	103	-	41,43,43	1.49	8 (19%)	50,54,54	2.34	17 (34%)
14	CRT	B7	102	-	41,43,43	1.86	8 (19%)	50,54,54	1.52	11 (22%)
15	PEF	AM	407	-	18,18,46	3.12	7 (38%)	21,23,51	1.96	6 (28%)
9	BCL	BM	401	-	64,74,74	1.42	10 (15%)	78,115,115	2.30	25 (32%)
15	PEF	AM	408	-	13,13,46	2.93	5 (38%)	15,16,51	1.16	1 (6%)
9	BCL	A1	102	-	64,74,74	2.59	18 (28%)	78,115,115	2.54	24 (30%)
9	BCL	BU	102	-	64,74,74	1.75	12 (18%)	78,115,115	2.36	22 (28%)
14	CRT	AM	406	-	41,43,43	1.61	6 (14%)	50,54,54	1.53	8 (16%)
9	BCL	AU	102	-	64,74,74	1.80	16 (25%)	78,115,115	2.97	32 (41%)
14	CRT	A7	102	-	41,43,43	3.31	10 (24%)	50,54,54	3.57	13 (26%)
7	HEM	AC	501	1	41,50,50	1.86	12 (29%)	45,82,82	1.74	9 (20%)
7	HEM	BC	504	1	41,50,50	1.92	9 (21%)	45,82,82	1.68	10 (22%)
9	BCL	AP	101	-	64,74,74	1.84	13 (20%)	78,115,115	2.47	25 (32%)
9	BCL	A6	101	-	64,74,74	2.17	14 (21%)	78,115,115	2.49	27 (34%)
9	BCL	AG	101	-	64,74,74	1.70	13 (20%)	78,115,115	2.30	24 (30%)
9	BCL	BV	101	-	64,74,74	1.70	15 (23%)	78,115,115	2.32	29 (37%)
10	BPH	BL	302	-	51,70,70	0.91	4 (7%)	52,101,101	1.13	5 (9%)
14	CRT	BO	103	-	41,43,43	1.41	7 (17%)	50,54,54	1.77	16 (32%)
9	BCL	AA	101	-	64,74,74	1.62	14 (21%)	78,115,115	2.25	22 (28%)
16	PO4	A3	101	-	4,4,4	1.67	0	6,6,6	0.43	0
9	BCL	BB	101	-	64,74,74	1.95	14 (21%)	78,115,115	2.53	26 (33%)
11	UQ8	AL	304	-	53,53,53	1.51	3 (5%)	64,67,67	1.80	14 (21%)
14	CRT	BV	102	-	41,43,43	2.07	11 (26%)	50,54,54	1.57	11 (22%)
14	CRT	B2	102	-	41,43,43	2.24	11 (26%)	50,54,54	1.73	15 (30%)
9	BCL	AS	103	-	64,74,74	1.86	11 (17%)	78,115,115	2.37	24 (30%)
14	CRT	BB	102	-	41,43,43	1.50	8 (19%)	50,54,54	1.87	17 (34%)
9	BCL	AZ	101	-	64,74,74	2.75	17 (26%)	78,115,115	3.32	26 (33%)
9	BCL	BL	303	-	64,74,74	1.42	9 (14%)	78,115,115	2.34	24 (30%)
9	BCL	BN	101	-	64,74,74	1.67	12 (18%)	78,115,115	2.23	26 (33%)
9	BCL	AN	101	-	64,74,74	1.80	15 (23%)	78,115,115	2.42	26 (33%)
9	BCL	AQ	102	-	64,74,74	1.58	15 (23%)	78,115,115	2.30	21 (26%)
7	HEM	AC	503	1	41,50,50	1.91	10 (24%)	45,82,82	1.60	6 (13%)
14	CRT	AB	102	-	41,43,43	1.34	5 (12%)	50,54,54	1.87	15 (30%)
15	PEF	AH	301	-	18,18,46	3.12	7 (38%)	21,23,51	1.96	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	CRT	B1	103	-	41,43,43	1.39	6 (14%)	50,54,54	1.73	18 (36%)
14	CRT	A2	102	-	41,43,43	1.74	9 (21%)	50,54,54	1.59	11 (22%)

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
14	CRT	AR	102	-	-	1/51/51/51	-
9	BCL	AO	102	-	-	17/37/137/137	-
9	BCL	B4	101	-	-	8/37/137/137	-
9	BCL	BW	102	-	-	17/37/137/137	-
9	BCL	AM	401	-	-	13/37/137/137	-
14	CRT	AN	102	-	-	1/51/51/51	-
14	CRT	A5	103	-	-	1/51/51/51	-
9	BCL	BA	101	-	-	12/37/137/137	-
14	CRT	AA	102	-	-	1/51/51/51	-
15	PEF	AM	409	-	-	20/50/50/50	-
9	BCL	AR	101	-	-	16/37/137/137	-
9	BCL	BX	101	-	-	12/37/137/137	-
9	BCL	AY	102	-	-	19/37/137/137	-
9	BCL	AI	102	-	-	14/37/137/137	-
9	BCL	AF	102	-	-	9/37/137/137	-
14	CRT	BA	102	-	-	1/51/51/51	-
9	BCL	BI	102	-	-	16/37/137/137	-
9	BCL	B5	102	-	-	16/37/137/137	-
14	CRT	B5	103	-	-	1/51/51/51	-
11	UQ8	BL	304	-	-	4/51/75/75	0/1/1/1
9	BCL	A8	101	-	-	10/37/137/137	-
9	BCL	A3	104	-	-	18/37/137/137	-
9	BCL	B6	101	-	-	19/37/137/137	-
9	BCL	BQ	103	-	-	15/37/137/137	-
7	HEM	BC	501	1	-	4/12/54/54	-
9	BCL	B1	102	-	-	14/37/137/137	-
9	BCL	AJ	101	-	-	11/37/137/137	-
9	BCL	AE	101	-	-	10/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	AT	101	-	-	11/37/137/137	-
9	BCL	BD	102	-	-	13/37/137/137	-
7	HEM	AC	502	1	-	7/12/54/54	-
9	BCL	BE	101	-	-	14/37/137/137	-
14	CRT	AJ	102	-	-	1/51/51/51	-
14	CRT	BU	103	-	-	2/51/51/51	-
9	BCL	BY	102	-	-	19/37/137/137	-
14	CRT	BW	103	-	-	0/51/51/51	-
9	BCL	AB	101	-	-	10/37/137/137	-
9	BCL	BF	102	-	-	13/37/137/137	-
9	BCL	BZ	101	-	-	13/37/137/137	-
9	BCL	AK	102	-	-	15/37/137/137	-
14	CRT	BP	102	-	-	2/51/51/51	-
9	BCL	AD	102	-	-	17/37/137/137	-
9	BCL	BK	102	-	-	13/37/137/137	-
9	BCL	A7	103	-	-	14/37/137/137	-
9	BCL	A2	101	-	-	16/37/137/137	-
14	CRT	BN	102	-	-	1/51/51/51	-
9	BCL	AW	101	-	-	17/37/137/137	-
10	BPH	BM	403	-	-	12/37/105/105	0/5/6/6
9	BCL	AL	303	-	-	12/37/137/137	-
7	HEM	AC	504	1	-	4/12/54/54	-
14	CRT	A0	101	-	-	2/51/51/51	-
14	CRT	BF	103	-	-	1/51/51/51	-
7	HEM	BC	503	1	-	8/12/54/54	-
9	BCL	A5	102	-	-	15/37/137/137	-
9	BCL	A9	102	-	-	19/37/137/137	-
14	CRT	BS	103	-	-	2/51/51/51	-
9	BCL	BG	101	-	-	11/37/137/137	-
9	BCL	BJ	101	-	-	8/37/137/137	-
14	CRT	AW	102	-	-	0/51/51/51	-
9	BCL	B7	103	-	-	11/37/137/137	-
14	CRT	B0	101	-	-	5/51/51/51	-
9	BCL	BS	102	-	-	14/37/137/137	-
14	CRT	AT	102	-	-	2/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MQ8	BM	405	-	-	14/47/67/67	0/2/2/2
15	PEF	AS	101	-	-	28/50/50/50	-
9	BCL	AL	301	-	-	10/37/137/137	-
9	BCL	B8	101	-	-	15/37/137/137	-
9	BCL	B2	101	-	-	11/37/137/137	-
9	BCL	B3	102	-	-	17/37/137/137	-
9	BCL	AV	102	-	-	14/37/137/137	-
10	BPH	AL	302	-	-	14/37/105/105	0/5/6/6
9	BCL	A0	102	-	-	16/37/137/137	-
15	PEF	BQ	101	-	-	23/50/50/50	-
9	BCL	BO	102	-	-	17/37/137/137	-
15	PEF	BM	407	-	-	12/20/20/50	-
9	BCL	BP	101	-	-	7/37/137/137	-
9	BCL	A3	103	-	-	17/37/137/137	-
9	BCL	B9	102	-	-	14/37/137/137	-
14	CRT	BM	406	-	-	0/51/51/51	-
9	BCL	AX	101	-	-	18/37/137/137	-
9	BCL	BT	101	-	-	6/37/137/137	-
9	BCL	B0	102	-	-	13/37/137/137	-
14	CRT	AX	102	-	-	1/51/51/51	-
9	BCL	AM	402	-	-	13/37/137/137	-
7	HEM	BC	502	1	-	4/12/54/54	-
10	BPH	AM	403	-	-	12/37/105/105	0/5/6/6
13	MQ8	AM	405	-	-	9/47/67/67	0/2/2/2
9	BCL	BQ	104	-	-	12/37/137/137	-
14	CRT	AS	104	-	-	2/51/51/51	-
9	BCL	BM	402	-	-	13/37/137/137	-
14	CRT	AP	102	-	-	2/51/51/51	-
14	CRT	AG	102	-	-	1/51/51/51	-
14	CRT	BG	102	-	-	2/51/51/51	-
9	BCL	BL	301	-	-	13/37/137/137	-
14	CRT	A1	103	-	-	2/51/51/51	-
14	CRT	B7	102	-	-	2/51/51/51	-
15	PEF	AM	407	-	-	14/20/20/50	-
9	BCL	BM	401	-	-	13/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PEF	AM	408	-	-	9/13/13/50	-
9	BCL	A1	102	-	-	16/37/137/137	-
9	BCL	BU	102	-	-	15/37/137/137	-
14	CRT	AM	406	-	-	0/51/51/51	-
9	BCL	AU	102	-	-	19/37/137/137	-
14	CRT	A7	102	-	-	4/51/51/51	-
7	HEM	AC	501	1	-	6/12/54/54	-
7	HEM	BC	504	1	-	7/12/54/54	-
9	BCL	AP	101	-	-	8/37/137/137	-
9	BCL	A6	101	-	-	21/37/137/137	-
9	BCL	AG	101	-	-	14/37/137/137	-
9	BCL	BV	101	-	-	15/37/137/137	-
10	BPH	BL	302	-	-	14/37/105/105	0/5/6/6
14	CRT	BO	103	-	-	1/51/51/51	-
9	BCL	AA	101	-	-	17/37/137/137	-
9	BCL	BB	101	-	-	9/37/137/137	-
11	UQ8	AL	304	-	-	10/51/75/75	0/1/1/1
14	CRT	BV	102	-	-	2/51/51/51	-
14	CRT	B2	102	-	-	2/51/51/51	-
9	BCL	AS	103	-	-	17/37/137/137	-
14	CRT	BB	102	-	-	2/51/51/51	-
9	BCL	AZ	101	-	-	20/37/137/137	-
9	BCL	BL	303	-	-	14/37/137/137	-
9	BCL	BN	101	-	-	12/37/137/137	-
9	BCL	AN	101	-	-	13/37/137/137	-
9	BCL	AQ	102	-	-	17/37/137/137	-
7	HEM	AC	503	1	-	8/12/54/54	-
14	CRT	AB	102	-	-	5/51/51/51	-
15	PEF	AH	301	-	-	9/20/20/50	-
14	CRT	B1	103	-	-	2/51/51/51	-
14	CRT	A2	102	-	-	1/51/51/51	-

The worst 5 of 1392 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AZ	101	BCL	O2A-C1	-17.34	0.97	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A1	102	BCL	O2A-C1	15.23	1.89	1.46
14	A7	102	CRT	C21-C20	13.68	1.71	1.36
14	A7	102	CRT	C21-C22	12.47	1.82	1.43
9	A6	101	BCL	O2A-C1	11.73	1.79	1.46

The worst 5 of 2419 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	AW	101	BCL	O2A-C1-C2	25.83	176.53	108.64
9	A0	102	BCL	O2A-C1-C2	21.78	165.88	108.64
9	A3	104	BCL	O2A-C1-C2	19.13	158.90	108.64
14	A7	102	CRT	C20-C21-C22	-18.09	86.41	123.47
9	AZ	101	BCL	O2A-C1-C2	15.71	149.94	108.64

There are no chirality outliers.

5 of 1314 torsion outliers are listed below:

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

There are no ring outliers.

131 monomers are involved in 3208 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	AR	102	CRT	20	0
9	AO	102	BCL	50	0
9	B4	101	BCL	24	0
9	BW	102	BCL	44	0
9	AM	401	BCL	18	0
14	AN	102	CRT	14	0
14	A5	103	CRT	29	0
9	BA	101	BCL	37	0
14	AA	102	CRT	24	0
15	AM	409	PEF	14	0
9	AR	101	BCL	34	0
9	BX	101	BCL	37	0
9	AY	102	BCL	47	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AI	102	BCL	41	0
9	AF	102	BCL	38	0
14	BA	102	CRT	26	0
9	BI	102	BCL	50	0
9	B5	102	BCL	25	0
14	B5	103	CRT	21	0
11	BL	304	UQ8	12	0
9	A8	101	BCL	46	0
9	A3	104	BCL	31	0
9	B6	101	BCL	26	0
9	BQ	103	BCL	33	0
7	BC	501	HEM	7	0
9	B1	102	BCL	40	0
9	AJ	101	BCL	44	0
9	AE	101	BCL	32	0
9	AT	101	BCL	25	0
9	BD	102	BCL	38	0
7	AC	502	HEM	11	0
9	BE	101	BCL	48	0
14	AJ	102	CRT	21	0
14	BU	103	CRT	61	0
9	BY	102	BCL	37	0
14	BW	103	CRT	21	0
9	AB	101	BCL	33	0
9	BF	102	BCL	41	0
9	BZ	101	BCL	30	0
9	AK	102	BCL	67	0
14	BP	102	CRT	28	0
9	AD	102	BCL	29	0
9	BK	102	BCL	32	0
9	A7	103	BCL	51	0
9	A2	101	BCL	31	0
14	BN	102	CRT	15	0
9	AW	101	BCL	40	0
10	BM	403	BPH	9	0
9	AL	303	BCL	27	0
7	AC	504	HEM	5	0
14	A0	101	CRT	27	0
14	BF	103	CRT	19	0
7	BC	503	HEM	10	0
9	A5	102	BCL	40	0
9	A9	102	BCL	35	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	BS	103	CRT	11	0
9	BG	101	BCL	44	0
9	BJ	101	BCL	30	0
14	AW	102	CRT	32	0
9	B7	103	BCL	41	0
14	B0	101	CRT	42	0
9	BS	102	BCL	25	0
14	AT	102	CRT	17	0
13	BM	405	MQ8	9	0
15	AS	101	PEF	37	0
9	AL	301	BCL	41	0
9	B8	101	BCL	37	0
9	B2	101	BCL	45	0
9	B3	102	BCL	51	0
9	AV	102	BCL	28	0
10	AL	302	BPH	17	0
9	A0	102	BCL	71	0
15	BQ	101	PEF	12	0
9	BO	102	BCL	50	0
15	BM	407	PEF	2	0
9	BP	101	BCL	40	0
9	A3	103	BCL	47	0
9	B9	102	BCL	35	0
14	BM	406	CRT	8	0
9	AX	101	BCL	36	0
9	BT	101	BCL	19	0
16	AH	302	PO4	1	0
9	B0	102	BCL	54	0
14	AX	102	CRT	46	0
9	AM	402	BCL	35	0
7	BC	502	HEM	7	0
10	AM	403	BPH	14	0
13	AM	405	MQ8	9	0
16	BH	301	PO4	1	0
9	BQ	104	BCL	33	0
14	AS	104	CRT	77	0
9	BM	402	BCL	39	0
14	AP	102	CRT	24	0
14	AG	102	CRT	11	0
14	BG	102	CRT	14	0
9	BL	301	BCL	37	0
14	A1	103	CRT	29	0

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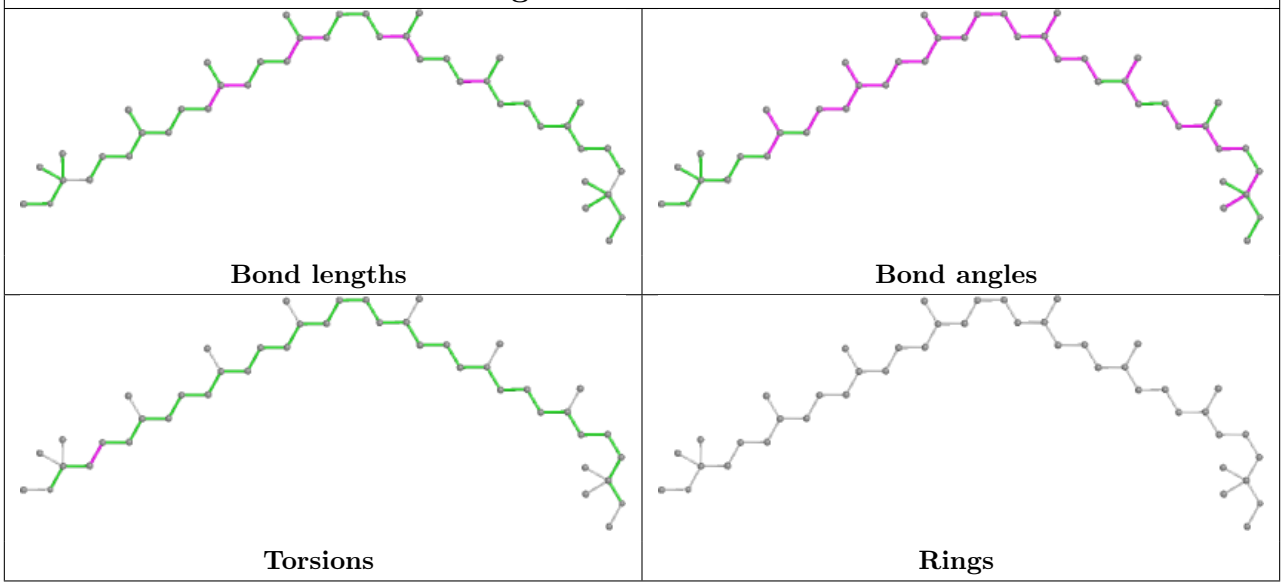
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B7	102	CRT	39	0
15	AM	407	PEF	3	0
9	BM	401	BCL	16	0
15	AM	408	PEF	6	0
9	A1	102	BCL	55	0
9	BU	102	BCL	41	0
14	AM	406	CRT	13	0
9	AU	102	BCL	46	0
14	A7	102	CRT	45	0
7	AC	501	HEM	9	0
7	BC	504	HEM	9	0
9	AP	101	BCL	41	0
9	A6	101	BCL	31	0
9	AG	101	BCL	37	0
9	BV	101	BCL	25	0
10	BL	302	BPH	11	0
14	BO	103	CRT	14	0
9	AA	101	BCL	41	0
9	BB	101	BCL	51	0
11	AL	304	UQ8	8	0
14	BV	102	CRT	59	0
14	B2	102	CRT	75	0
9	AS	103	BCL	32	0
14	BB	102	CRT	27	0
9	AZ	101	BCL	41	0
9	BL	303	BCL	15	0
9	BN	101	BCL	31	0
9	AN	101	BCL	57	0
9	AQ	102	BCL	26	0
7	AC	503	HEM	11	0
14	AB	102	CRT	45	0
15	AH	301	PEF	8	0
14	B1	103	CRT	40	0
14	A2	102	CRT	51	0

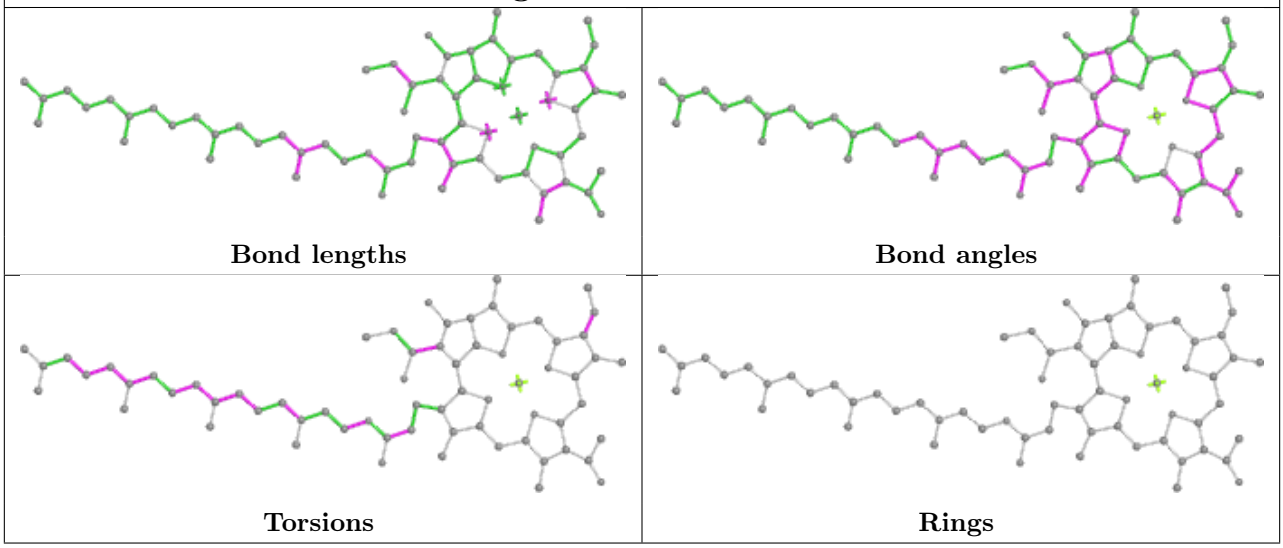
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 CRT AR 102



Ligand BCL AO 102



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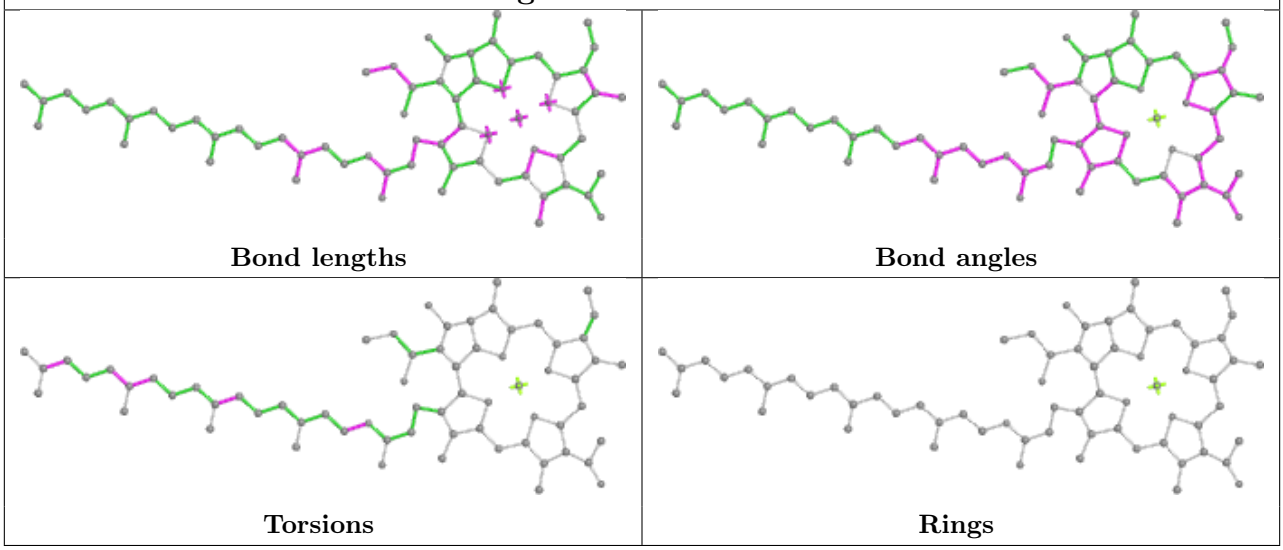
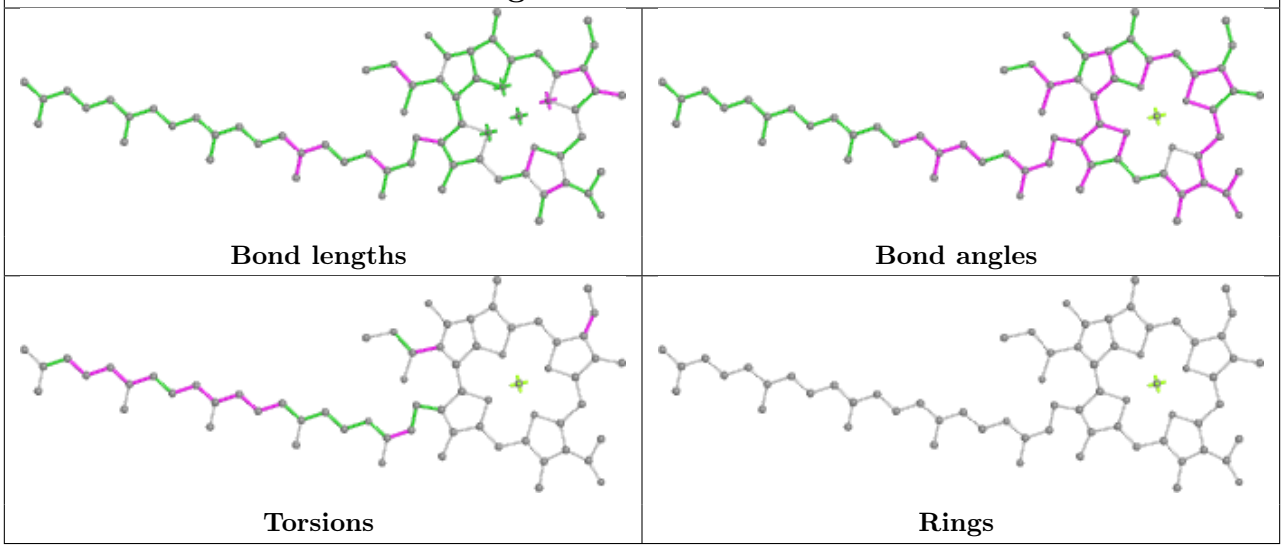
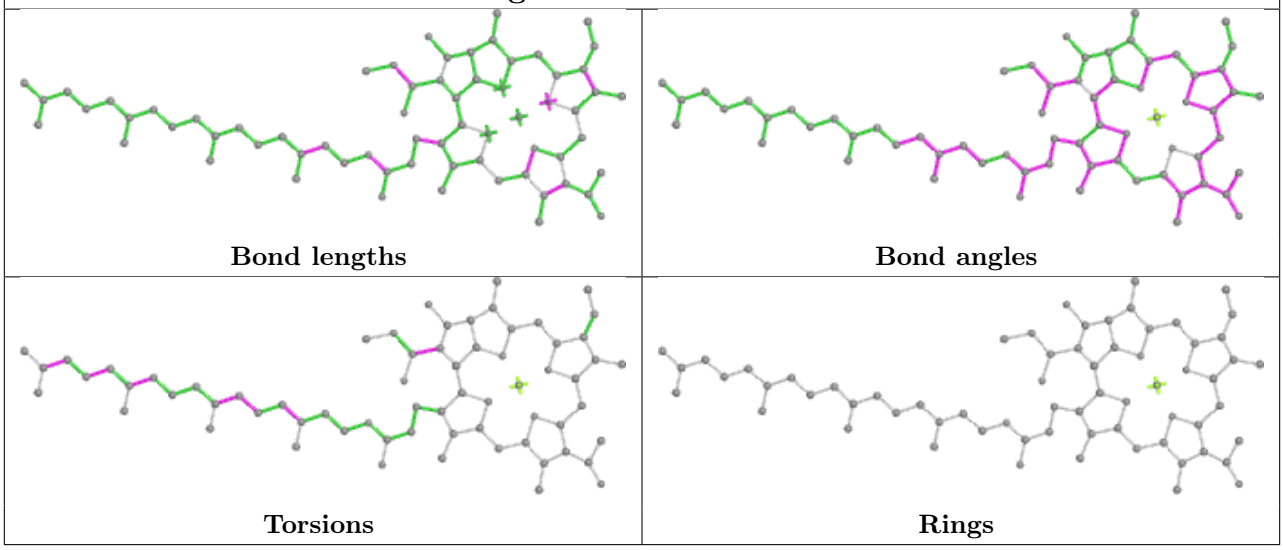


Ligand BCL BW 102



Ligand BCL AM 401



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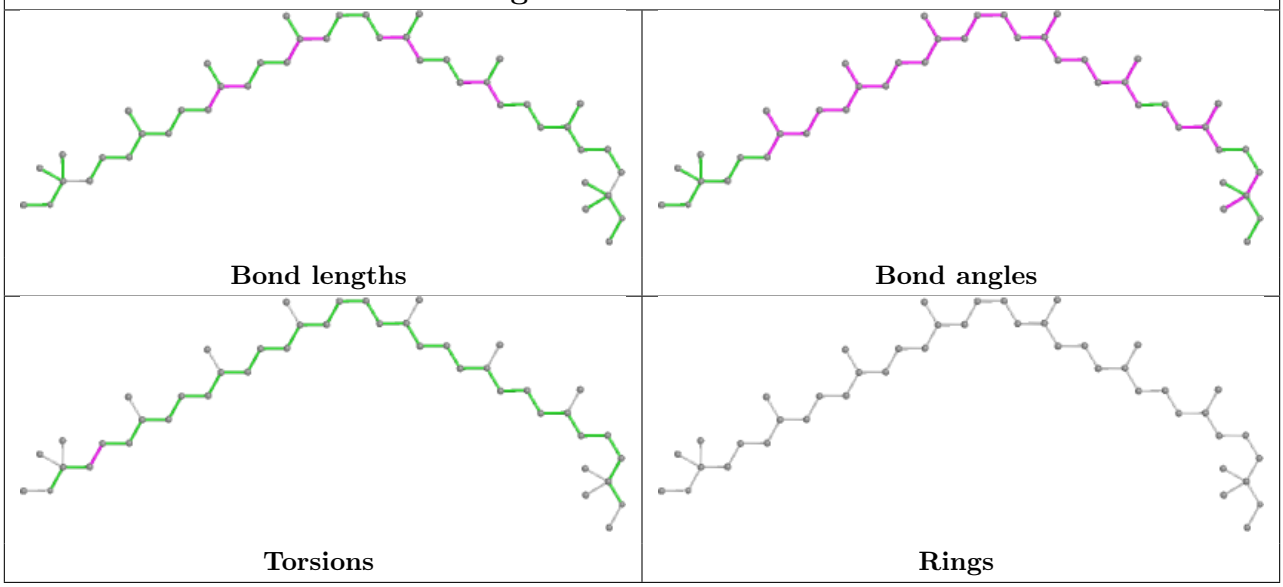
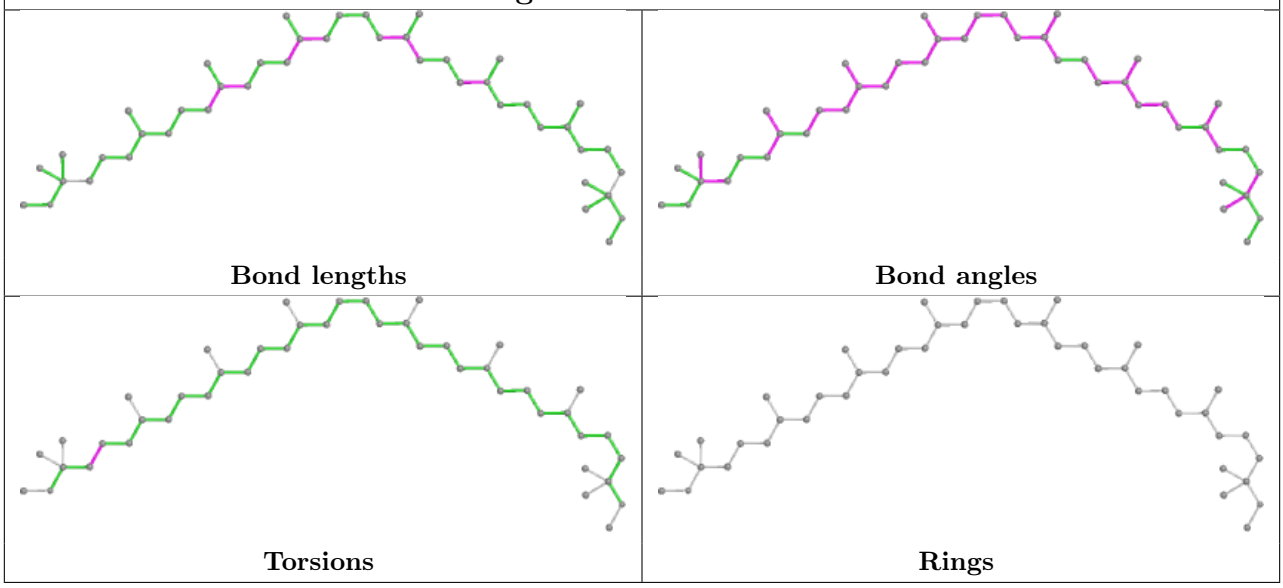


Ligand CRT A5 103



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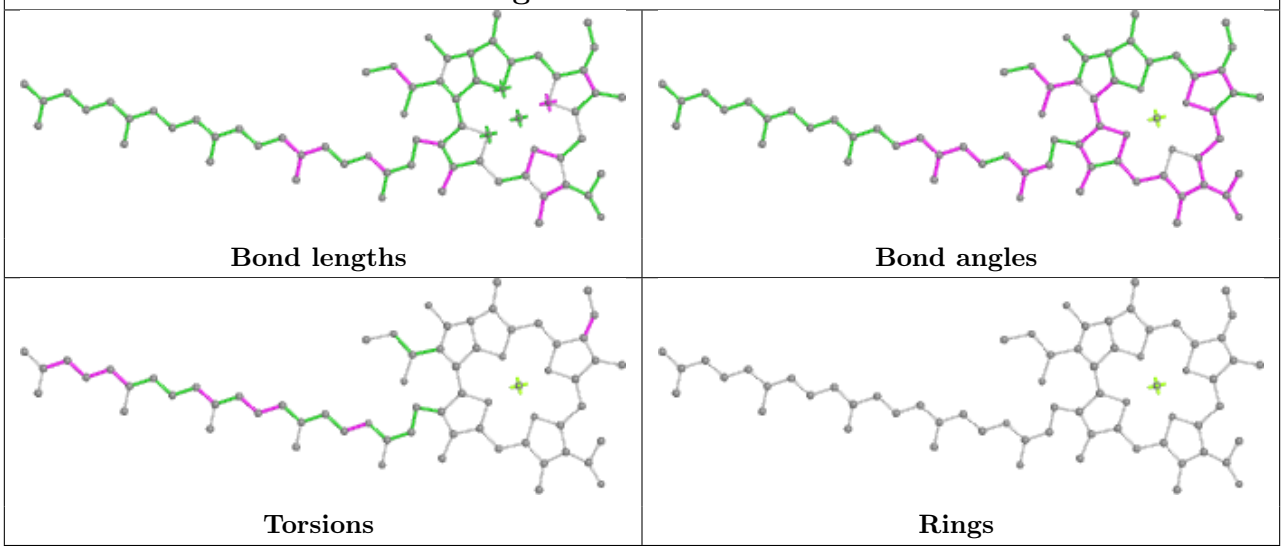

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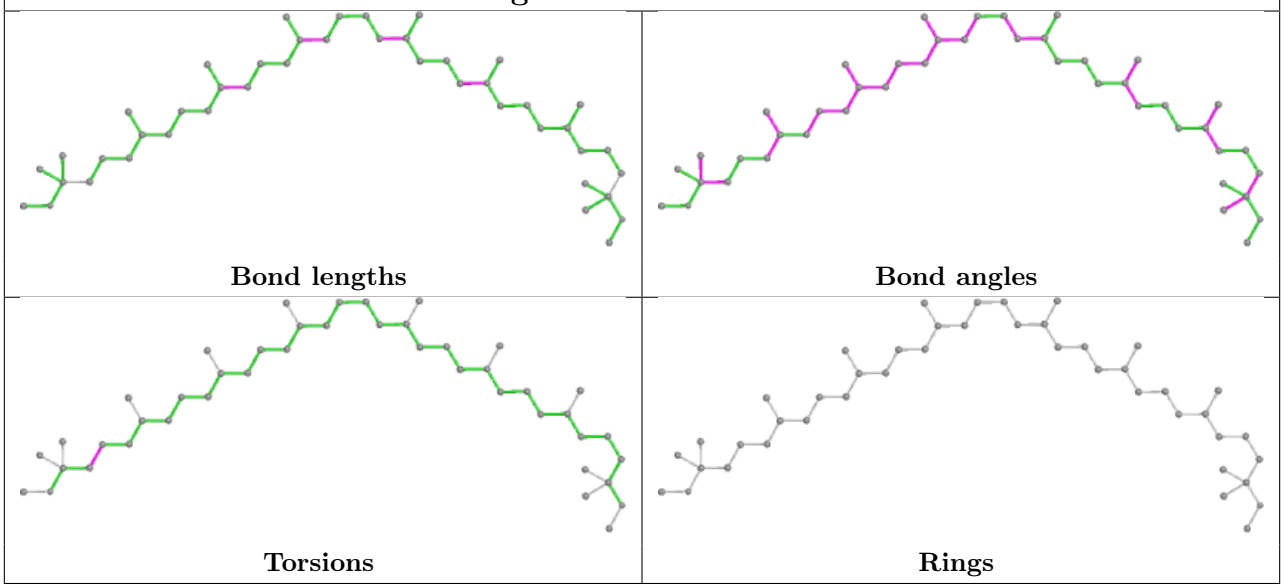
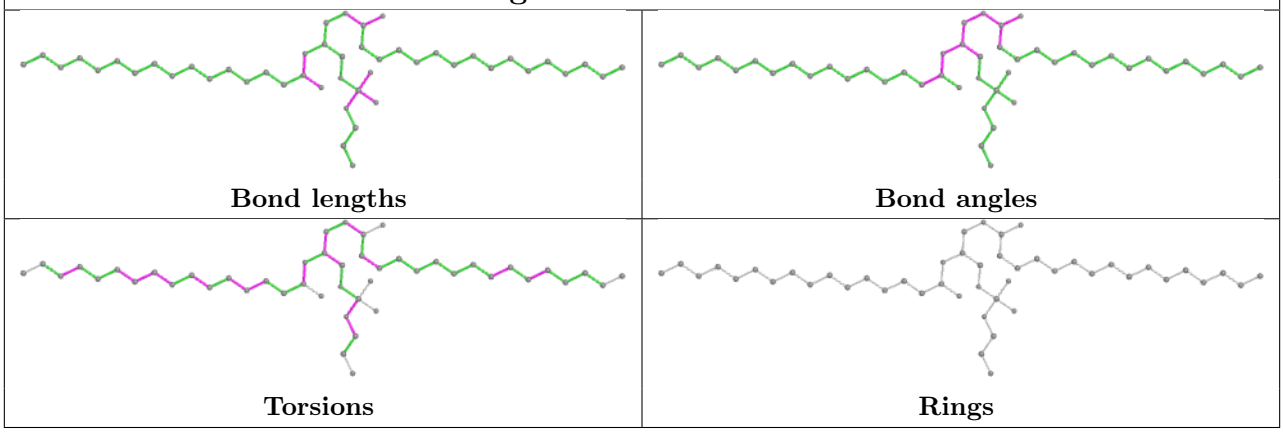


Ligand PEF AM 409



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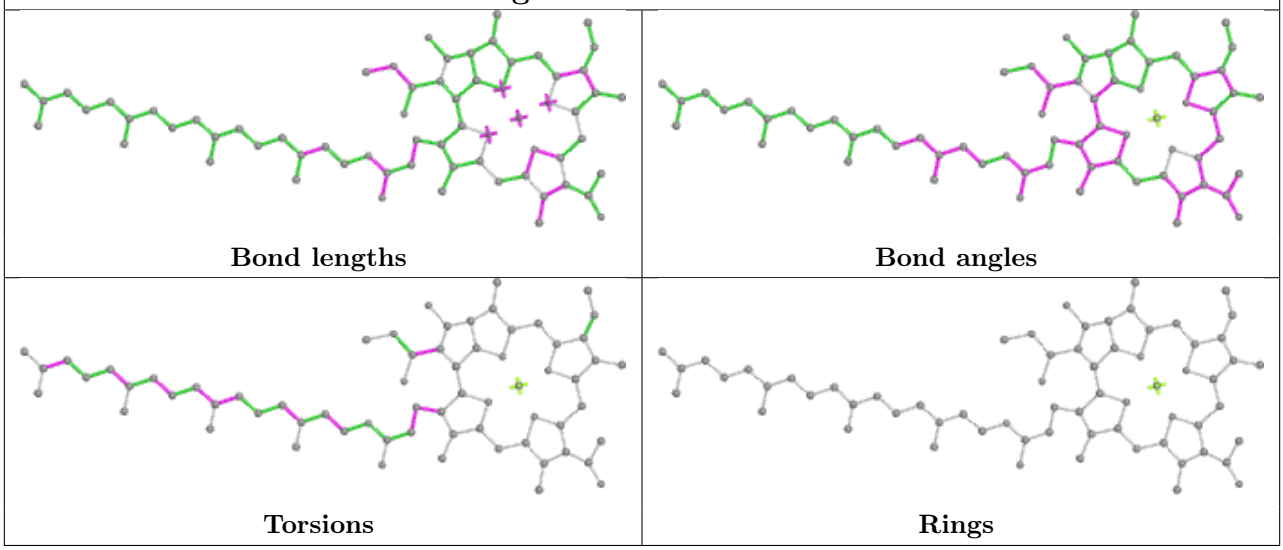

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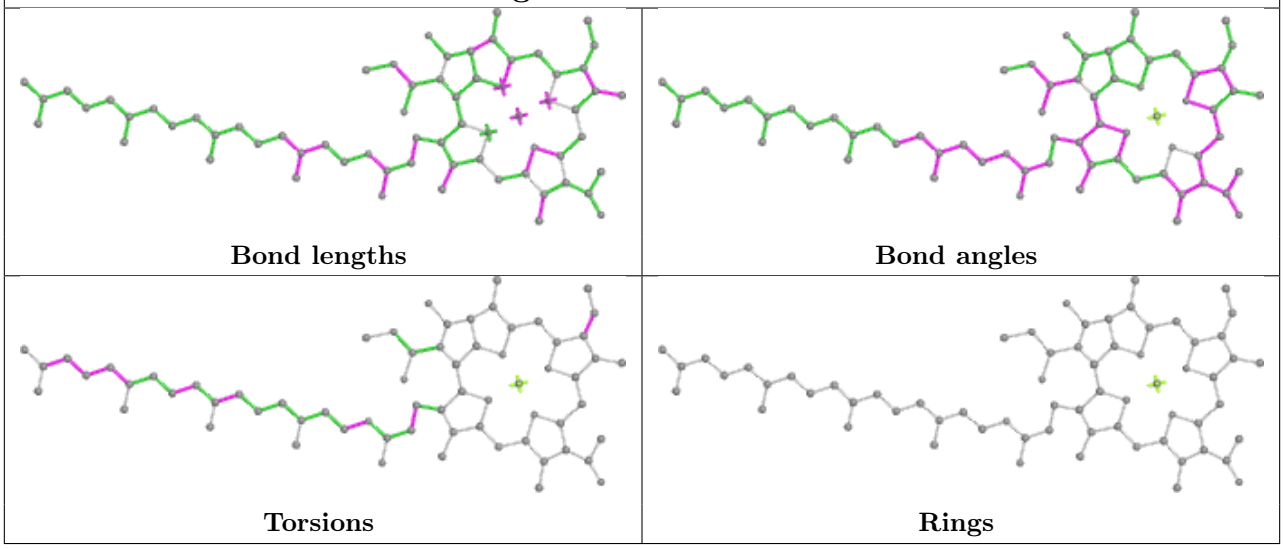
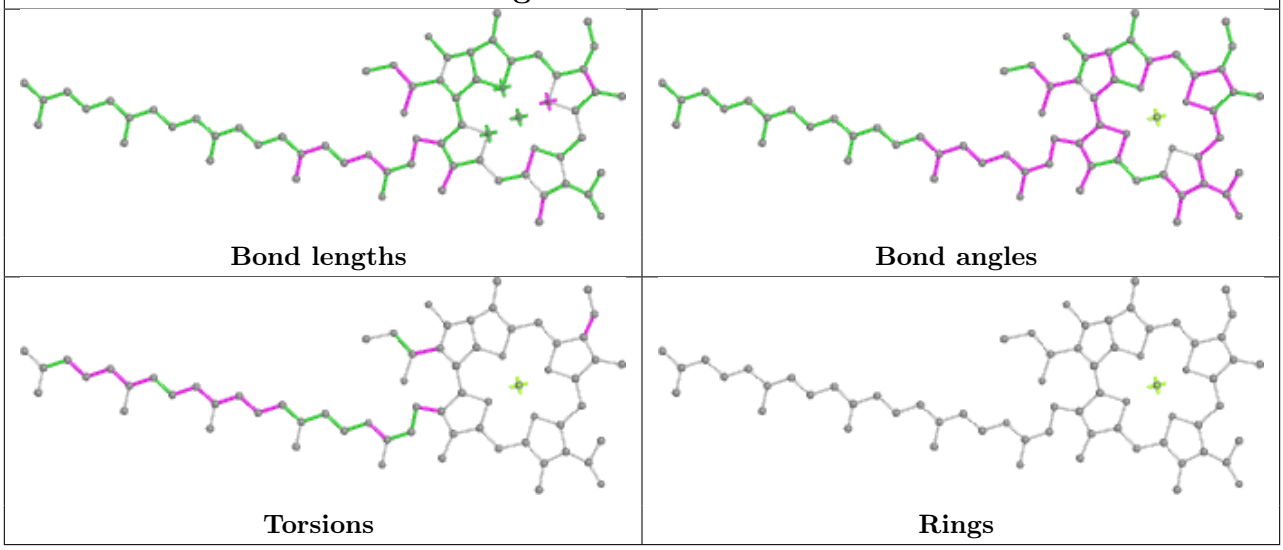


Ligand BCL AY 102



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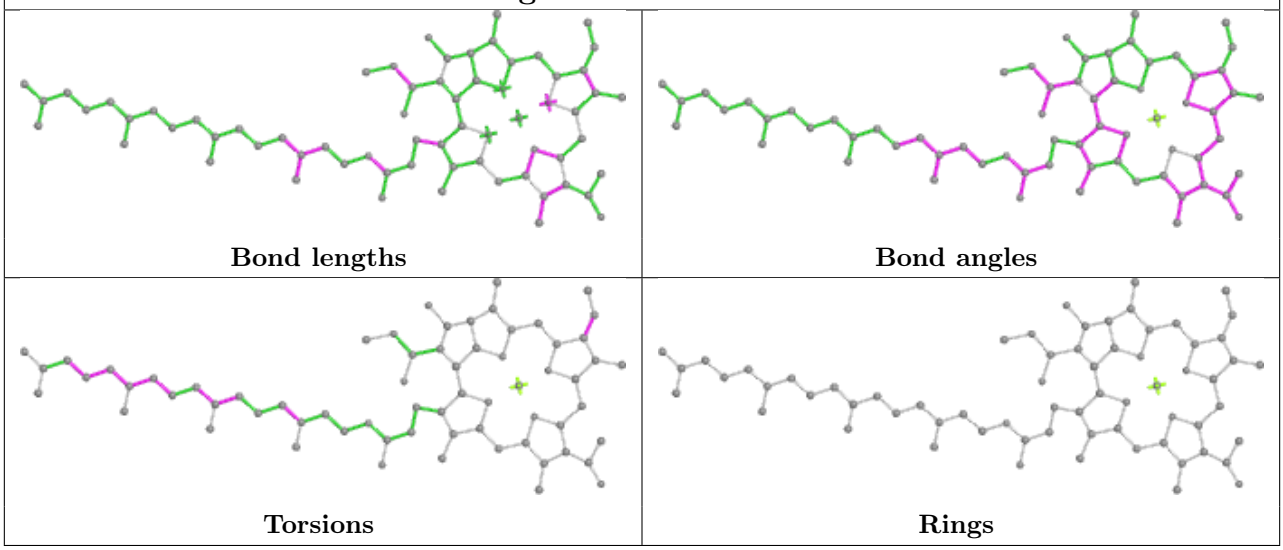

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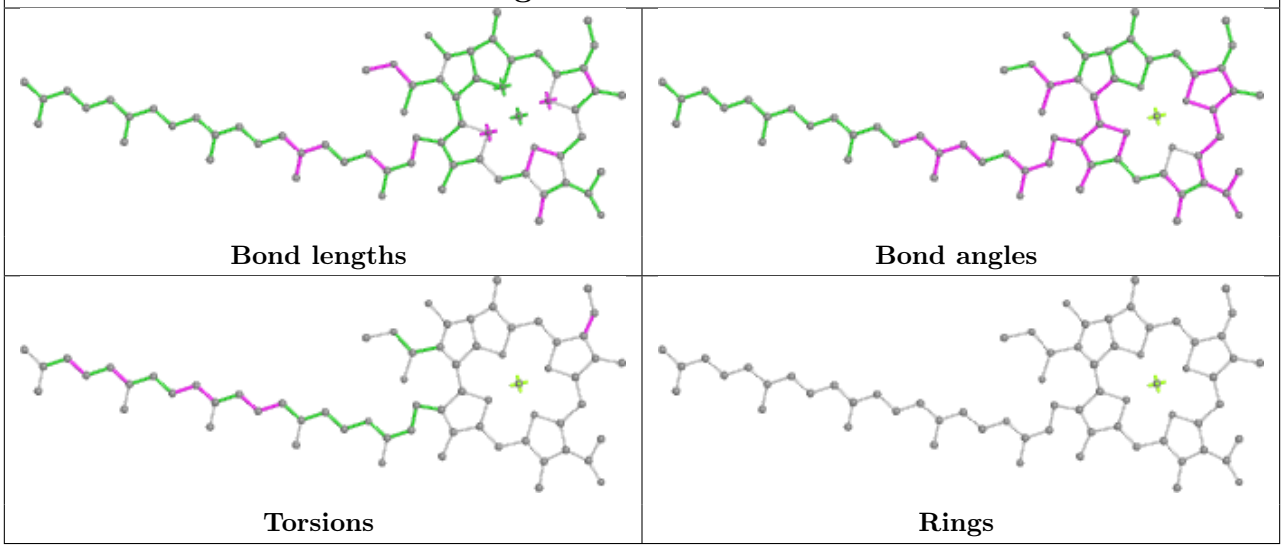

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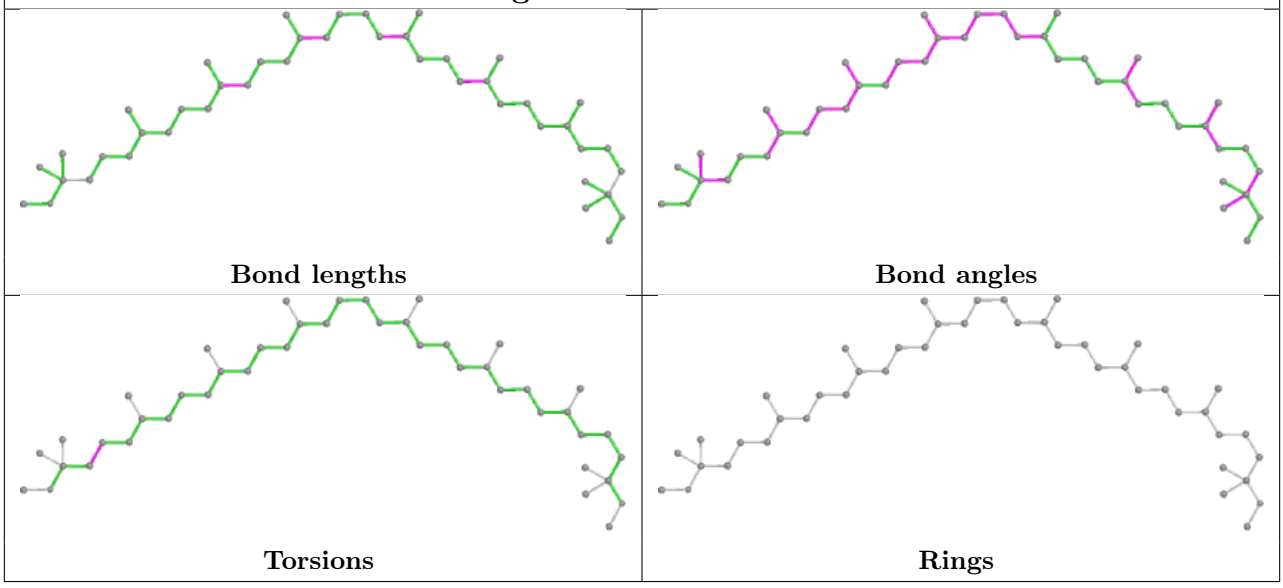

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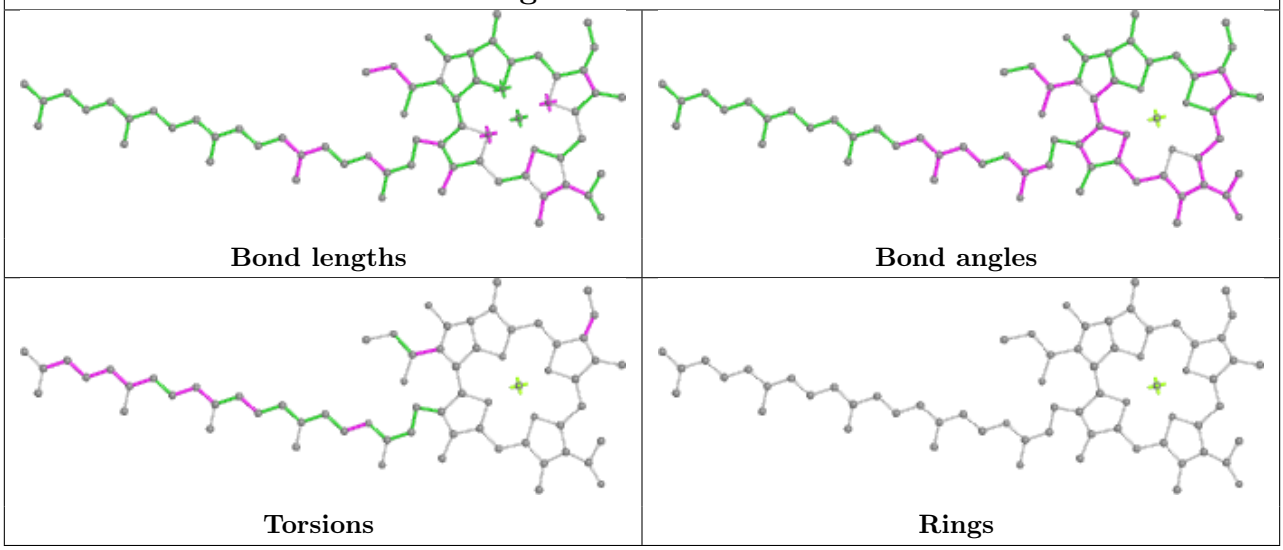

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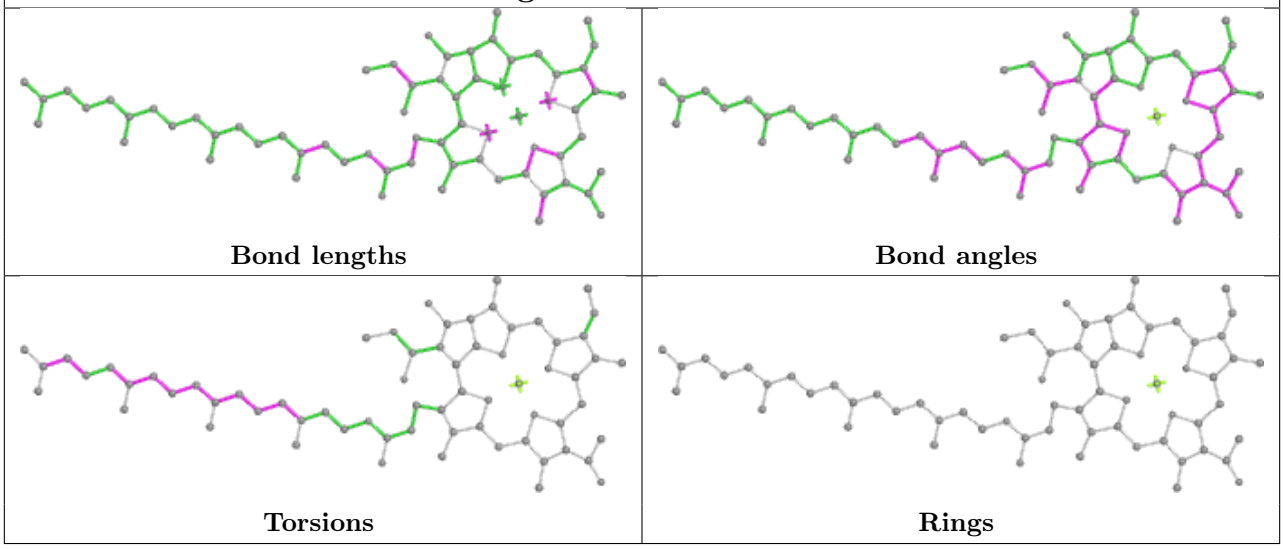

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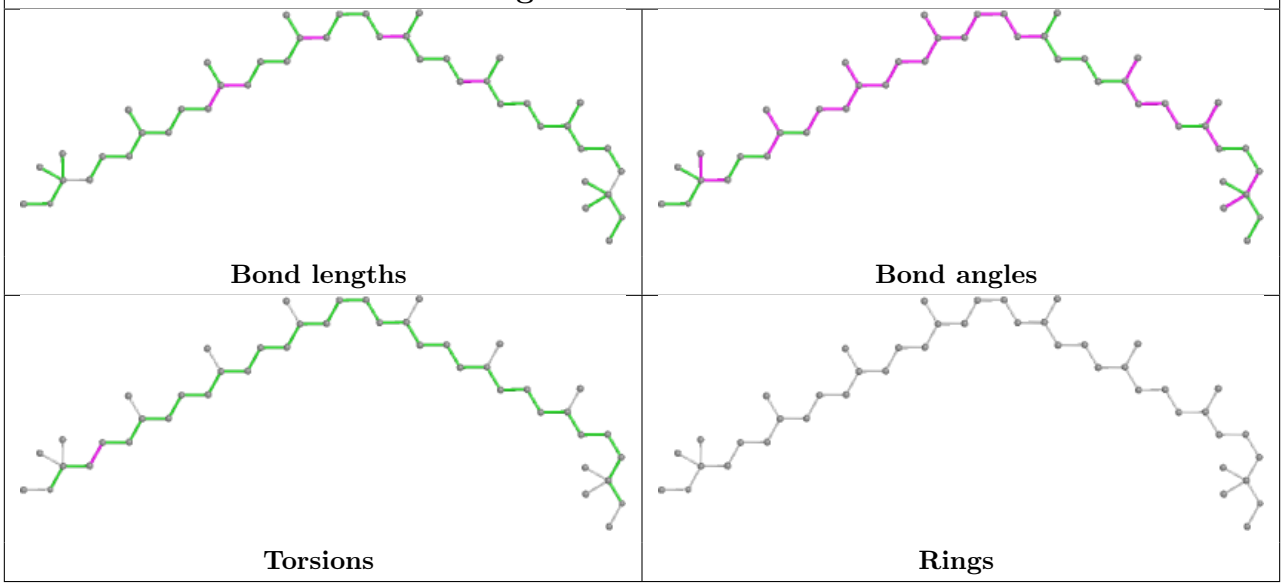
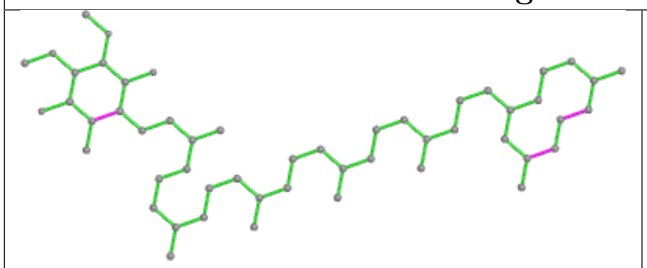
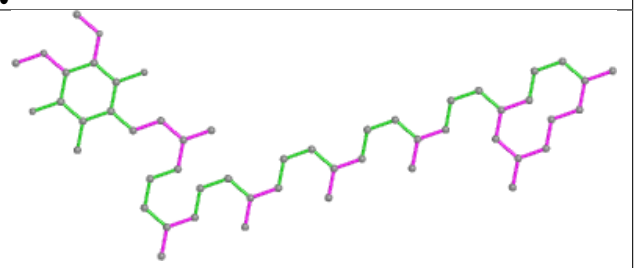


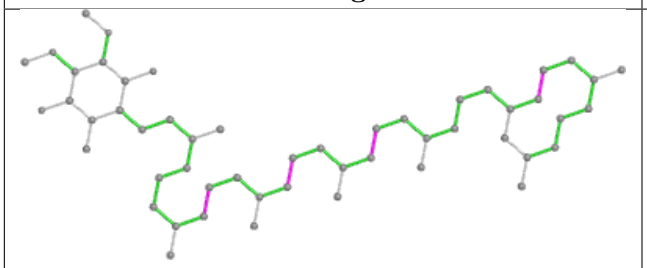
Ligand UQ8 BL 304



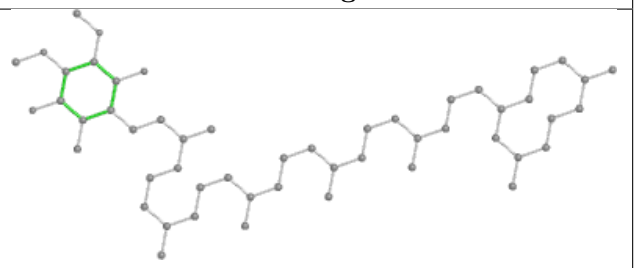
Bond lengths



Bond angles

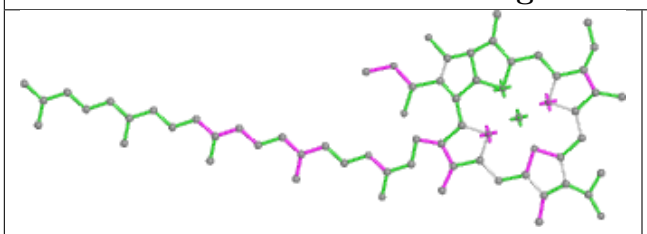


Torsions

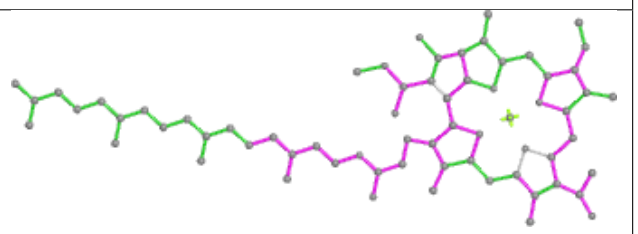


Rings

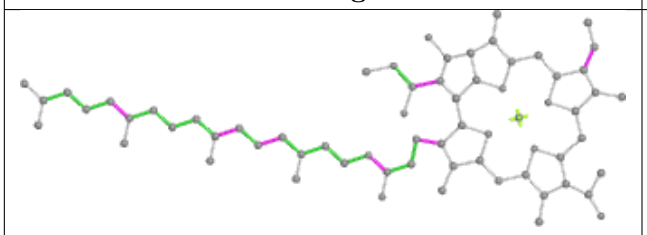
Ligand BCL A8 101



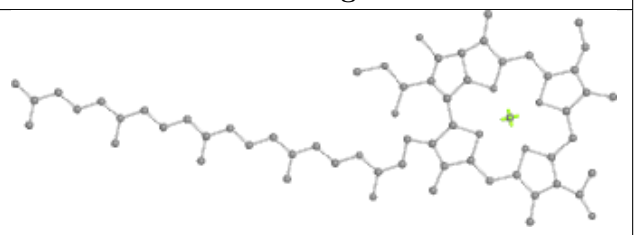
Bond lengths



Bond angles

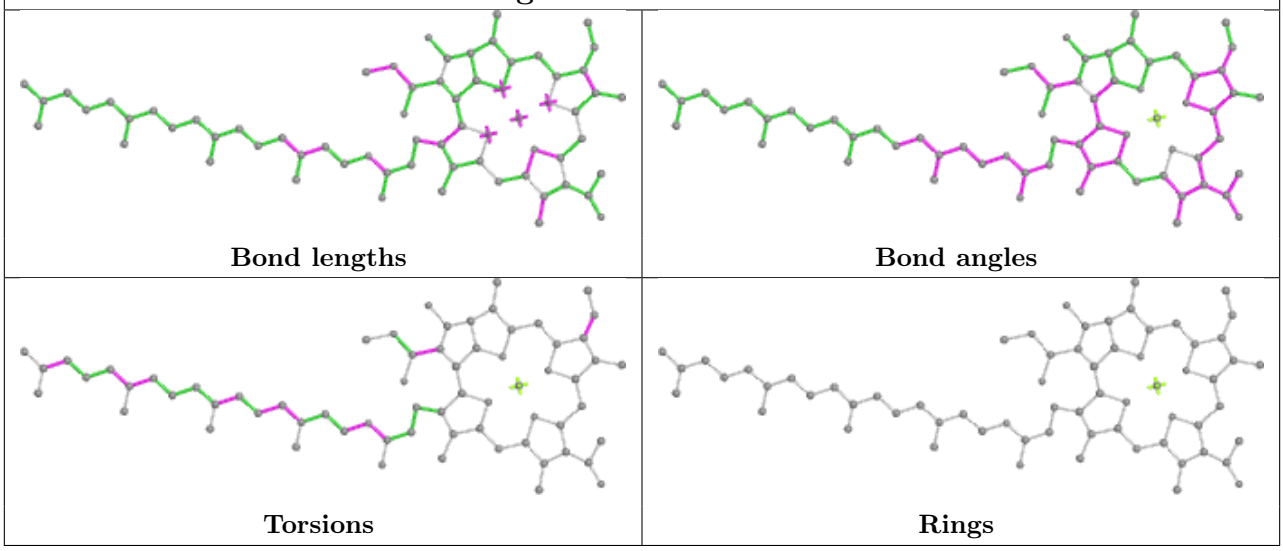


Torsions

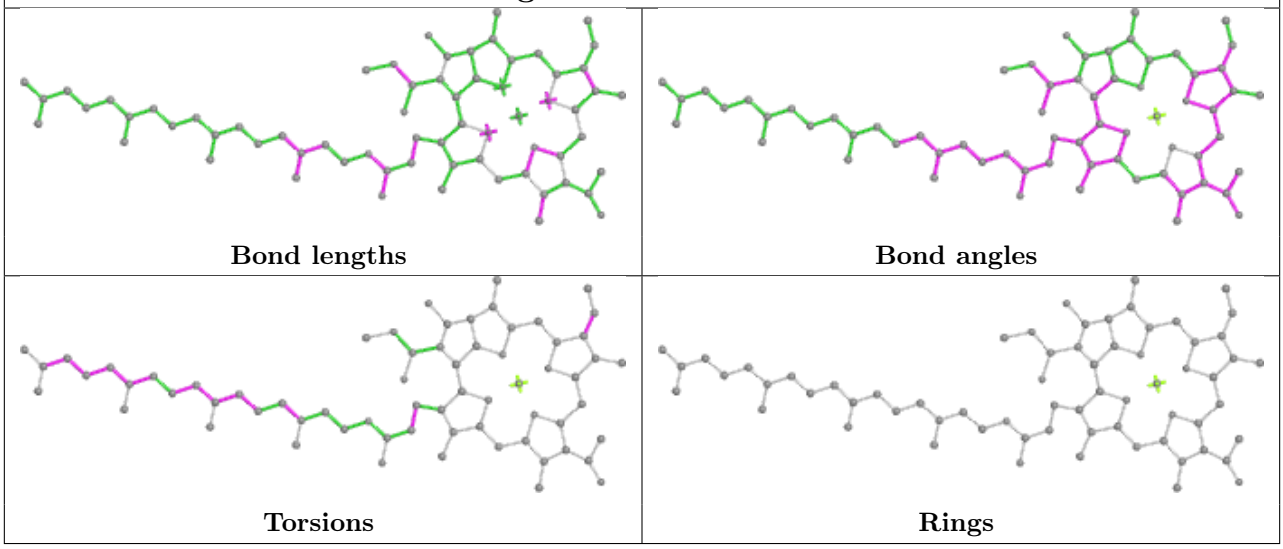


Rings

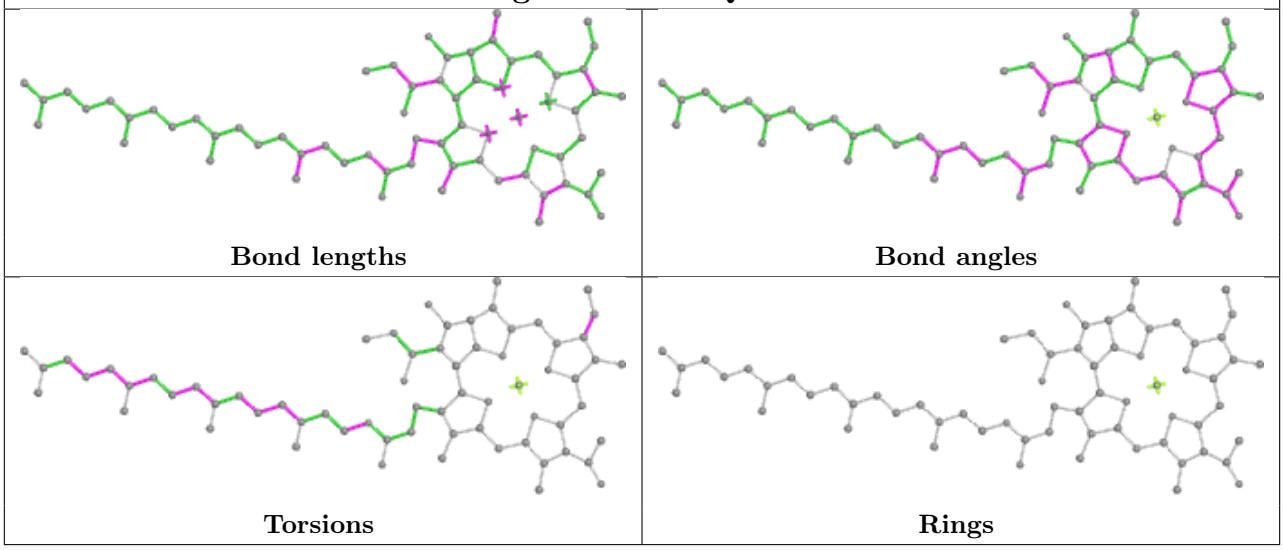
Ligand BCL A3 104



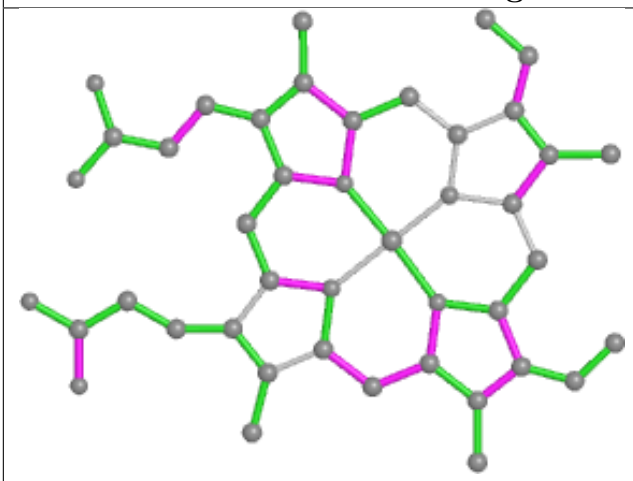
Ligand BCL B6 101



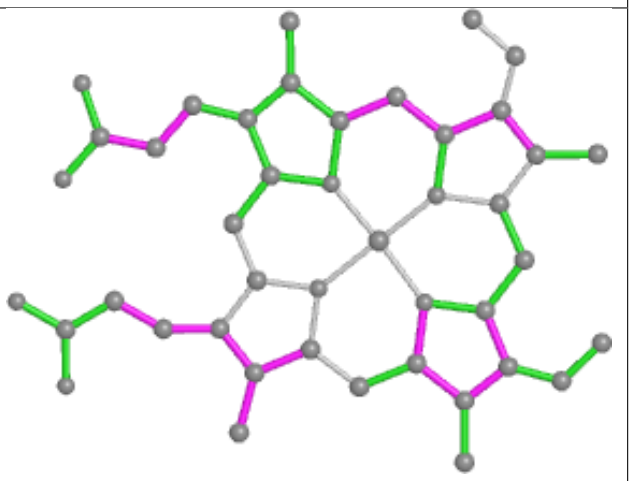
Ligand BCL BQ 103



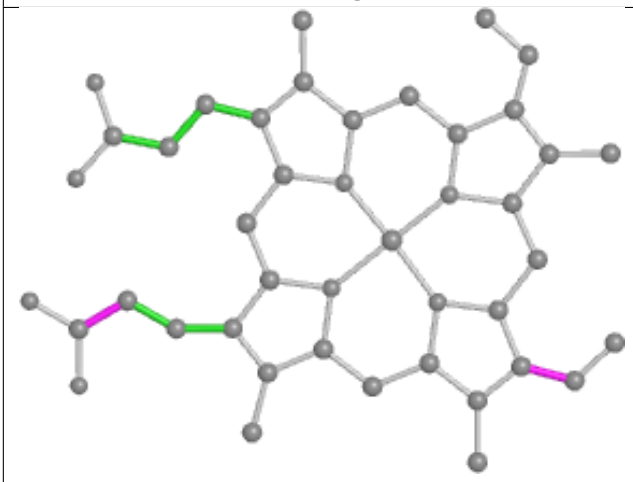
Ligand HEM BC 501



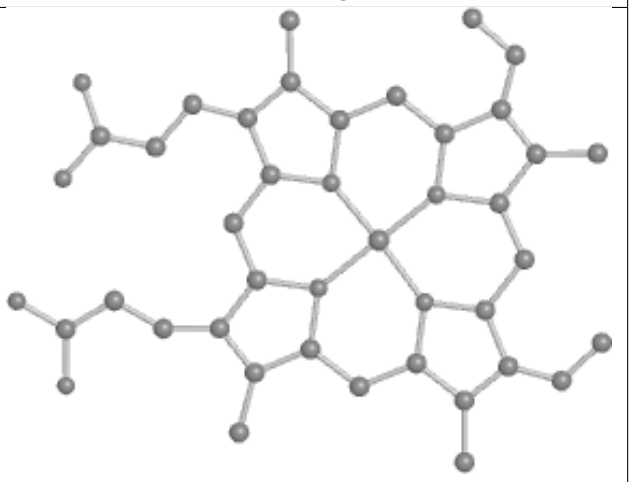
Bond lengths



Bond angles

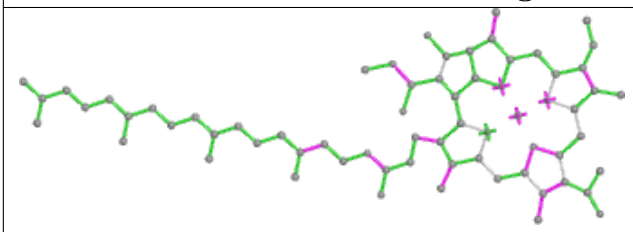


Torsions

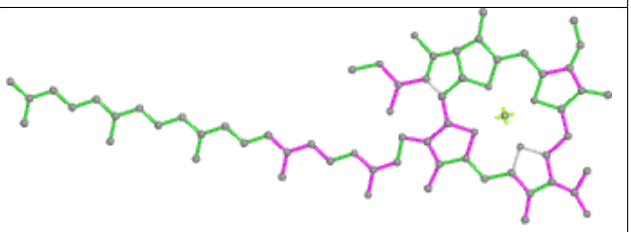


Rings

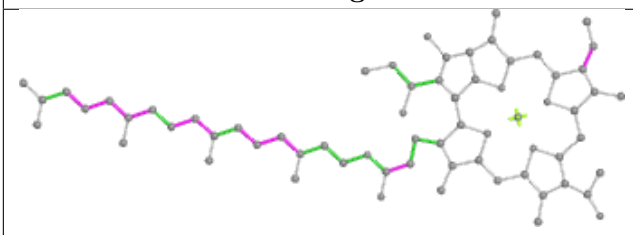
Ligand BCL B1 102



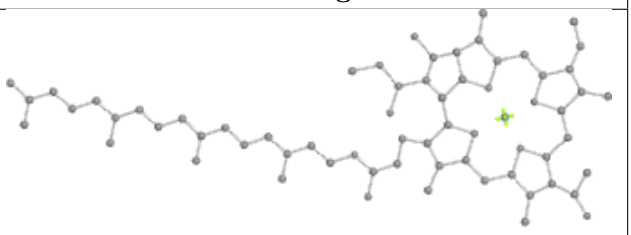
Bond lengths



Bond angles

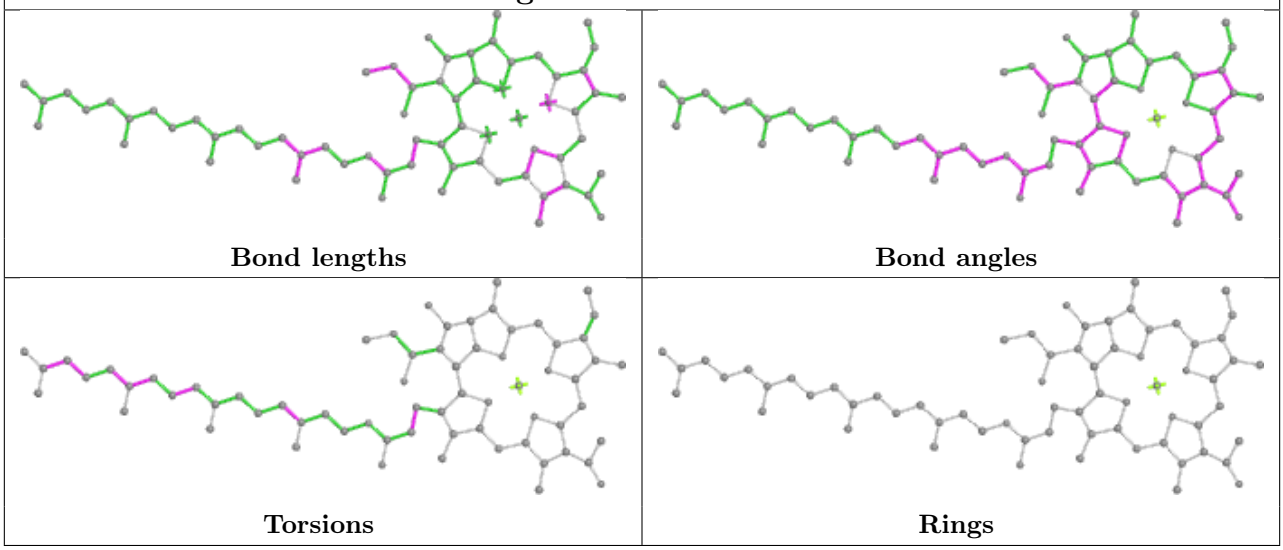


Torsions

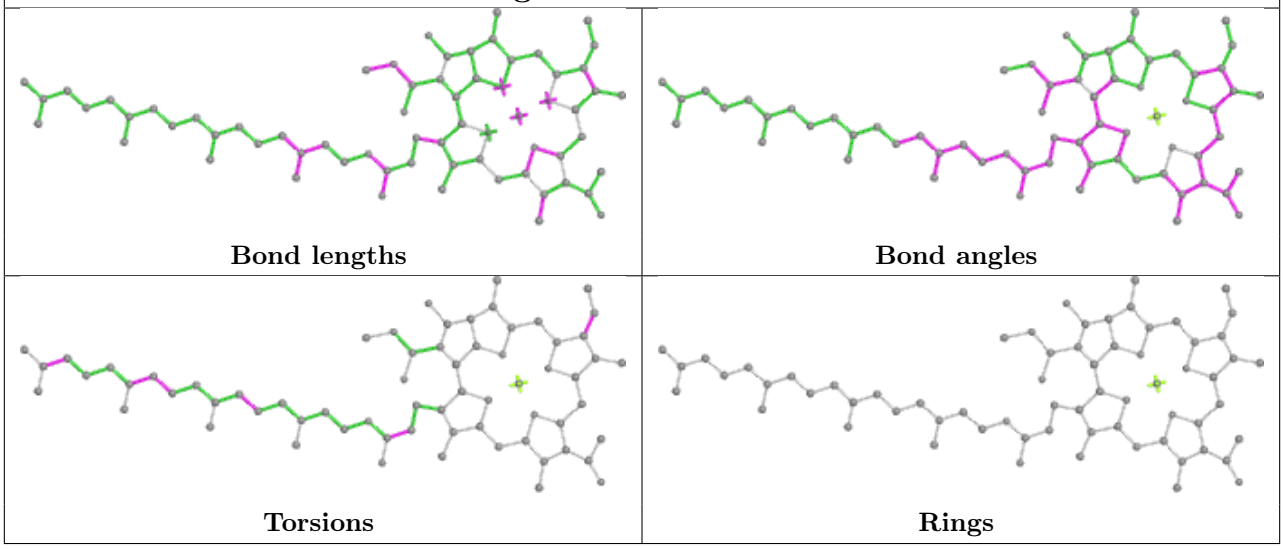


Rings

Ligand BCL AJ 101



Ligand BCL AE 101



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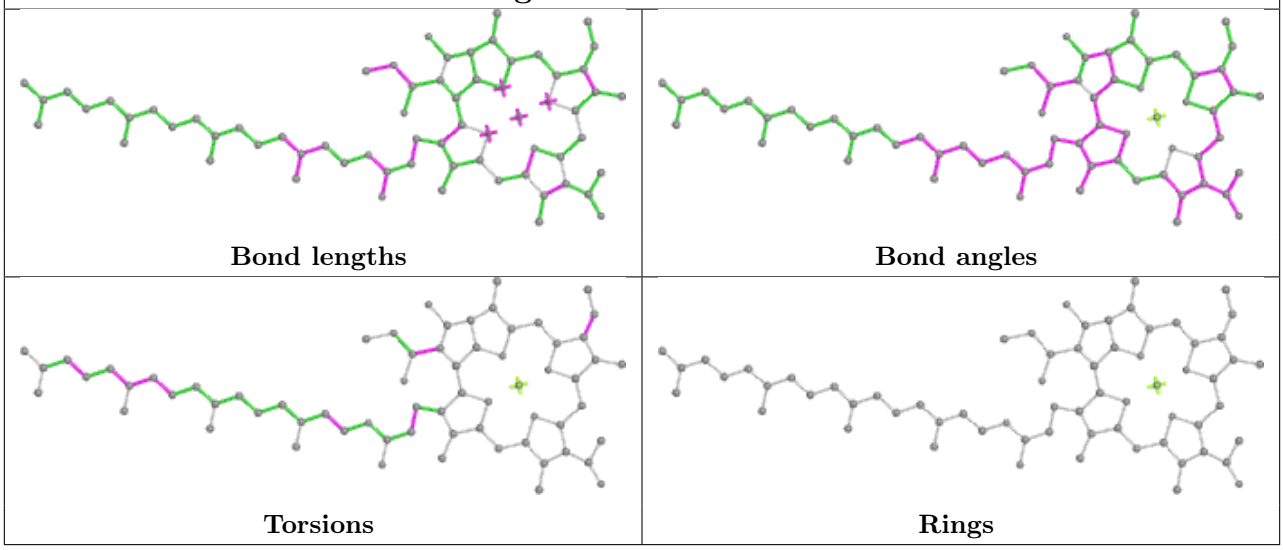

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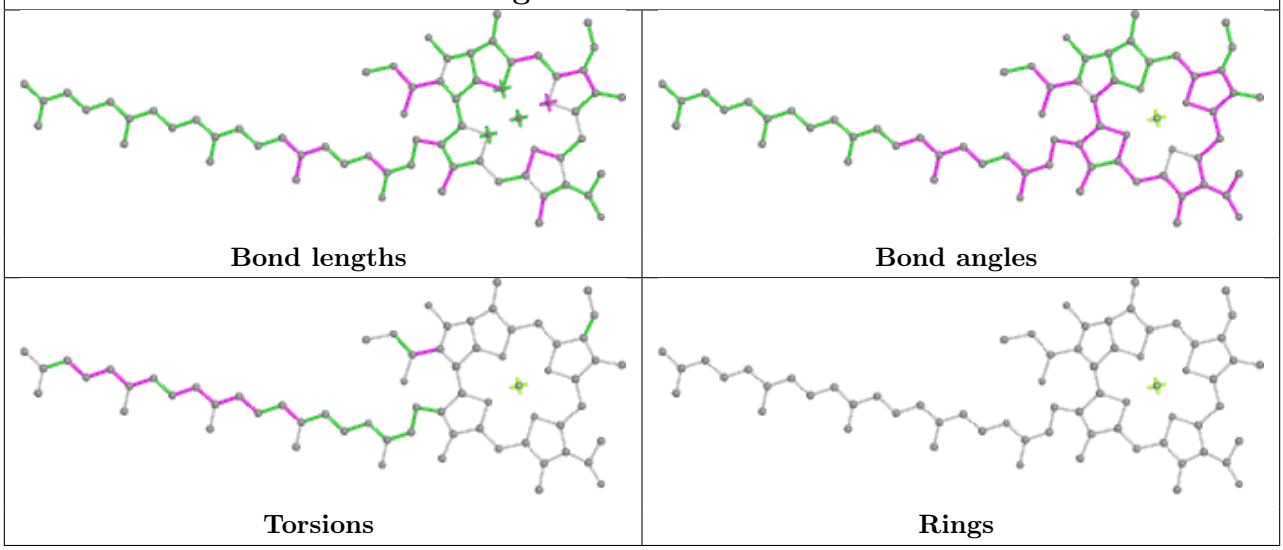
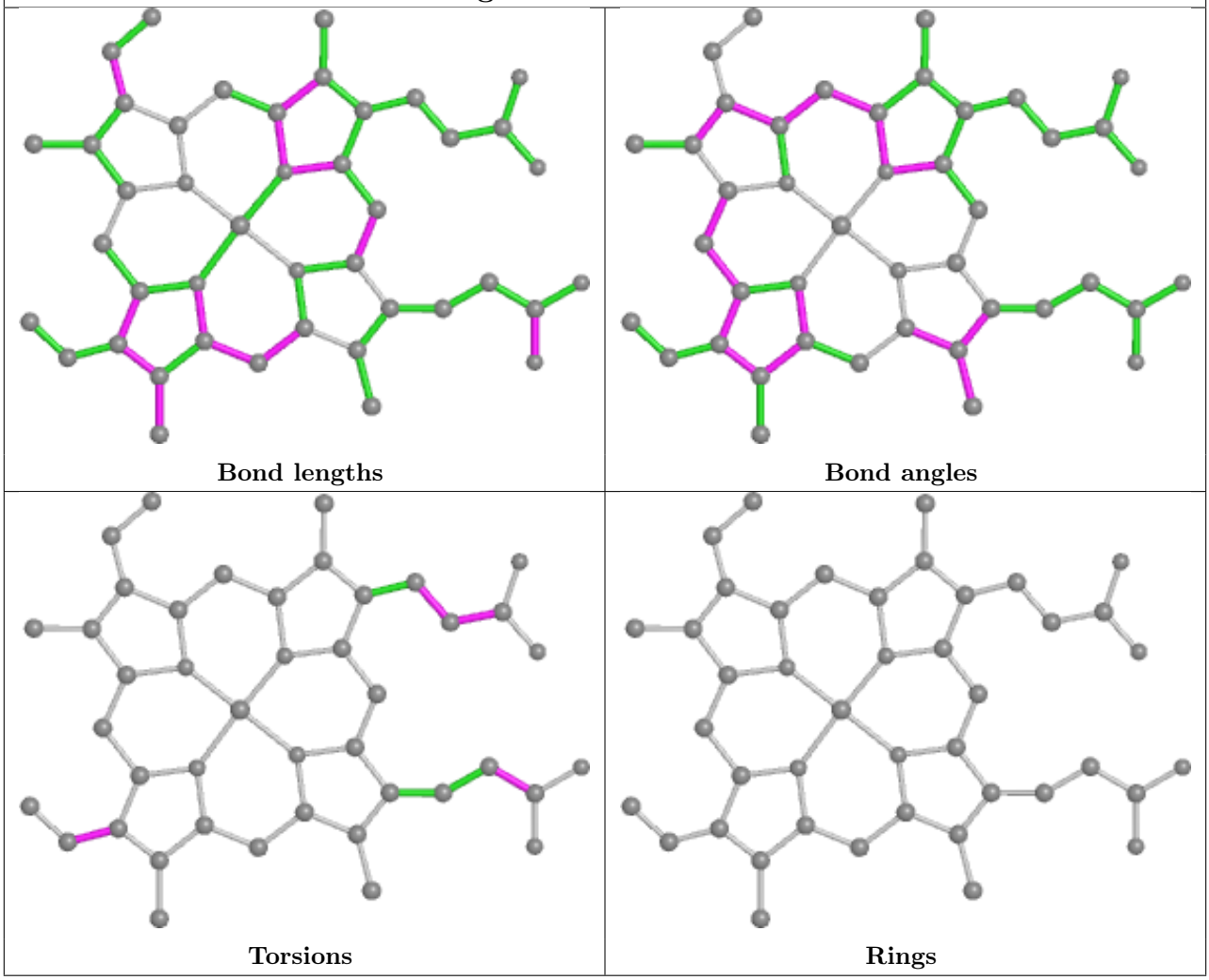


Ligand HEM AC 502



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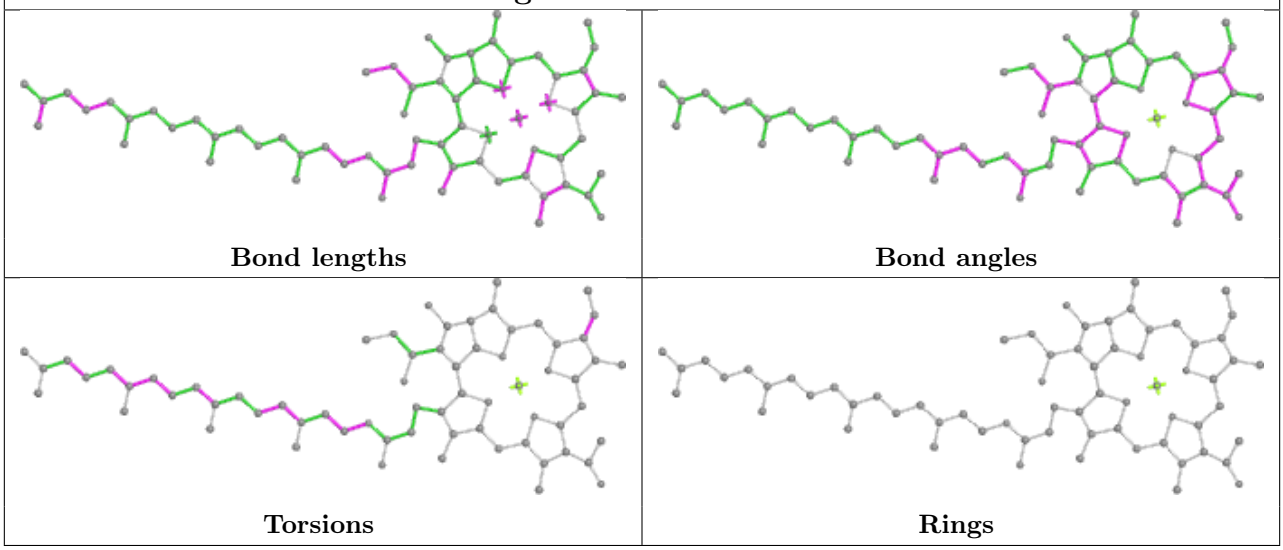
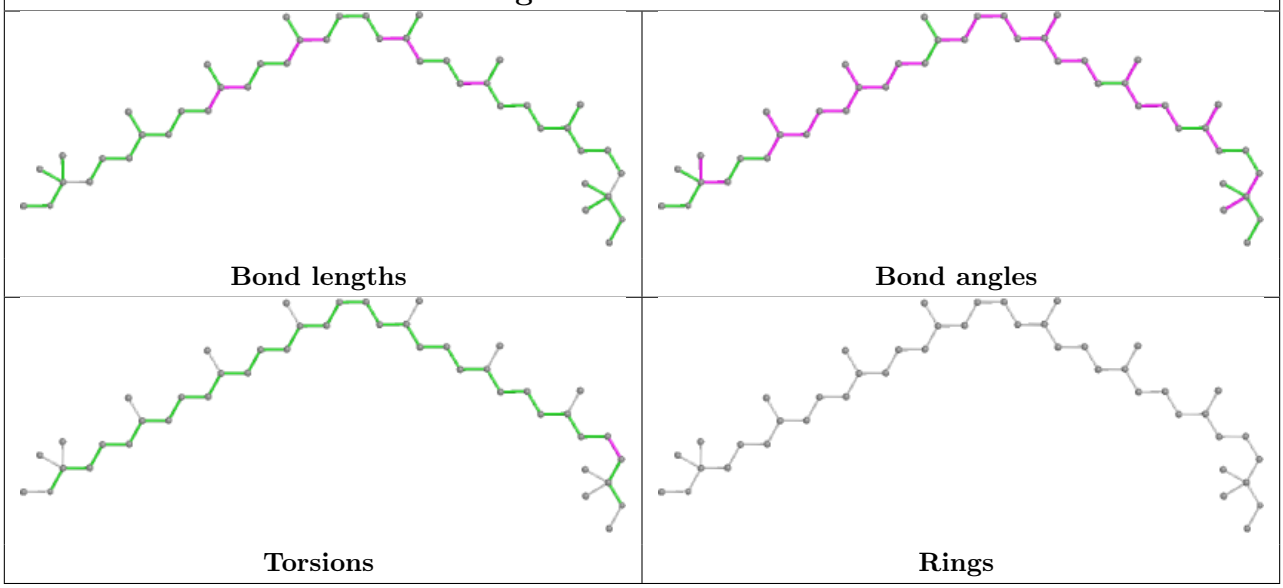
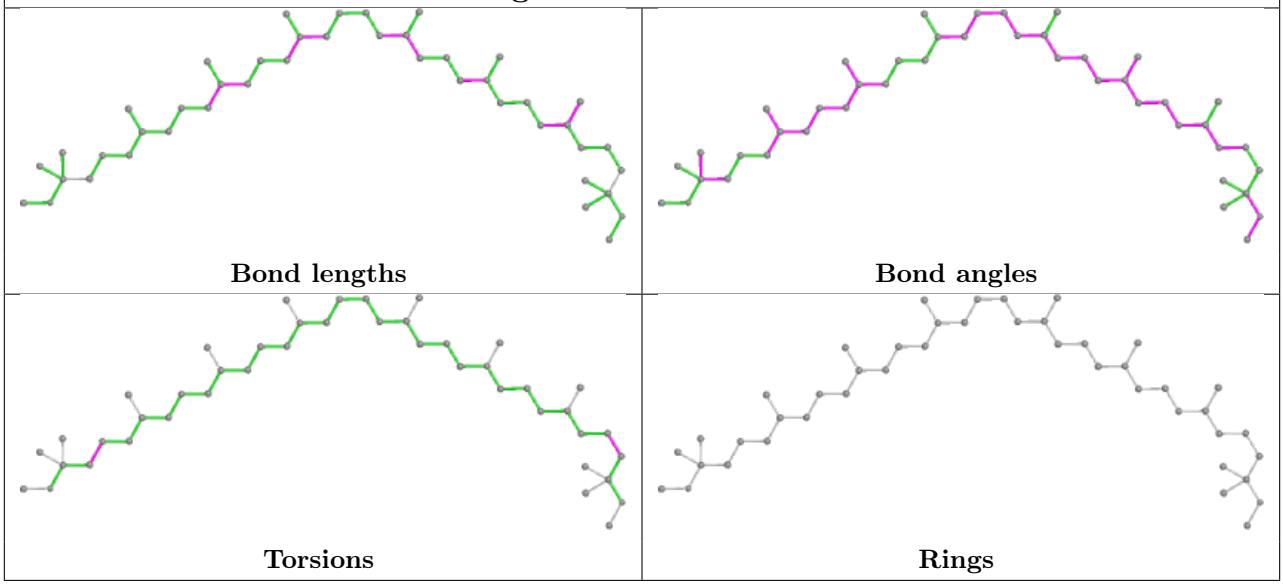


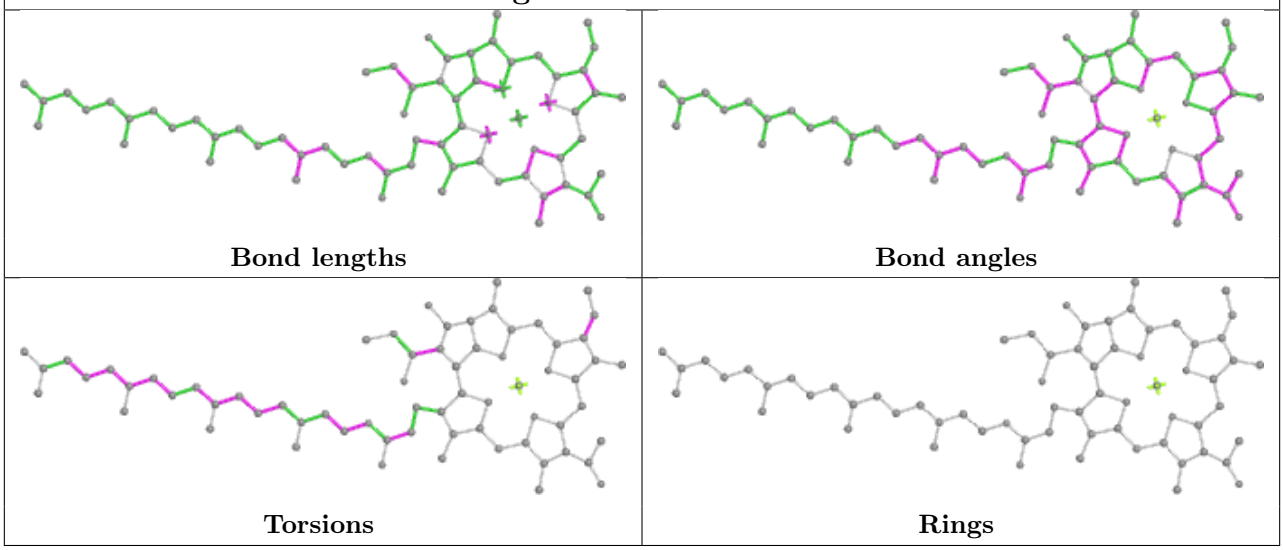
Ligand CRT AJ 102



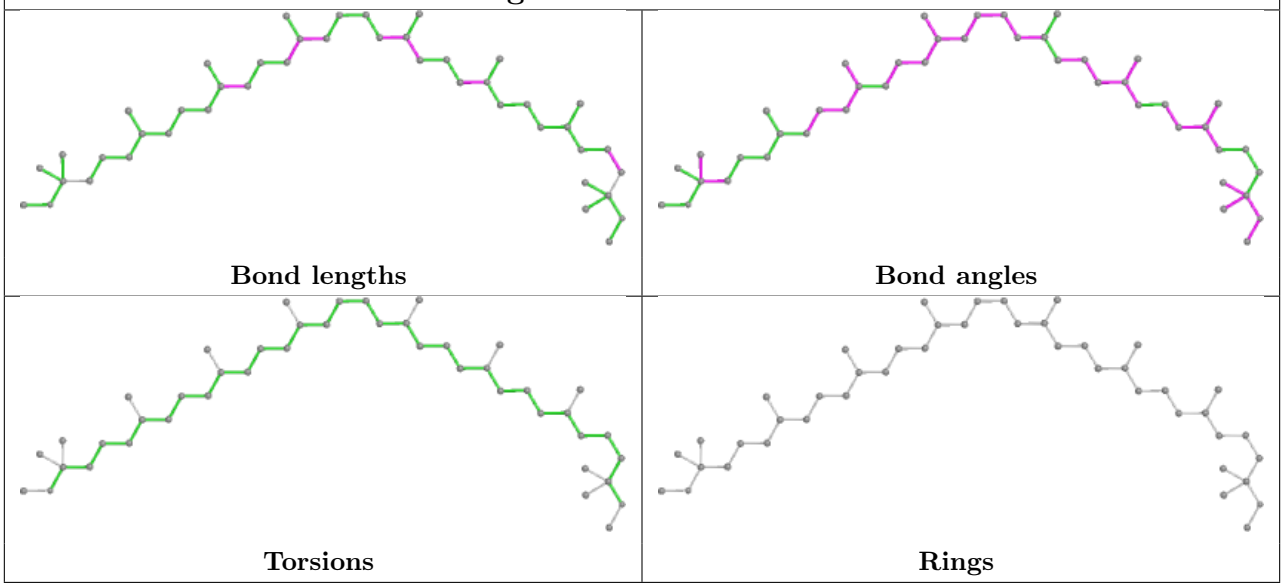
Ligand CRT BU 103



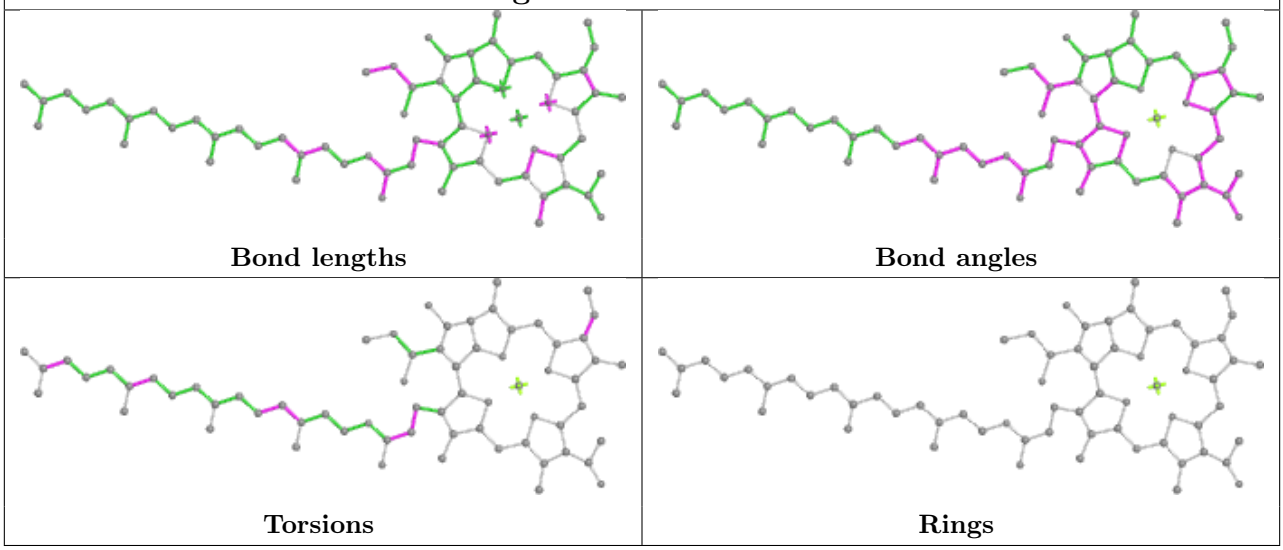
Ligand BCL BY 102



Ligand CRT BW 103



Ligand BCL AB 101



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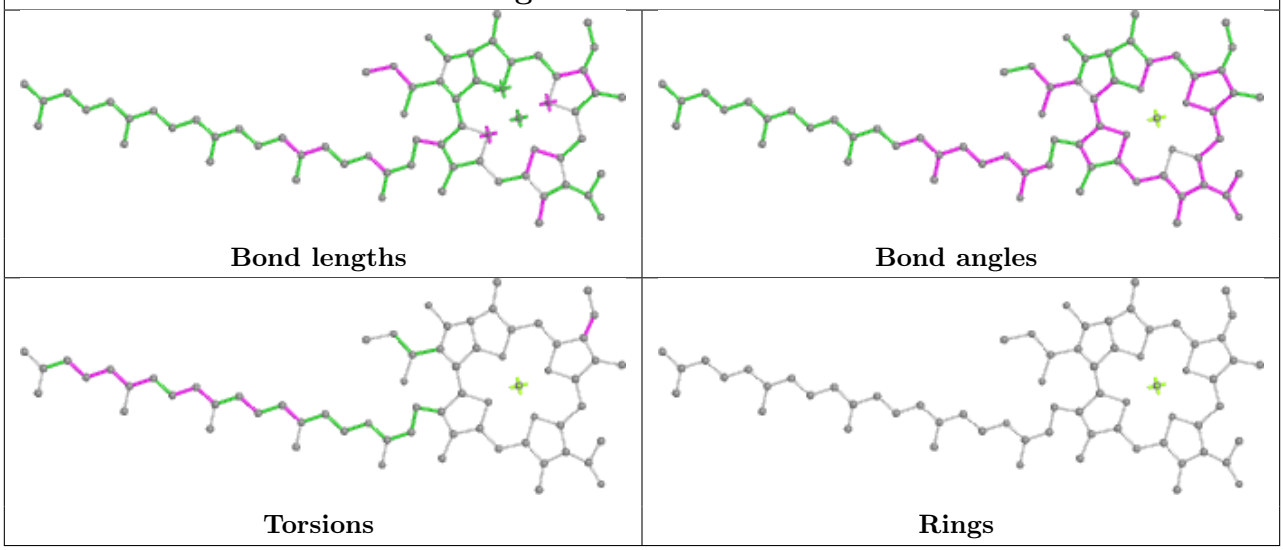

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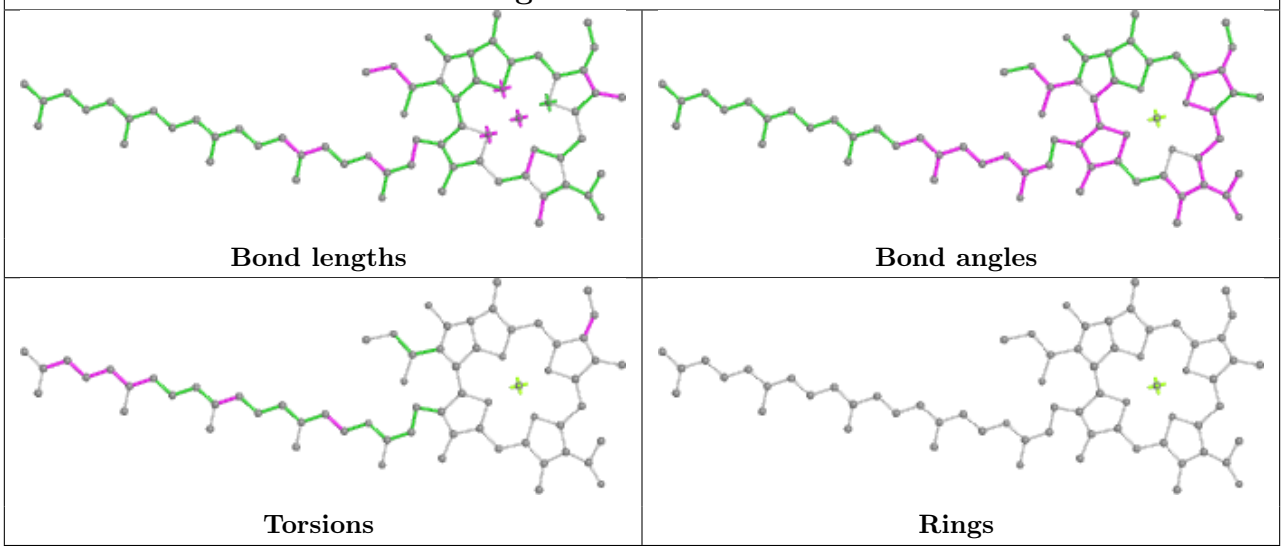
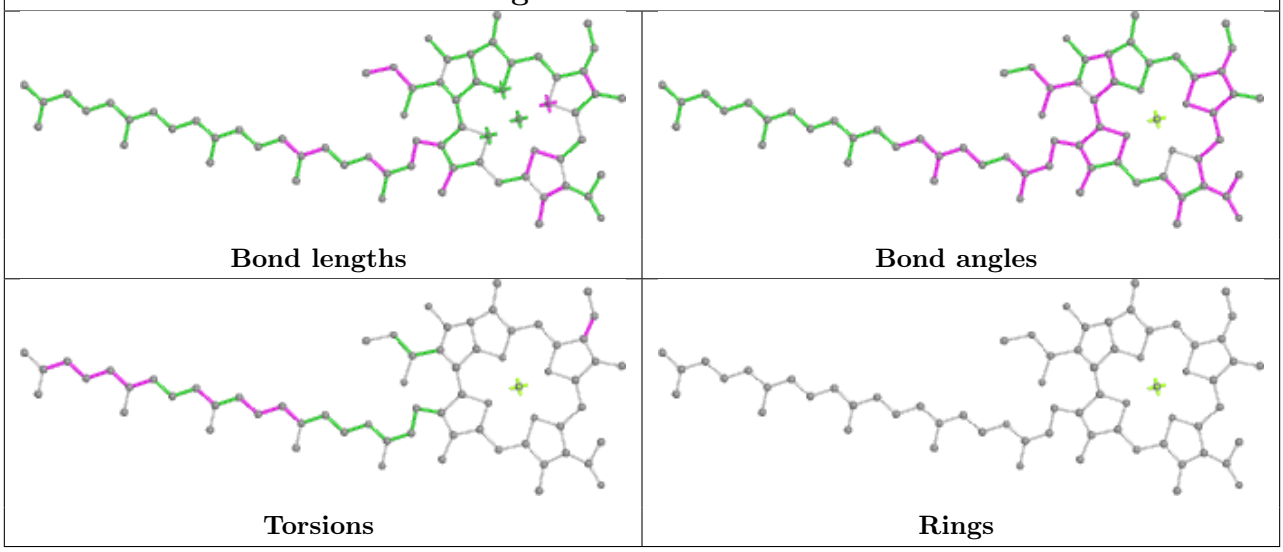


Ligand BCL AK 102



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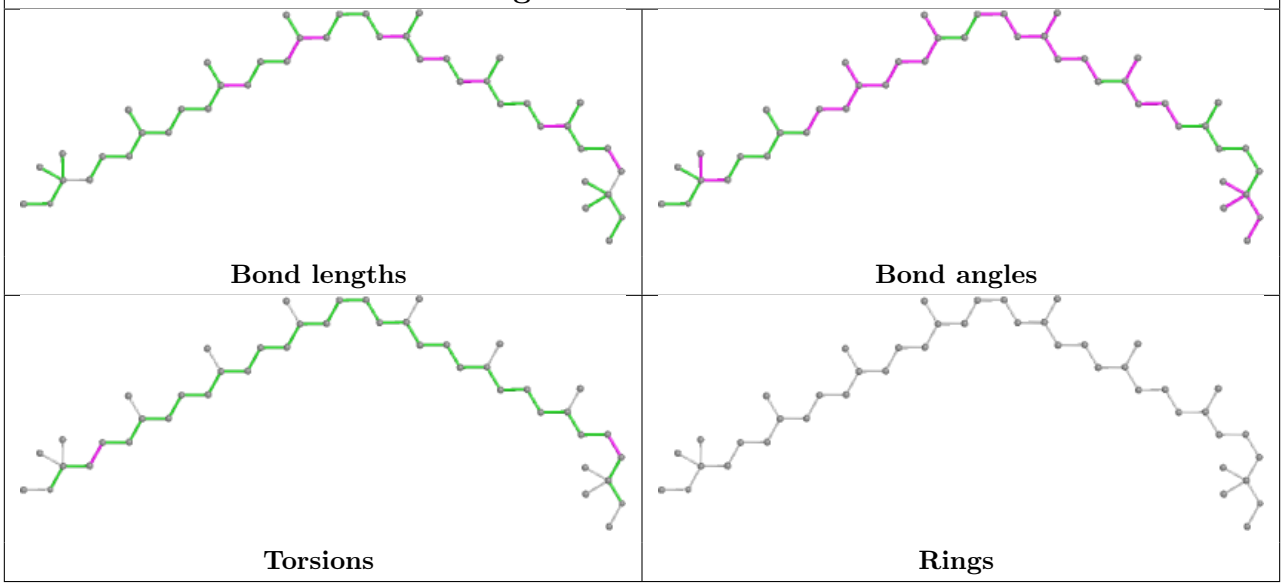
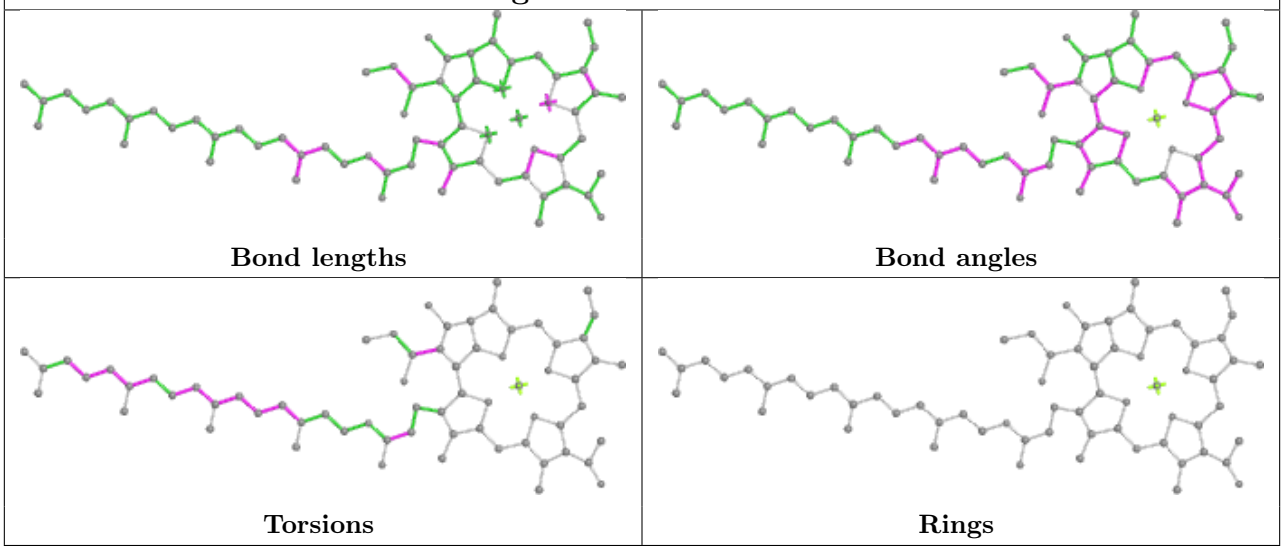


Ligand BCL AD 102



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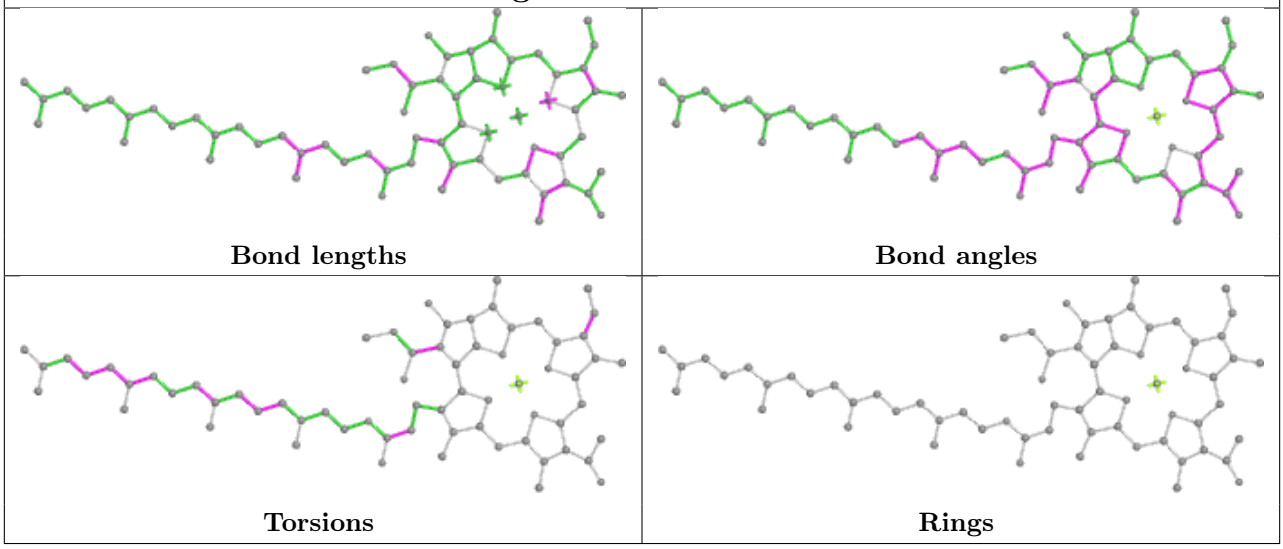
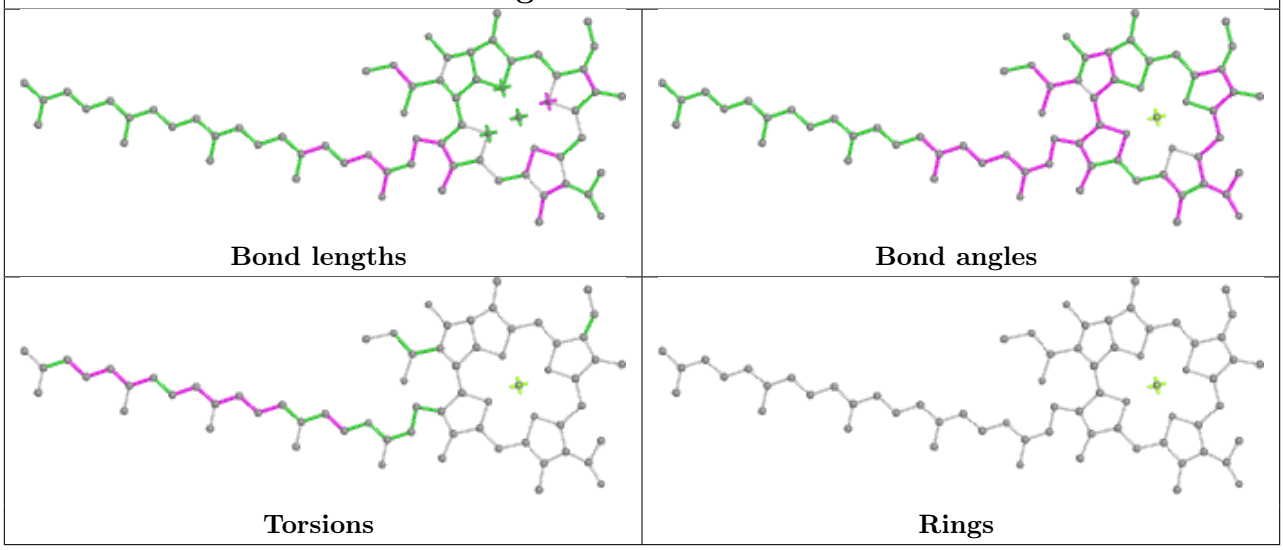


Ligand BCL A7 103



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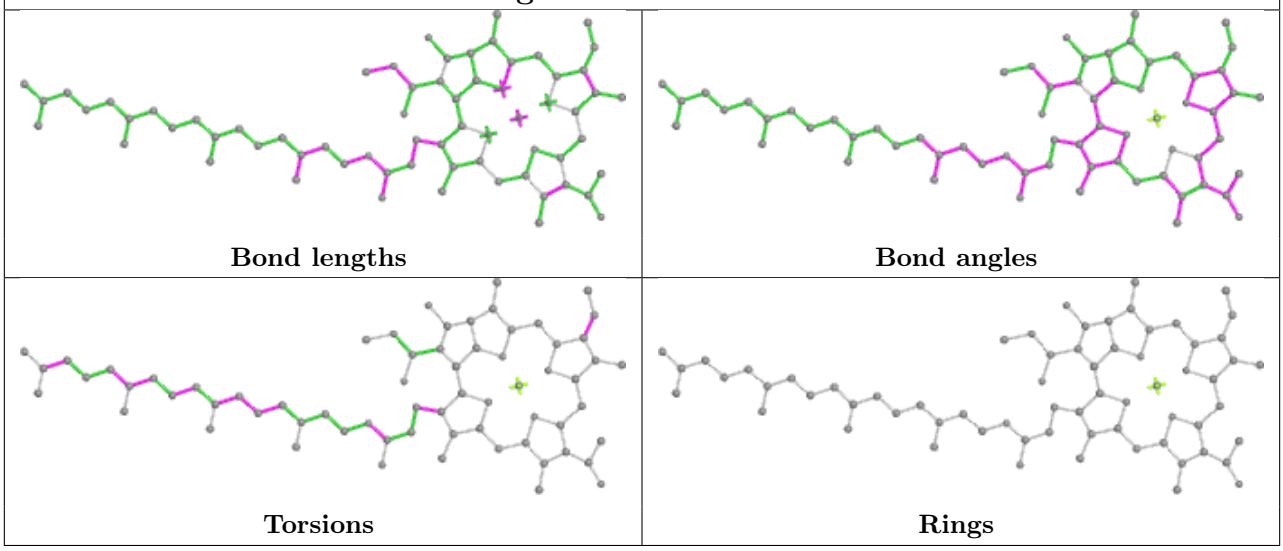
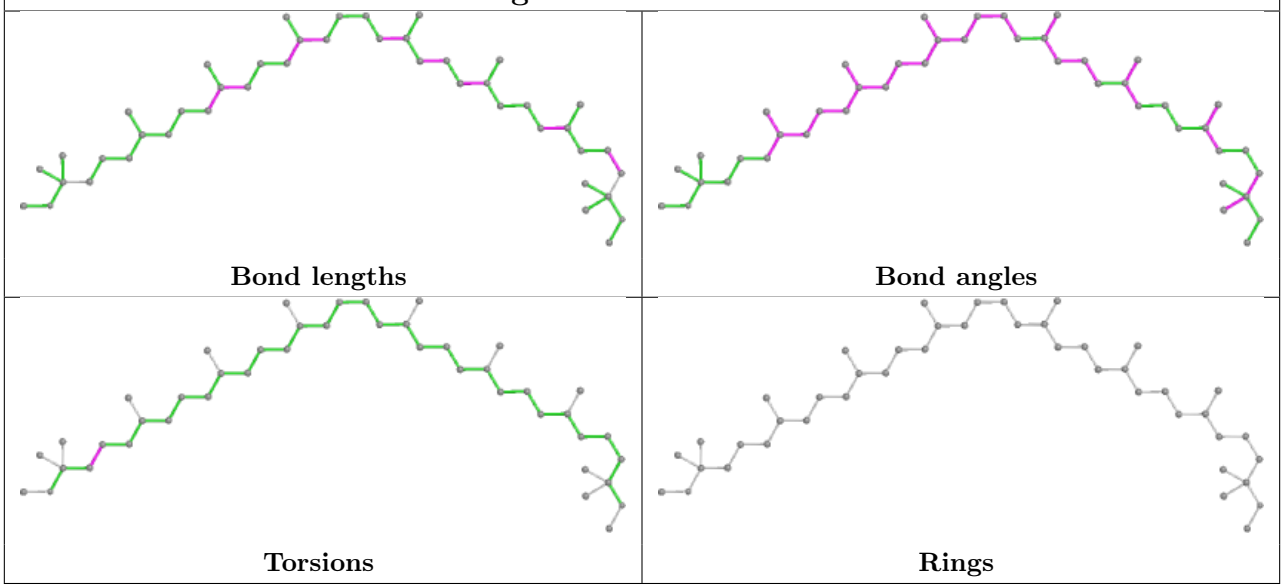


Ligand CRT BN 102



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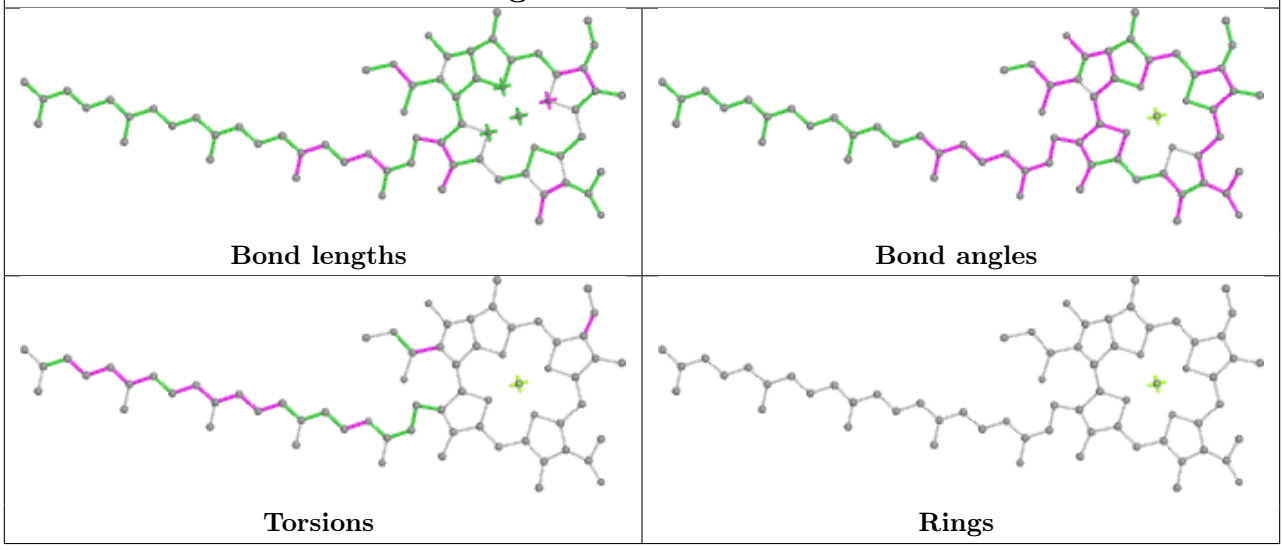
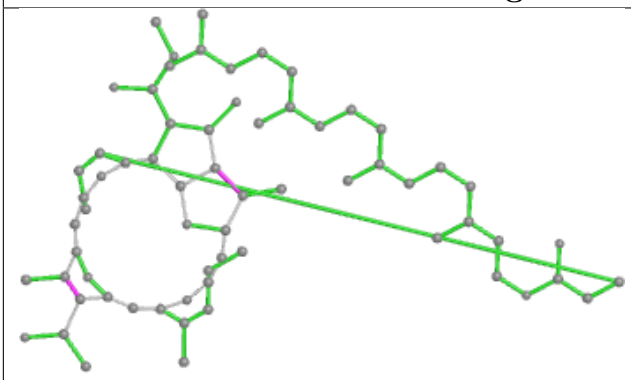
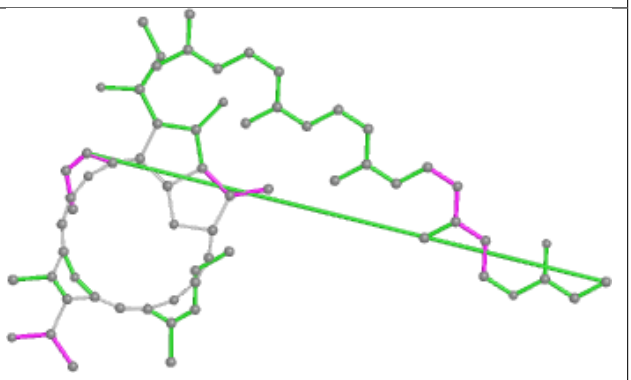


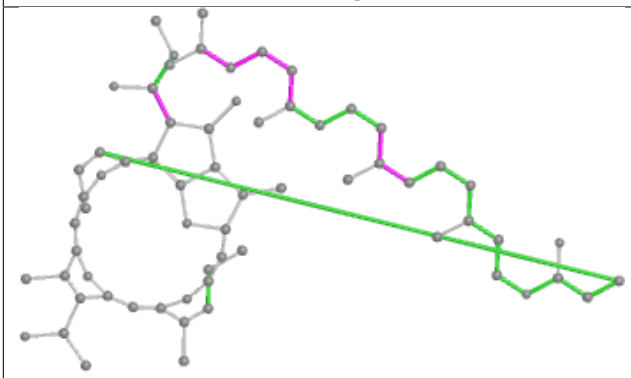
Ligand BPH BM 403



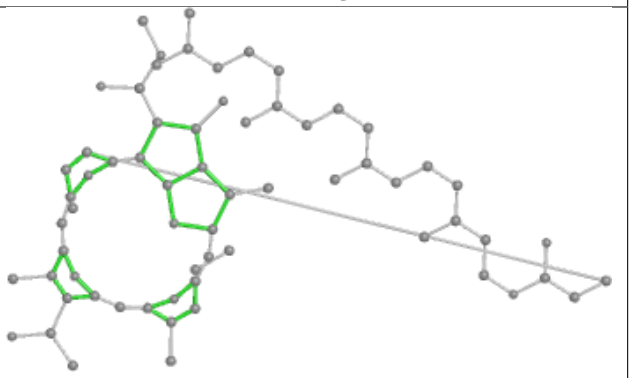
Bond lengths



Bond angles

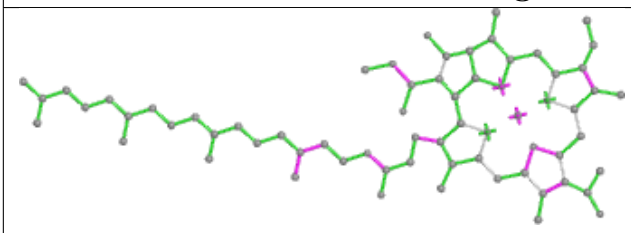


Torsions

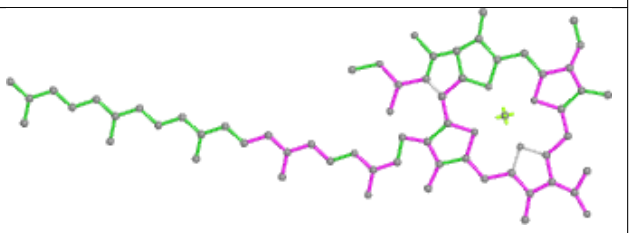


Rings

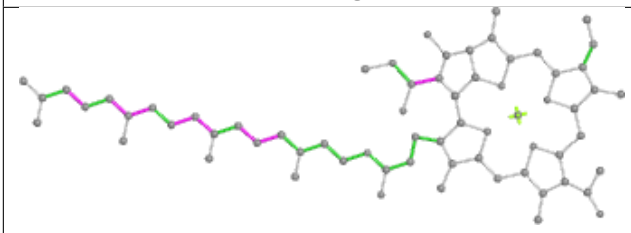
Ligand BCL AL 303



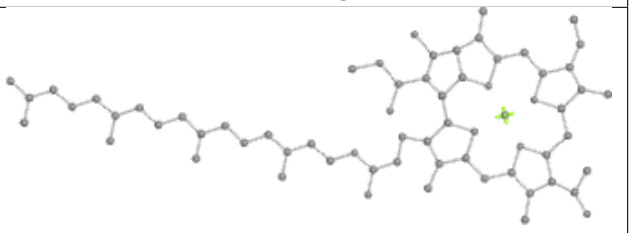
Bond lengths



Bond angles

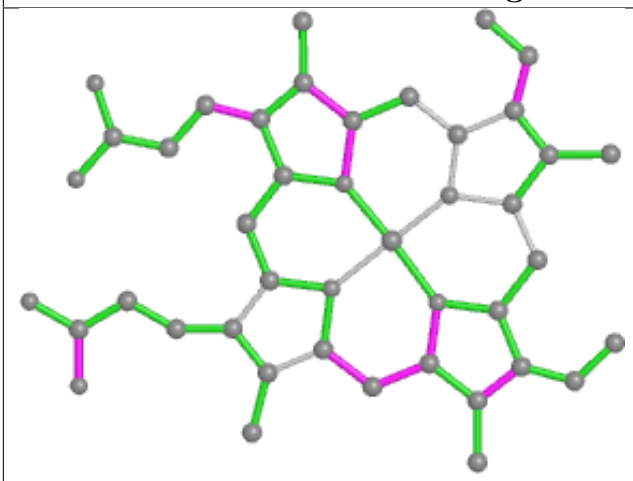


Torsions

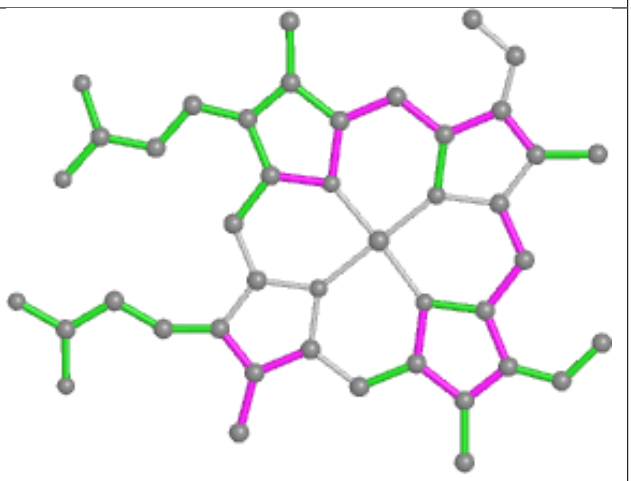


Rings

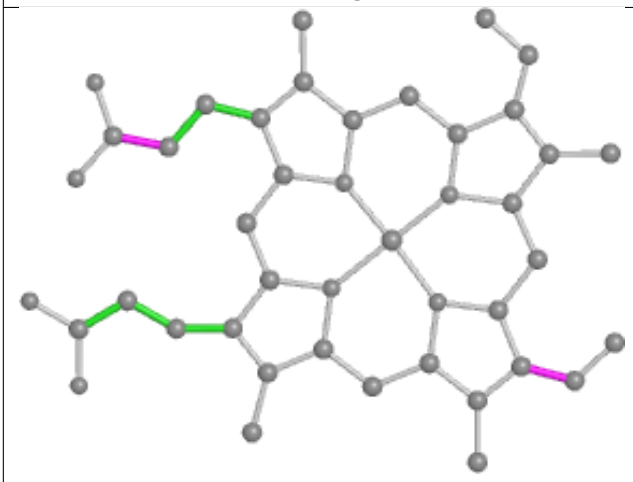
Ligand HEM AC 504



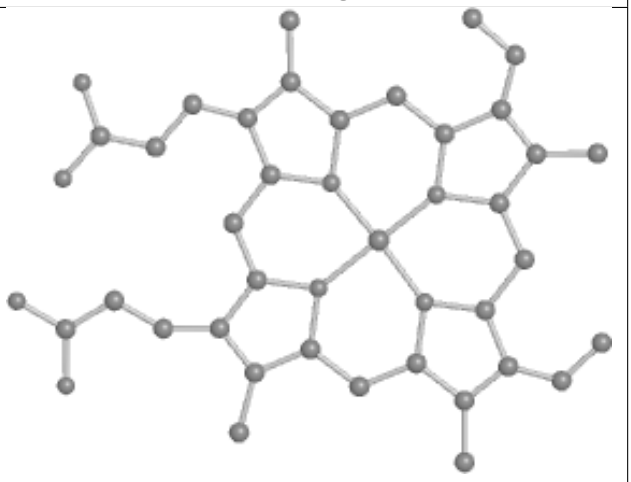
Bond lengths



Bond angles

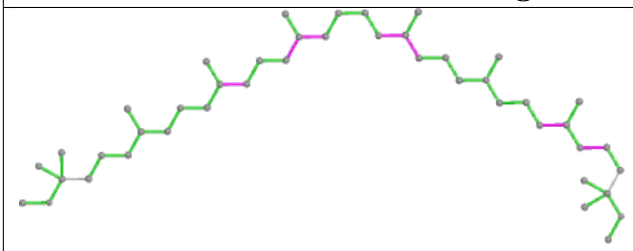


Torsions

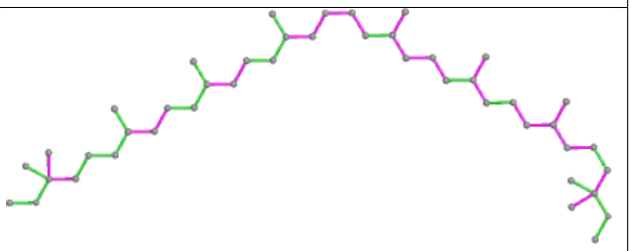


Rings

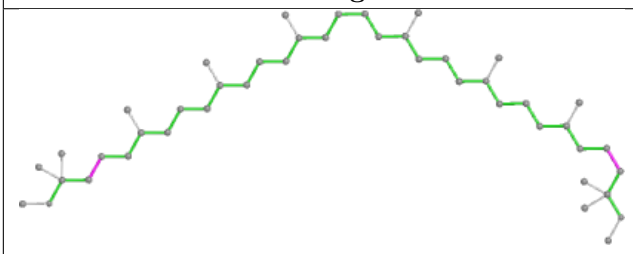
Ligand CRT A0 101



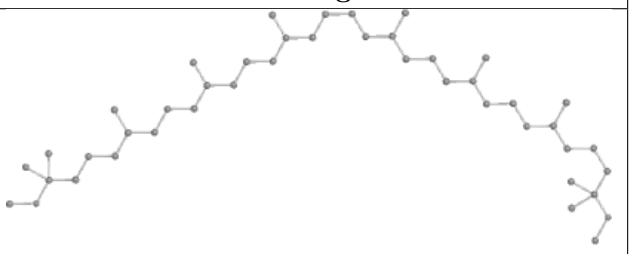
Bond lengths



Bond angles

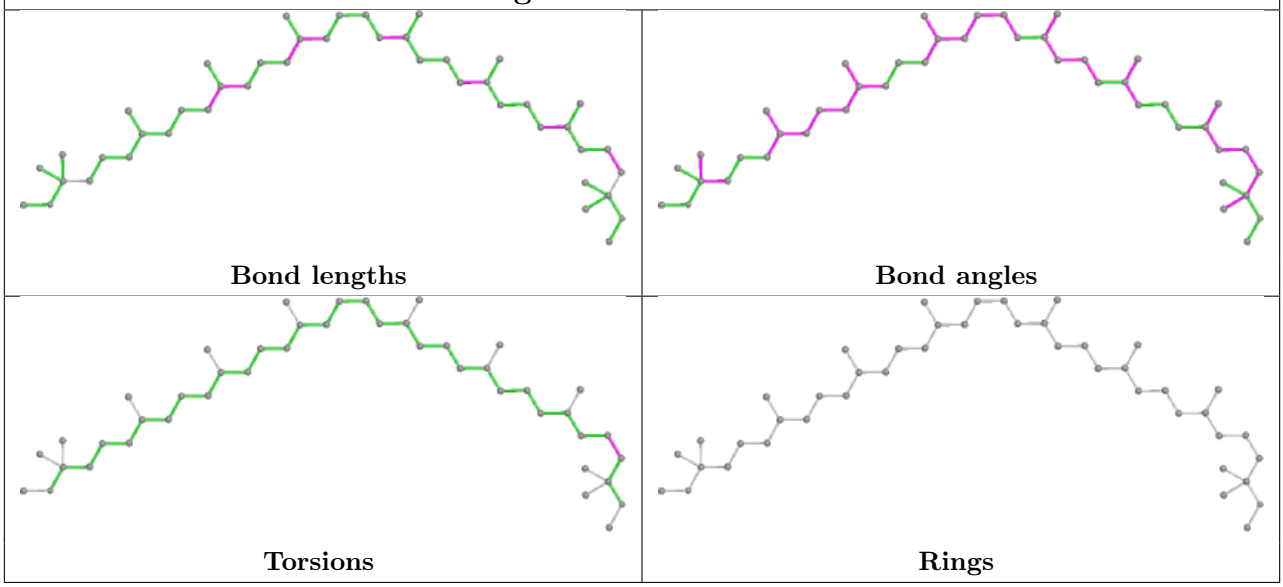


Torsions

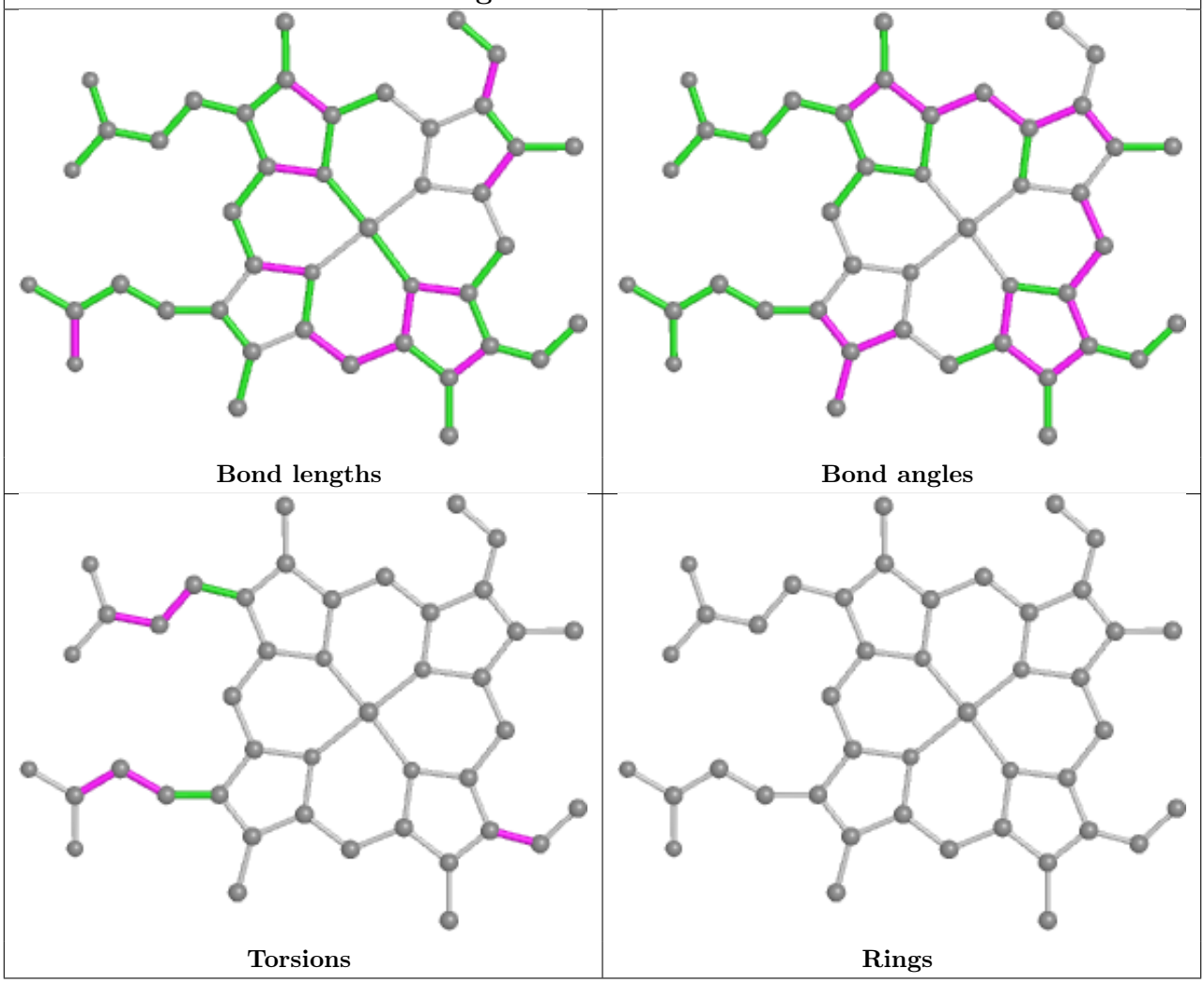


Rings

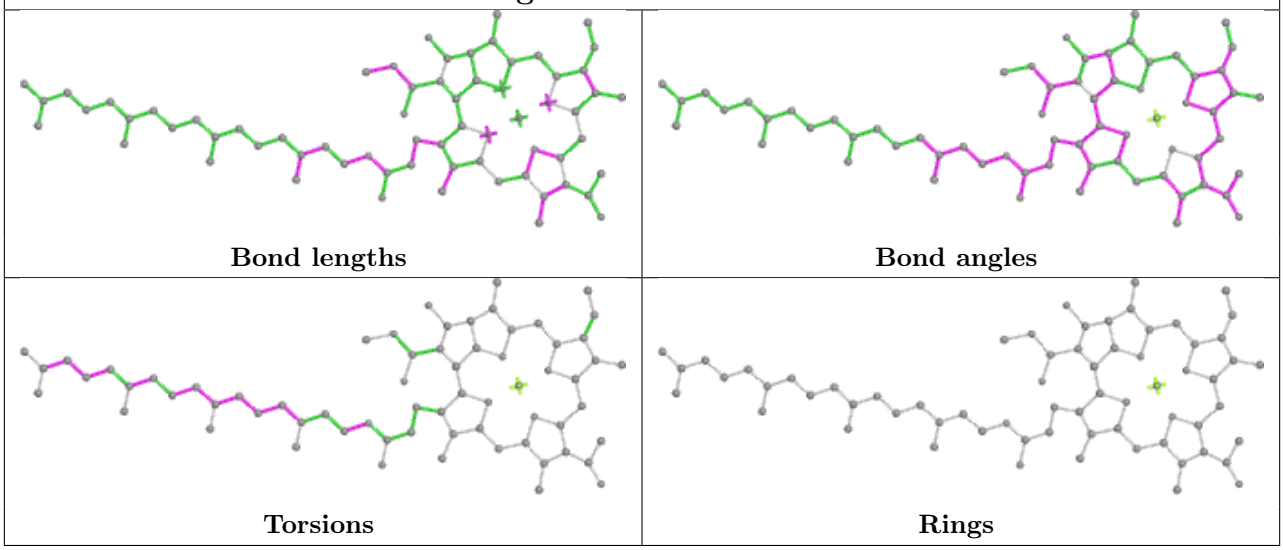
Ligand CRT BF 103



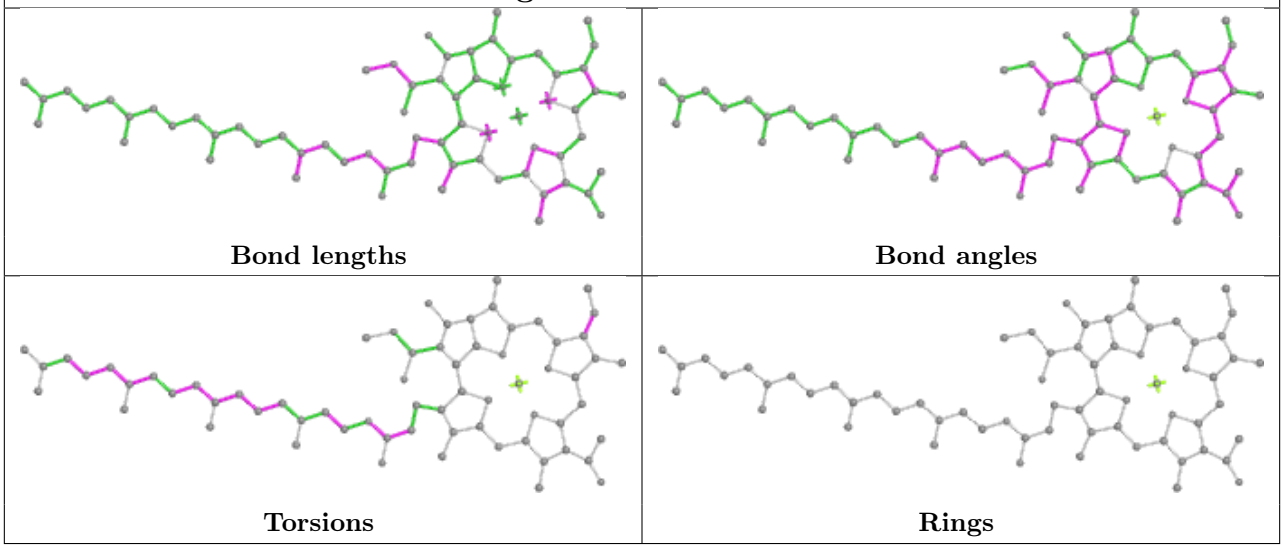
Ligand HEM BC 503



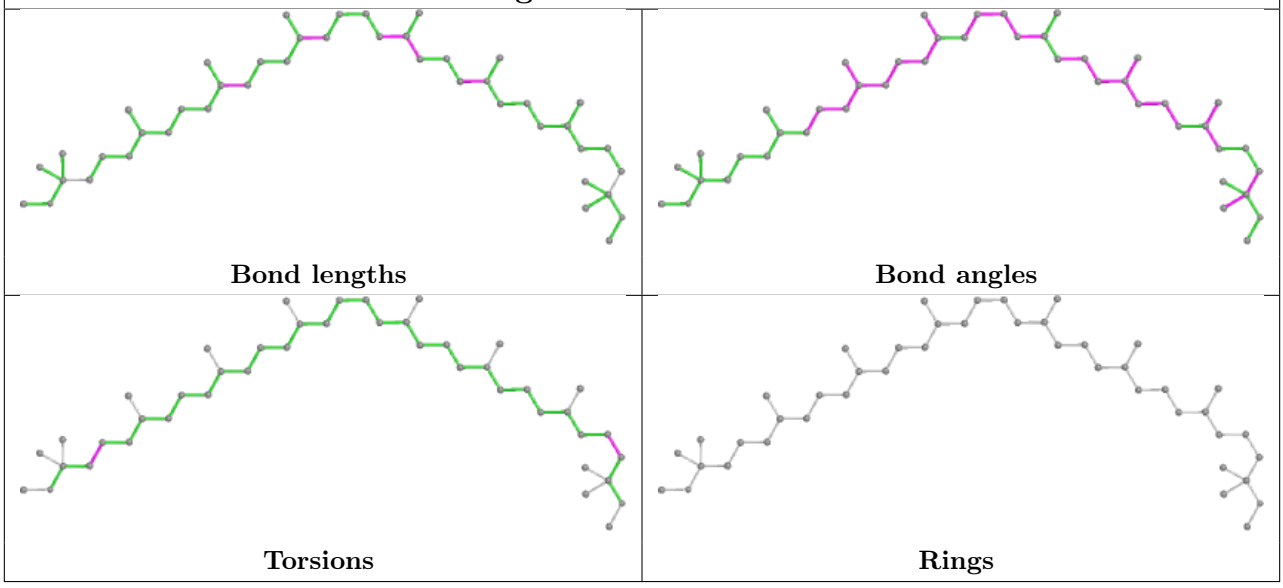
Ligand BCL A5 102



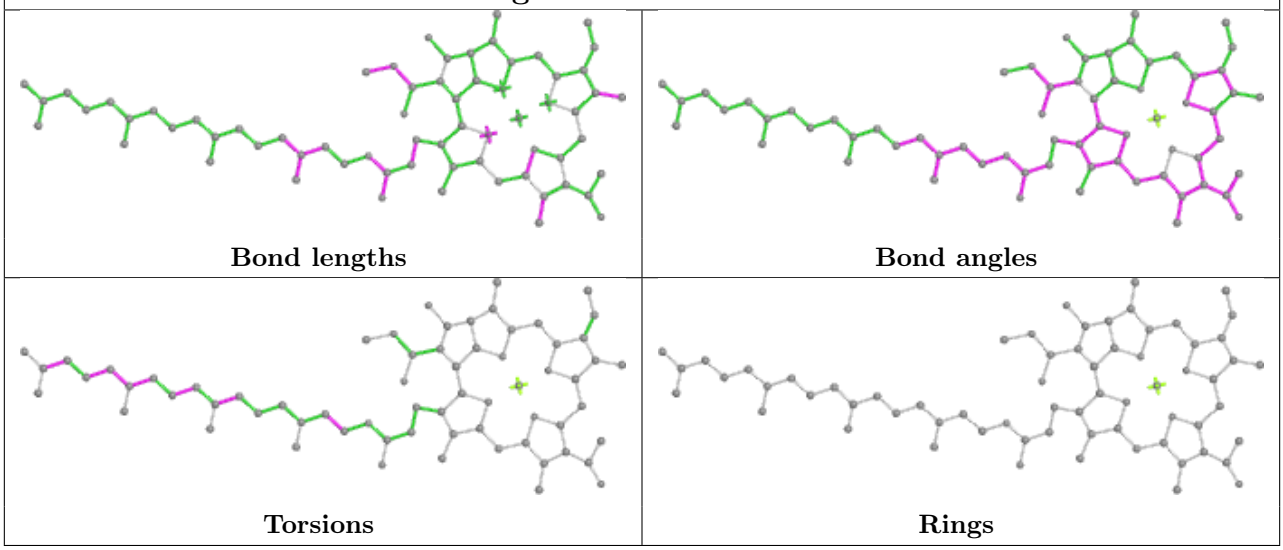
Ligand BCL A9 102



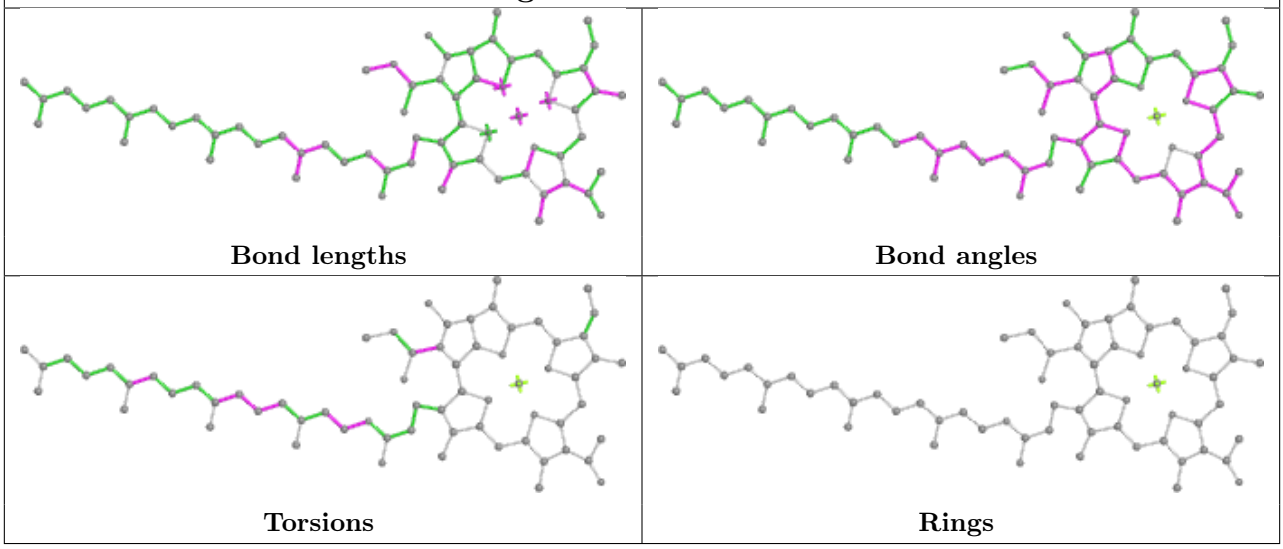
Ligand CRT BS 103



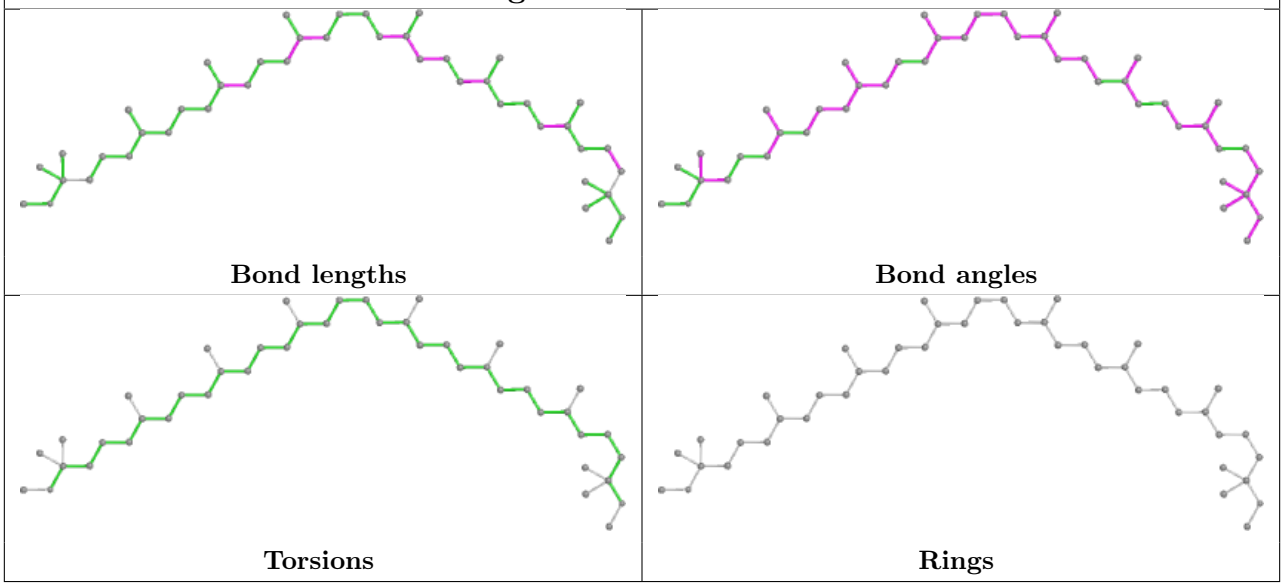
Ligand BCL BG 101



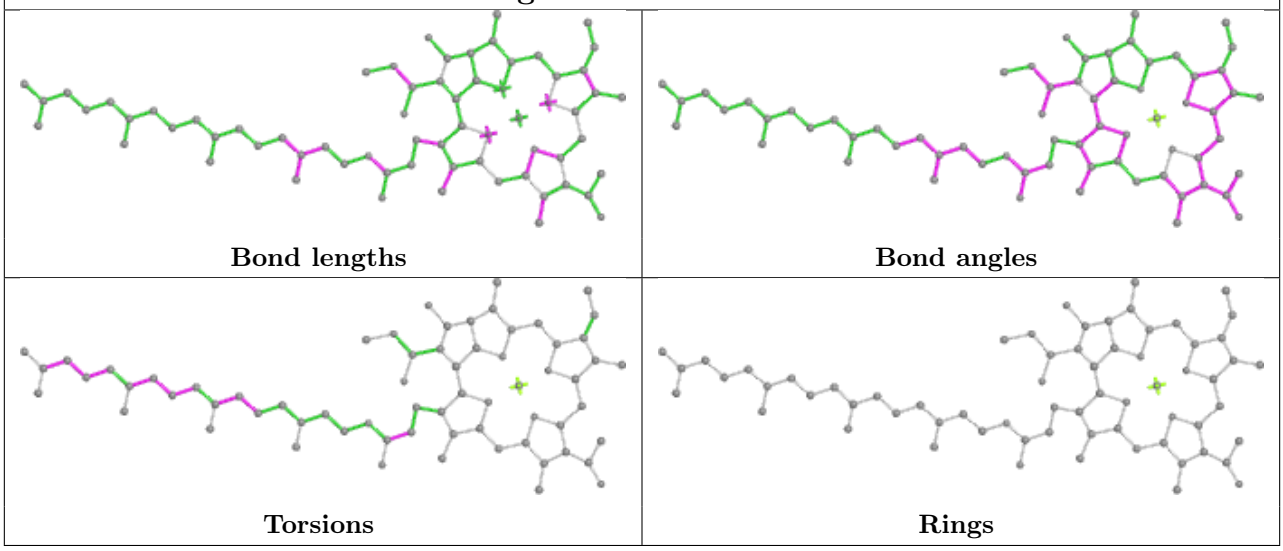
Ligand BCL BJ 101



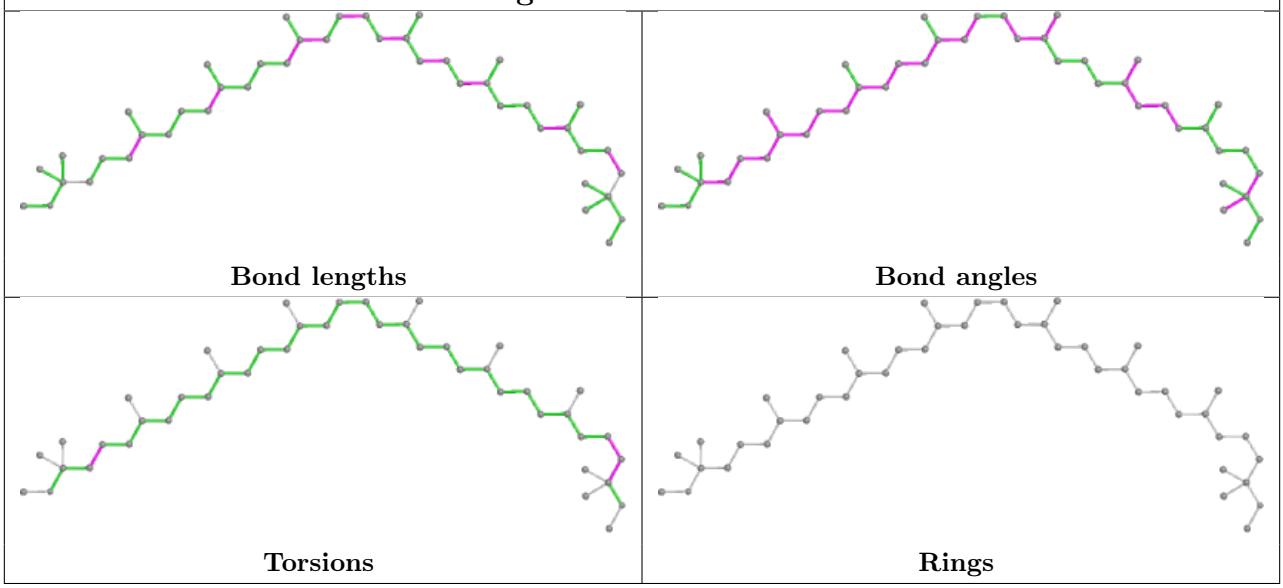
Ligand CRT AW 102



Ligand BCL B7 103



Ligand CRT B0 101



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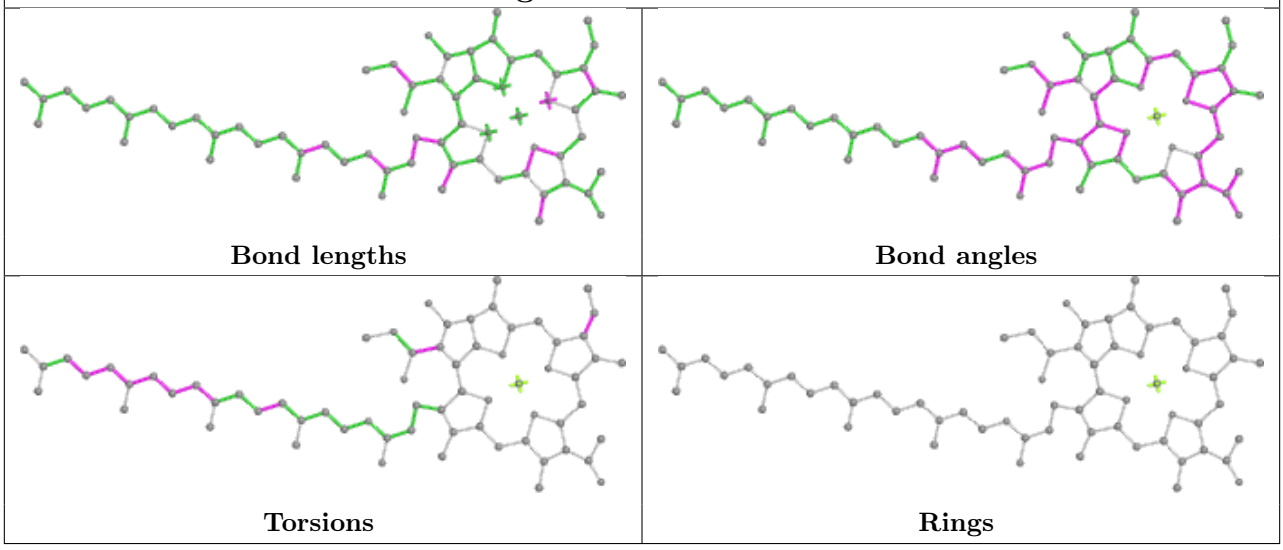

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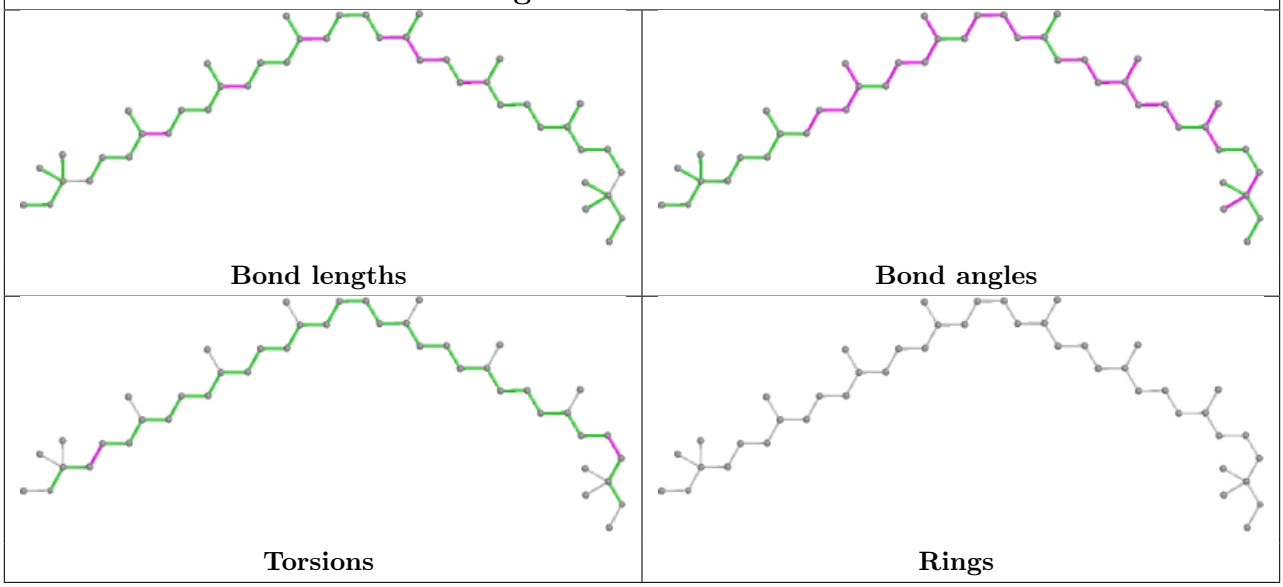
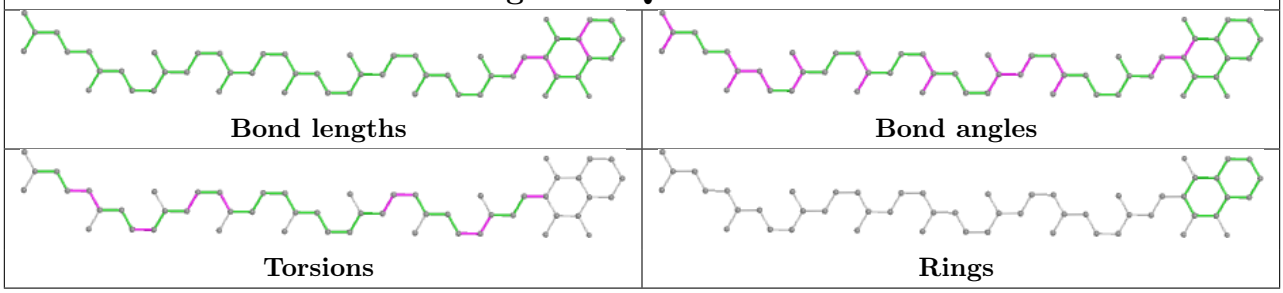
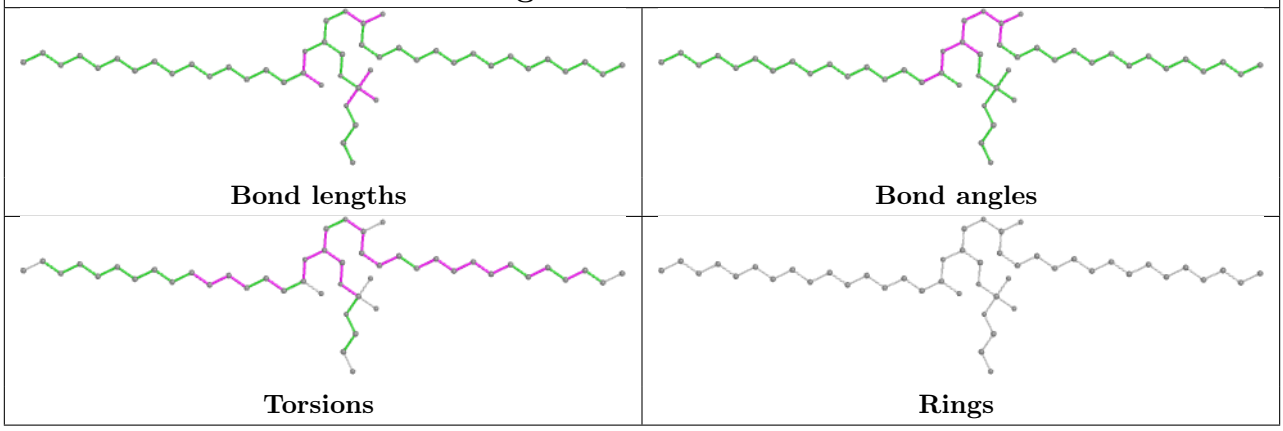


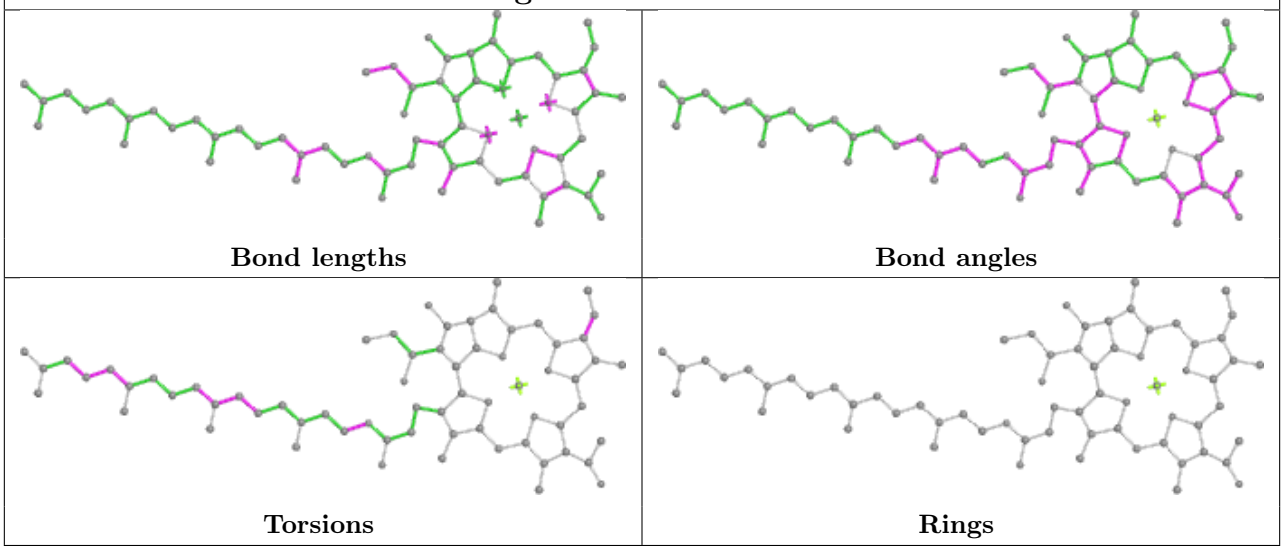
Ligand MQ8 BM 405



Ligand PEF AS 101



Ligand BCL AL 301



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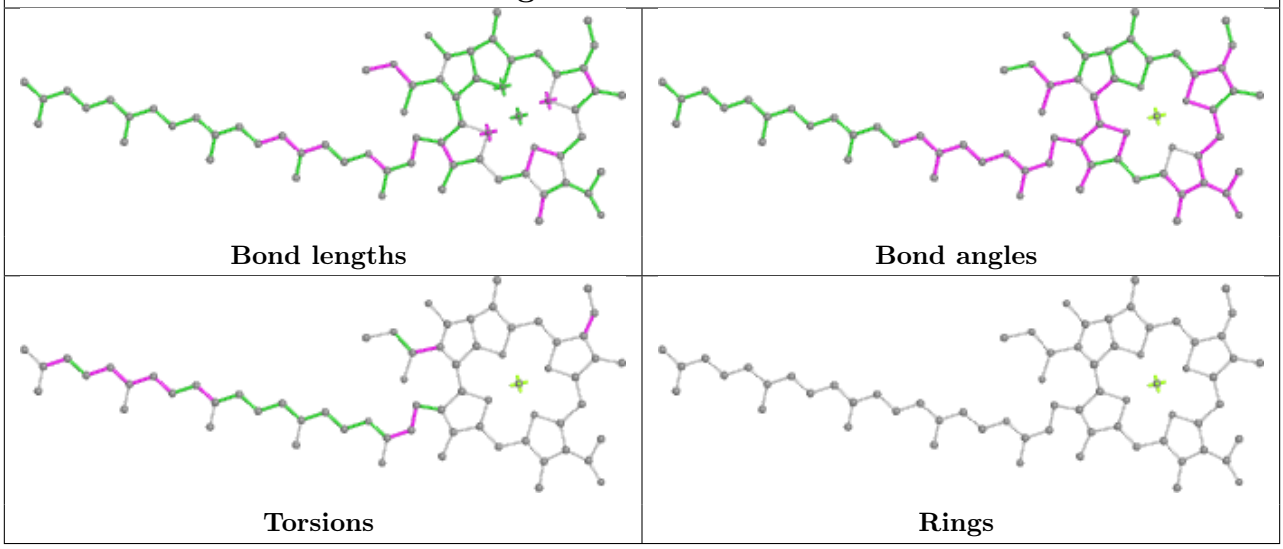

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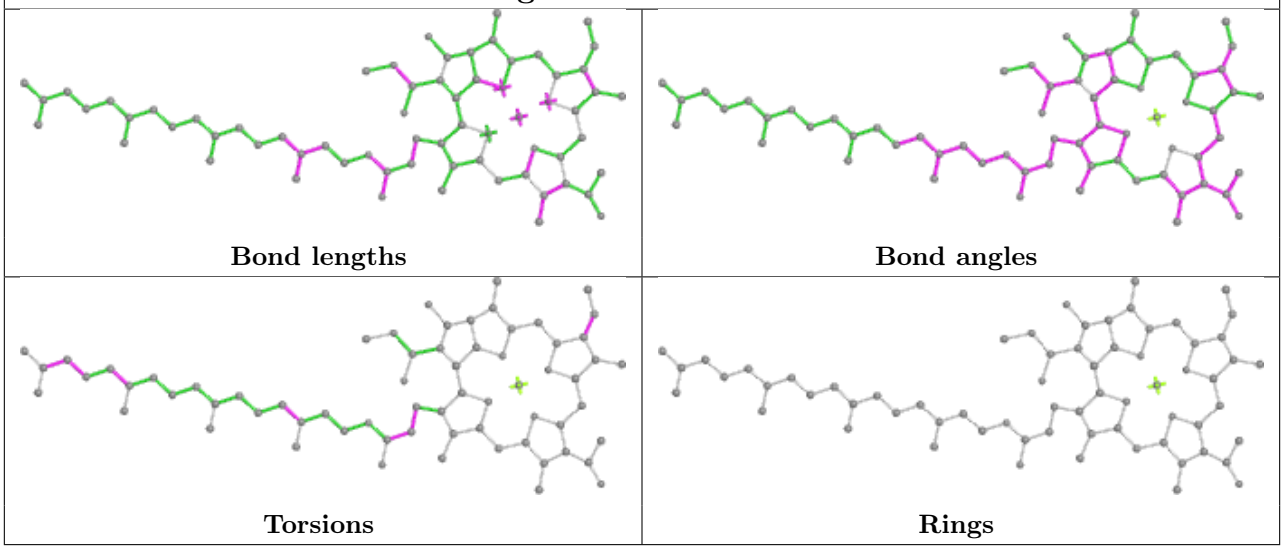

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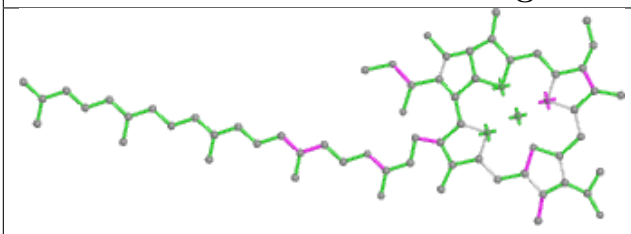
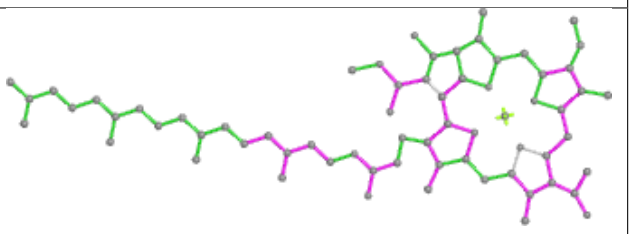
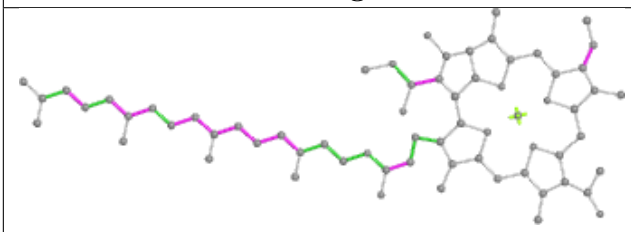
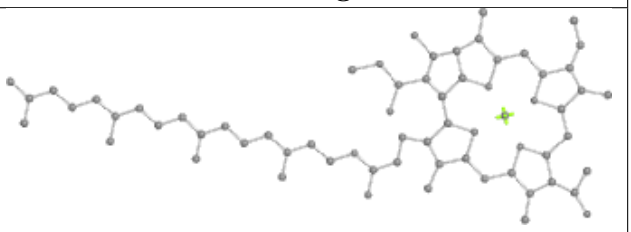
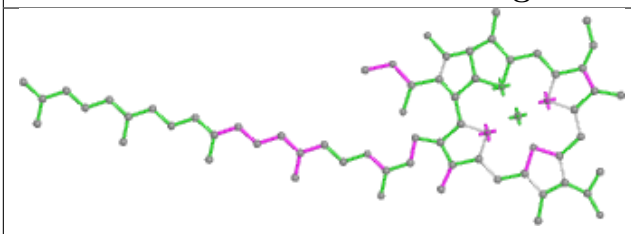
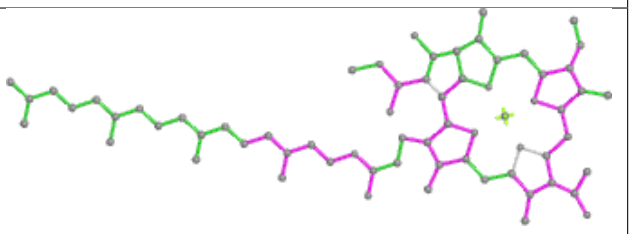
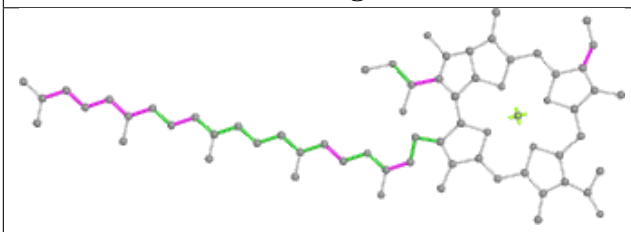
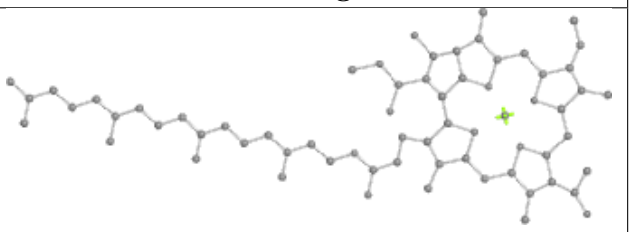
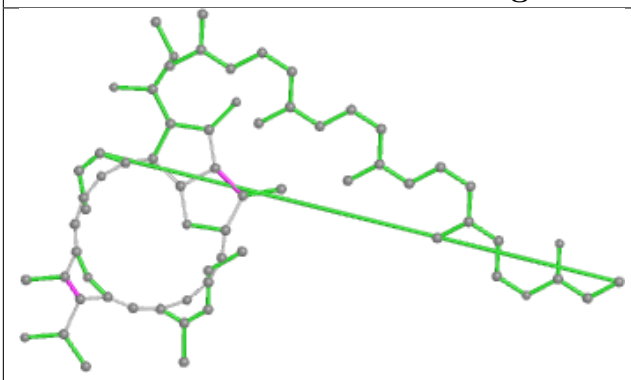
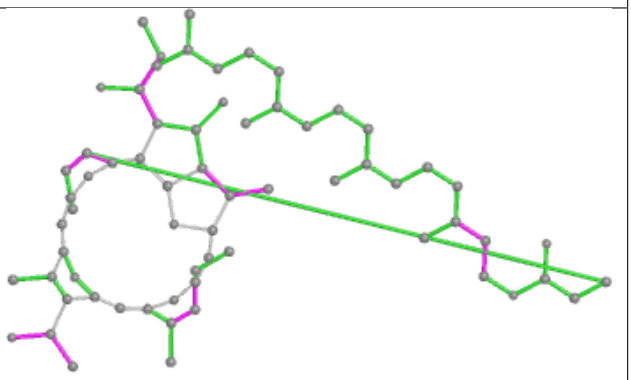
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL AV 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

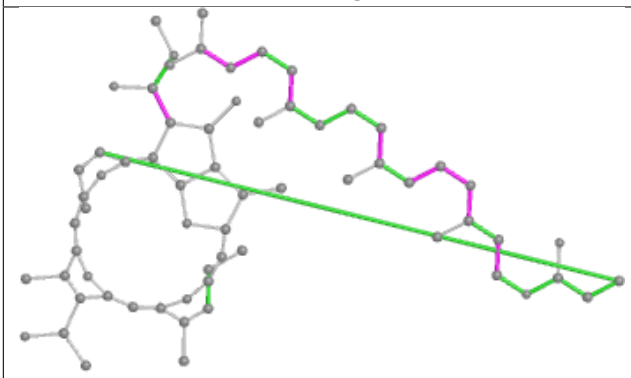
Ligand BPH AL 302



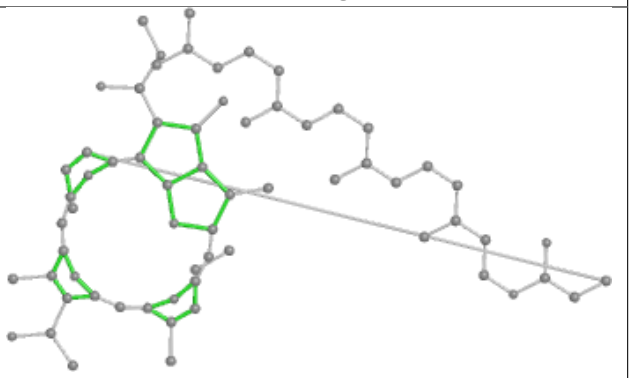
Bond lengths



Bond angles

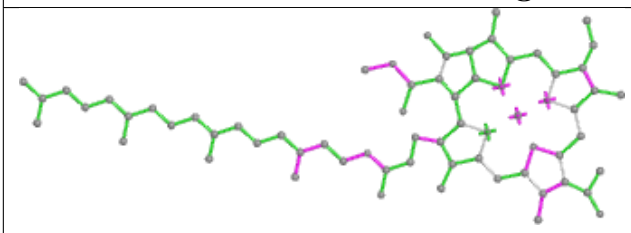


Torsions



Rings

Ligand BCL A0 102



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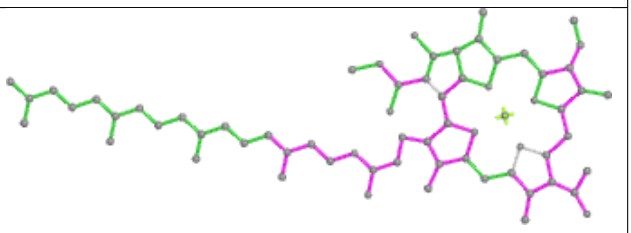

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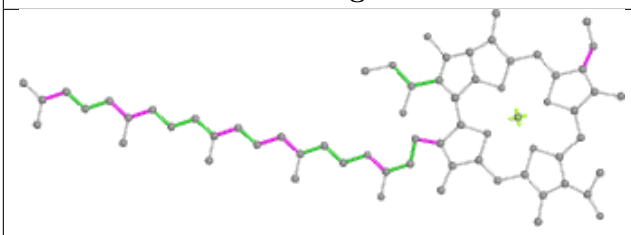

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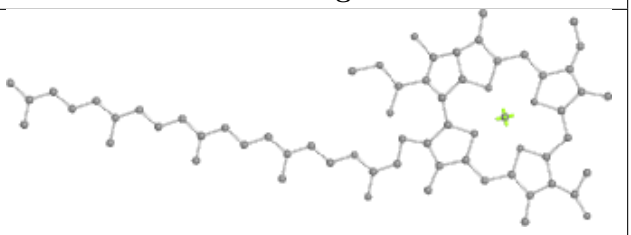
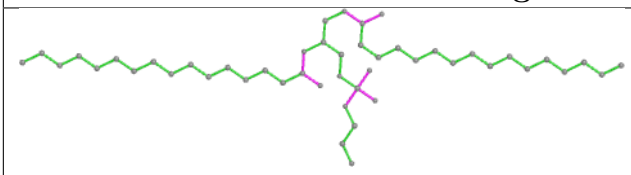
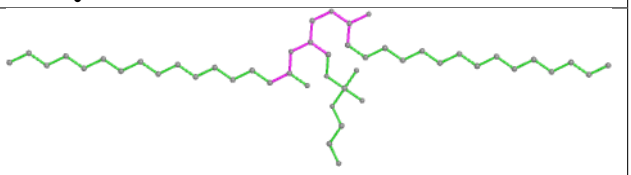
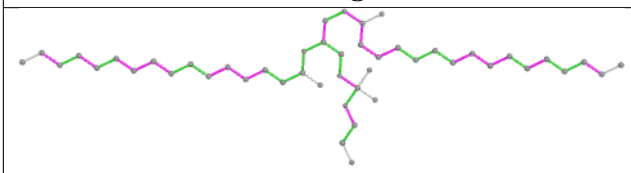
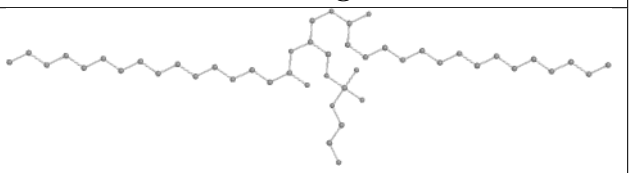


Rings

Ligand PEF BQ 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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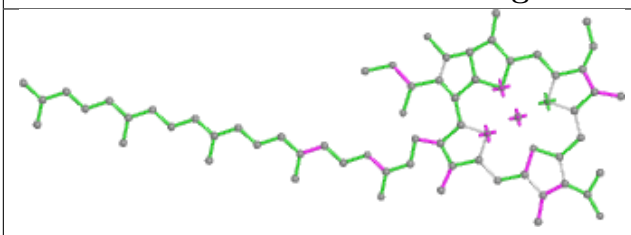
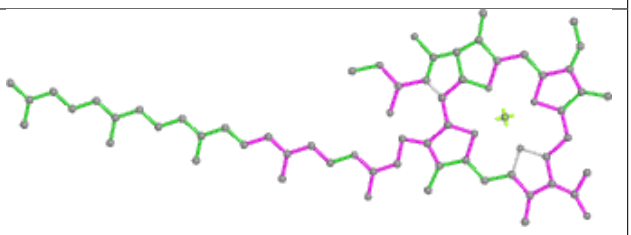
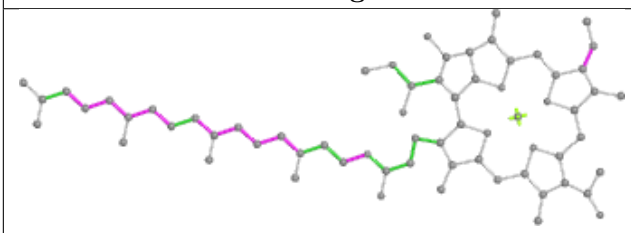
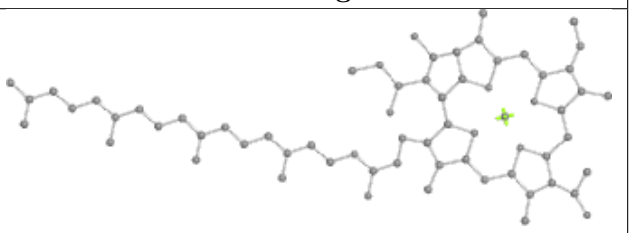
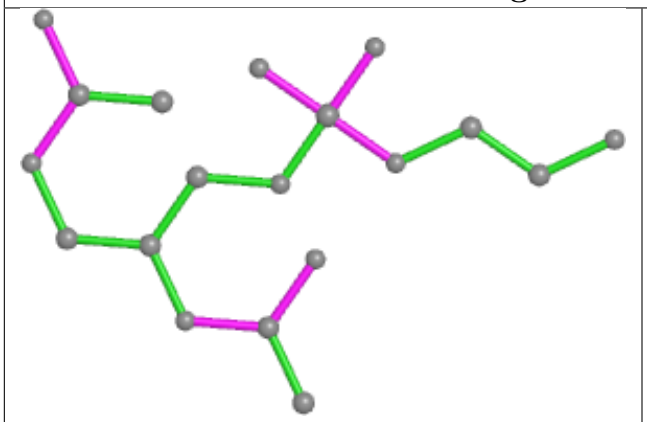
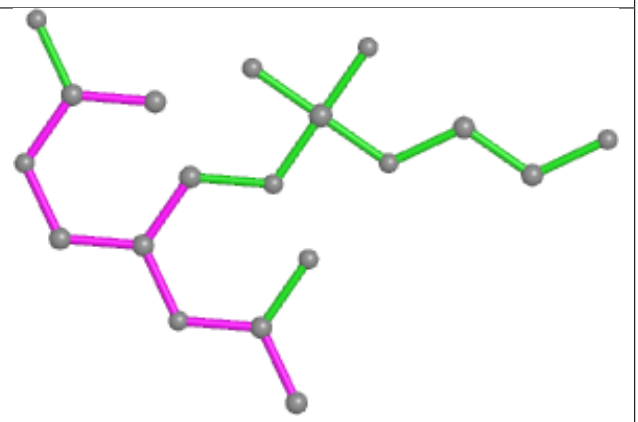
 Bond lengths	 Bond angles
 Torsions	 Rings

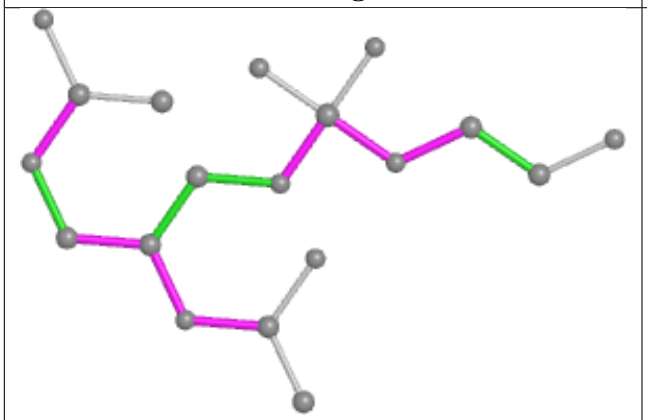
Ligand PEF BM 407



Bond lengths



Bond angles



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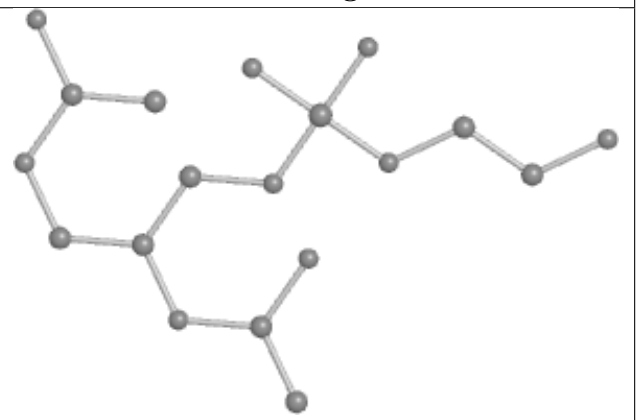

Rings

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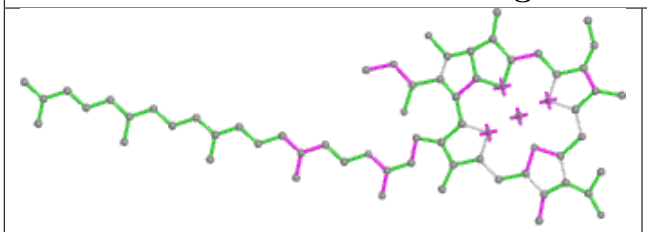

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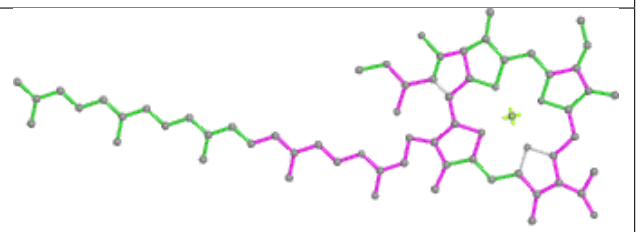
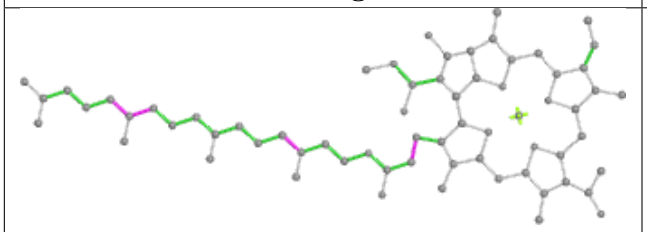


Bond angles



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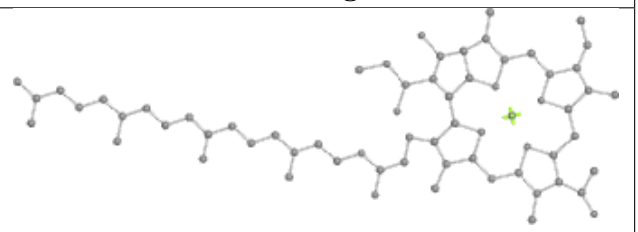
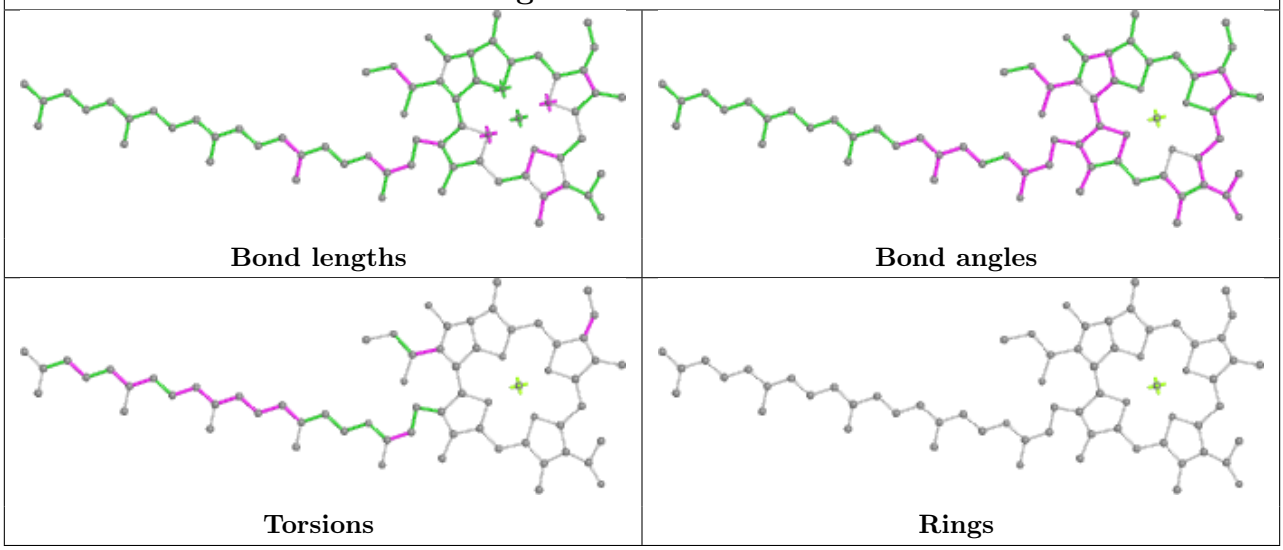
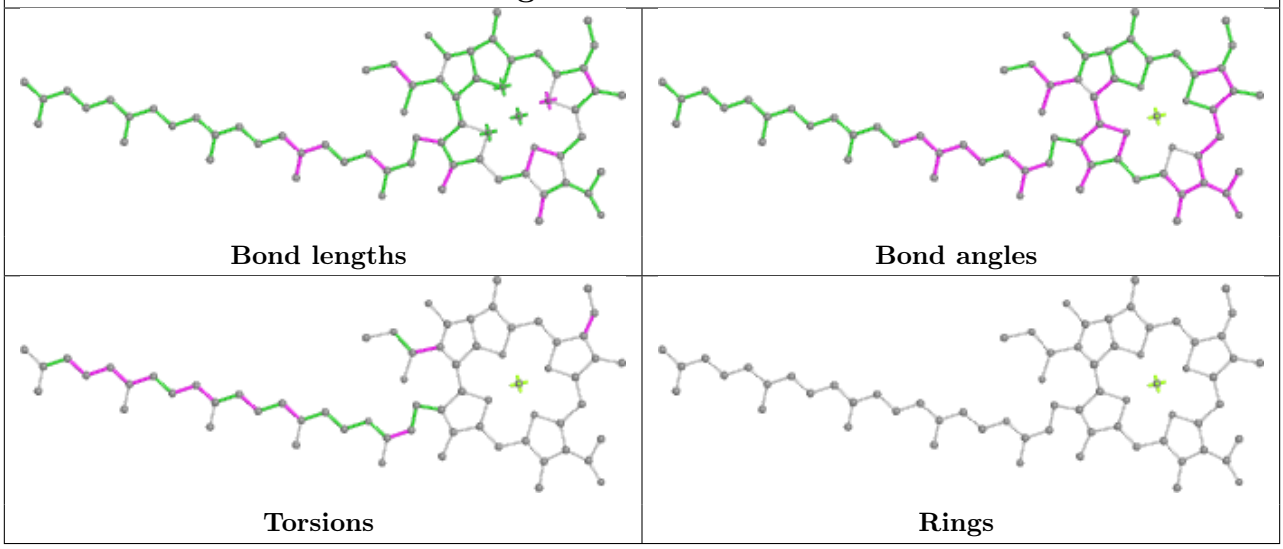


Rings

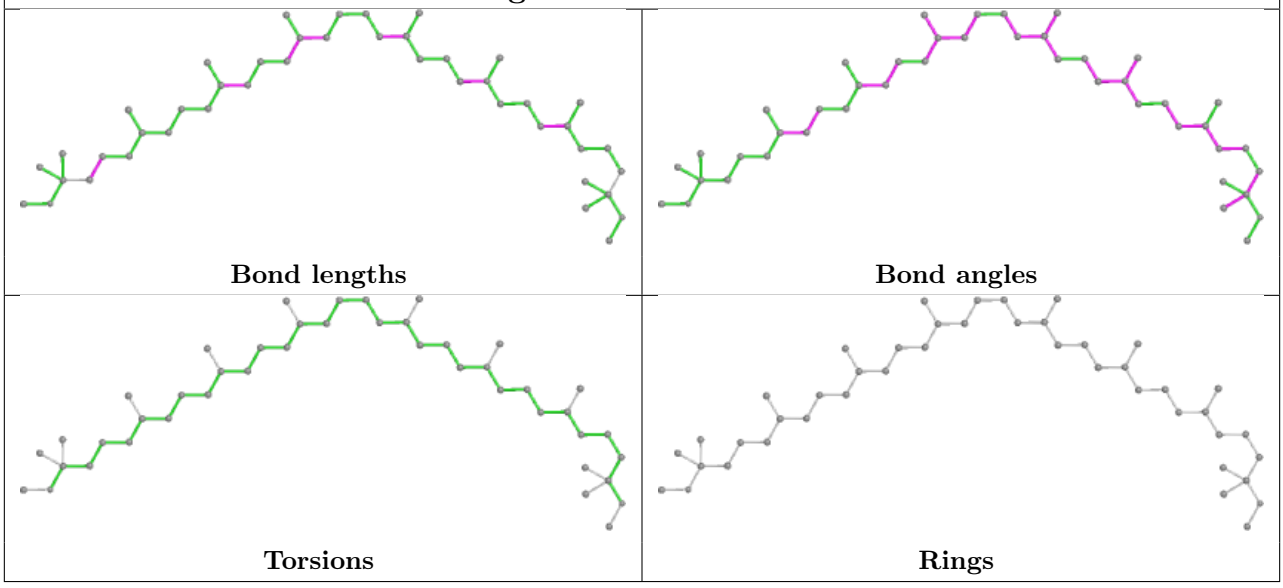
Ligand BCL A3 103



Ligand BCL B9 102



Ligand CRT BM 406



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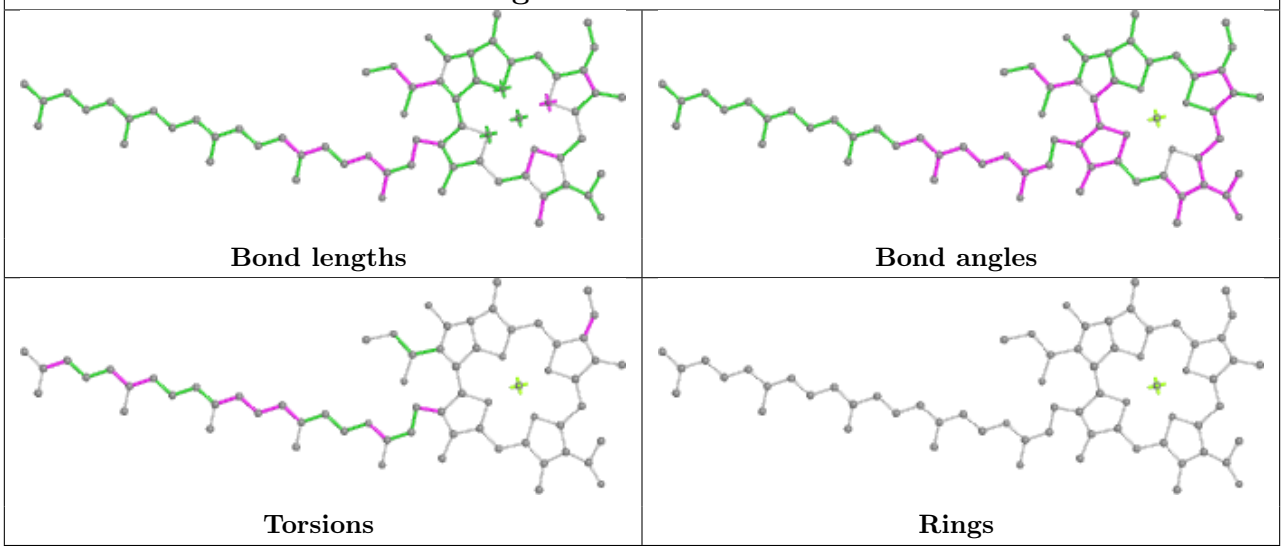
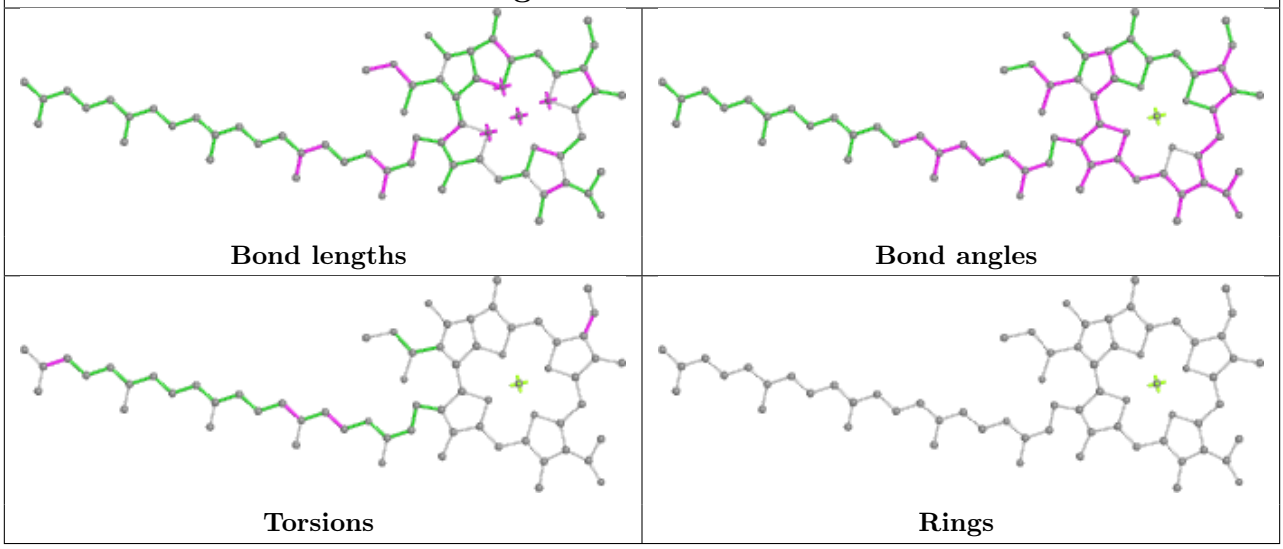
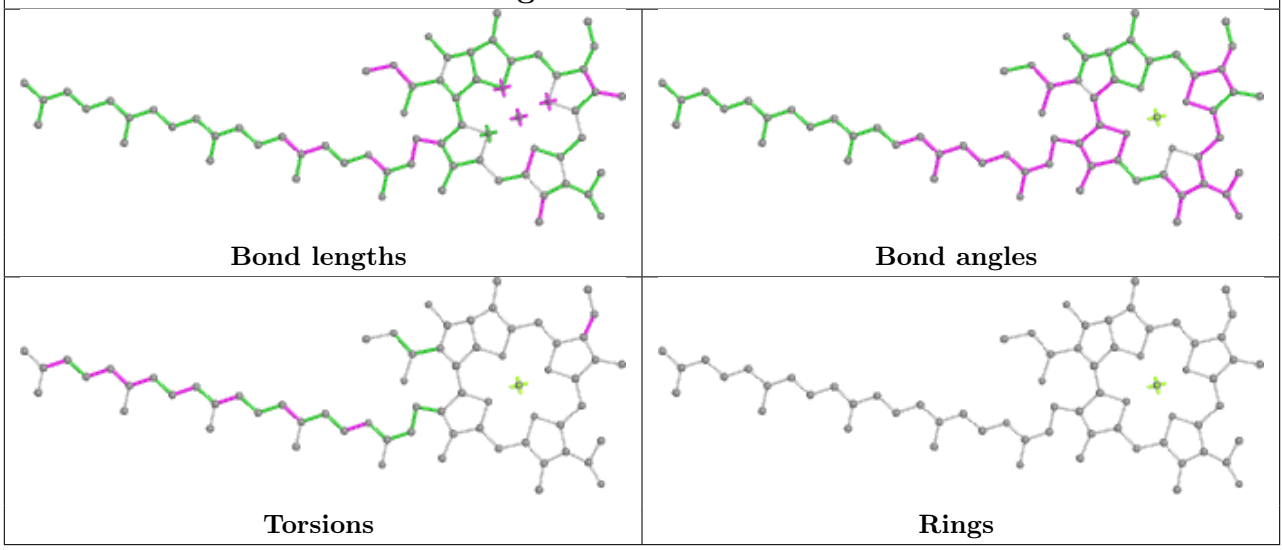


Ligand BCL BT 101



Ligand BCL B0 102



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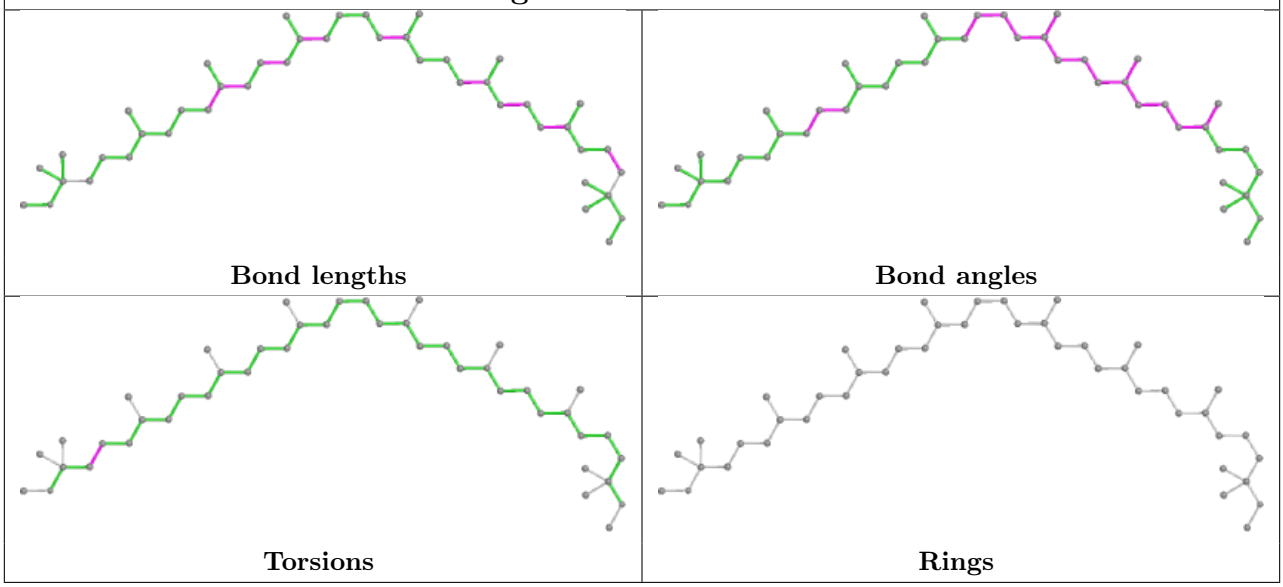
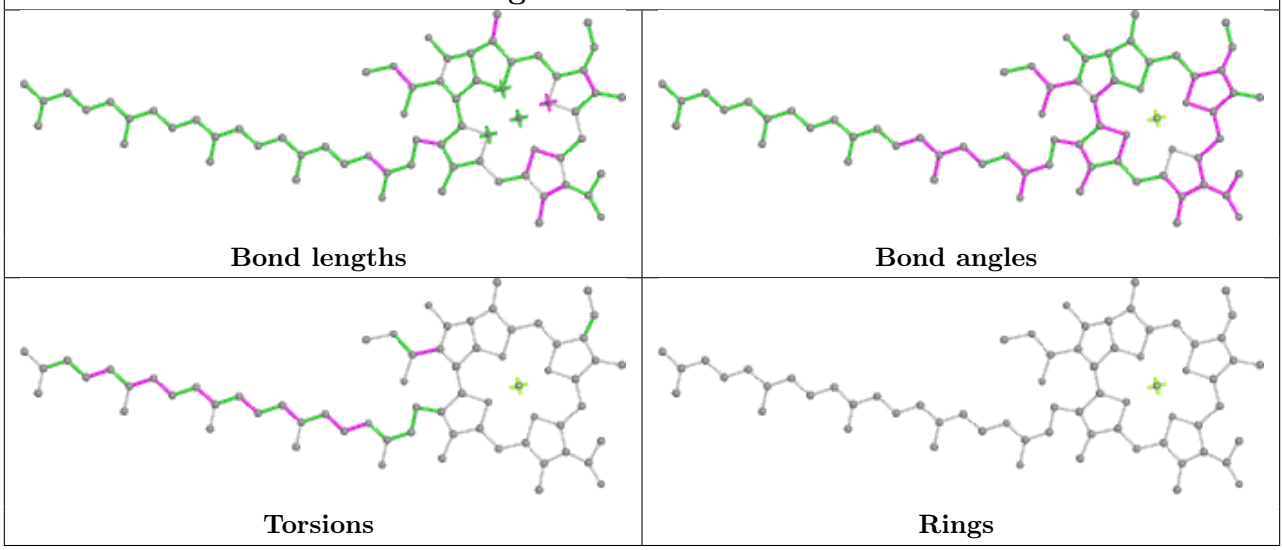
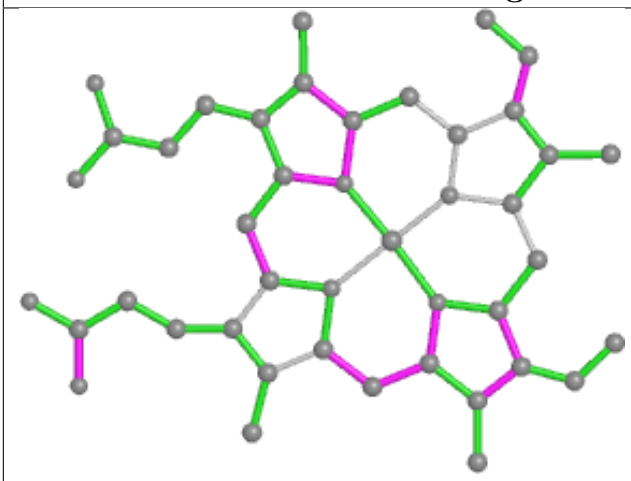


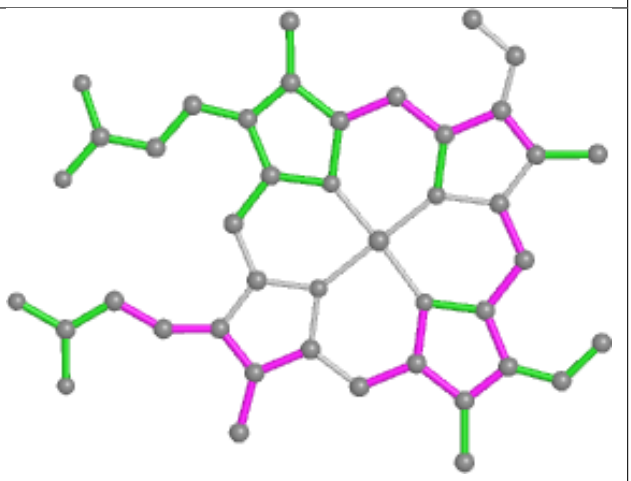
Ligand BCL AM 402



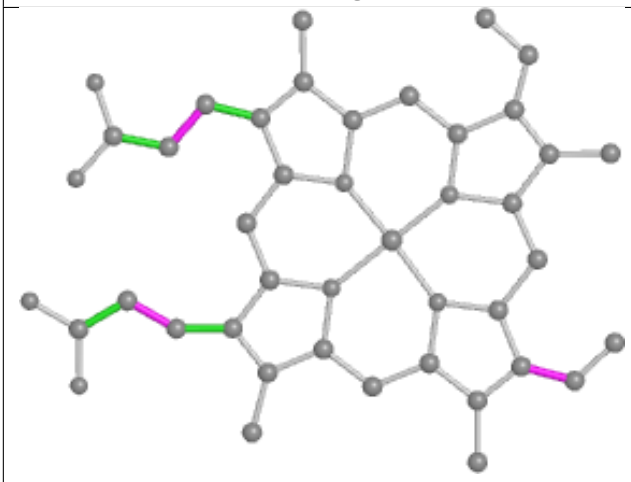
Ligand HEM BC 502



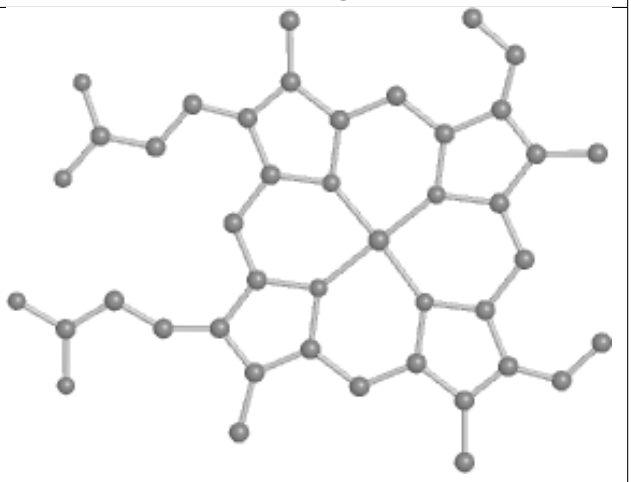
Bond lengths



Bond angles

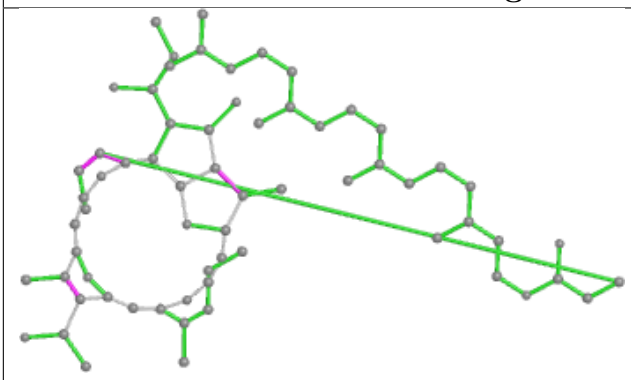


Torsions

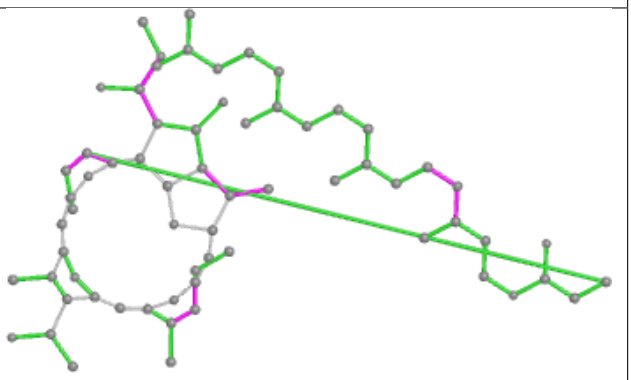


Rings

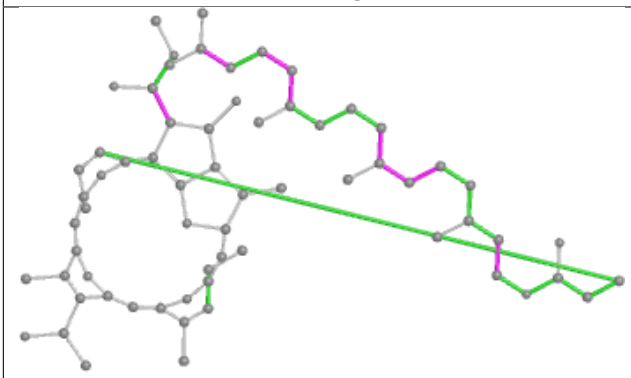
Ligand BPH AM 403



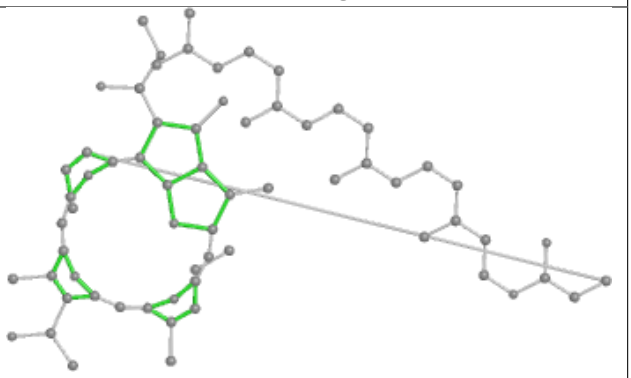
Bond lengths



Bond angles

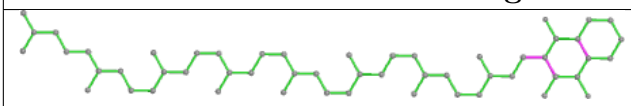


Torsions

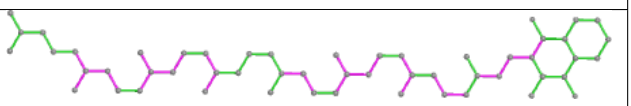


Rings

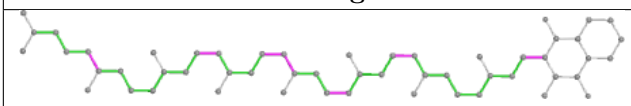
Ligand MQ8 AM 405



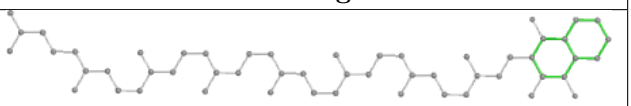
Bond lengths



Bond angles

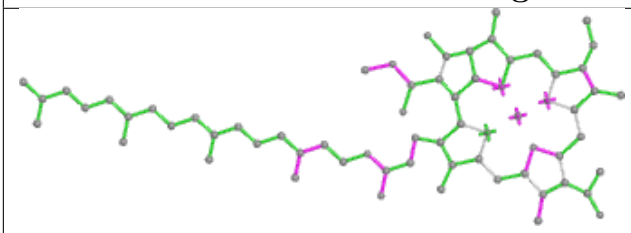


Torsions

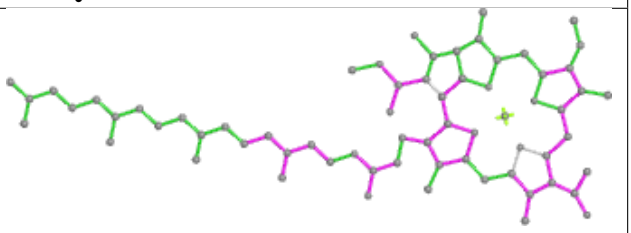


Rings

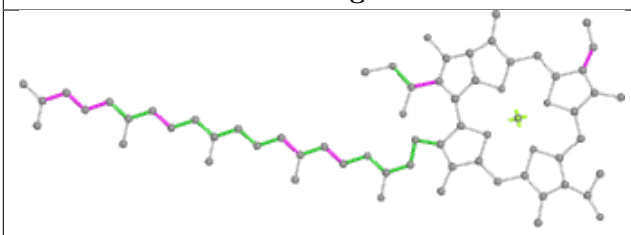
Ligand BCL BQ 104



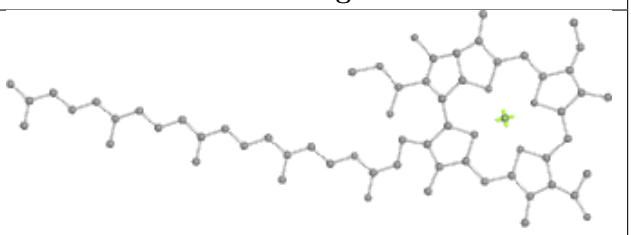
Bond lengths



Bond angles

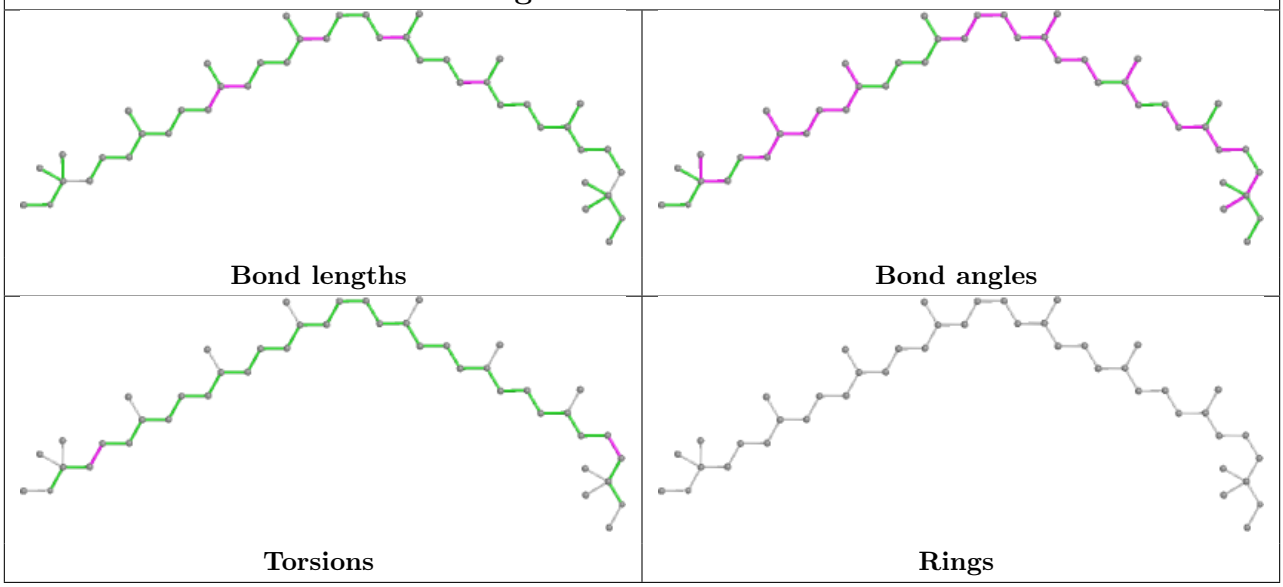


Torsions

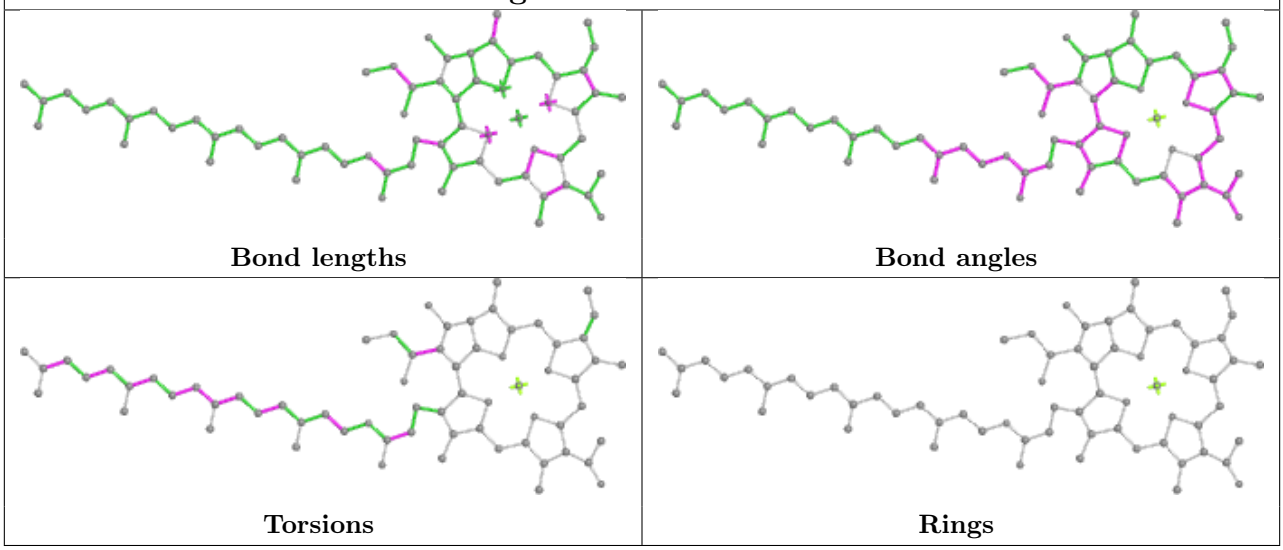


Rings

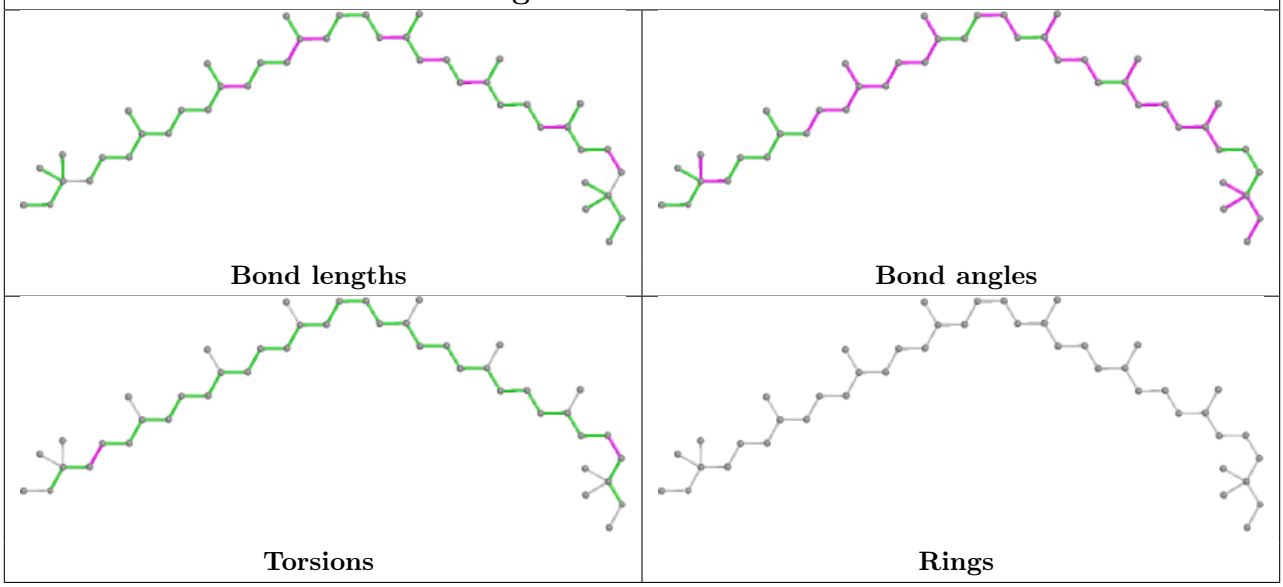
Ligand CRT AS 104



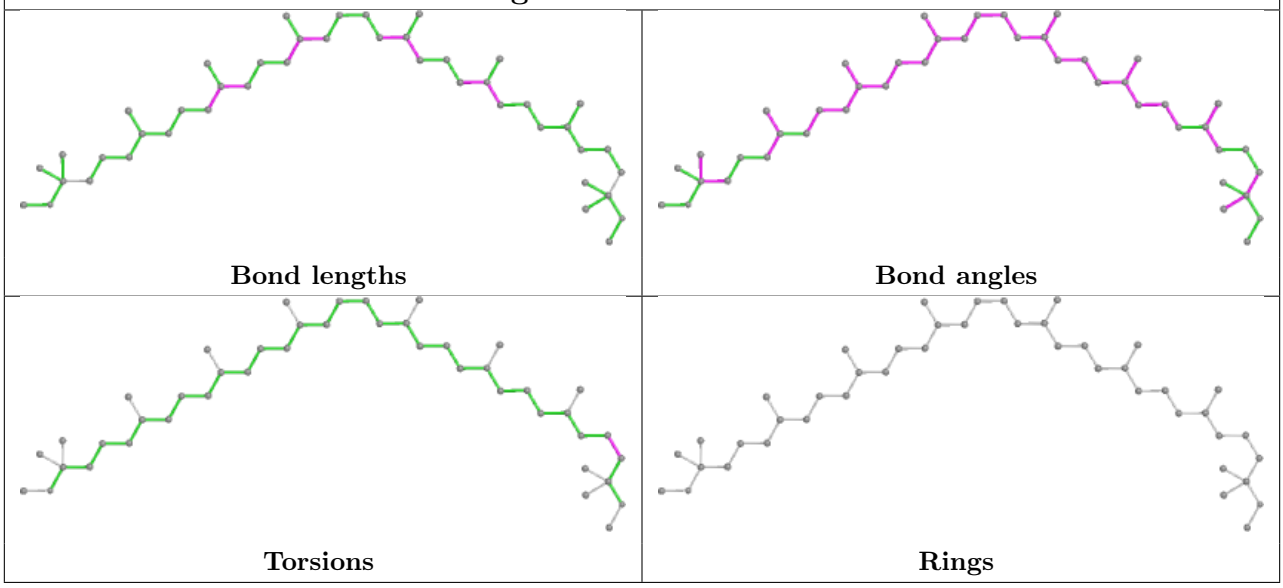
Ligand BCL BM 402



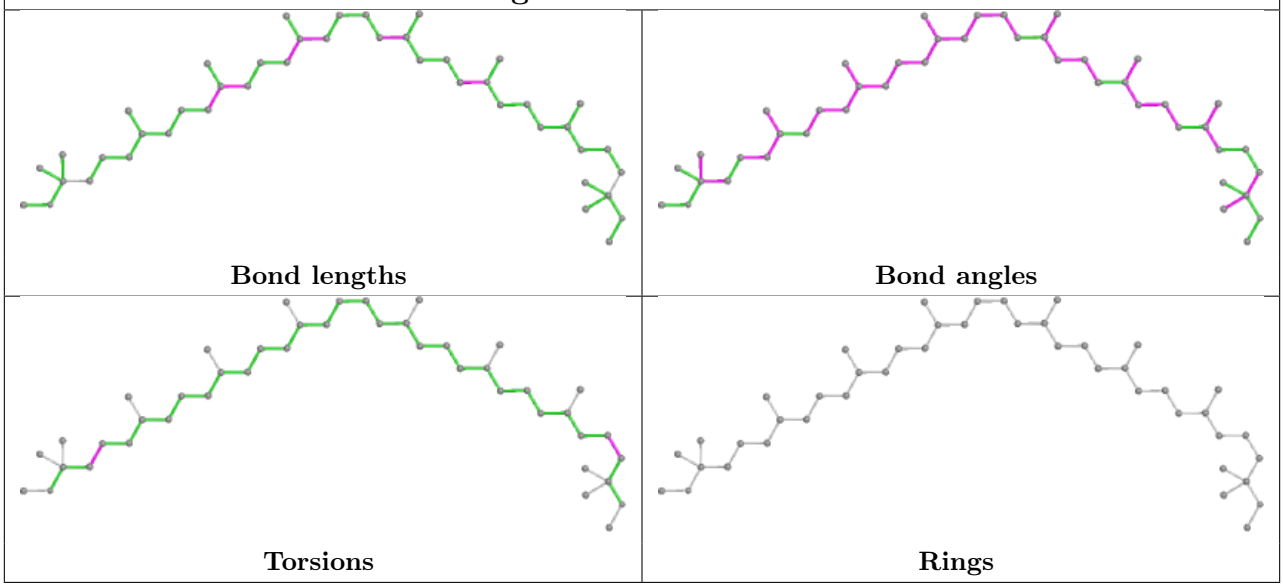
Ligand CRT AP 102



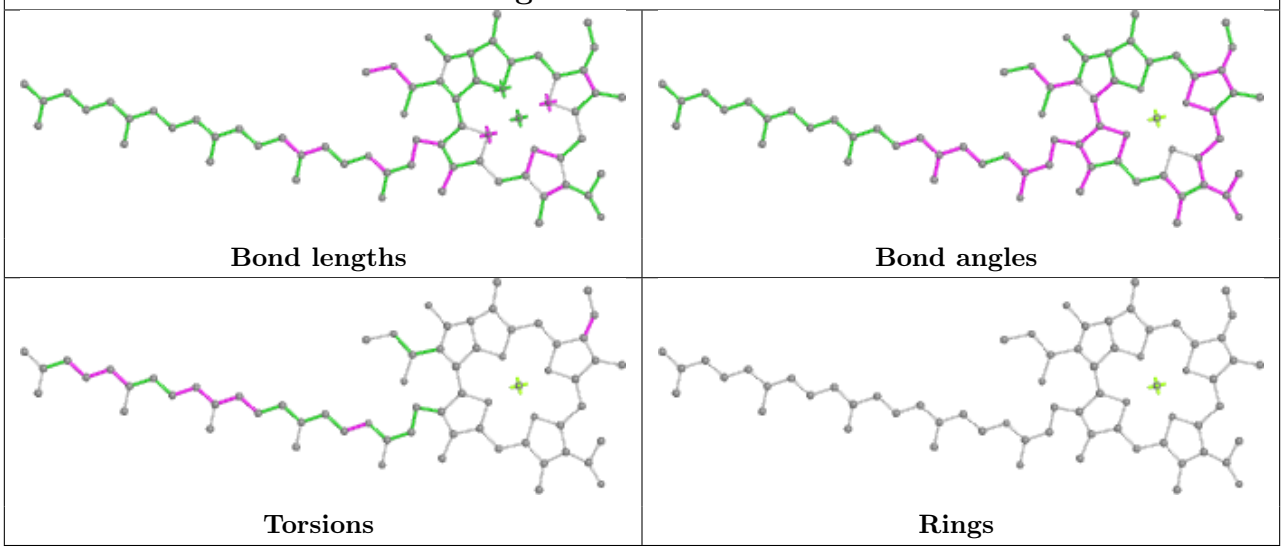
Ligand CRT AG 102



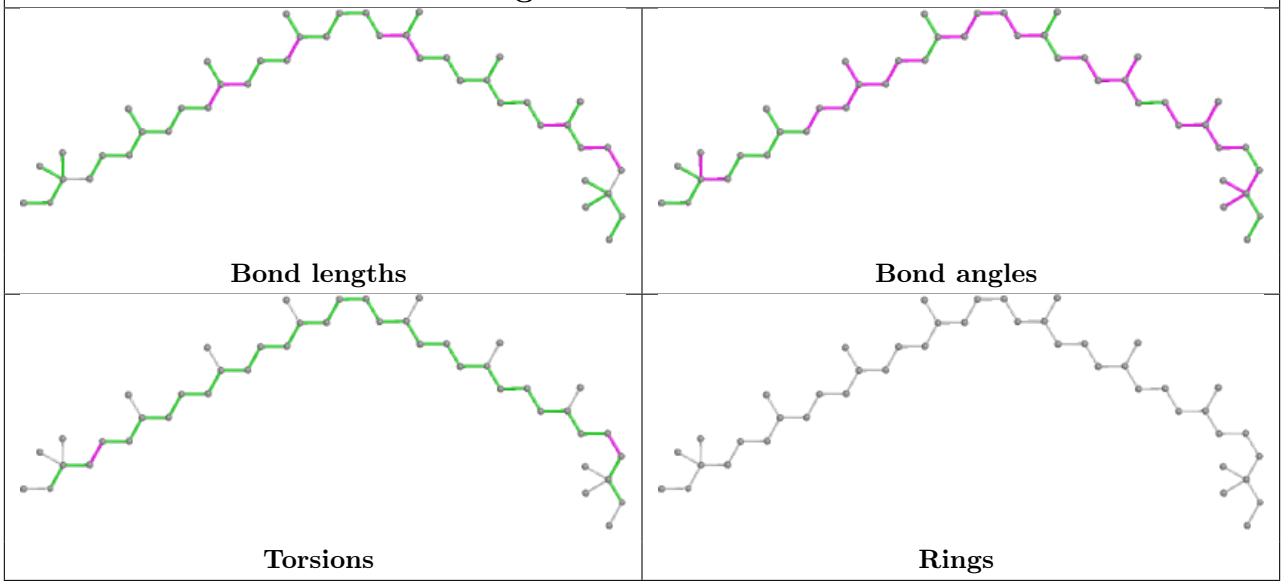
Ligand CRT BG 102



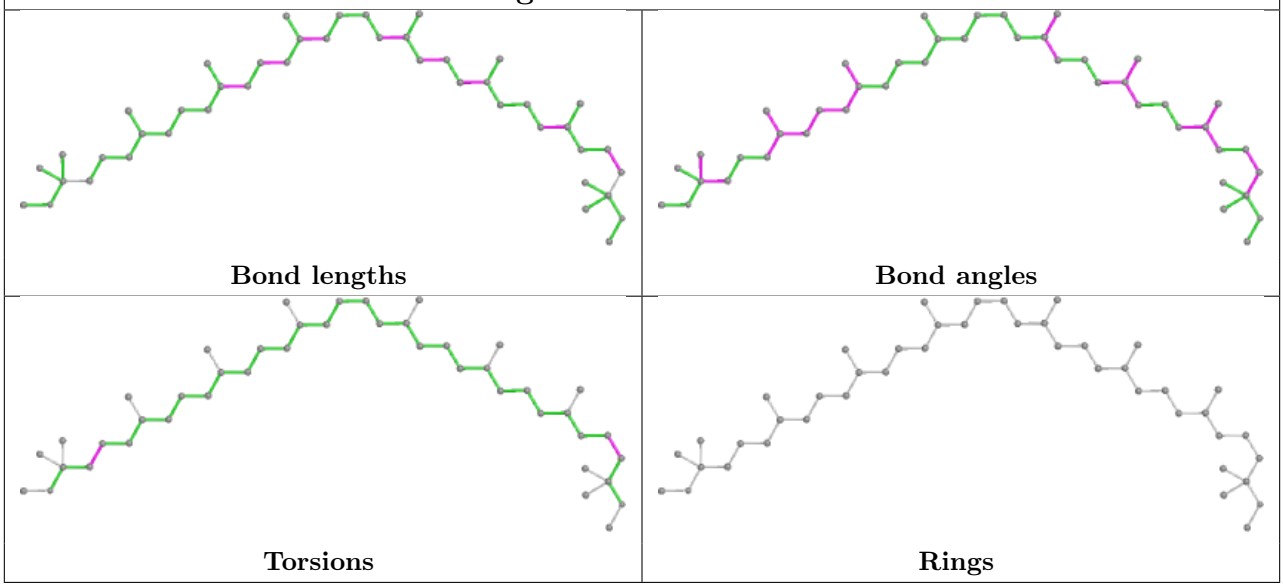
Ligand BCL BL 301



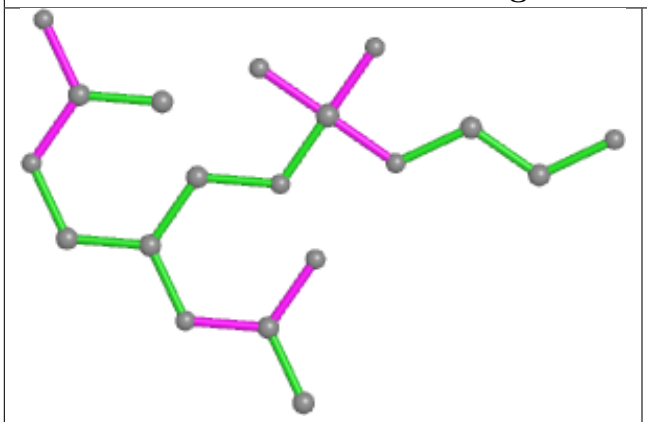
Ligand CRT A1 103



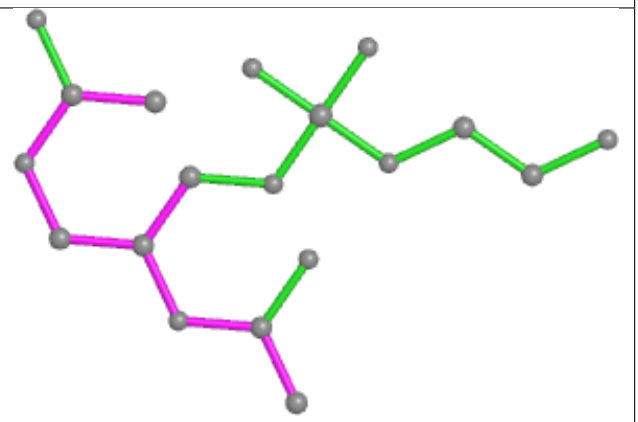
Ligand CRT B7 102



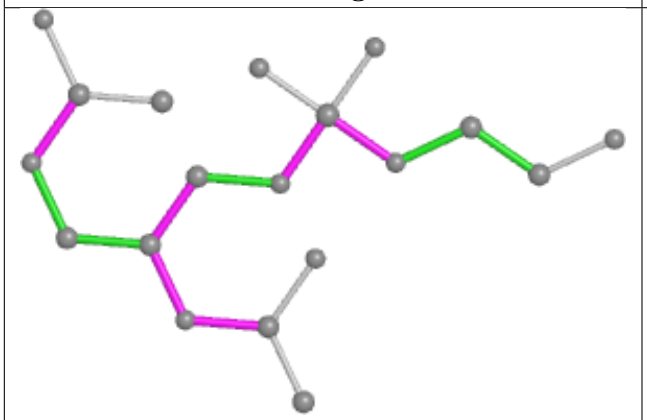
Ligand PEF AM 407



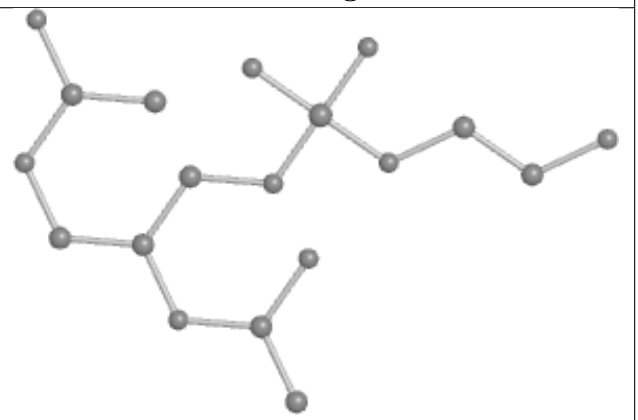
Bond lengths



Bond angles

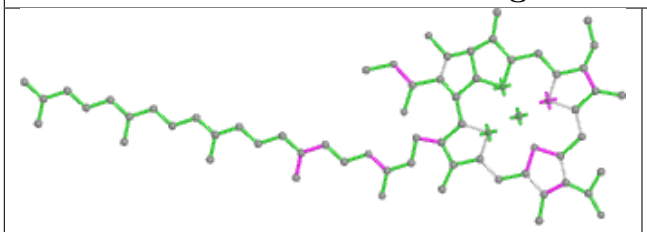


Torsions

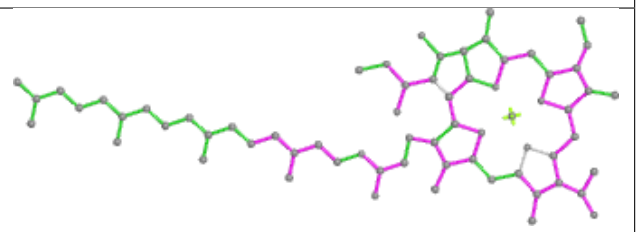


Rings

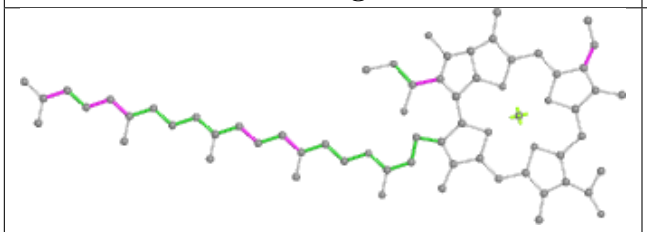
Ligand BCL BM 401



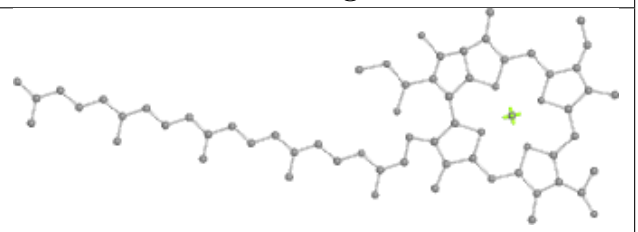
Bond lengths



Bond angles

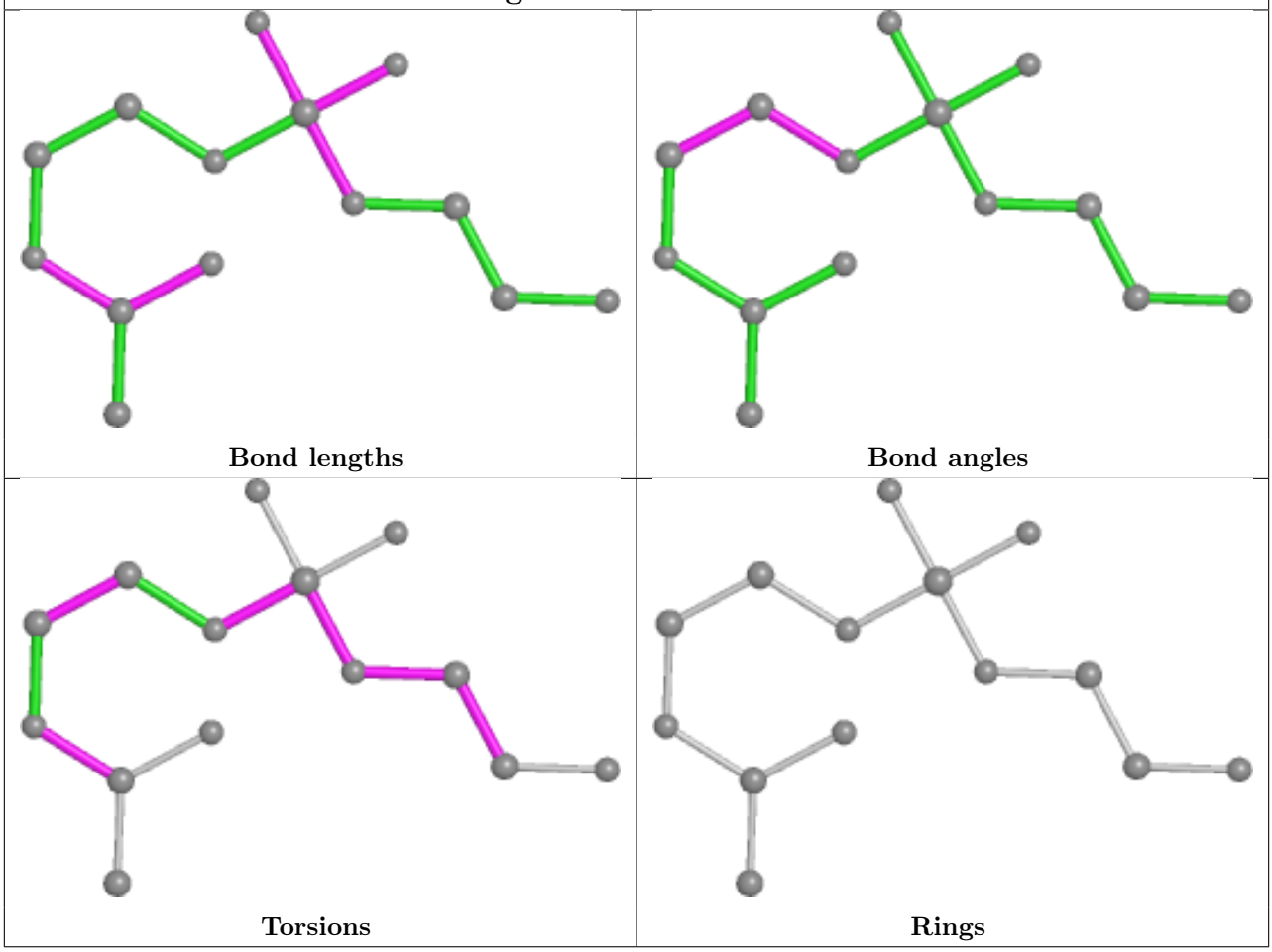


Torsions

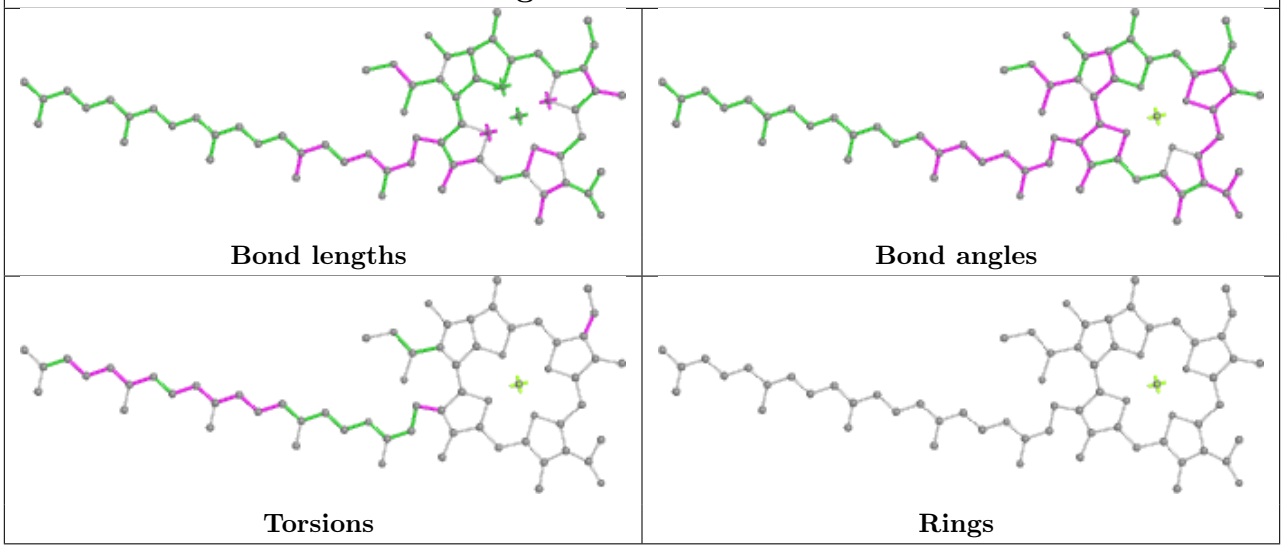


Rings

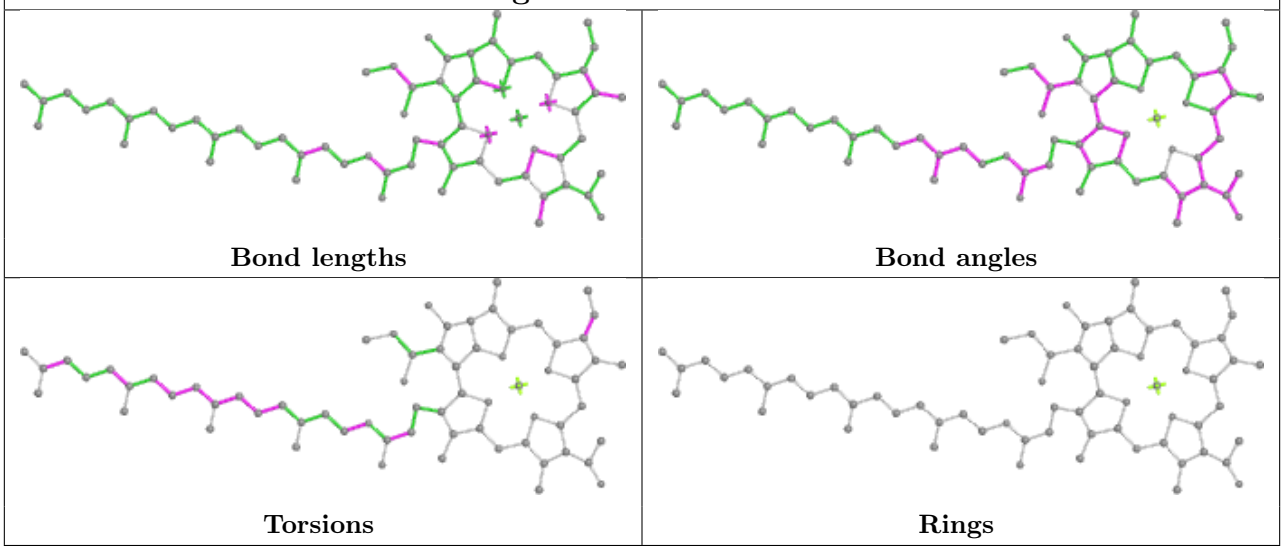
Ligand PEF AM 408



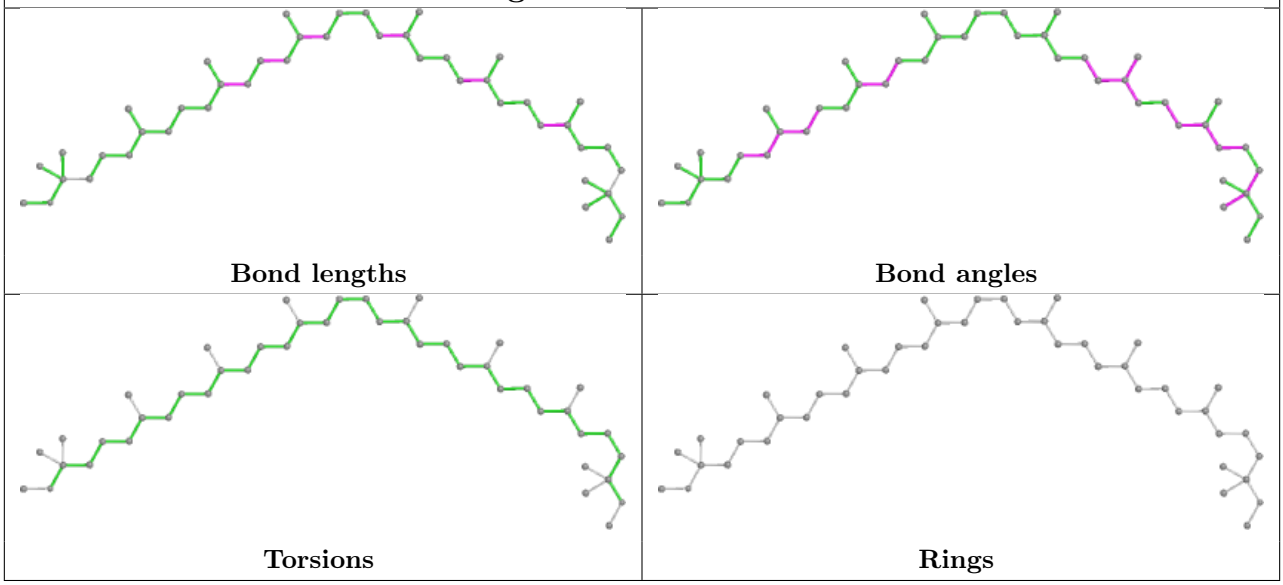
Ligand BCL A1 102



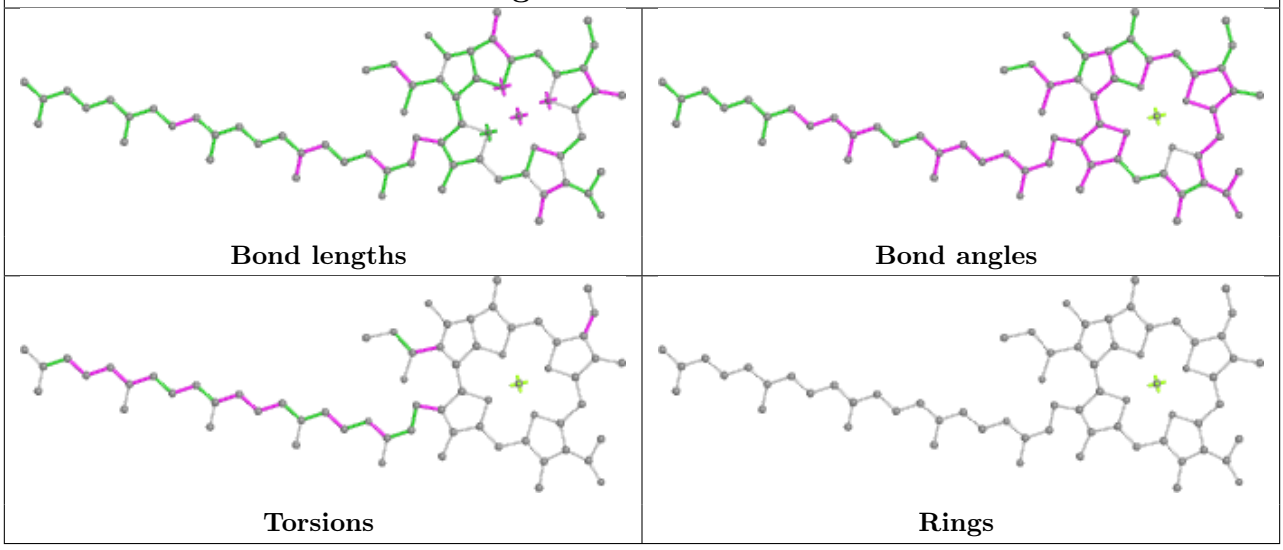
Ligand BCL BU 102



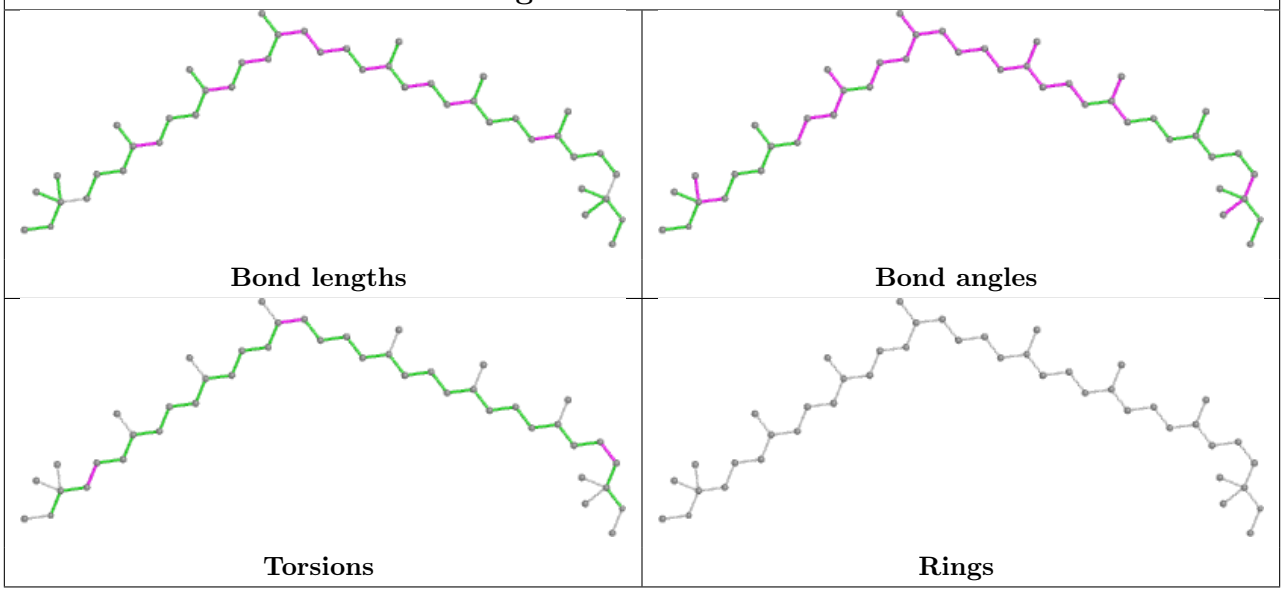
Ligand CRT AM 406



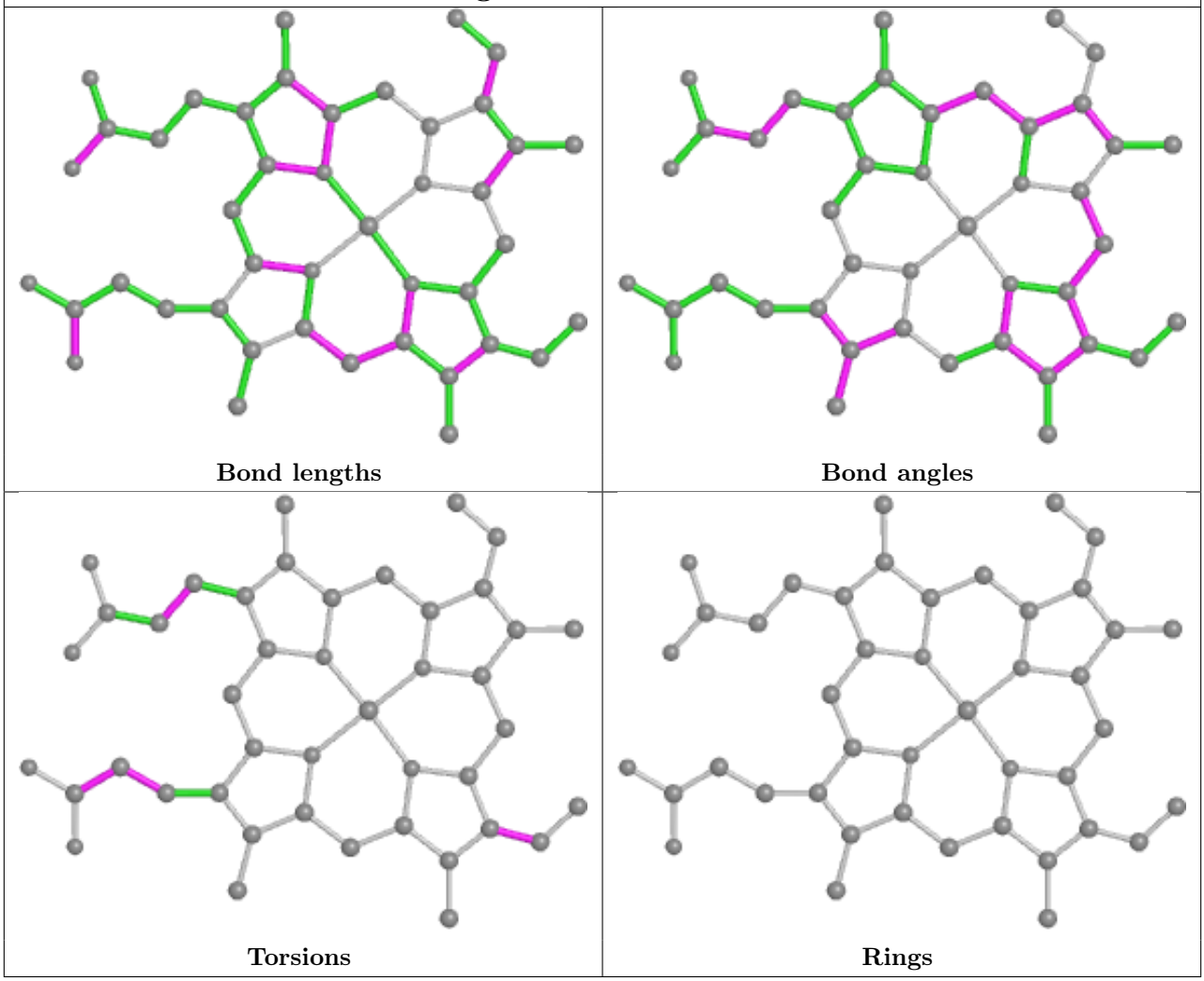
Ligand BCL AU 102



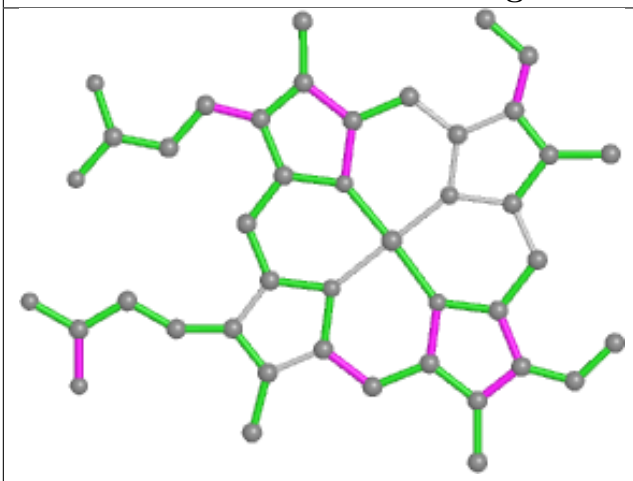
Ligand CRT A7 102



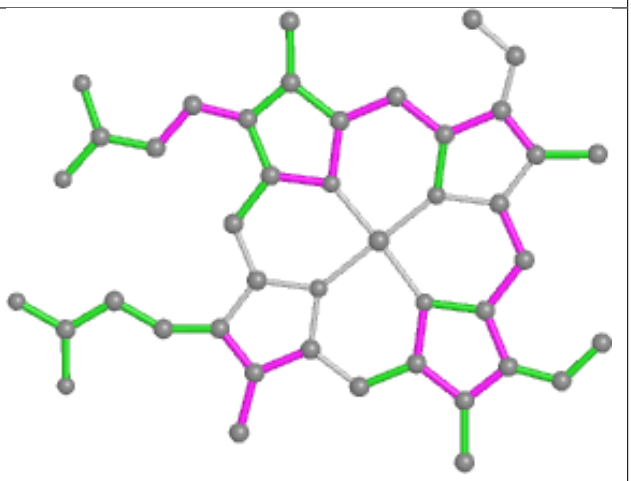
Ligand HEM AC 501



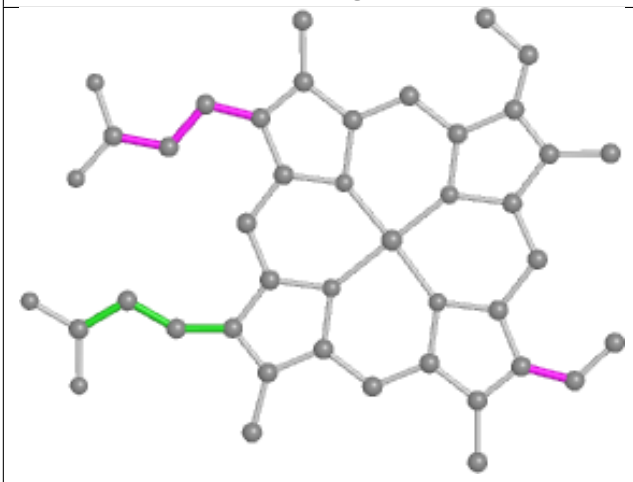
Ligand HEM BC 504



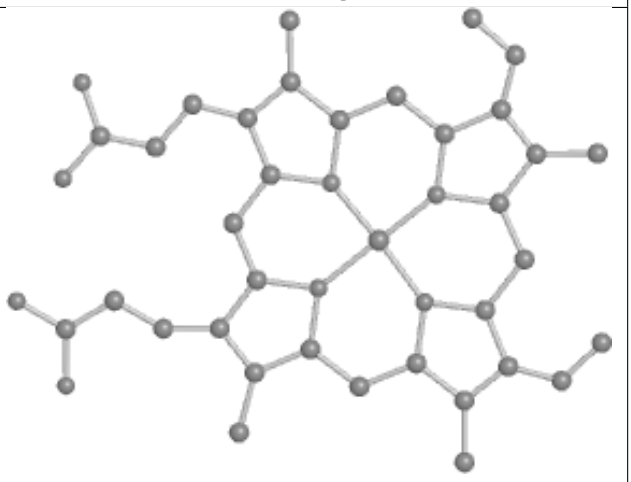
Bond lengths



Bond angles

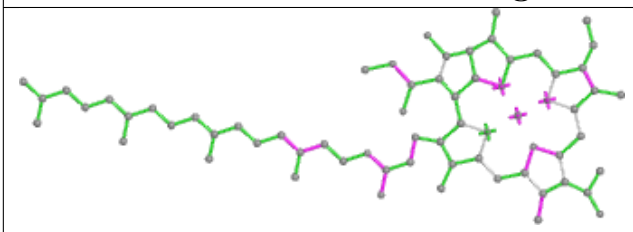


Torsions

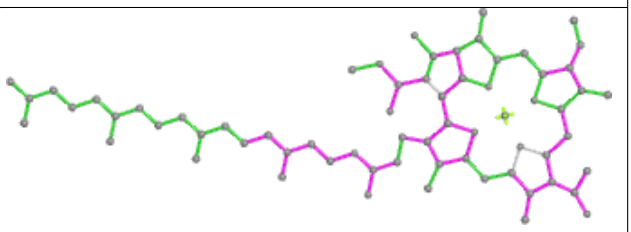


Rings

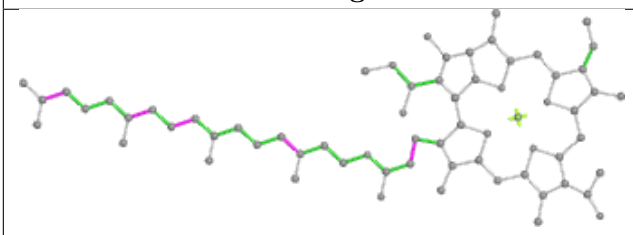
Ligand BCL AP 101



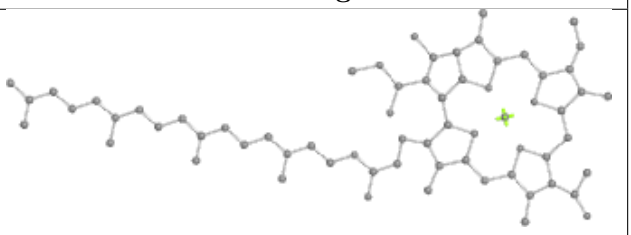
Bond lengths



Bond angles

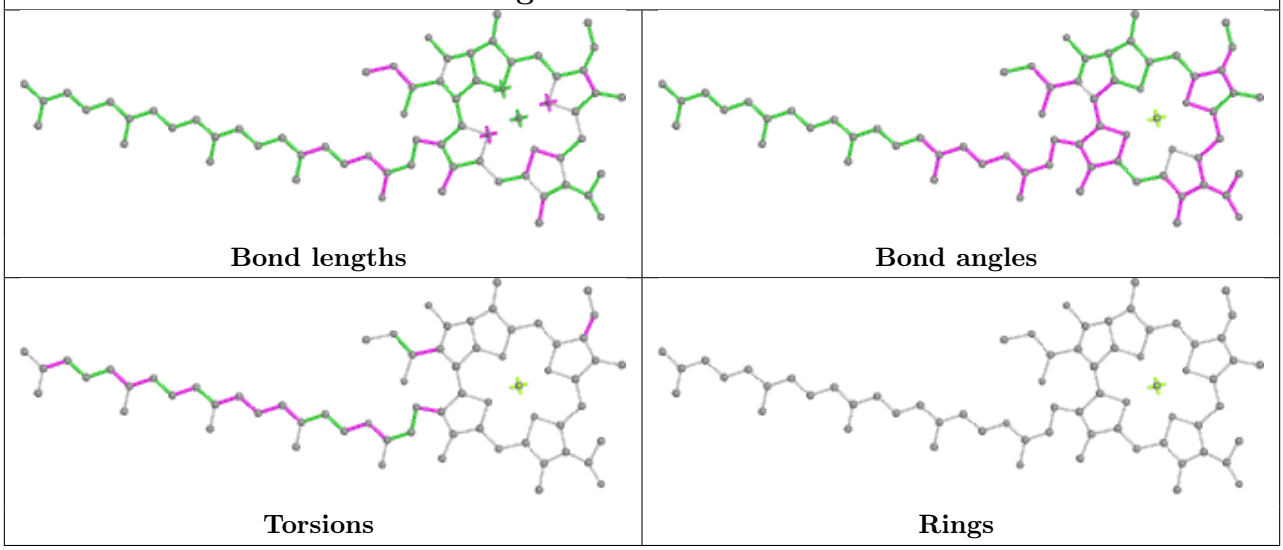


Torsions

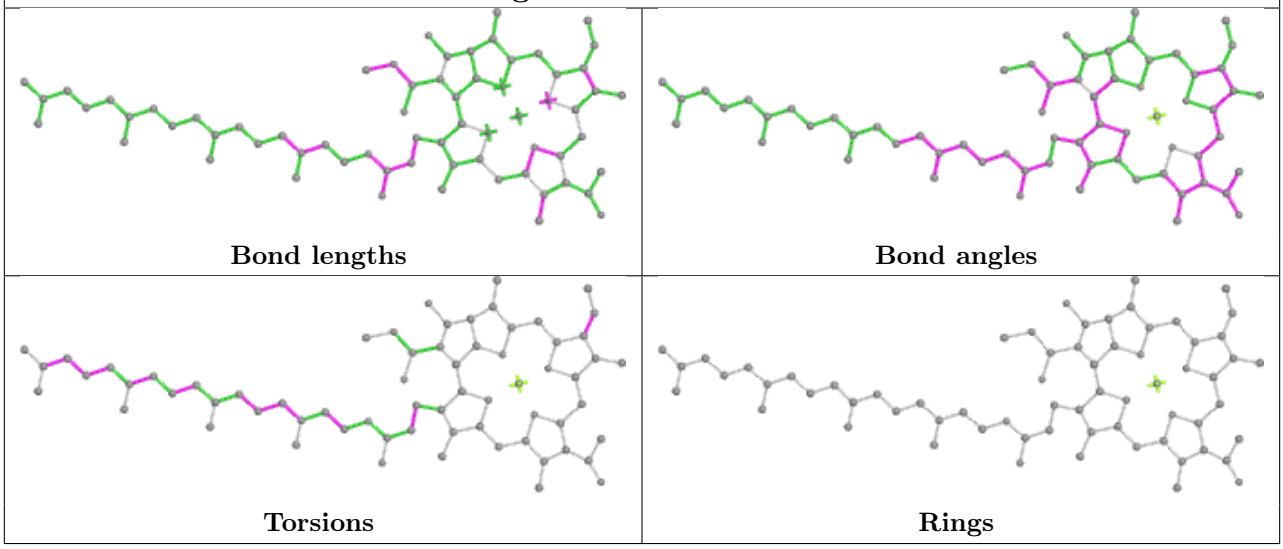


Rings

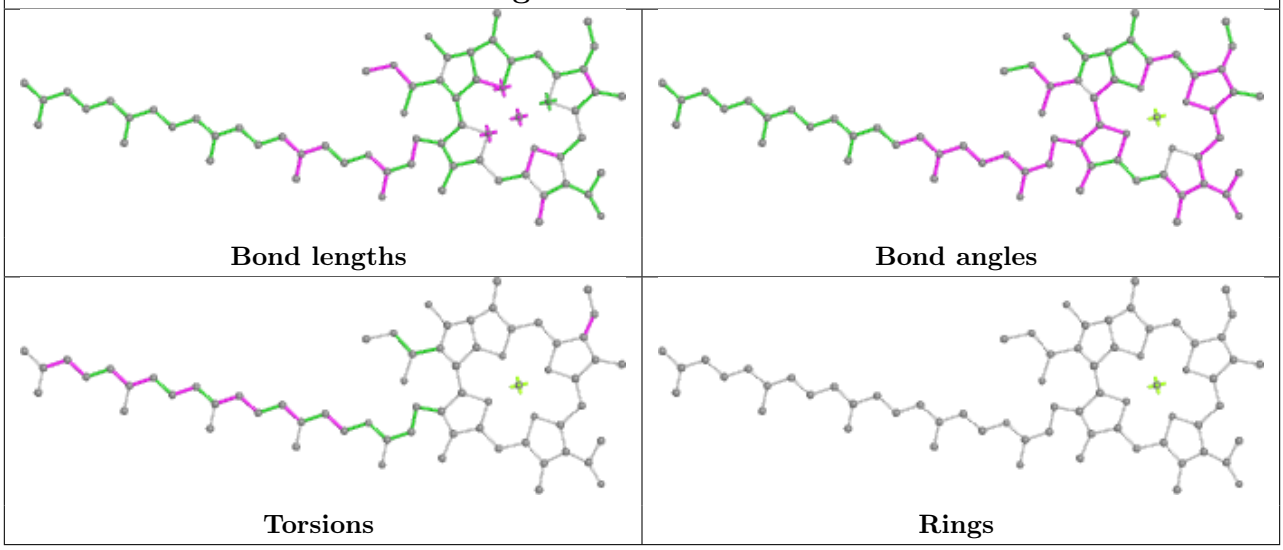
Ligand BCL A6 101



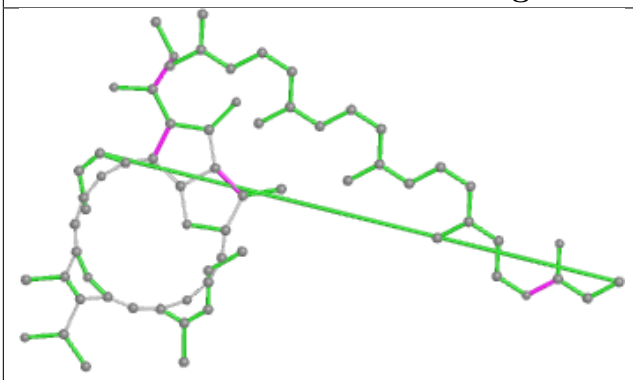
Ligand BCL AG 101



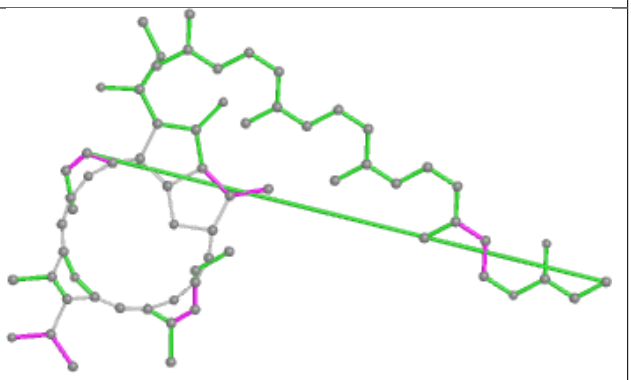
Ligand BCL BV 101



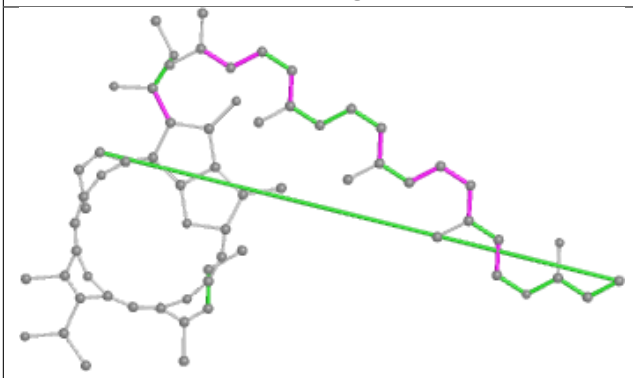
Ligand BPH BL 302



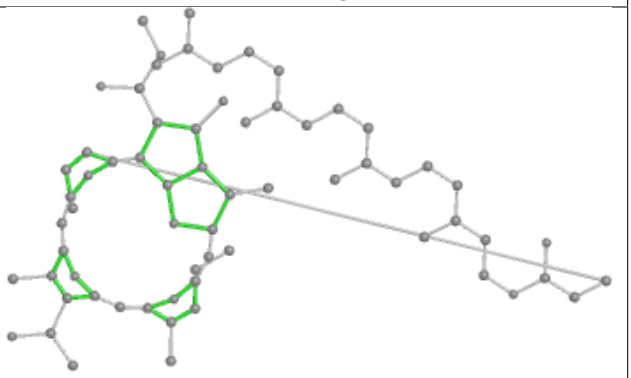
Bond lengths



Bond angles

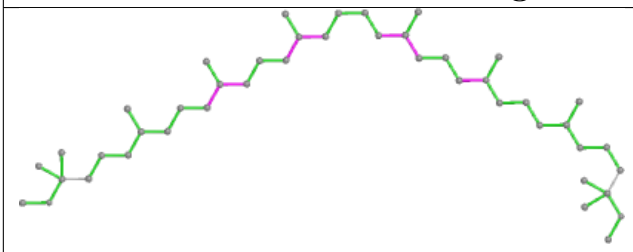


Torsions

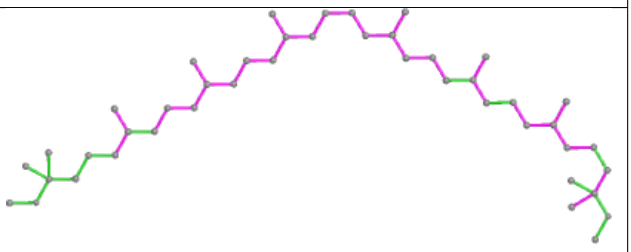


Rings

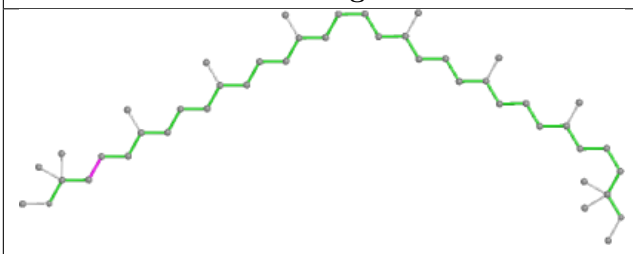
Ligand CRT BO 103



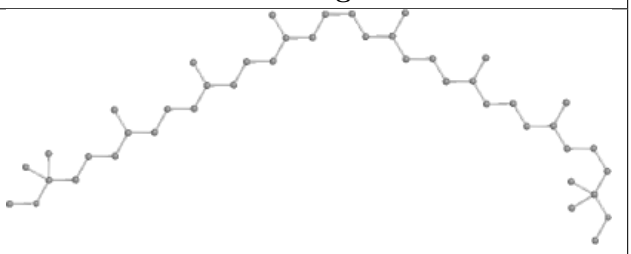
Bond lengths



Bond angles

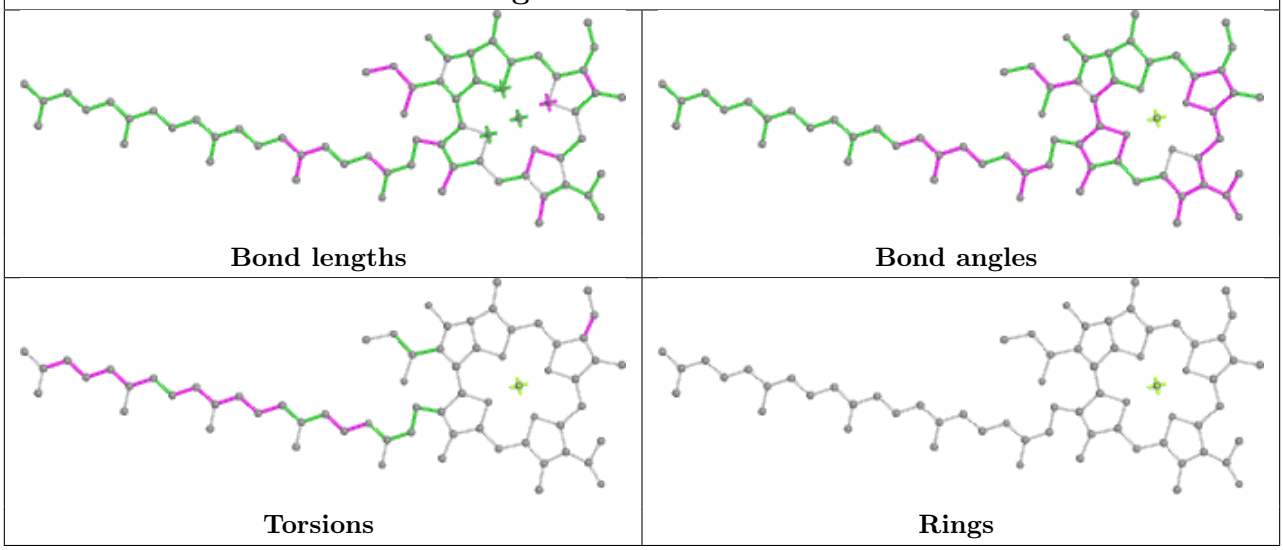


Torsions

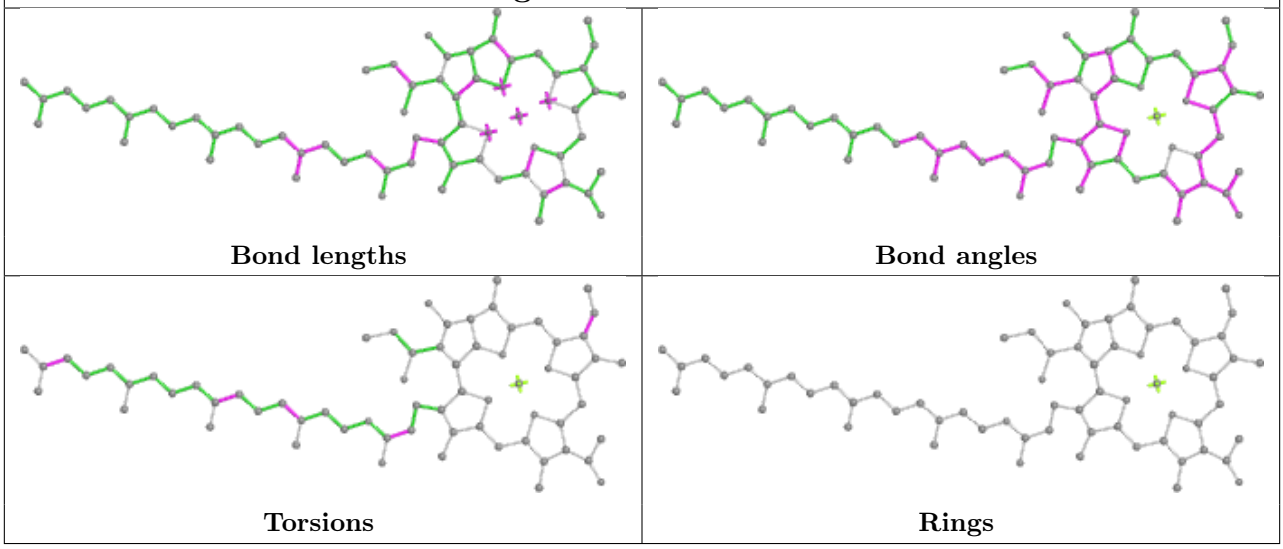


Rings

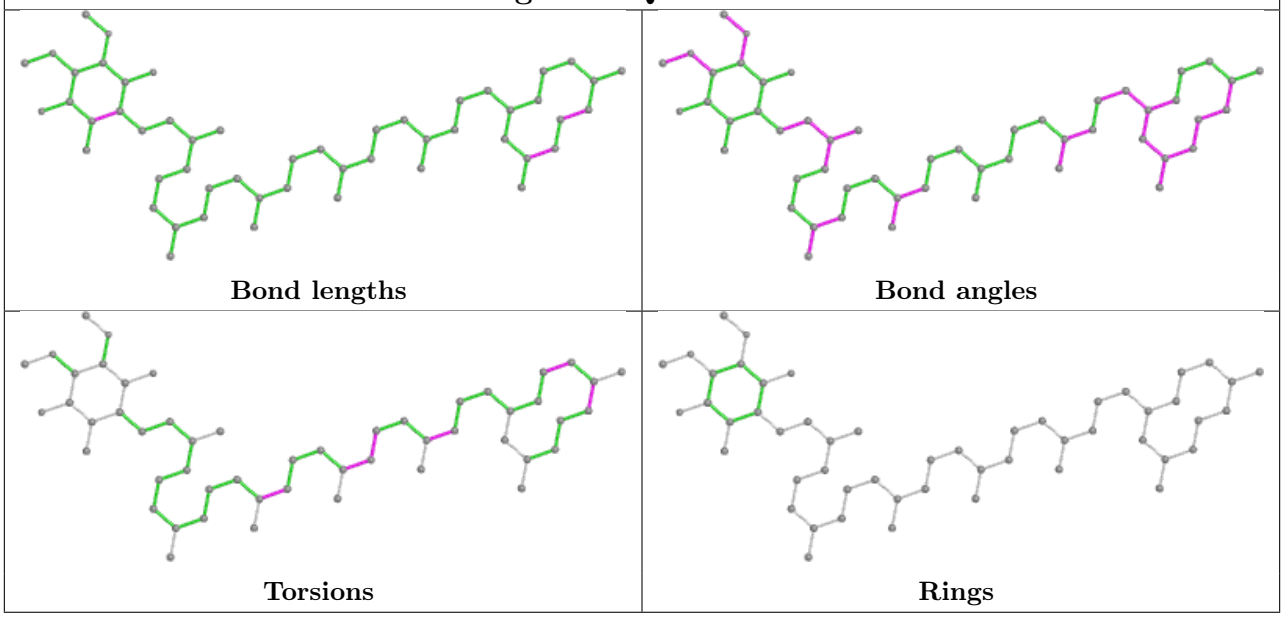
Ligand BCL AA 101



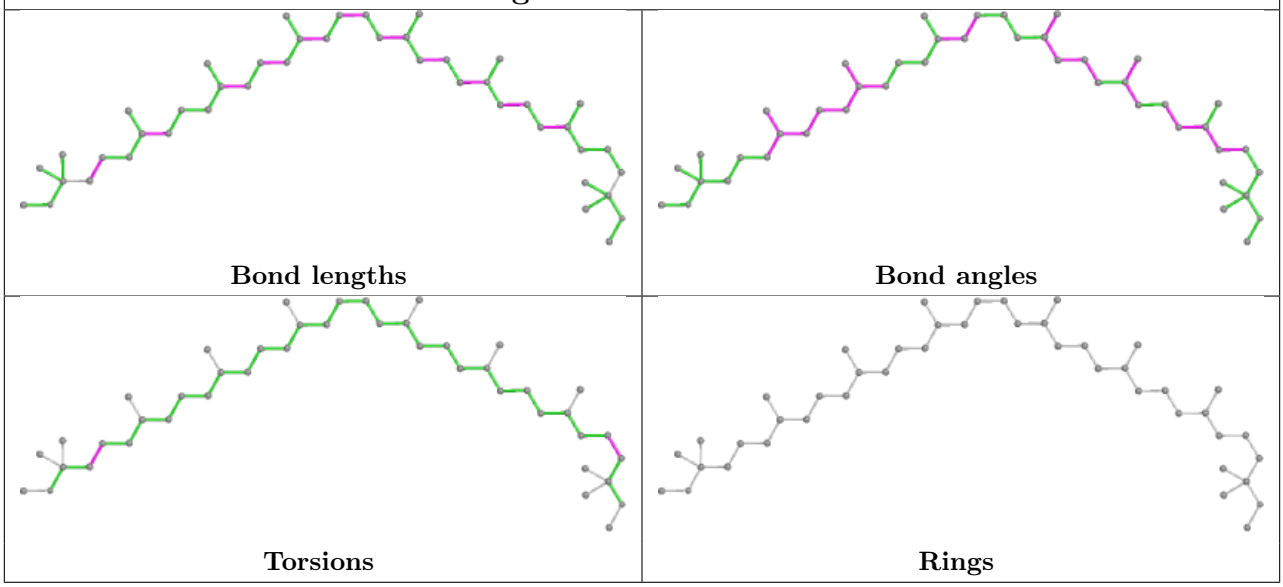
Ligand BCL BB 101



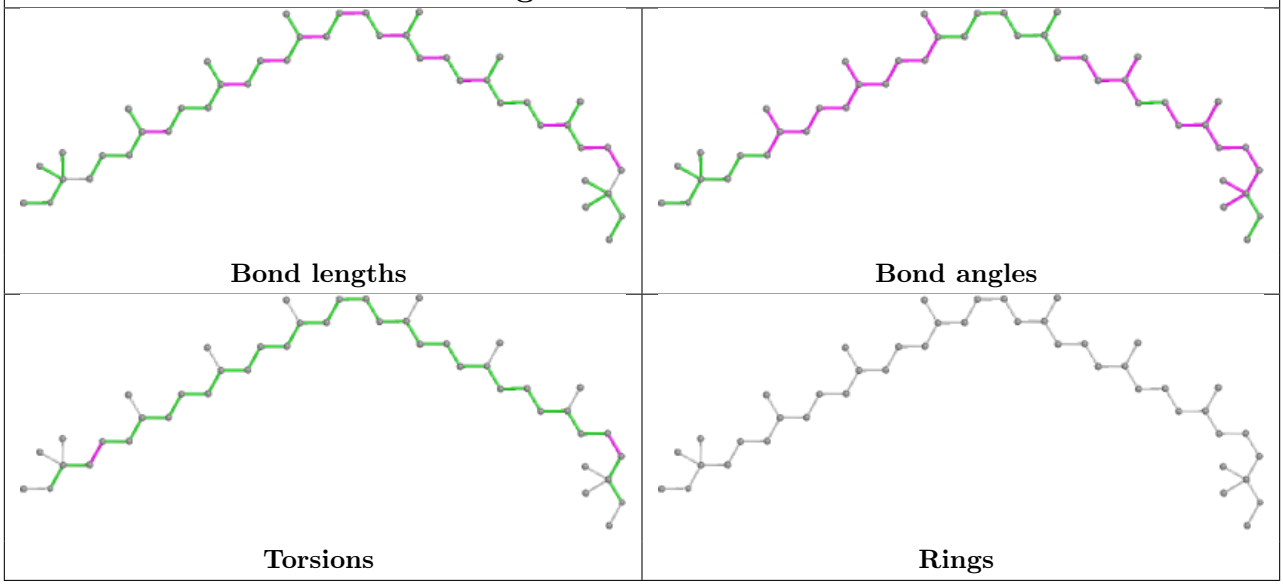
Ligand UQ8 AL 304



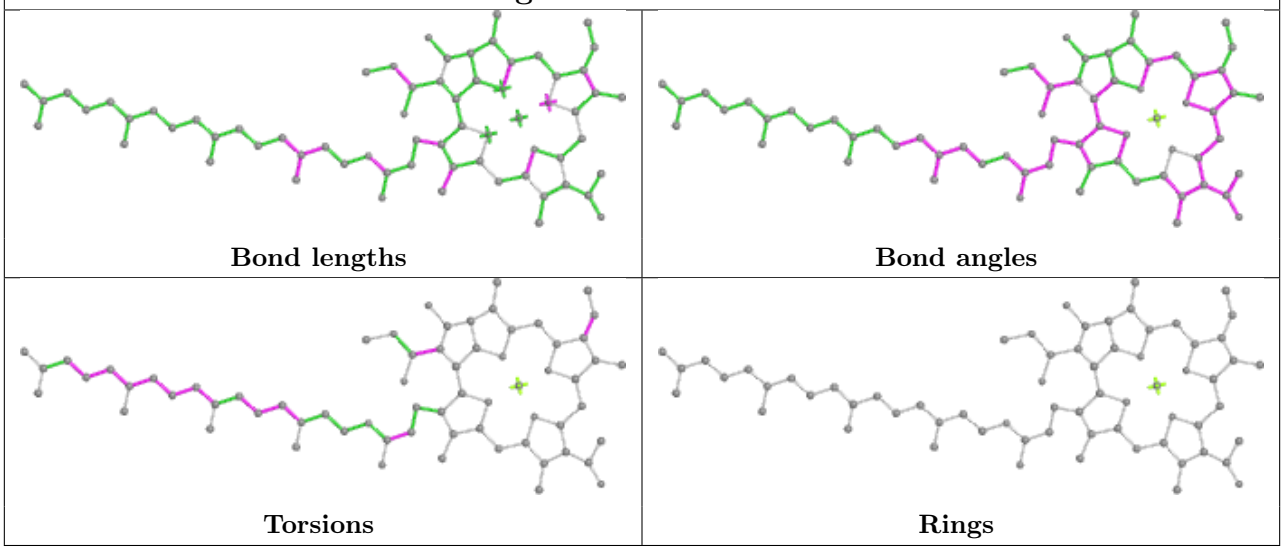
Ligand CRT BV 102



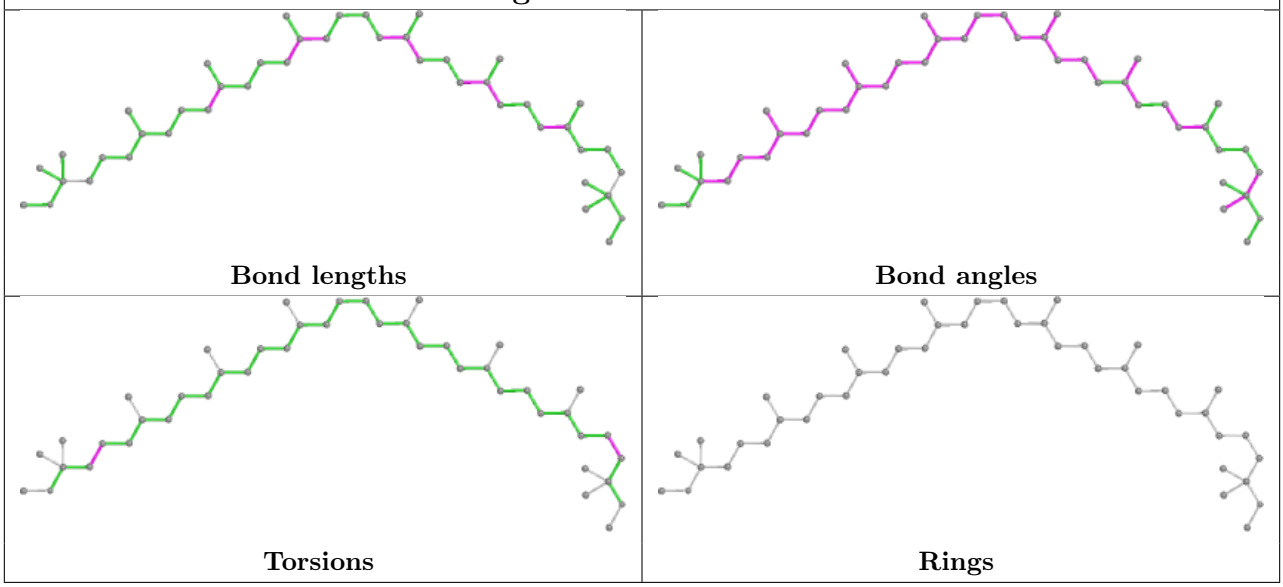
Ligand CRT B2 102



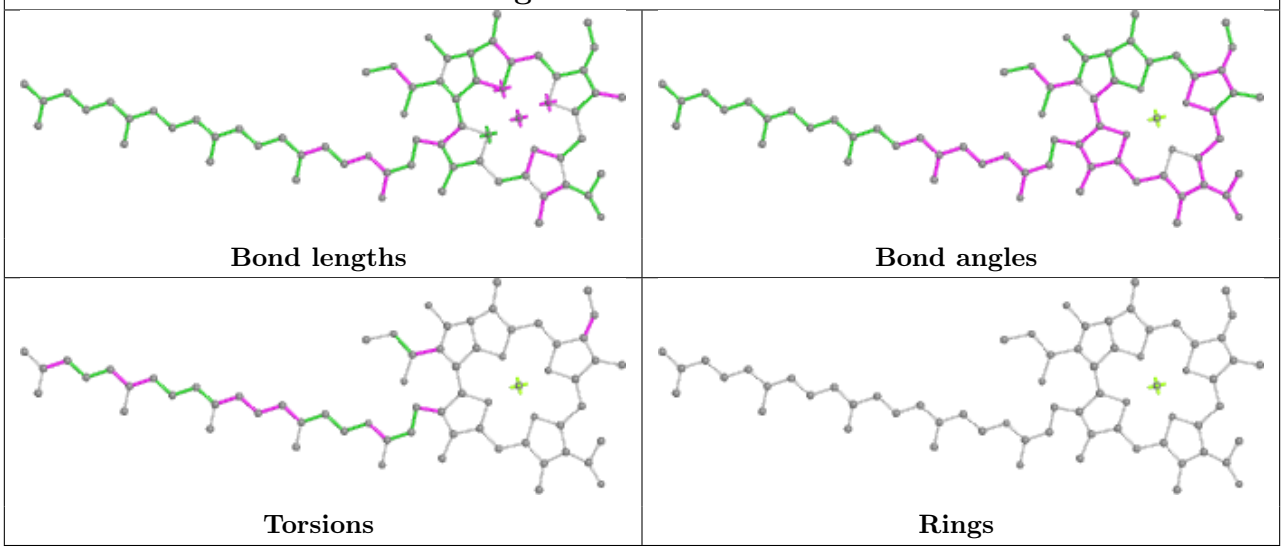
Ligand BCL AS 103



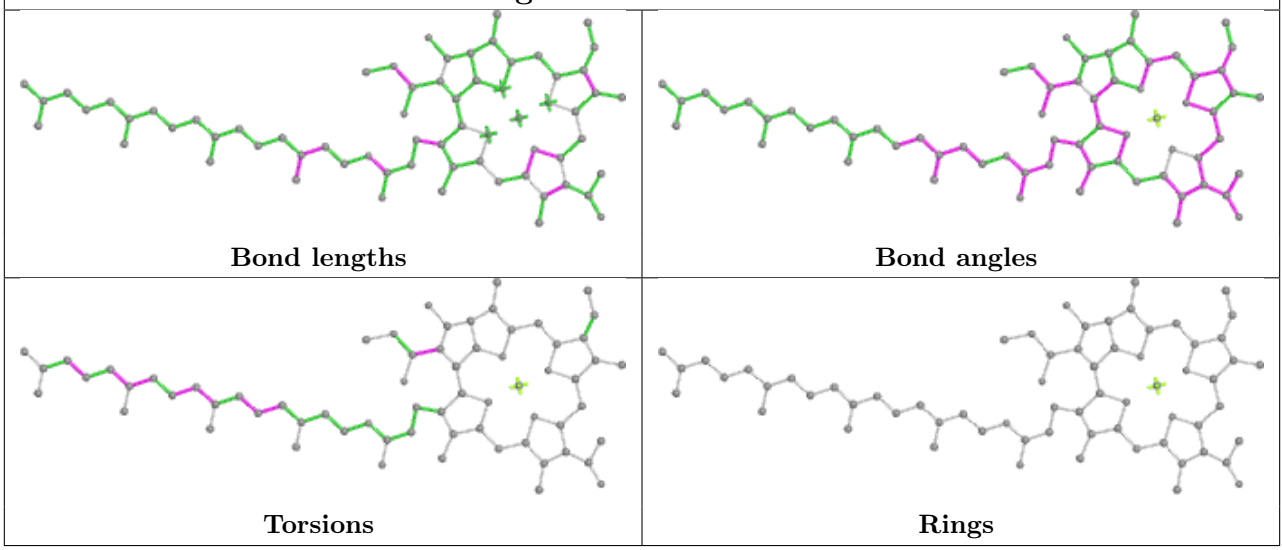
Ligand CRT BB 102



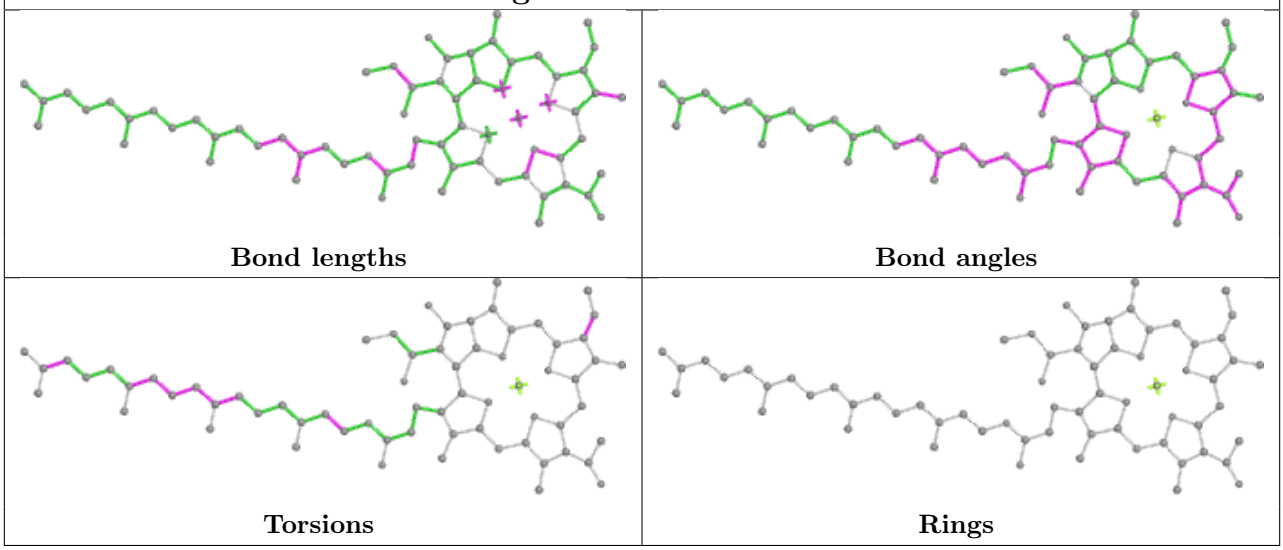
Ligand BCL AZ 101



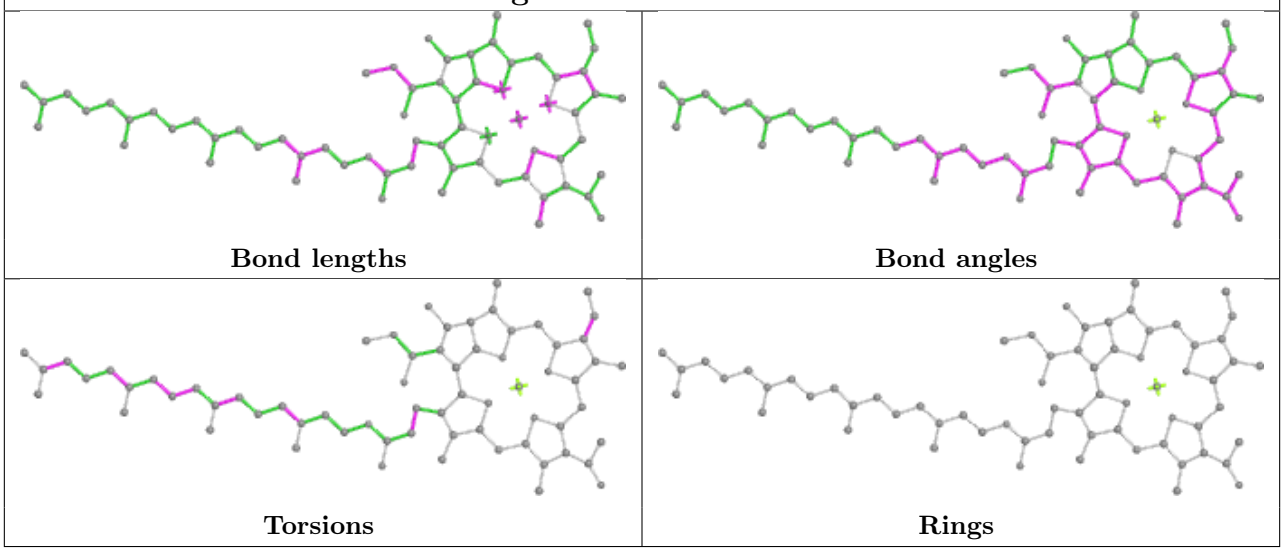
Ligand BCL BL 303



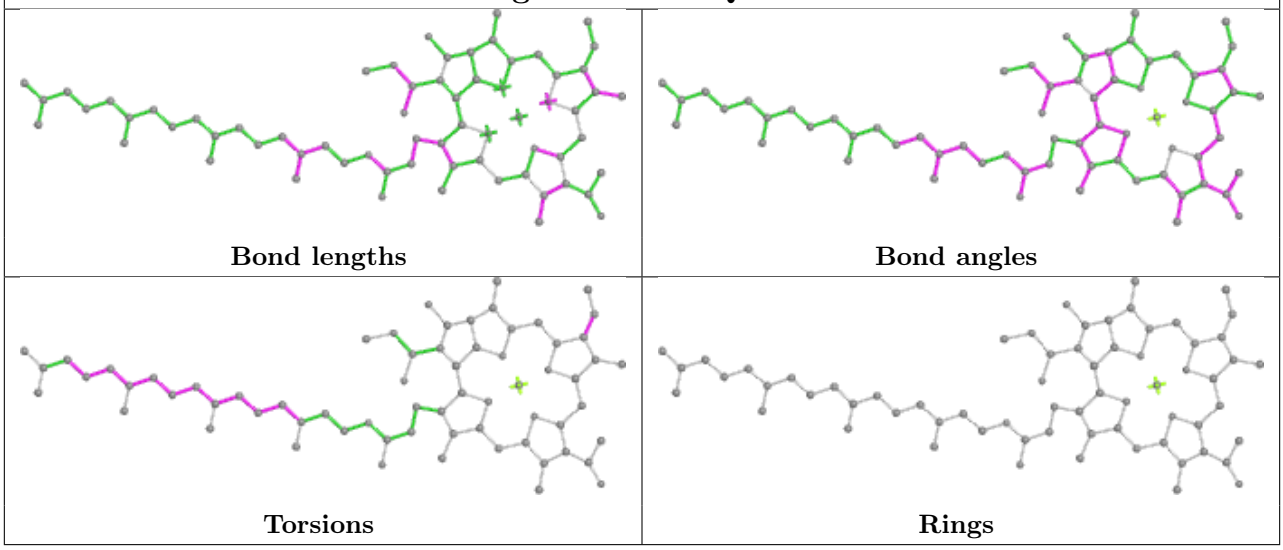
Ligand BCL BN 101



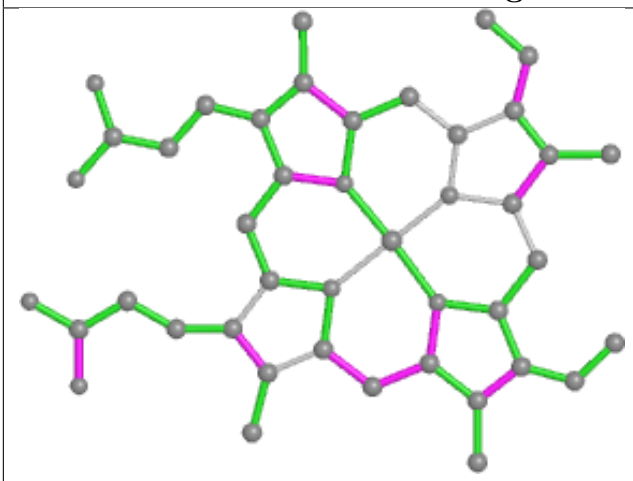
Ligand BCL AN 101



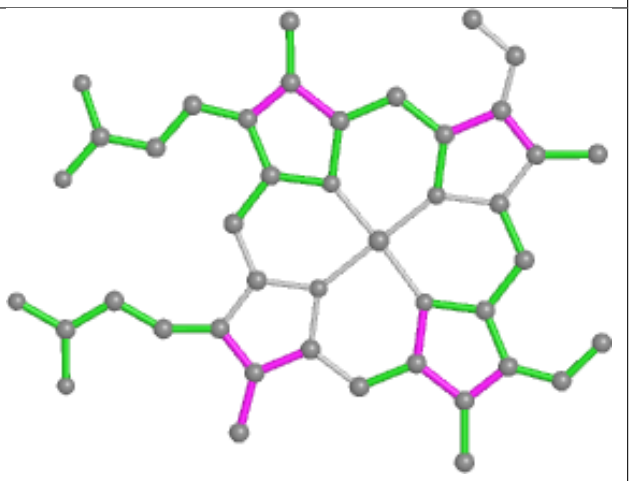
Ligand BCL AQ 102



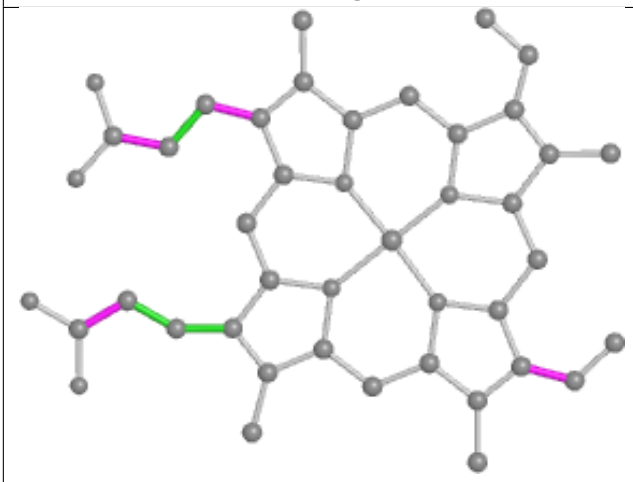
Ligand HEM AC 503



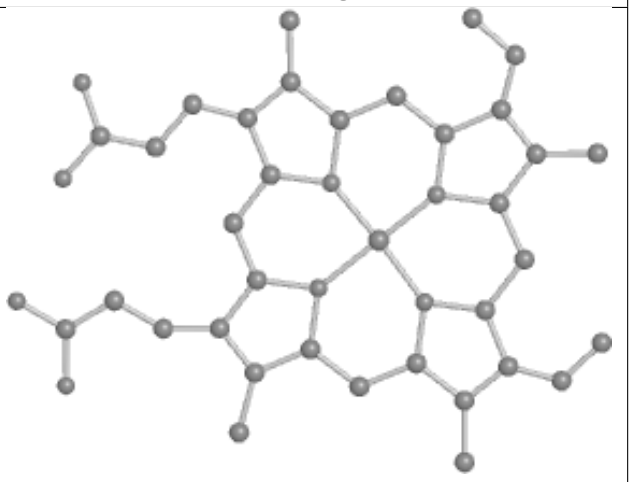
Bond lengths



Bond angles

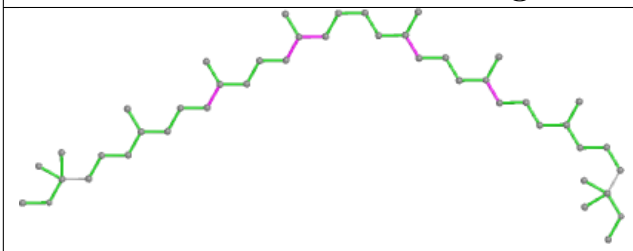


Torsions

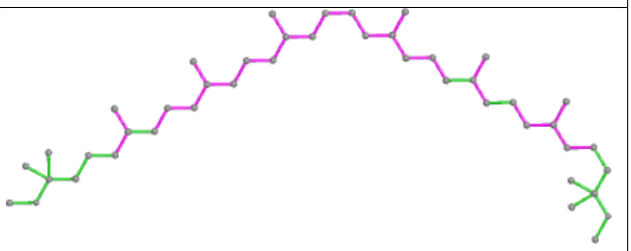


Rings

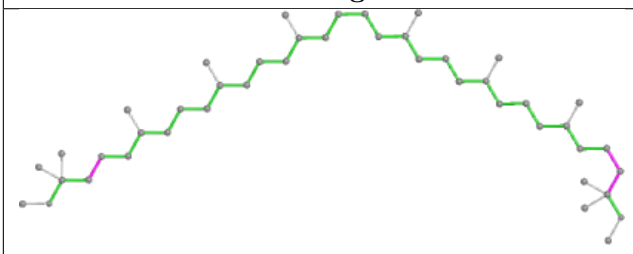
Ligand CRT AB 102



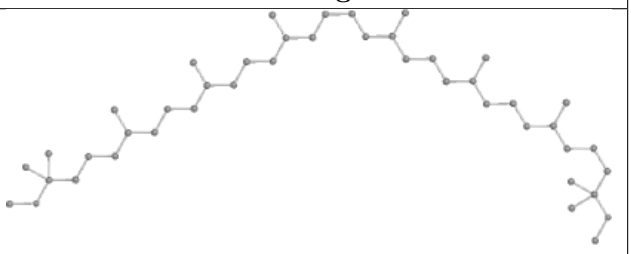
Bond lengths



Bond angles

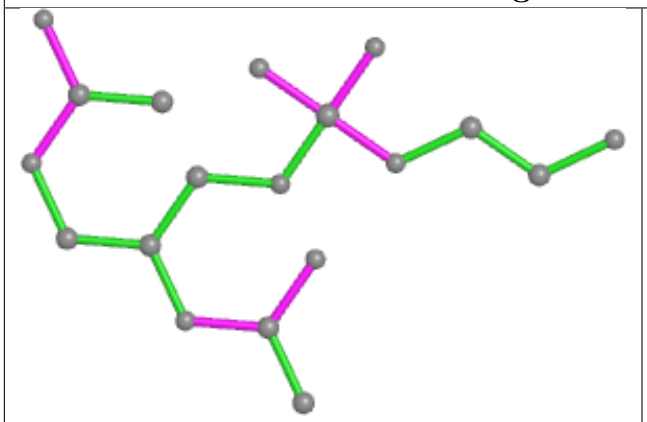


Torsions

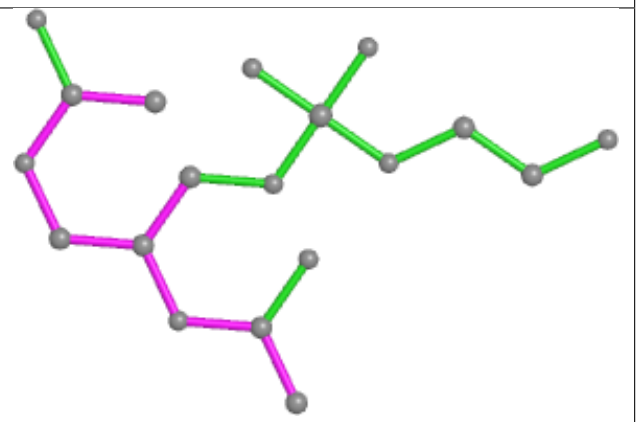


Rings

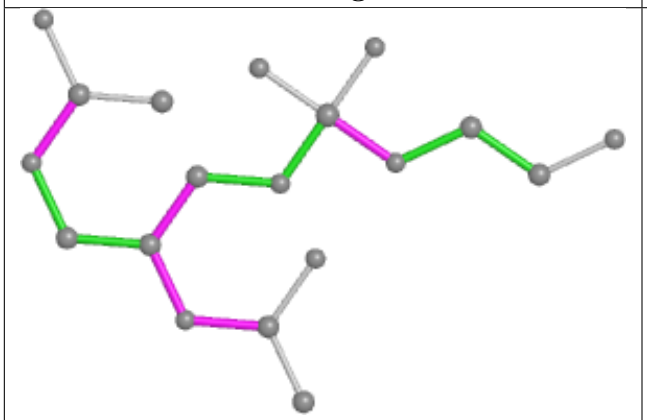
Ligand PEF AH 301



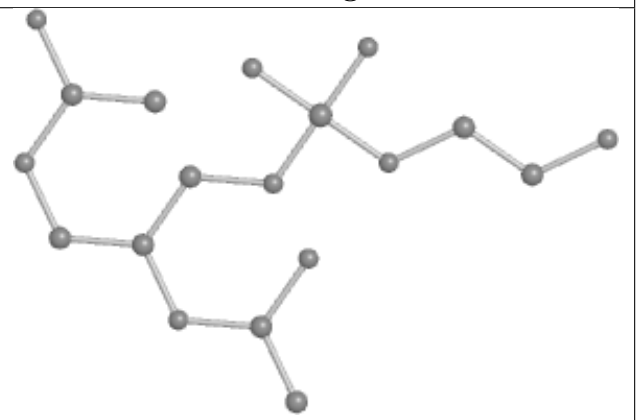
Bond lengths



Bond angles

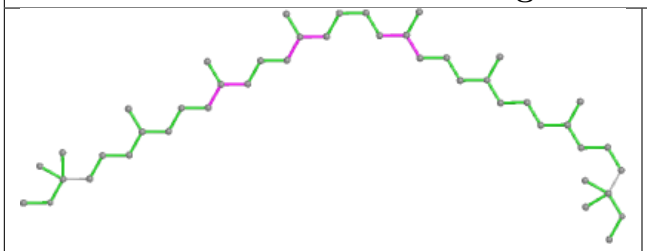


Torsions

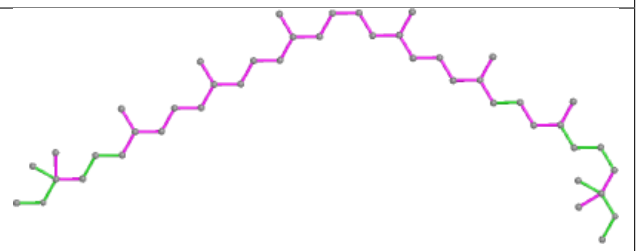


Rings

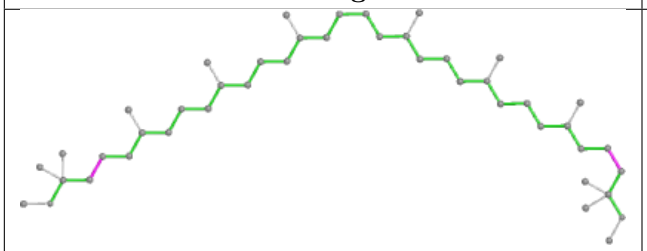
Ligand CRT B1 103



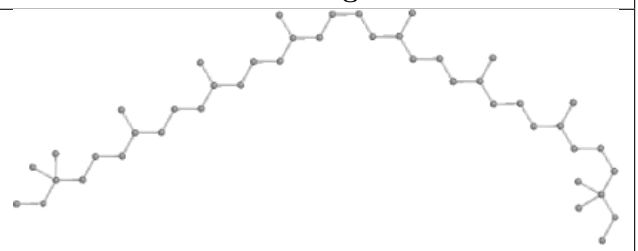
Bond lengths



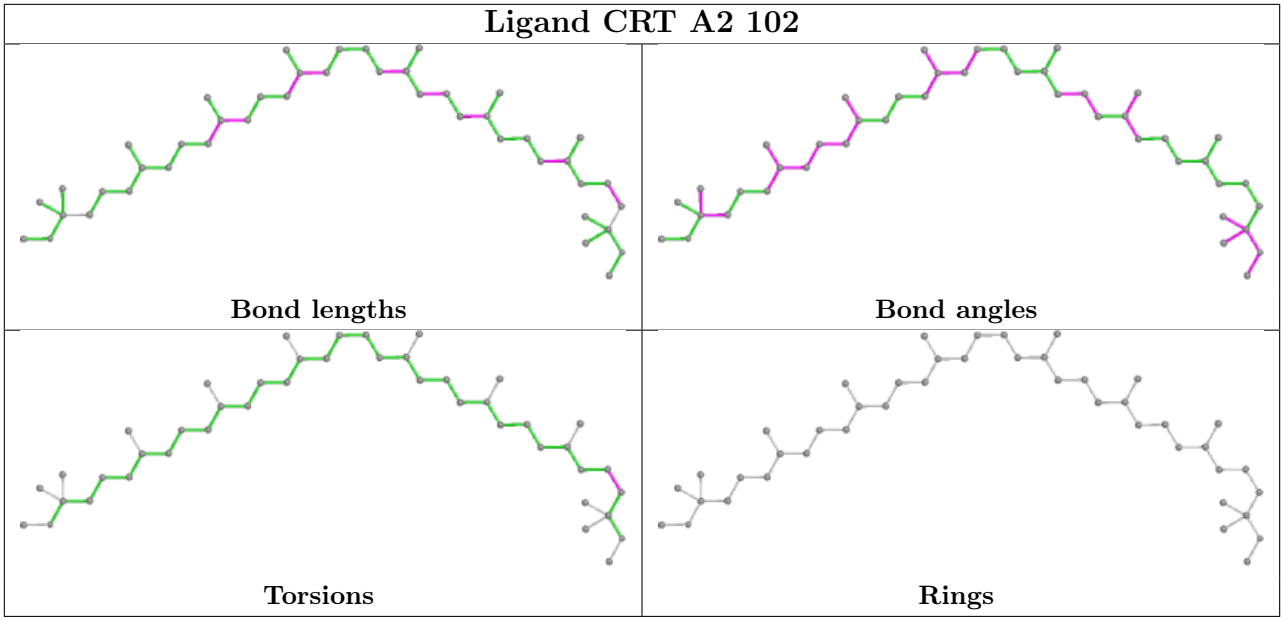
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AC	317/404 (78%)	0.06	19 (5%)	21	7	41, 84, 141, 197	1 (0%)
1	BC	317/404 (78%)	0.15	24 (7%)	13	4	58, 91, 139, 165	1 (0%)
2	AL	280/281 (99%)	-0.15	8 (2%)	51	23	21, 58, 119, 145	0
2	BL	280/281 (99%)	-0.02	16 (5%)	23	8	33, 77, 136, 156	0
3	AM	319/325 (98%)	-0.13	9 (2%)	53	25	19, 65, 107, 121	0
3	BM	319/325 (98%)	-0.11	10 (3%)	49	21	37, 80, 125, 184	0
4	AH	258/259 (99%)	0.25	16 (6%)	20	7	46, 95, 149, 183	0
4	BH	258/259 (99%)	0.23	24 (9%)	8	3	57, 104, 164, 183	0
5	A1	58/61 (95%)	0.62	10 (17%)	1	0	73, 163, 300, 305	0
5	A3	57/61 (93%)	0.40	6 (10%)	6	2	117, 162, 318, 320	0
5	A5	56/61 (91%)	1.36	13 (23%)	0	0	70, 165, 320, 321	0
5	A7	51/61 (83%)	0.51	9 (17%)	1	0	111, 148, 234, 251	0
5	A9	60/61 (98%)	0.73	13 (21%)	0	0	96, 151, 319, 319	0
5	AA	48/61 (78%)	0.71	10 (20%)	1	0	92, 144, 241, 257	0
5	AD	57/61 (93%)	0.99	12 (21%)	1	0	97, 145, 222, 239	0
5	AF	59/61 (96%)	0.37	6 (10%)	6	2	99, 130, 226, 235	0
5	AI	59/61 (96%)	0.91	11 (18%)	1	0	81, 143, 236, 267	0
5	AK	58/61 (95%)	0.08	5 (8%)	10	3	81, 140, 226, 261	0
5	AO	59/61 (96%)	0.88	10 (16%)	1	0	88, 158, 258, 262	0
5	AQ	57/61 (93%)	0.17	4 (7%)	16	5	56, 135, 277, 280	0
5	AS	59/61 (96%)	0.50	6 (10%)	6	2	86, 158, 300, 309	0
5	AU	60/61 (98%)	0.88	13 (21%)	0	0	144, 167, 252, 254	0
5	AW	60/61 (98%)	0.18	5 (8%)	11	3	68, 135, 239, 250	0
5	AY	60/61 (98%)	0.68	8 (13%)	3	1	128, 152, 278, 284	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
5	B1	54/61 (88%)	0.14	3 (5%) 24 8	88, 126, 237, 238	0
5	B3	60/61 (98%)	0.51	7 (11%) 4 1	103, 151, 262, 263	0
5	B5	51/61 (83%)	1.72	20 (39%) 0 0	131, 174, 234, 237	0
5	B7	54/61 (88%)	0.49	6 (11%) 5 1	120, 191, 255, 261	0
5	B9	51/61 (83%)	0.39	5 (9%) 7 2	101, 150, 240, 241	0
5	BA	55/61 (90%)	0.81	9 (16%) 1 0	112, 161, 261, 269	0
5	BD	45/61 (73%)	1.04	6 (13%) 3 1	135, 140, 226, 247	0
5	BF	56/61 (91%)	0.69	10 (17%) 1 0	135, 168, 237, 251	0
5	BI	50/61 (81%)	0.36	7 (14%) 2 1	107, 134, 223, 229	0
5	BK	60/61 (98%)	0.96	13 (21%) 0 0	152, 166, 314, 318	0
5	BO	59/61 (96%)	0.52	10 (16%) 1 0	76, 129, 292, 295	0
5	BQ	59/61 (96%)	1.04	11 (18%) 1 0	150, 168, 266, 274	0
5	BS	59/61 (96%)	1.07	14 (23%) 0 0	91, 159, 250, 253	0
5	BU	58/61 (95%)	1.13	13 (22%) 0 0	109, 150, 280, 282	0
5	BW	58/61 (95%)	0.87	12 (20%) 1 0	49, 114, 230, 232	0
5	BY	54/61 (88%)	0.18	3 (5%) 24 8	46, 95, 222, 230	0
6	A0	40/47 (85%)	0.03	2 (5%) 28 10	166, 177, 205, 220	0
6	A2	40/47 (85%)	0.64	8 (20%) 1 0	122, 146, 202, 211	0
6	A4	40/47 (85%)	-0.04	3 (7%) 14 4	147, 151, 221, 222	0
6	A6	40/47 (85%)	-0.20	2 (5%) 28 10	140, 155, 199, 213	0
6	A8	40/47 (85%)	0.85	10 (25%) 0 0	129, 187, 225, 229	0
6	AB	40/47 (85%)	0.33	6 (15%) 2 1	122, 162, 189, 190	0
6	AE	40/47 (85%)	0.49	9 (22%) 0 0	120, 145, 169, 184	0
6	AG	40/47 (85%)	-0.07	1 (2%) 57 29	74, 116, 140, 145	0
6	AJ	40/47 (85%)	0.18	4 (10%) 7 2	118, 129, 154, 159	0
6	AN	40/47 (85%)	-0.03	2 (5%) 28 10	101, 121, 155, 161	0
6	AP	40/47 (85%)	0.09	4 (10%) 7 2	106, 142, 245, 248	0
6	AR	40/47 (85%)	0.81	10 (25%) 0 0	122, 157, 194, 199	0
6	AT	40/47 (85%)	0.23	3 (7%) 14 4	119, 148, 198, 205	0
6	AV	40/47 (85%)	0.79	7 (17%) 1 0	130, 167, 222, 225	0
6	AX	40/47 (85%)	0.24	4 (10%) 7 2	157, 167, 194, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
6	AZ	40/47 (85%)	0.62	7 (17%)	1	0	111, 137, 238, 240	0
6	B0	40/47 (85%)	0.89	8 (20%)	1	0	197, 208, 220, 221	0
6	B2	40/47 (85%)	-0.07	0	100	100	116, 127, 158, 162	0
6	B4	40/47 (85%)	0.59	4 (10%)	7	2	134, 156, 191, 199	0
6	B6	40/47 (85%)	1.14	10 (25%)	0	0	115, 152, 213, 215	0
6	B8	40/47 (85%)	0.48	4 (10%)	7	2	123, 199, 232, 234	0
6	BB	40/47 (85%)	0.66	8 (20%)	1	0	155, 164, 228, 231	0
6	BE	40/47 (85%)	0.43	6 (15%)	2	1	148, 170, 194, 212	0
6	BG	40/47 (85%)	0.87	7 (17%)	1	0	185, 204, 218, 220	0
6	BJ	40/47 (85%)	0.87	6 (15%)	2	1	199, 204, 208, 209	0
6	BN	40/47 (85%)	0.38	4 (10%)	7	2	152, 160, 194, 200	0
6	BP	40/47 (85%)	0.13	5 (12%)	3	1	124, 149, 226, 230	0
6	BR	40/47 (85%)	0.64	4 (10%)	7	2	138, 171, 206, 213	0
6	BT	40/47 (85%)	0.29	3 (7%)	14	4	132, 157, 227, 233	0
6	BV	40/47 (85%)	-0.07	2 (5%)	28	10	91, 143, 170, 174	0
6	BX	40/47 (85%)	-0.16	1 (2%)	57	29	100, 127, 169, 172	0
6	BZ	40/47 (85%)	0.46	4 (10%)	7	2	121, 135, 178, 186	0
All	All	5429/5994 (90%)	0.33	574 (10%)	6	2	19, 123, 236, 321	2 (0%)

The worst 5 of 574 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AC	17	SER	21.5
5	BD	41	SER	17.9
5	A5	5	ASN	16.8
1	AC	18	VAL	15.7
4	AH	51	GLY	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
8	CA	AO	101	1/1	-0.72	0.43	267,267,267,267	0
8	CA	BA	103	1/1	-0.45	0.09	283,283,283,283	0
8	CA	AF	101	1/1	0.16	0.13	254,254,254,254	0
8	CA	BO	101	1/1	0.18	0.15	238,238,238,238	0
8	CA	B1	101	1/1	0.32	0.12	184,184,184,184	0
8	CA	B5	101	1/1	0.32	0.15	226,226,226,226	0
14	CRT	BB	102	44/44	0.35	1.06	169,185,201,205	0
14	CRT	BV	102	44/44	0.39	0.80	208,214,218,220	0
14	CRT	AR	102	44/44	0.40	1.09	189,193,200,201	0
14	CRT	BO	103	44/44	0.41	1.22	179,182,185,186	0
14	CRT	AW	102	44/44	0.42	1.32	127,136,144,147	0
14	CRT	AA	102	44/44	0.43	1.03	164,164,167,167	0
8	CA	A3	102	1/1	0.43	0.09	256,256,256,256	0
14	CRT	AB	102	44/44	0.44	1.19	170,172,177,178	0
14	CRT	B5	103	44/44	0.44	1.62	178,198,221,226	0
14	CRT	A0	101	44/44	0.45	0.63	179,184,194,195	0
14	CRT	BP	102	44/44	0.46	0.87	149,151,153,154	0
8	CA	AS	102	1/1	0.46	0.11	190,190,190,190	0
14	CRT	AT	102	44/44	0.46	1.13	200,205,209,210	0
14	CRT	AP	102	44/44	0.48	1.21	137,140,147,148	0
14	CRT	BS	103	44/44	0.49	1.26	193,197,199,200	0
14	CRT	AX	102	44/44	0.50	1.79	218,225,227,229	0
8	CA	BQ	102	1/1	0.51	0.07	249,249,249,249	0
14	CRT	AJ	102	44/44	0.51	0.72	138,140,144,147	0
14	CRT	BA	102	44/44	0.51	0.85	143,157,171,174	0
14	CRT	A5	103	44/44	0.52	1.51	167,174,185,187	0
14	CRT	A7	102	44/44	0.53	0.64	126,137,150,152	0
14	CRT	B7	102	44/44	0.53	0.75	173,194,212,217	0
15	PEF	AS	101	47/47	0.55	0.43	178,225,225,225	0
15	PEF	BM	407	19/47	0.55	0.41	102,136,173,178	0
14	CRT	BU	103	44/44	0.58	1.30	161,173,176,176	0
14	CRT	B0	101	44/44	0.58	1.48	202,220,238,242	0
15	PEF	AM	409	47/47	0.58	0.62	129,183,183,183	0
8	CA	AK	101	1/1	0.58	0.10	216,216,216,216	0
8	CA	BD	101	1/1	0.58	0.08	236,236,236,236	0
14	CRT	AN	102	44/44	0.59	0.78	133,135,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	CRT	B1	103	44/44	0.59	1.04	205,224,238,240	0
14	CRT	BF	103	44/44	0.59	0.86	134,141,147,149	0
14	CRT	A1	103	44/44	0.59	1.00	110,123,135,138	0
8	CA	AU	101	1/1	0.60	0.12	223,223,223,223	0
8	CA	BI	101	1/1	0.60	0.12	236,236,236,236	0
14	CRT	B2	102	44/44	0.60	1.53	132,151,166,171	0
8	CA	BS	101	1/1	0.62	0.06	222,222,222,222	0
14	CRT	BG	102	44/44	0.62	0.52	122,130,143,145	0
8	CA	AY	101	1/1	0.62	0.14	197,197,197,197	0
14	CRT	BN	102	44/44	0.64	0.66	134,135,140,141	0
8	CA	BW	101	1/1	0.64	0.09	204,204,204,204	0
8	CA	A5	101	1/1	0.65	0.08	255,255,255,255	0
8	CA	A9	101	1/1	0.65	0.07	268,268,268,268	0
14	CRT	AG	102	44/44	0.66	0.84	126,127,135,138	0
8	CA	BU	101	1/1	0.66	0.09	237,237,237,237	0
8	CA	AA	103	1/1	0.67	0.18	275,275,275,275	0
8	CA	AI	101	1/1	0.67	0.08	224,224,224,224	0
15	PEF	BQ	101	47/47	0.67	0.88	121,145,161,161	0
14	CRT	A2	102	44/44	0.68	0.99	107,117,146,149	0
8	CA	AV	101	1/1	0.68	0.10	168,168,168,168	0
14	CRT	BW	103	44/44	0.68	0.93	129,145,156,161	0
14	CRT	AS	104	44/44	0.69	0.93	165,170,177,180	0
9	BCL	BV	101	66/66	0.71	0.45	172,194,218,220	0
8	CA	BY	101	1/1	0.72	0.16	148,148,148,148	0
9	BCL	BK	102	66/66	0.75	0.50	194,257,267,269	0
9	BCL	B9	102	66/66	0.75	0.53	205,229,236,237	0
11	UQ8	BL	304	53/53	0.75	0.42	66,137,159,166	0
9	BCL	BQ	104	66/66	0.76	0.37	181,191,253,254	0
8	CA	B7	101	1/1	0.77	0.13	259,259,259,259	0
14	CRT	BM	406	44/44	0.77	0.48	69,74,96,109	0
11	UQ8	AL	304	53/53	0.77	0.36	74,107,143,151	0
15	PEF	AM	407	19/47	0.77	0.42	114,165,177,177	0
9	BCL	BA	101	66/66	0.79	0.46	206,224,237,238	0
10	BPH	BM	403	65/65	0.79	0.26	72,96,164,176	0
14	CRT	AM	406	44/44	0.80	0.40	58,70,105,107	0
9	BCL	AS	103	66/66	0.81	0.67	206,220,229,233	0
9	BCL	BP	101	66/66	0.81	0.40	156,173,208,209	0
9	BCL	A3	103	66/66	0.81	0.50	127,137,178,178	0
8	CA	B9	101	1/1	0.81	0.25	150,150,150,150	0
15	PEF	AH	301	19/47	0.81	0.24	128,144,161,167	0
9	BCL	BZ	101	66/66	0.81	0.30	125,139,192,193	0
9	BCL	B8	101	66/66	0.81	0.37	226,245,252,258	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	BD	102	66/66	0.81	0.44	147,182,237,238	0
9	BCL	BS	102	66/66	0.82	0.38	152,193,231,231	0
9	BCL	BT	101	66/66	0.82	0.43	176,191,253,254	0
9	BCL	AR	101	66/66	0.82	0.36	187,200,230,231	0
9	BCL	BJ	101	66/66	0.82	0.41	202,204,207,208	0
9	BCL	A7	103	66/66	0.82	0.35	239,243,267,268	0
9	BCL	BM	402	66/66	0.82	0.35	41,58,73,79	0
9	BCL	A2	101	66/66	0.82	0.40	122,133,201,203	0
13	MQ8	AM	405	53/53	0.83	0.49	76,93,128,137	0
13	MQ8	BM	405	53/53	0.83	0.38	68,99,166,168	0
9	BCL	BF	102	66/66	0.83	0.43	143,168,206,210	0
9	BCL	AQ	102	66/66	0.83	0.52	187,198,210,221	0
9	BCL	A3	104	66/66	0.83	0.38	151,177,223,224	0
9	BCL	BN	101	66/66	0.83	0.51	153,170,192,193	0
8	CA	B3	101	1/1	0.83	0.07	222,222,222,222	0
9	BCL	AA	101	66/66	0.84	0.42	235,252,257,260	0
9	BCL	B7	103	66/66	0.84	0.47	232,250,259,260	0
9	BCL	AI	102	66/66	0.84	0.50	148,163,190,191	0
9	BCL	AV	102	66/66	0.84	0.39	183,194,249,250	0
9	BCL	BI	102	66/66	0.84	0.38	131,159,208,208	0
9	BCL	A9	102	66/66	0.84	0.43	213,227,251,252	0
8	CA	AQ	101	1/1	0.84	0.05	207,207,207,207	0
9	BCL	A5	102	66/66	0.85	0.41	152,159,199,200	0
9	BCL	AN	101	66/66	0.85	0.31	106,126,157,171	0
9	BCL	B0	102	66/66	0.85	0.47	198,202,205,207	0
9	BCL	AU	102	66/66	0.85	0.57	161,175,231,234	0
9	BCL	A6	101	66/66	0.86	0.36	238,254,268,272	0
9	BCL	AD	102	66/66	0.86	0.44	179,196,260,263	0
8	CA	BK	101	1/1	0.86	0.20	275,275,275,275	0
9	BCL	BO	102	66/66	0.86	0.34	153,180,189,193	0
9	BCL	AT	101	66/66	0.86	0.36	187,198,247,248	0
9	BCL	B4	101	66/66	0.86	0.42	149,166,212,214	0
9	BCL	B6	101	66/66	0.86	0.39	238,251,261,264	0
9	BCL	BB	101	66/66	0.87	0.43	187,209,245,245	0
9	BCL	BU	102	66/66	0.87	0.36	144,161,240,240	0
9	BCL	AK	102	66/66	0.87	0.34	142,154,184,184	0
9	BCL	BW	102	66/66	0.87	0.39	129,145,213,213	0
9	BCL	BE	101	66/66	0.87	0.36	146,170,225,227	0
9	BCL	AB	101	66/66	0.87	0.28	124,158,224,224	0
9	BCL	AY	102	66/66	0.87	0.48	133,140,195,196	0
9	BCL	AJ	101	66/66	0.87	0.43	134,165,191,193	0
16	PO4	A3	101	5/5	0.87	0.20	153,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	B2	101	66/66	0.88	0.41	136,152,203,204	0
9	BCL	AX	101	66/66	0.88	0.41	157,171,252,255	0
8	CA	BF	101	1/1	0.88	0.07	276,276,276,276	0
8	CA	AD	101	1/1	0.88	0.09	238,238,238,238	0
9	BCL	AL	301	66/66	0.88	0.27	38,50,92,96	0
8	CA	A1	101	1/1	0.88	0.07	212,212,212,212	0
8	CA	A7	101	1/1	0.88	0.05	213,213,213,213	0
10	BPH	AL	302	65/65	0.88	0.25	31,54,75,84	0
9	BCL	AO	102	66/66	0.88	0.43	199,207,214,219	0
9	BCL	A0	102	66/66	0.89	0.29	199,210,239,240	0
15	PEF	AM	408	14/47	0.89	0.23	12,90,119,125	0
9	BCL	B5	102	66/66	0.89	0.28	154,171,221,221	0
10	BPH	BL	302	65/65	0.89	0.23	36,63,98,116	0
9	BCL	BG	101	66/66	0.89	0.33	201,207,214,217	0
9	BCL	BY	102	66/66	0.89	0.36	110,129,169,169	0
9	BCL	AW	101	66/66	0.89	0.51	143,191,243,243	0
9	BCL	AE	101	66/66	0.89	0.30	135,156,211,212	0
10	BPH	AM	403	65/65	0.90	0.26	43,61,150,153	0
9	BCL	BX	101	66/66	0.90	0.36	126,139,204,205	0
9	BCL	AF	102	66/66	0.90	0.39	156,175,222,222	0
7	HEM	BC	502	43/43	0.90	0.28	50,80,94,103	0
9	BCL	AM	402	66/66	0.90	0.25	40,48,81,101	0
9	BCL	BQ	103	66/66	0.90	0.51	168,191,225,226	0
9	BCL	A8	101	66/66	0.90	0.26	201,214,245,247	0
9	BCL	B1	102	66/66	0.91	0.38	87,118,185,186	0
9	BCL	BM	401	66/66	0.91	0.21	33,56,137,146	0
9	BCL	B3	102	66/66	0.91	0.37	104,112,169,170	0
9	BCL	A1	102	66/66	0.91	0.40	96,135,194,194	0
16	PO4	AM	410	5/5	0.91	0.20	83,84,84,84	0
9	BCL	AG	101	66/66	0.91	0.37	105,132,177,178	0
9	BCL	AM	401	66/66	0.92	0.23	19,34,93,96	0
7	HEM	BC	501	43/43	0.92	0.24	52,60,117,131	0
7	HEM	AC	501	43/43	0.92	0.26	86,86,86,96	0
7	HEM	BC	503	43/43	0.92	0.24	84,110,135,146	0
9	BCL	BL	301	66/66	0.92	0.23	36,53,94,100	0
7	HEM	BC	504	43/43	0.93	0.22	55,78,92,106	0
7	HEM	AC	502	43/43	0.93	0.25	53,68,81,88	0
7	HEM	AC	503	43/43	0.93	0.28	71,84,106,112	0
7	HEM	AC	504	43/43	0.93	0.26	39,76,101,104	0
9	BCL	AP	101	66/66	0.94	0.34	107,127,189,190	0
9	BCL	AL	303	66/66	0.94	0.22	32,54,95,104	0
9	BCL	BL	303	66/66	0.94	0.20	39,55,82,90	0

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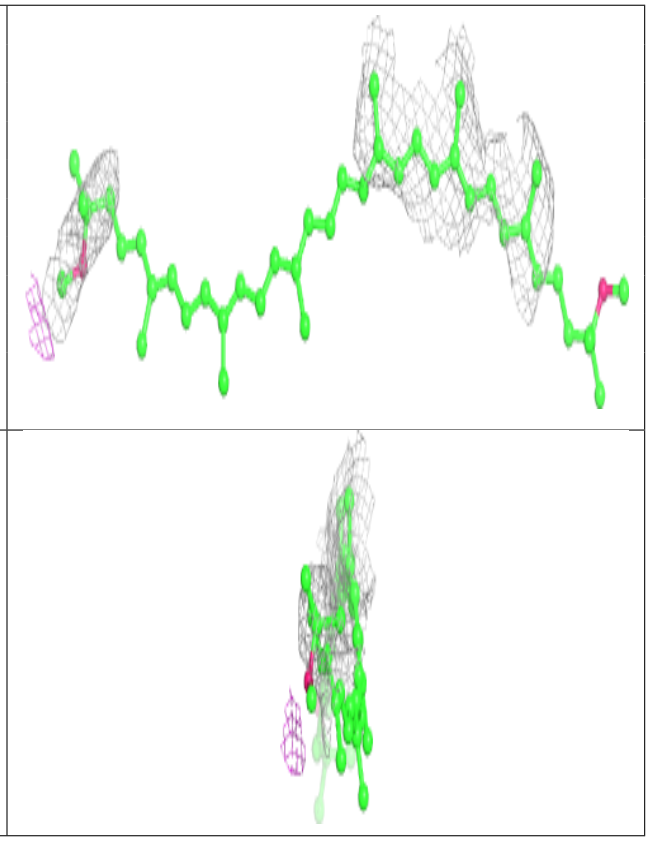
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	PO4	AH	302	5/5	0.94	0.13	102,103,104,104	0
9	BCL	AZ	101	66/66	0.94	0.36	120,142,217,218	0
16	PO4	BH	301	5/5	0.94	0.13	108,109,109,110	0
12	FE	BM	404	1/1	0.98	0.07	44,44,44,44	0
8	CA	BC	505	1/1	0.98	0.07	69,69,69,69	0
8	CA	AC	505	1/1	0.99	0.07	30,30,30,30	0
12	FE	AM	404	1/1	0.99	0.09	47,47,47,47	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.

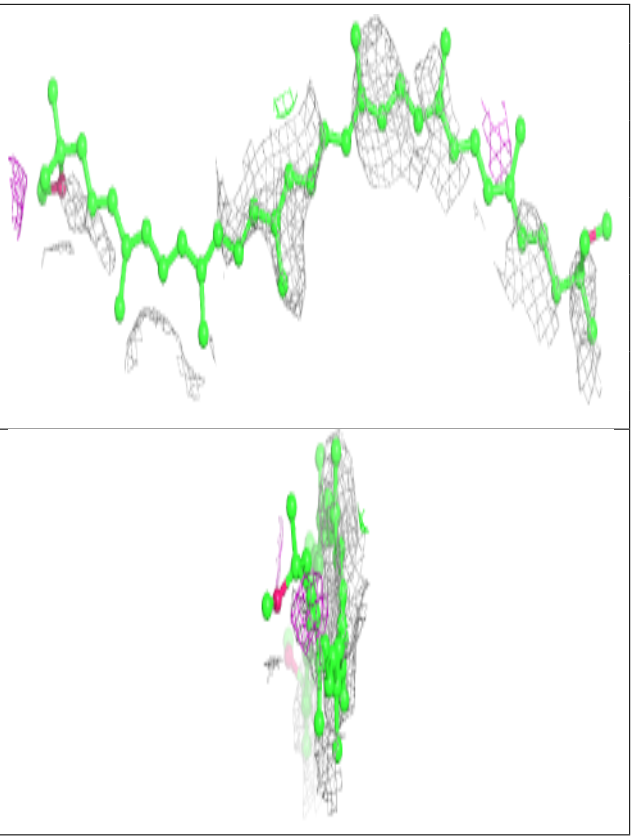
Electron density around CRT BB 102:

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



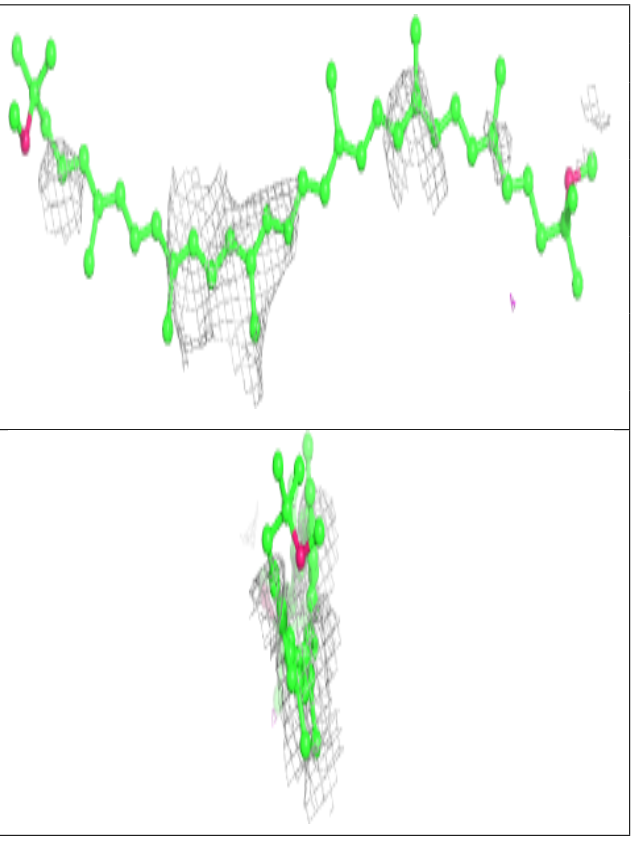
Electron density around CRT BV 102:

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



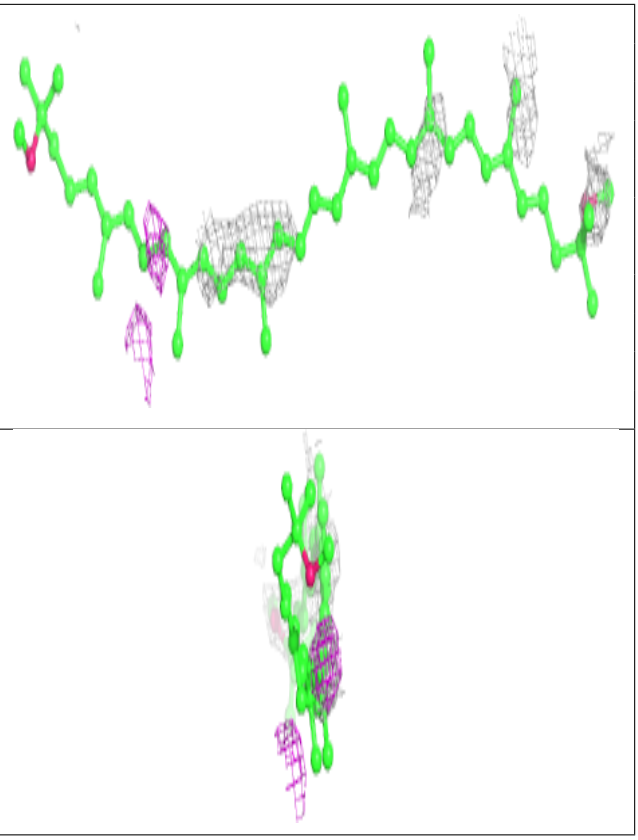
Electron density around CRT AR 102:

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



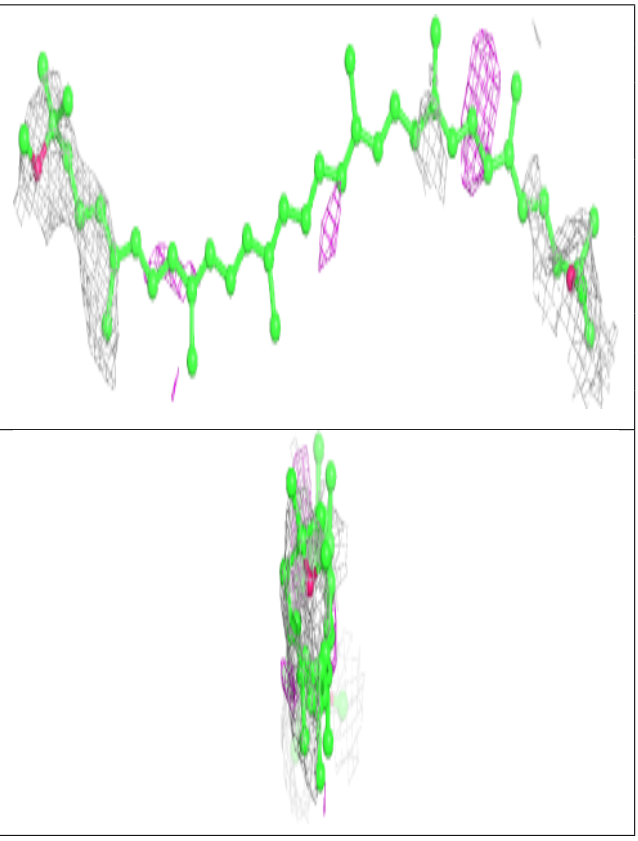
Electron density around CRT BO 103:

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



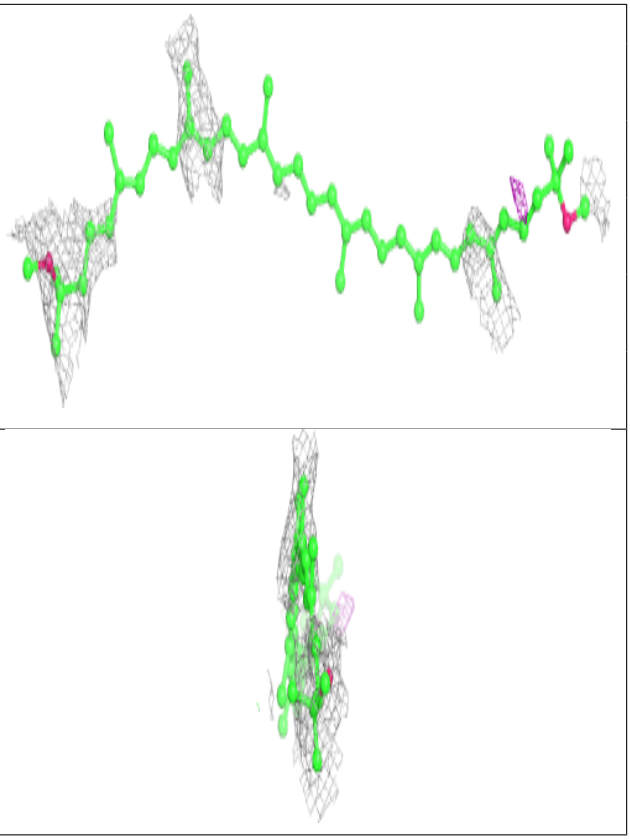
Electron density around CRT AW 102:

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



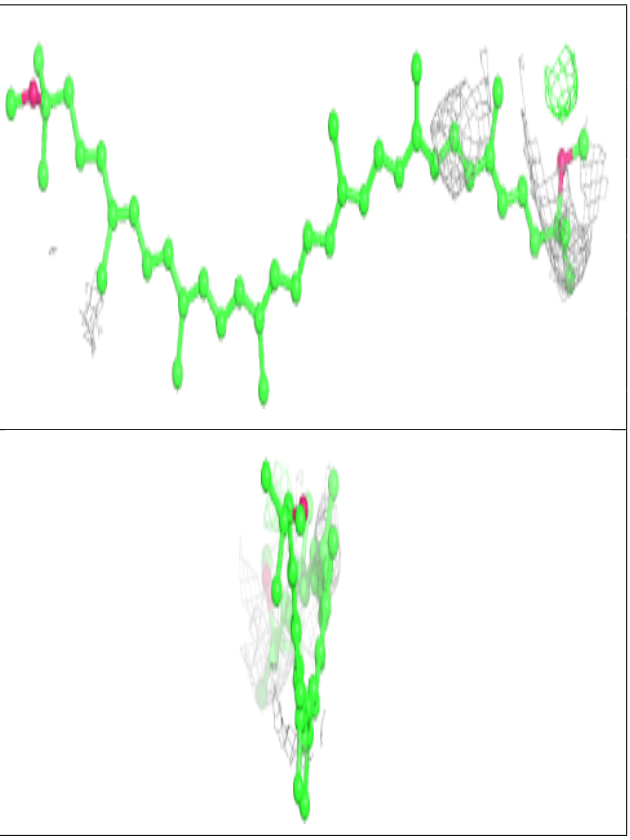
Electron density around CRT AA 102:

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



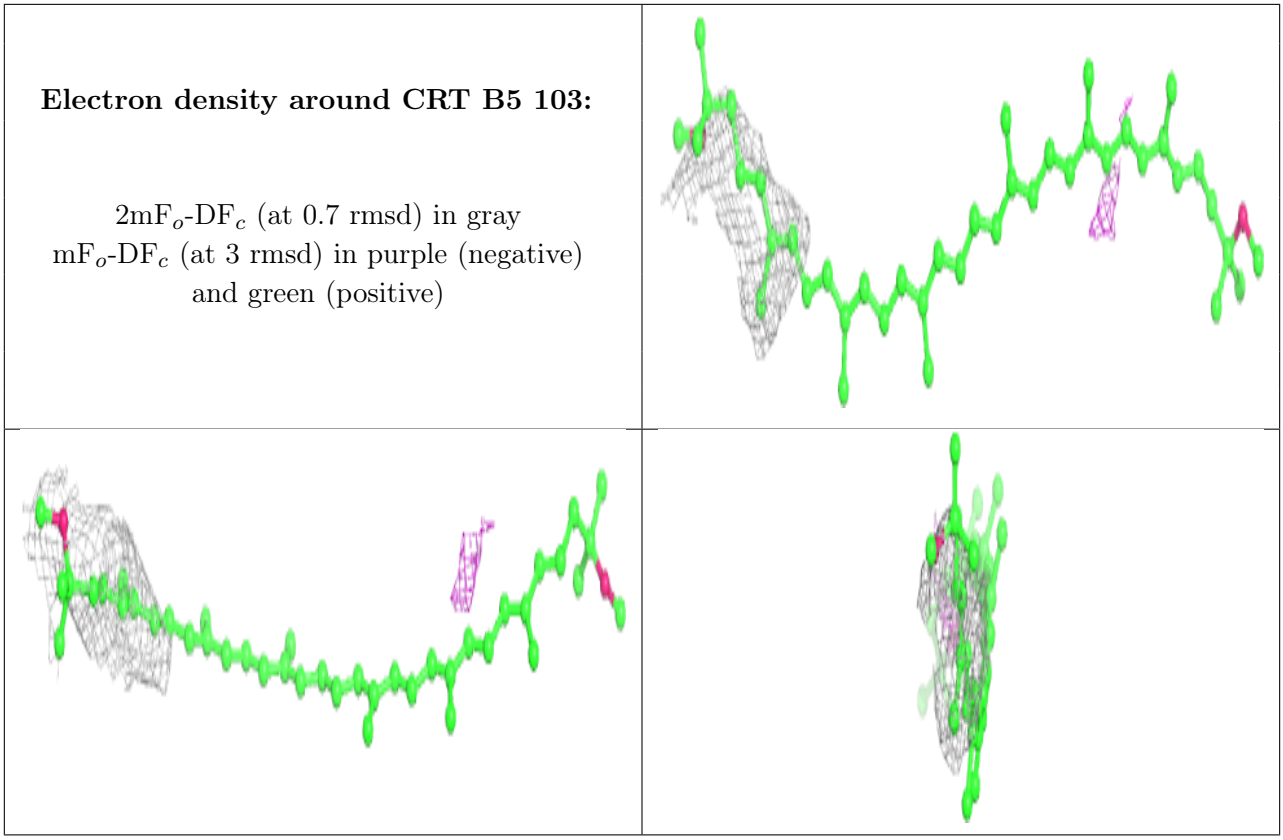
Electron density around CRT AB 102:

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



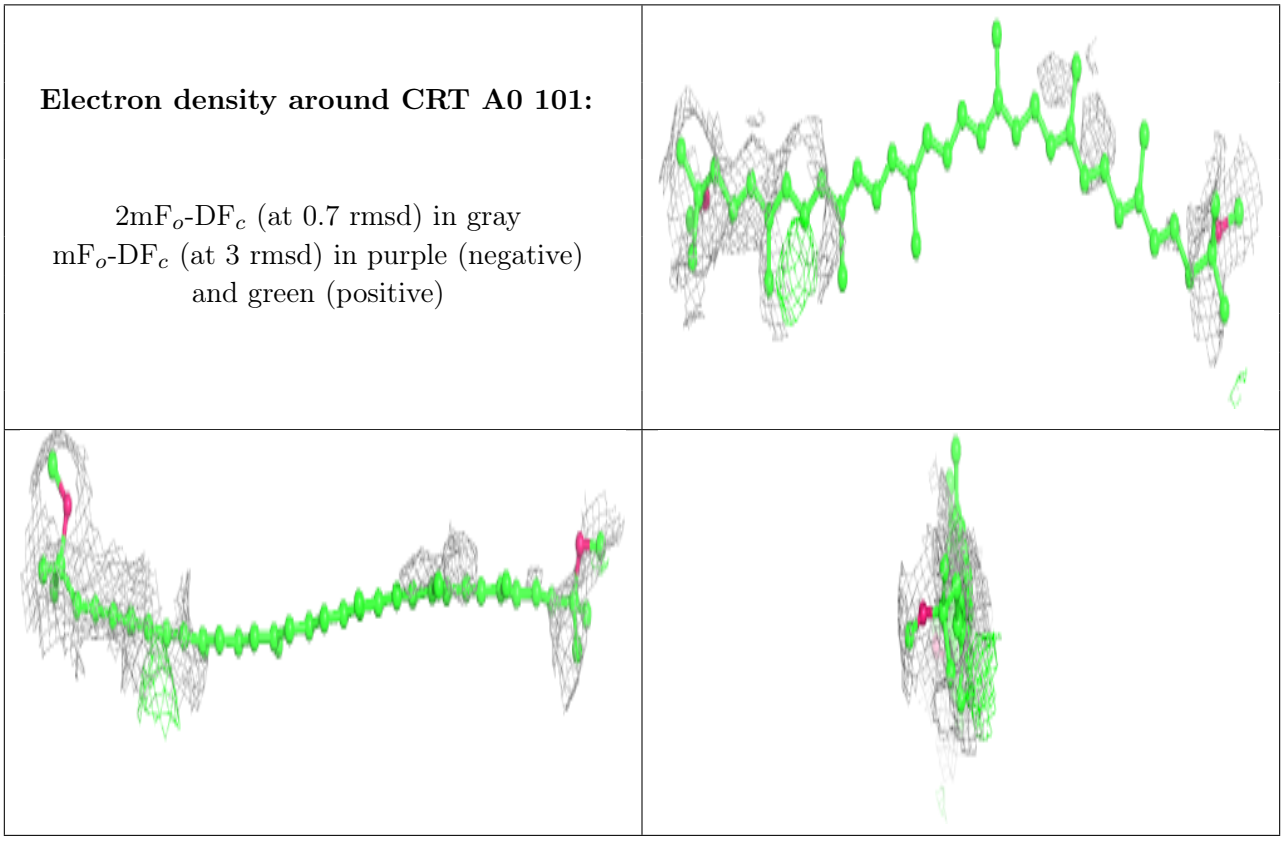
Electron density around CRT B5 103:

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



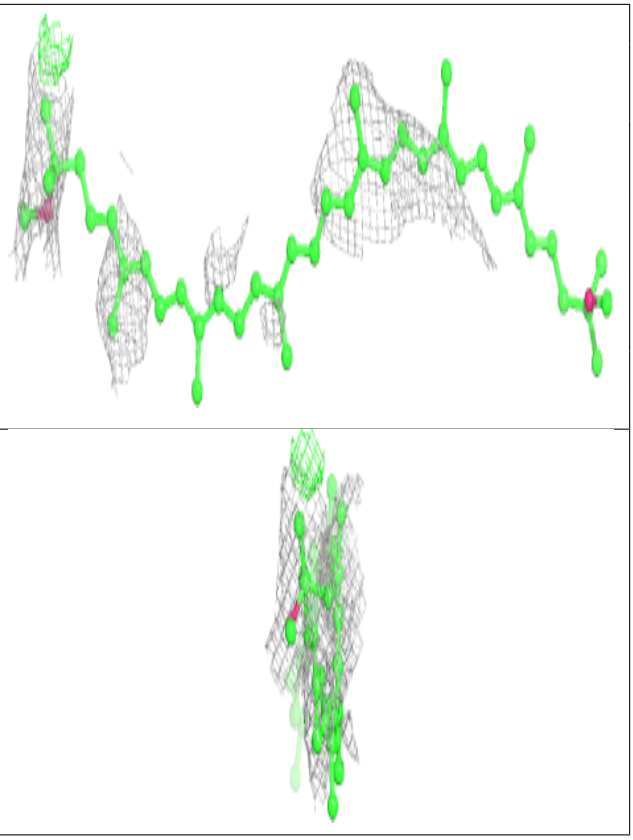
Electron density around CRT A0 101:

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



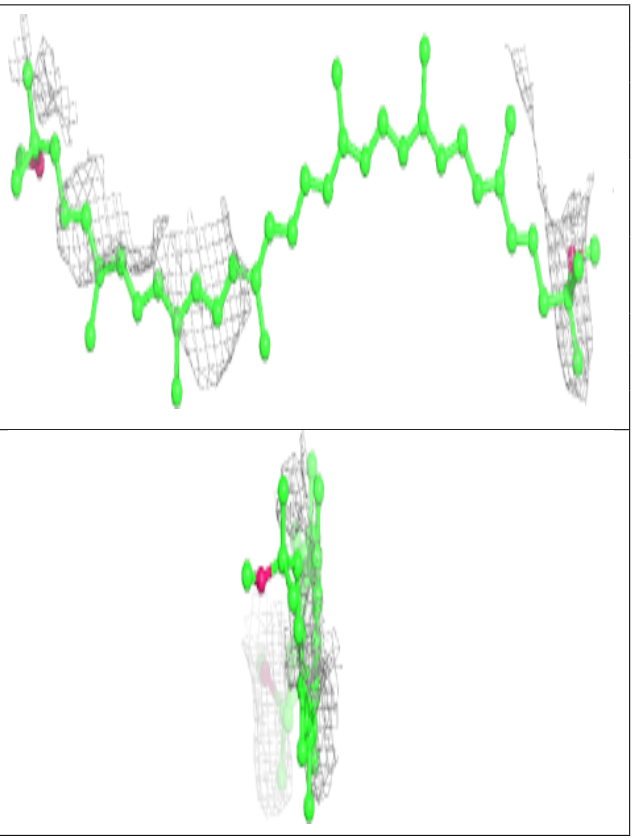
Electron density around CRT BP 102:

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



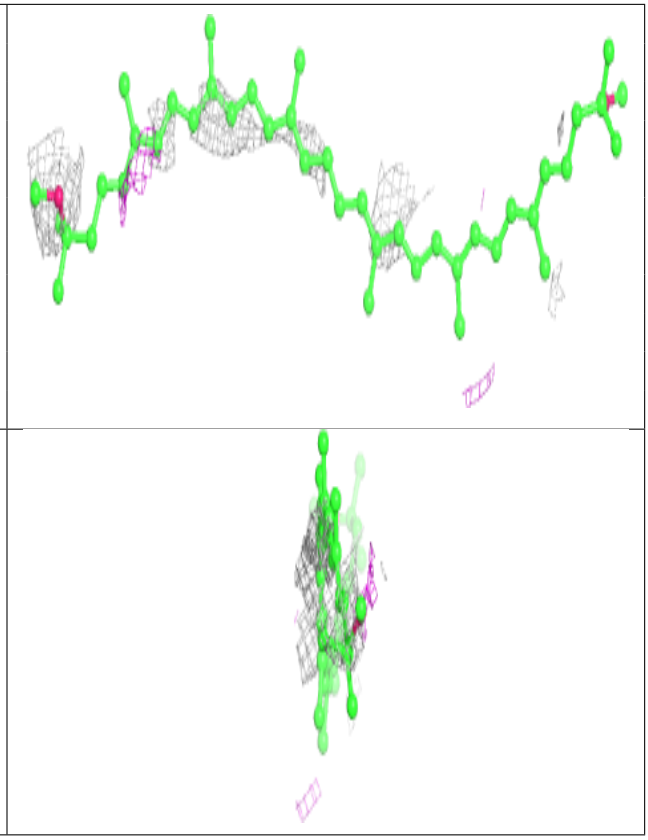
Electron density around CRT AT 102:

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



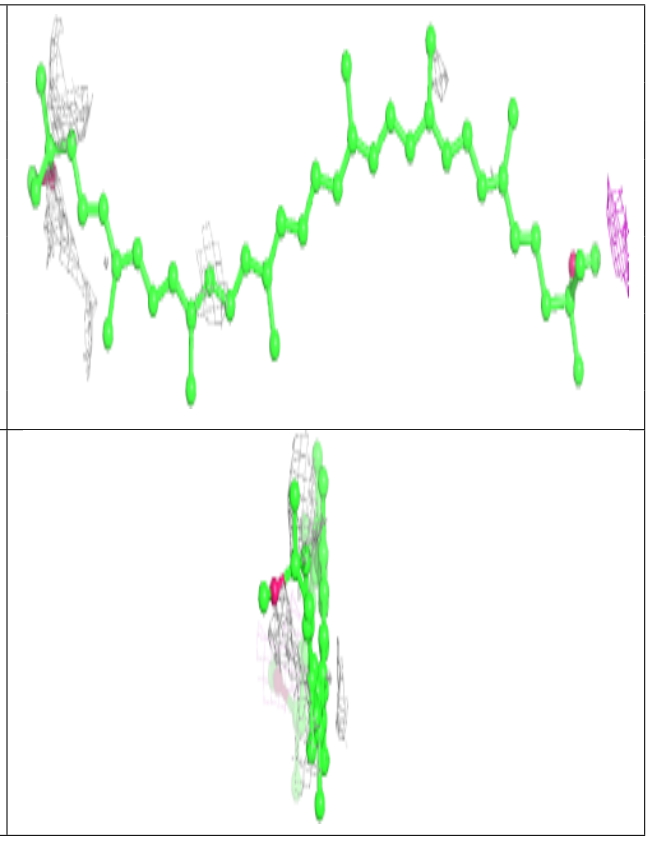
Electron density around CRT AP 102:

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



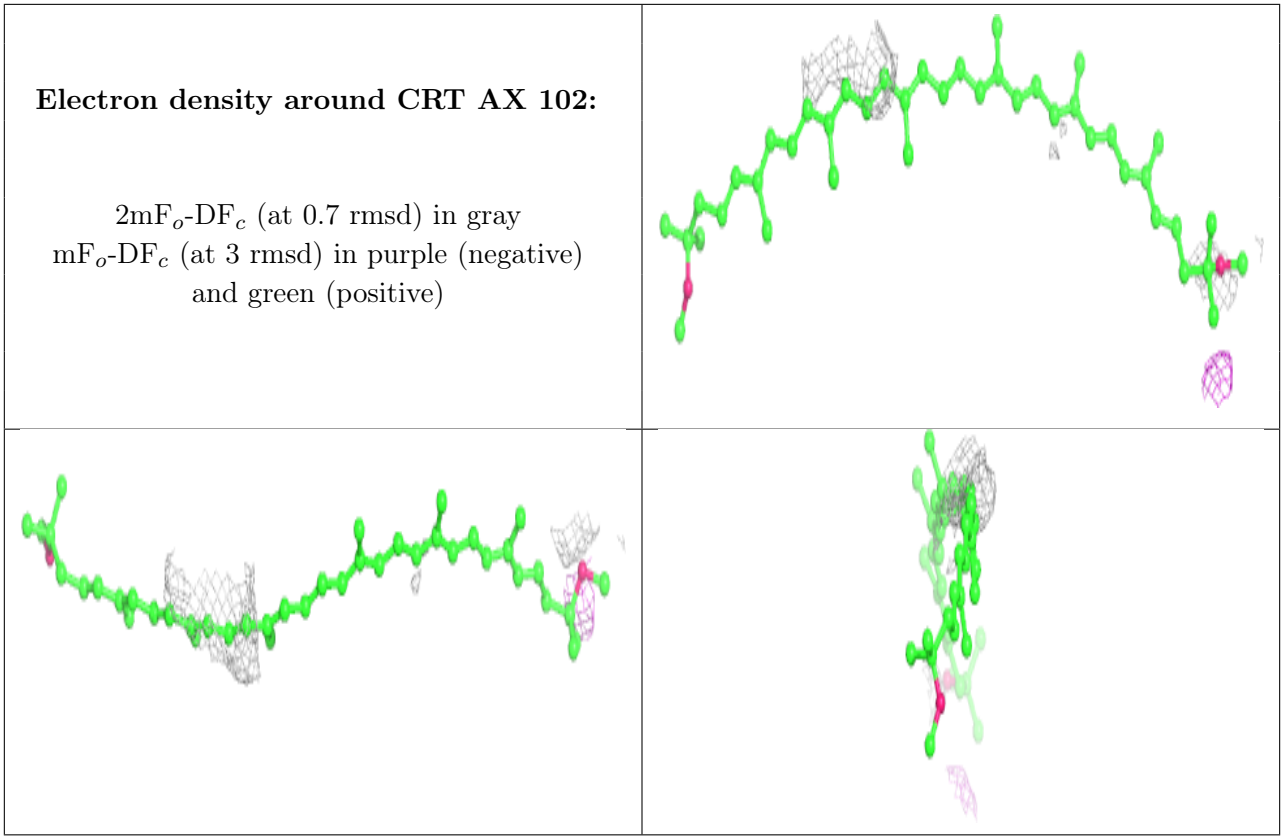
Electron density around CRT BS 103:

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



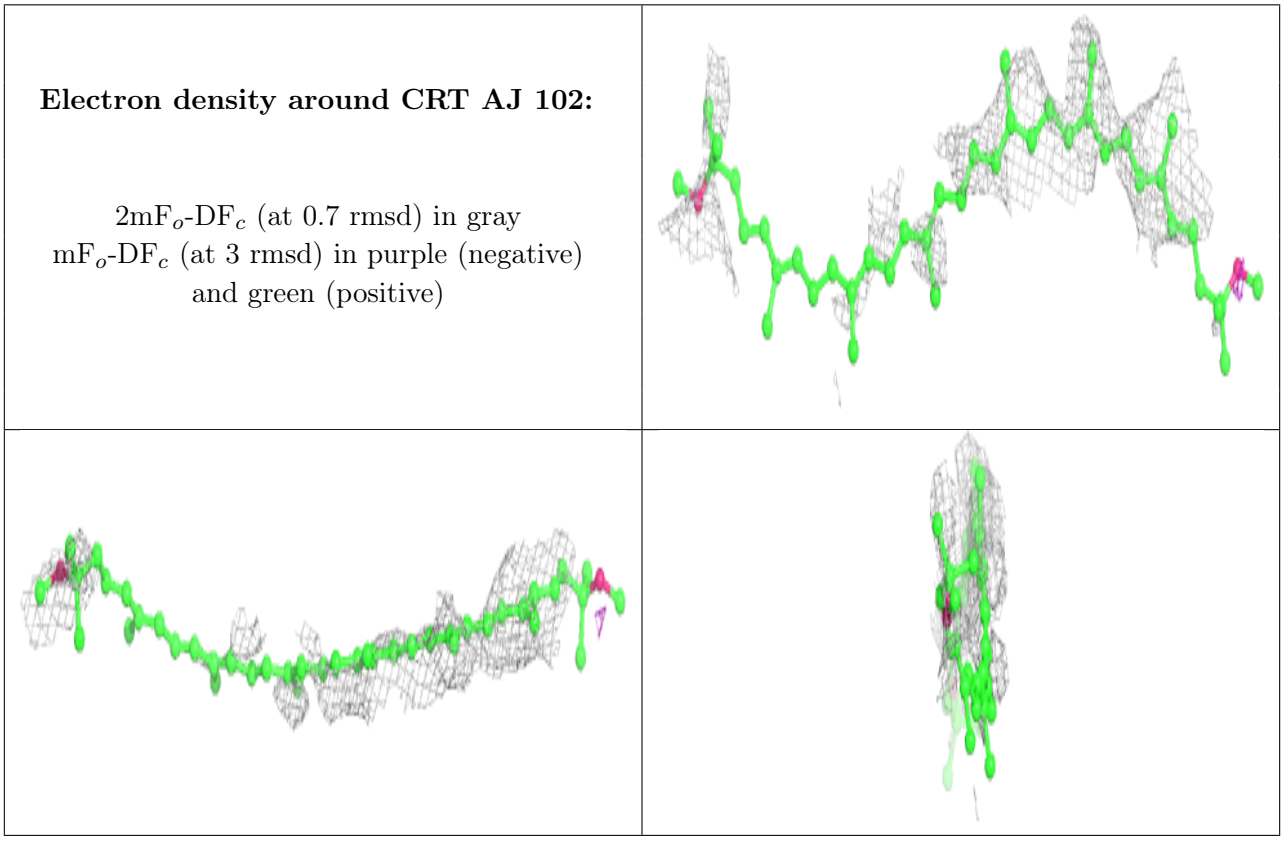
Electron density around CRT AX 102:

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



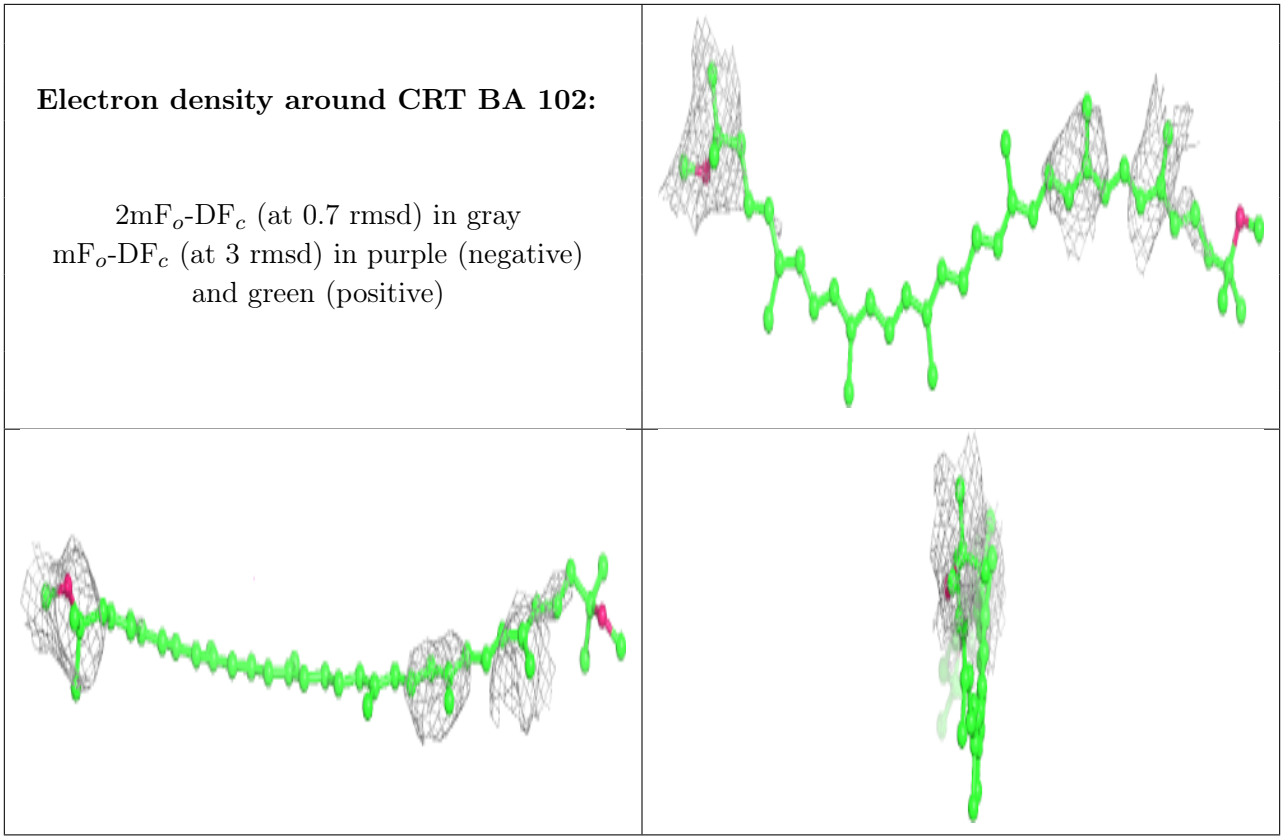
Electron density around CRT AJ 102:

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



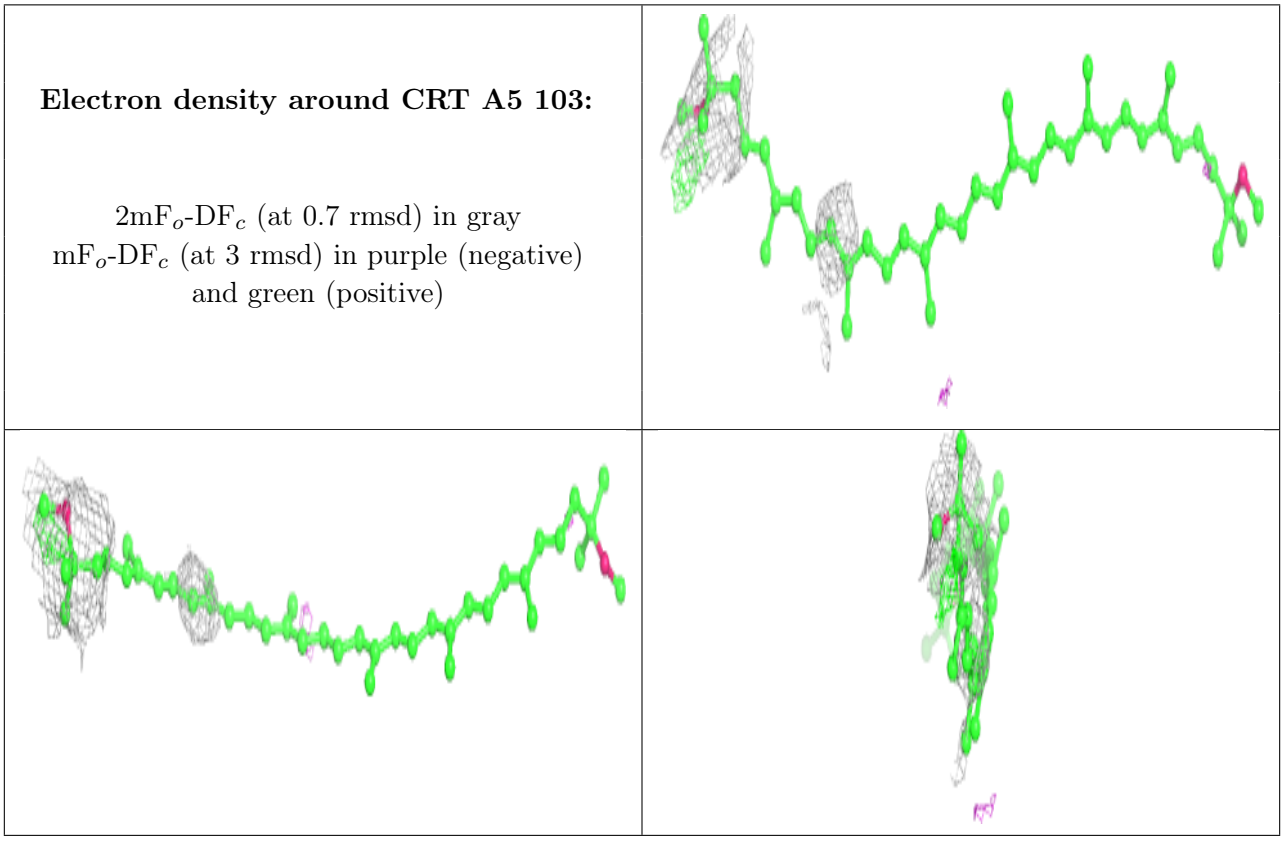
Electron density around CRT BA 102:

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



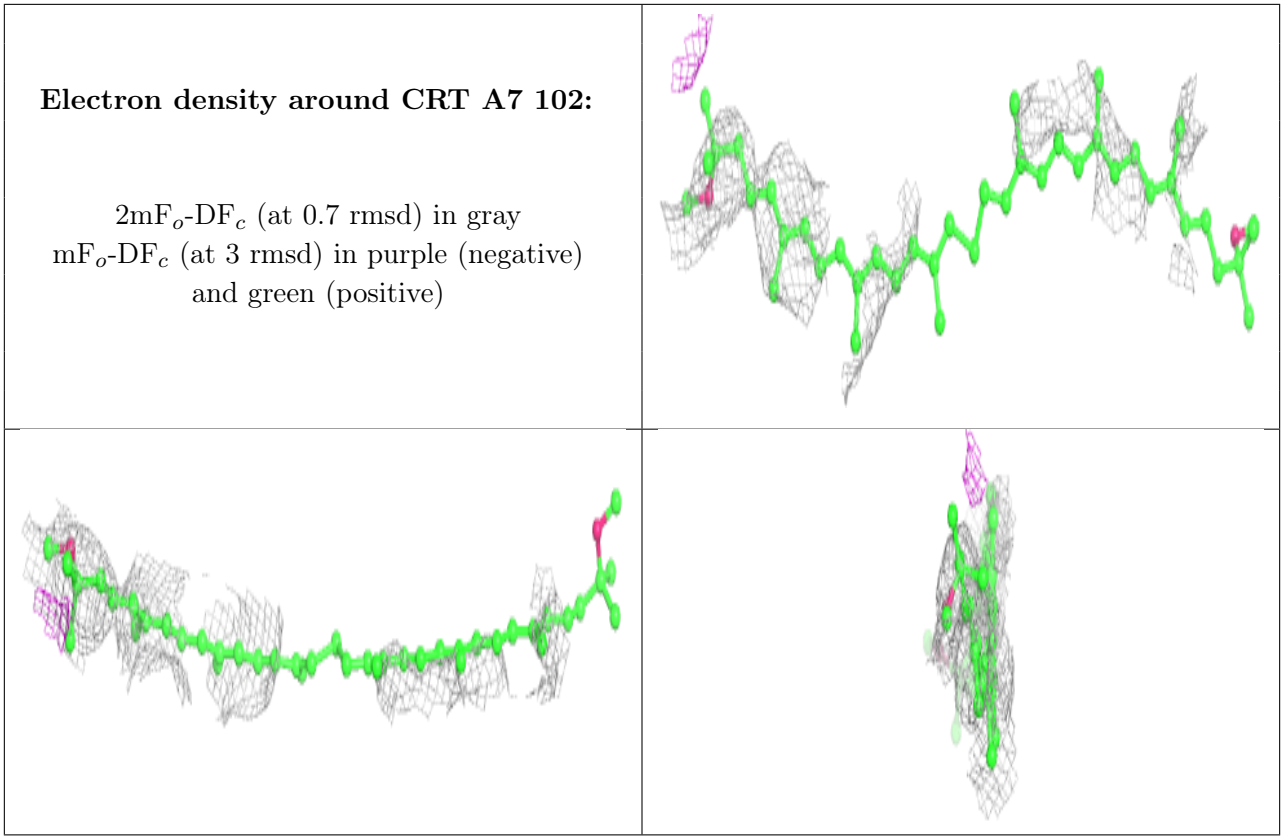
Electron density around CRT A5 103:

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



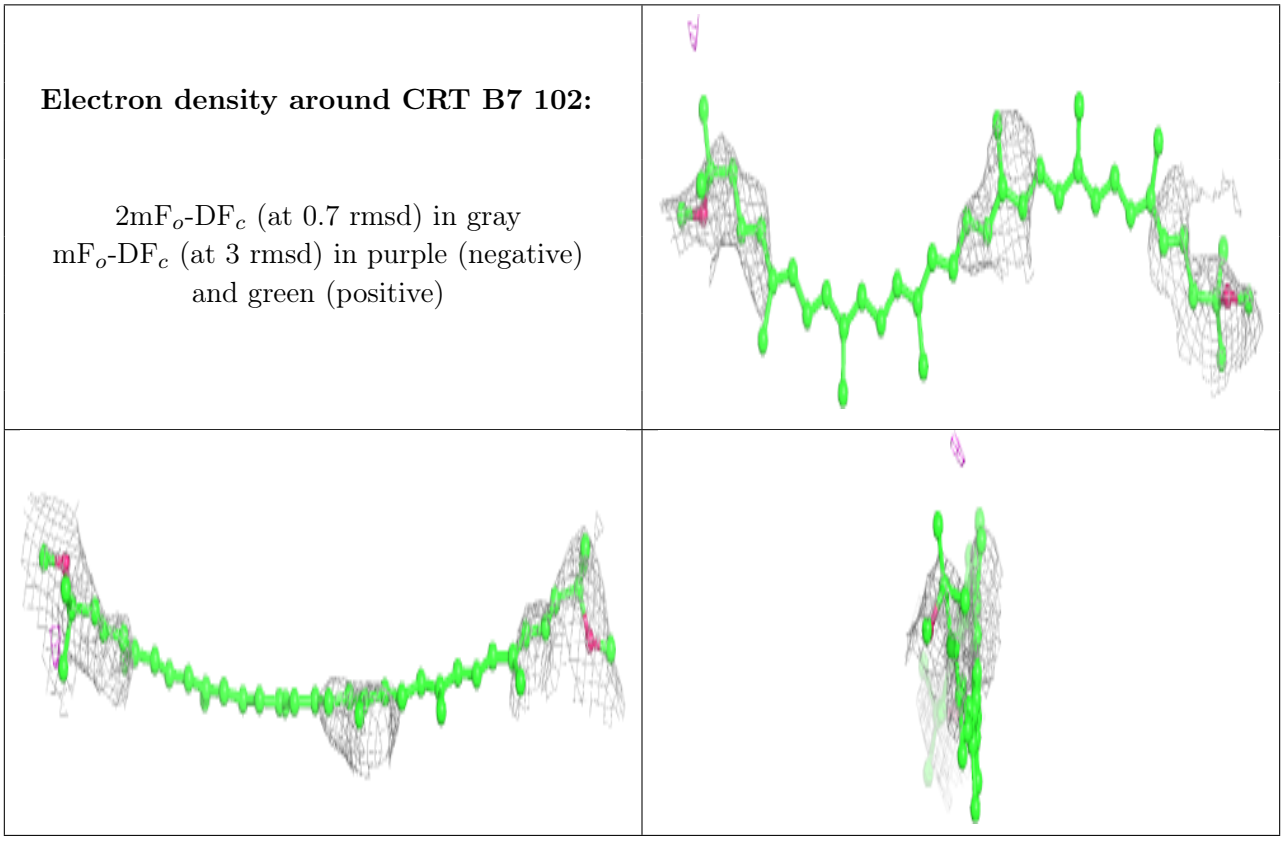
Electron density around CRT A7 102:

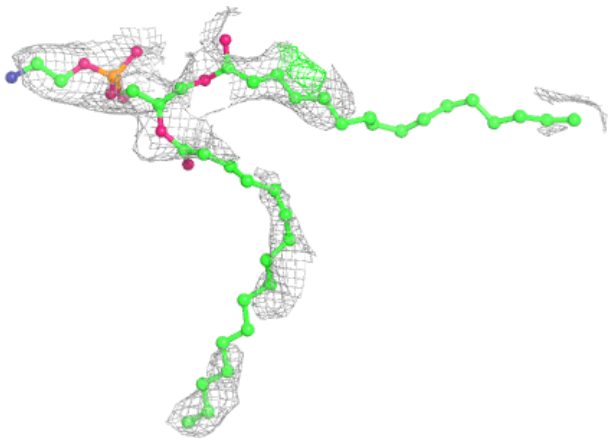
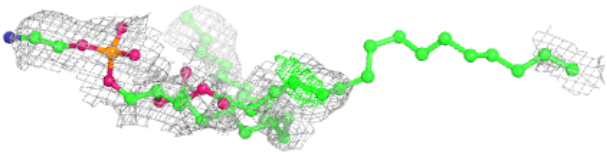
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CRT B7 102:

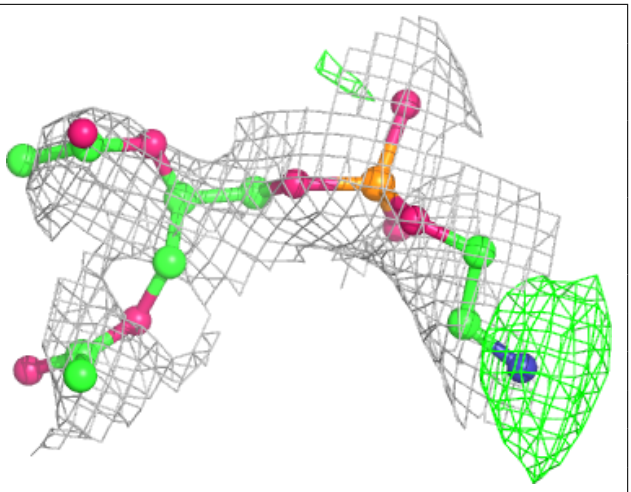
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

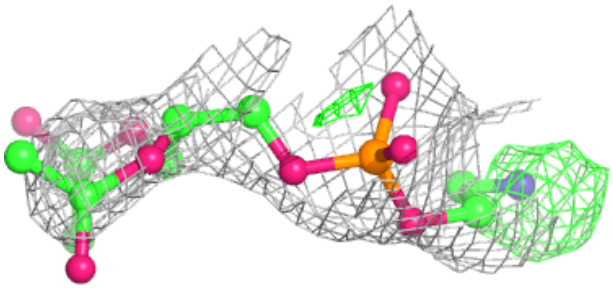


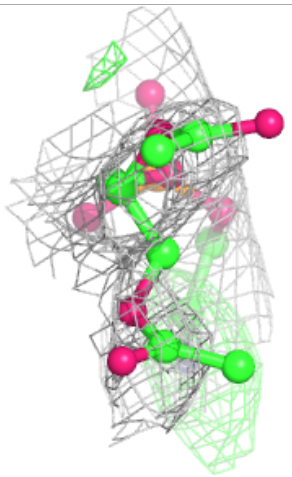
Electron density around PEF AS 101: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around PEF BM 407:

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

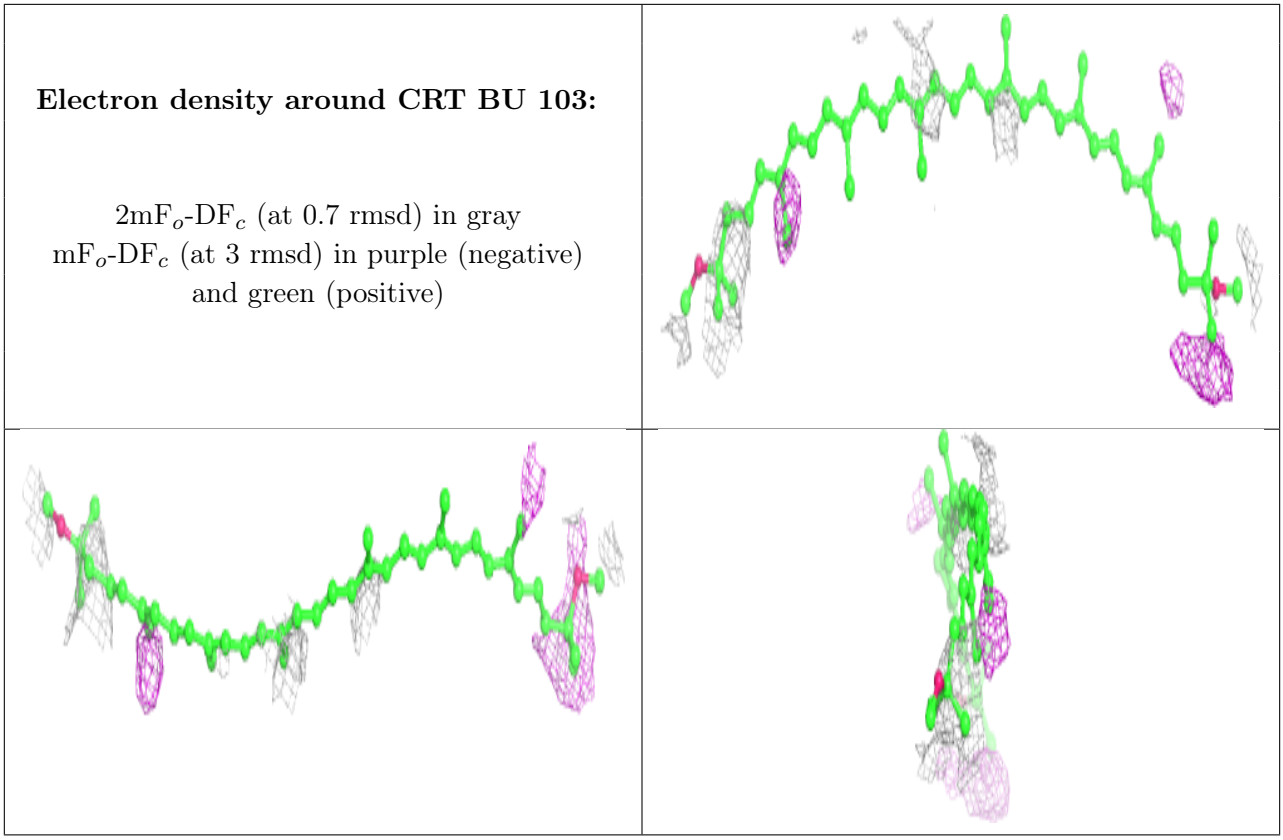






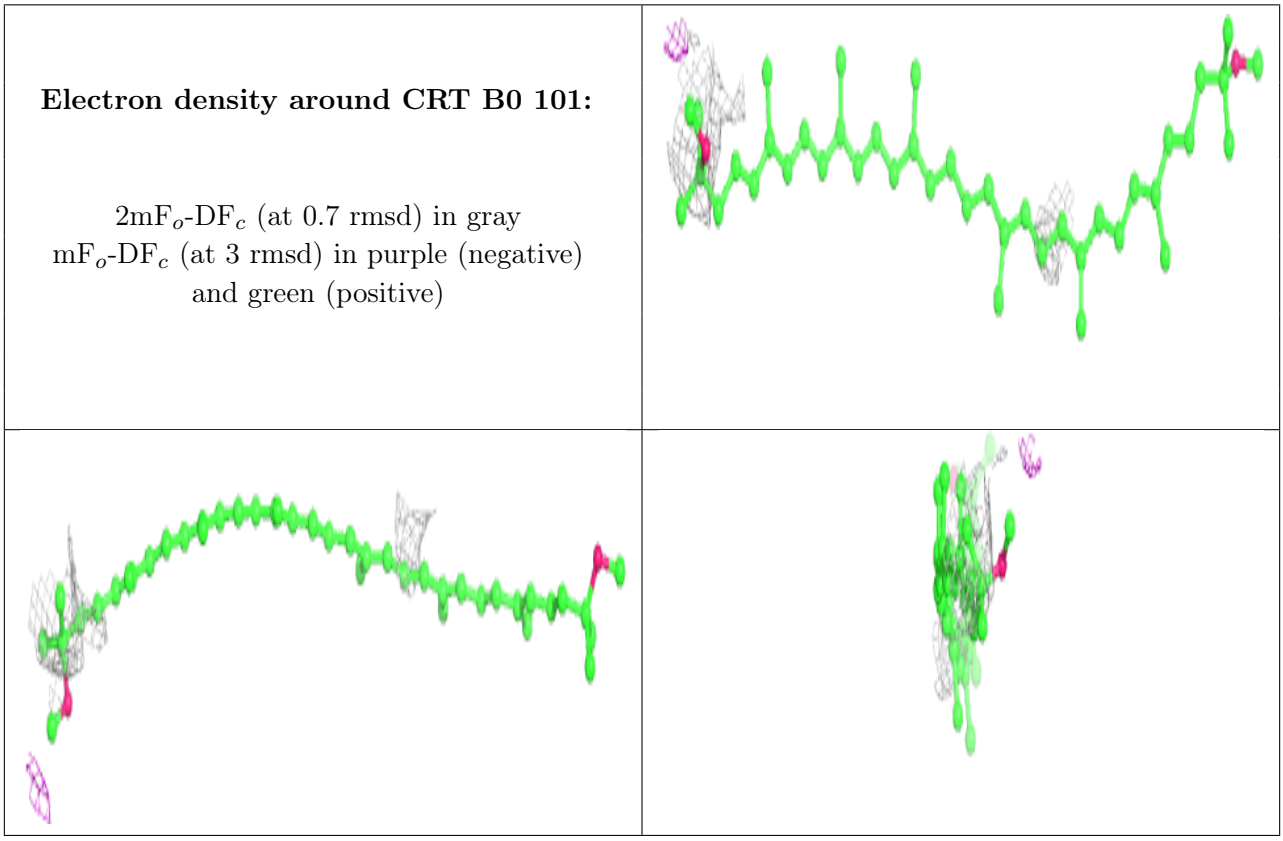
Electron density around CRT BU 103:

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



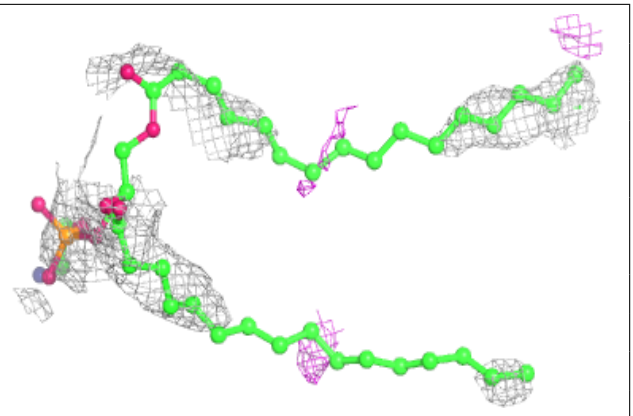
Electron density around CRT B0 101:

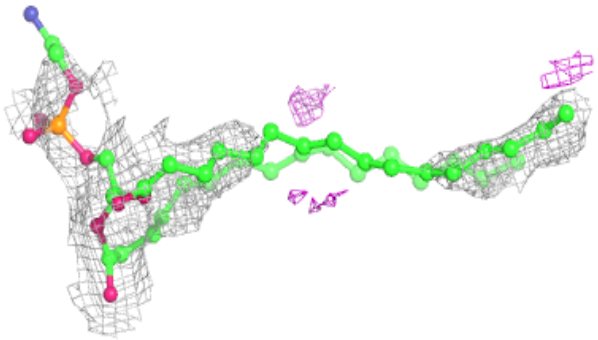
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

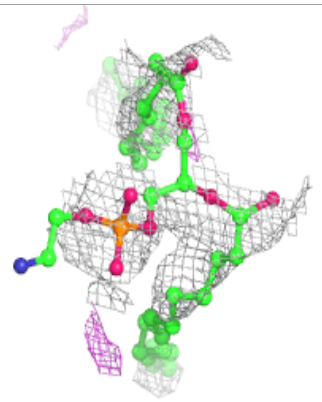


Electron density around PEF AM 409:

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

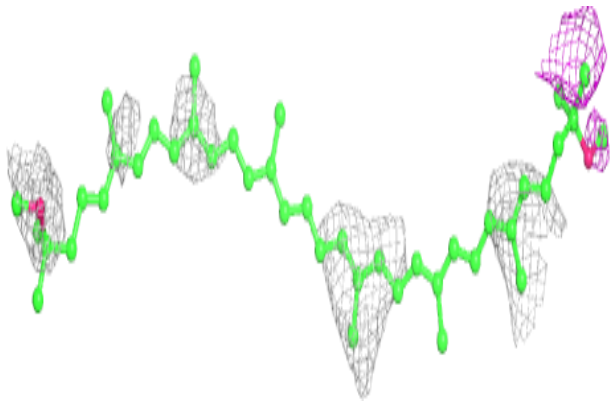


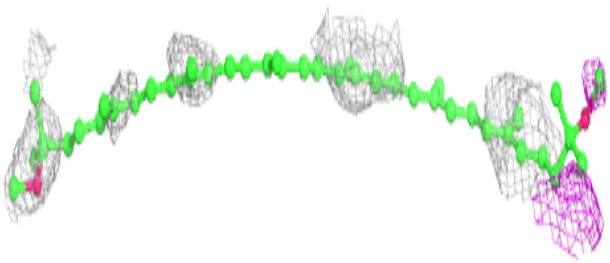


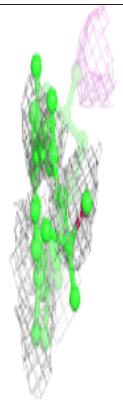


Electron density around CRT AN 102:

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

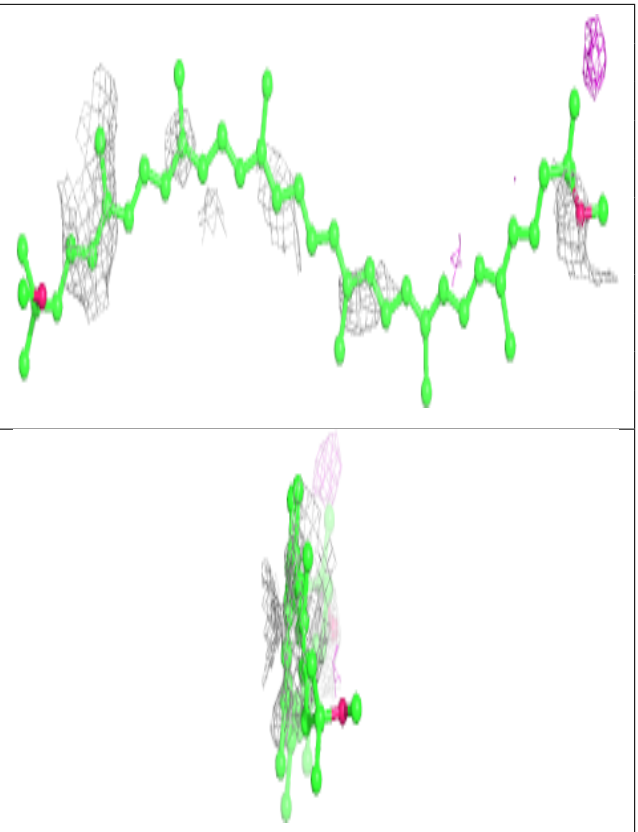


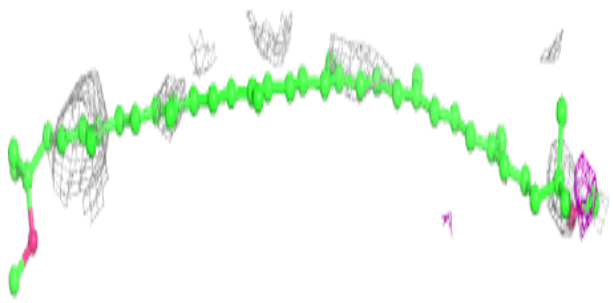




Electron density around CRT B1 103:

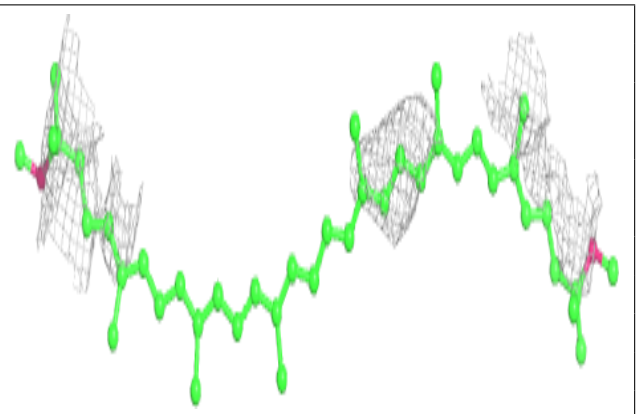
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

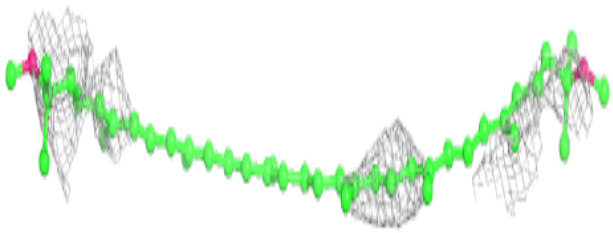


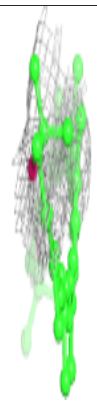


Electron density around CRT BF 103:

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

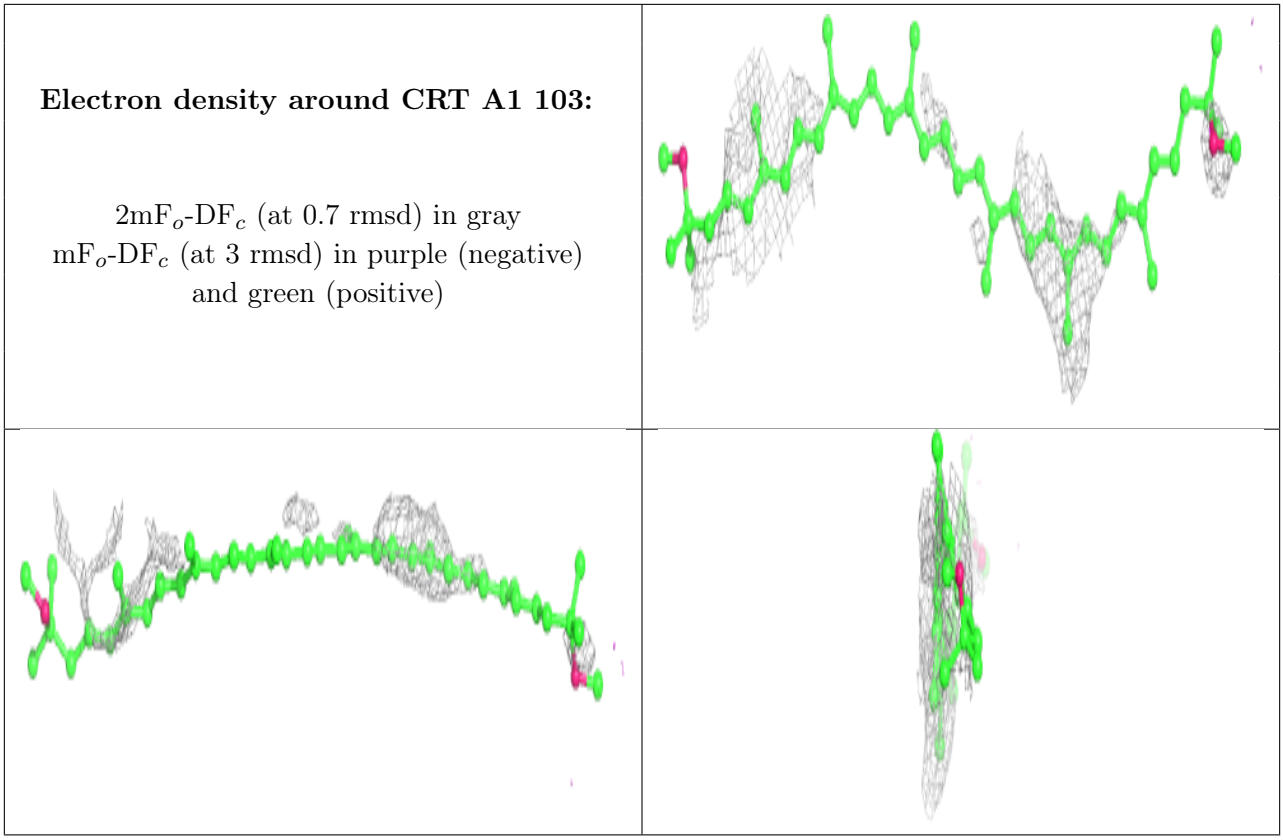






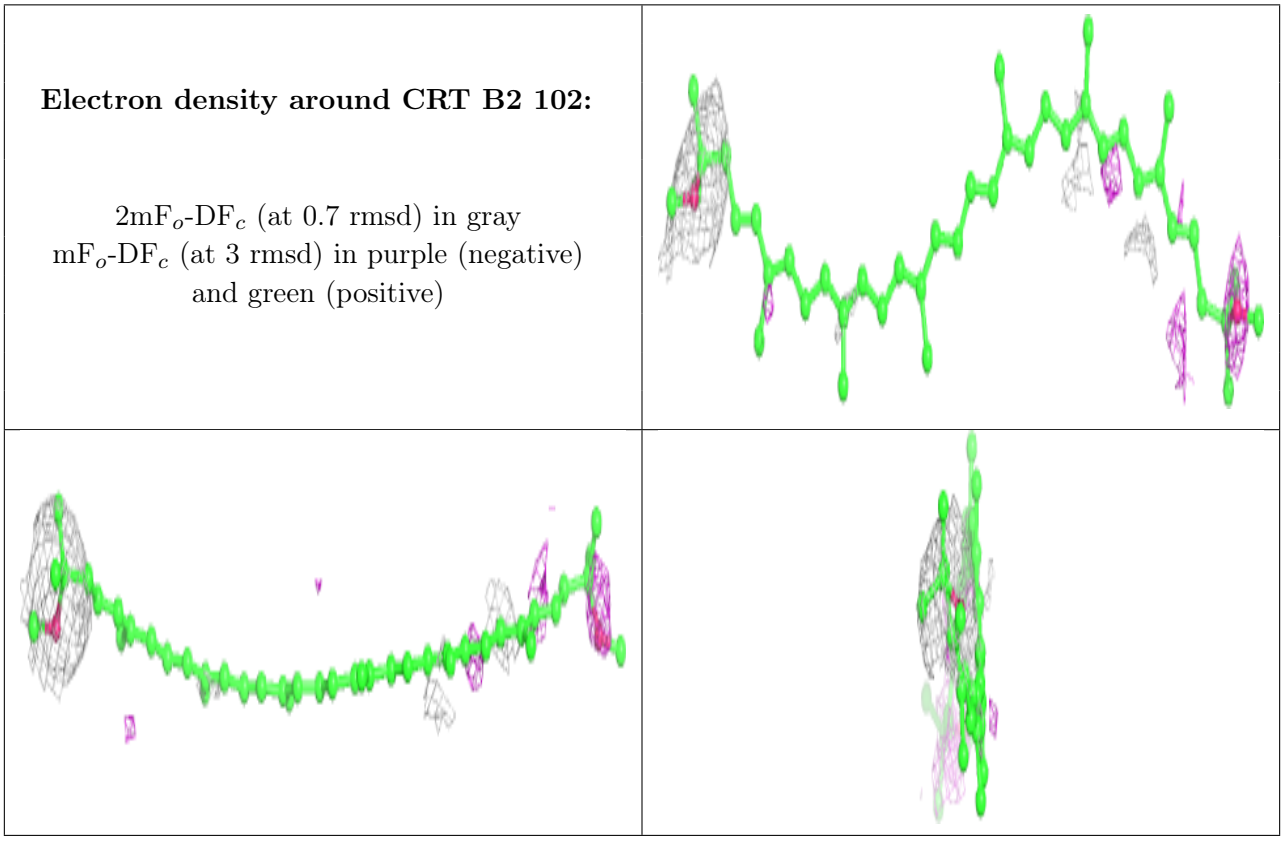
Electron density around CRT A1 103:

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



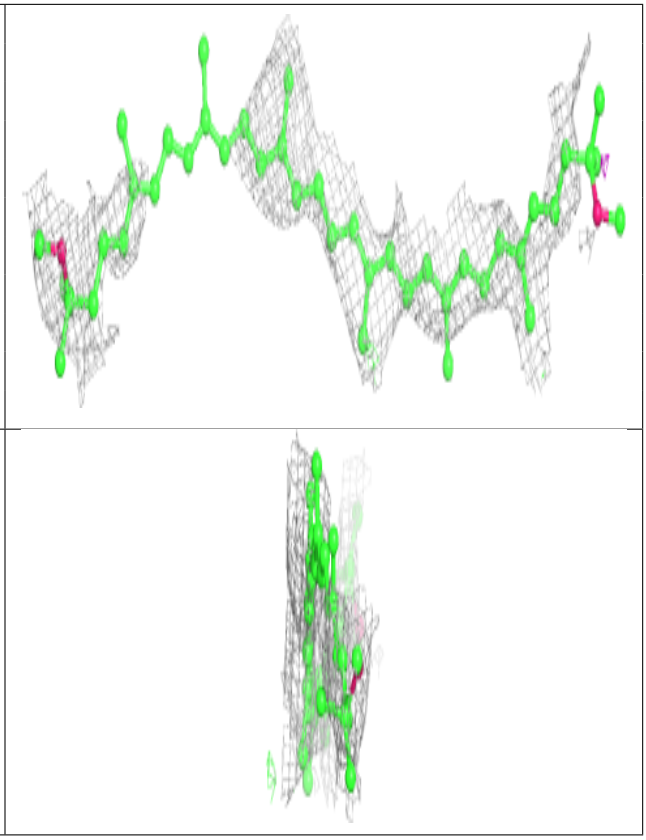
Electron density around CRT B2 102:

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



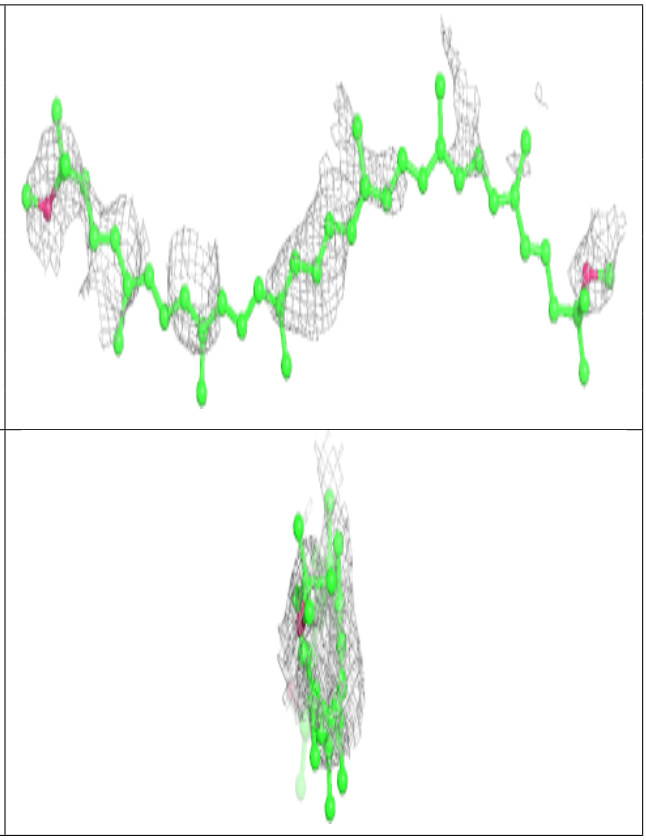
Electron density around CRT BG 102:

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



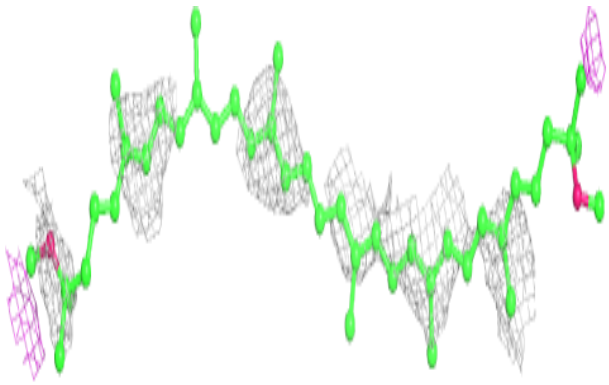
Electron density around CRT BN 102:

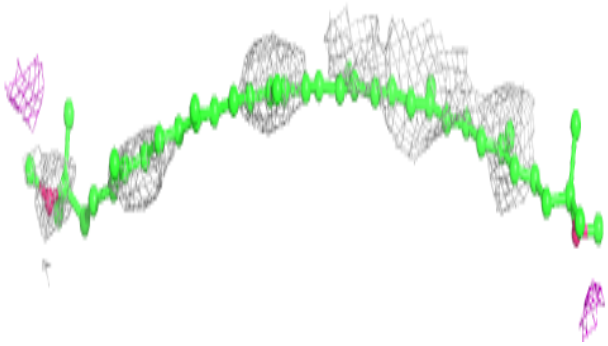
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

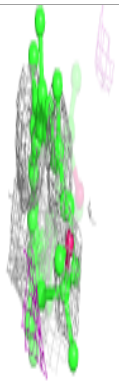


Electron density around CRT AG 102:

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

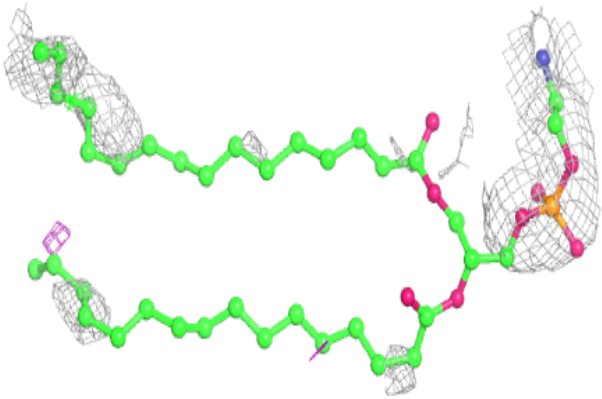


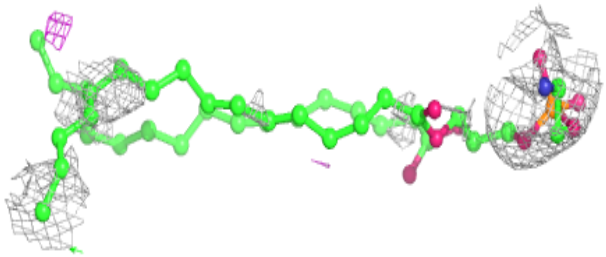


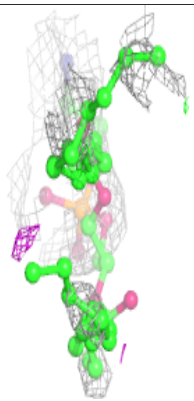


Electron density around PEF BQ 101:

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

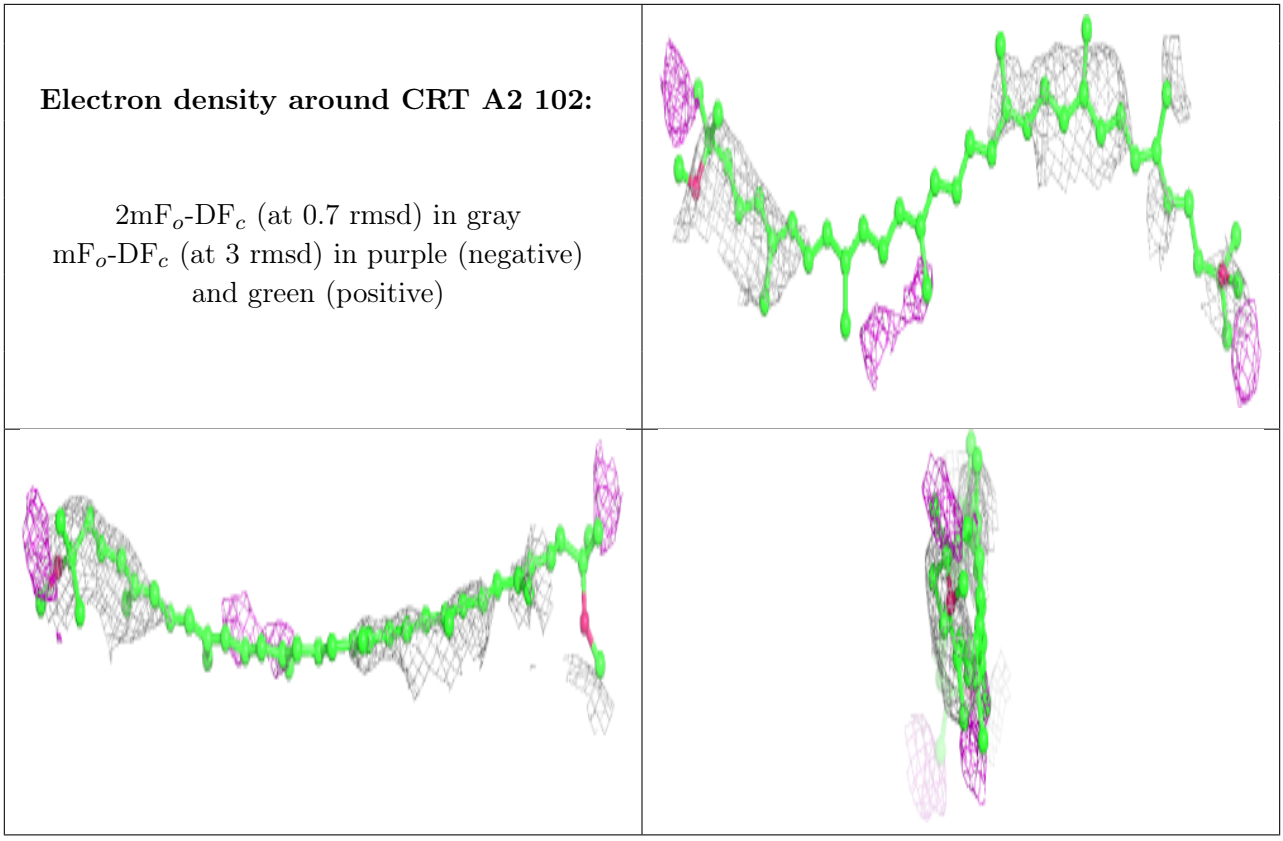






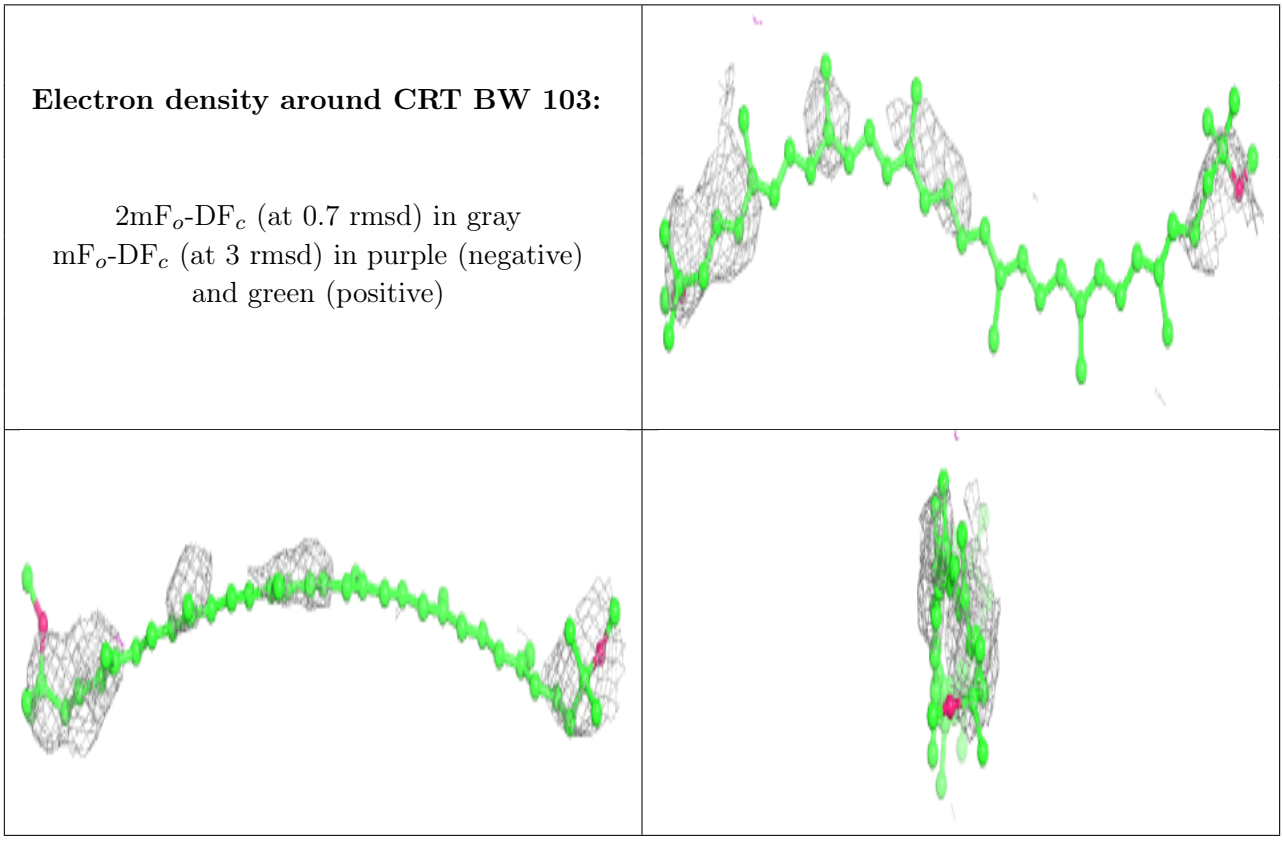
Electron density around CRT A2 102:

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



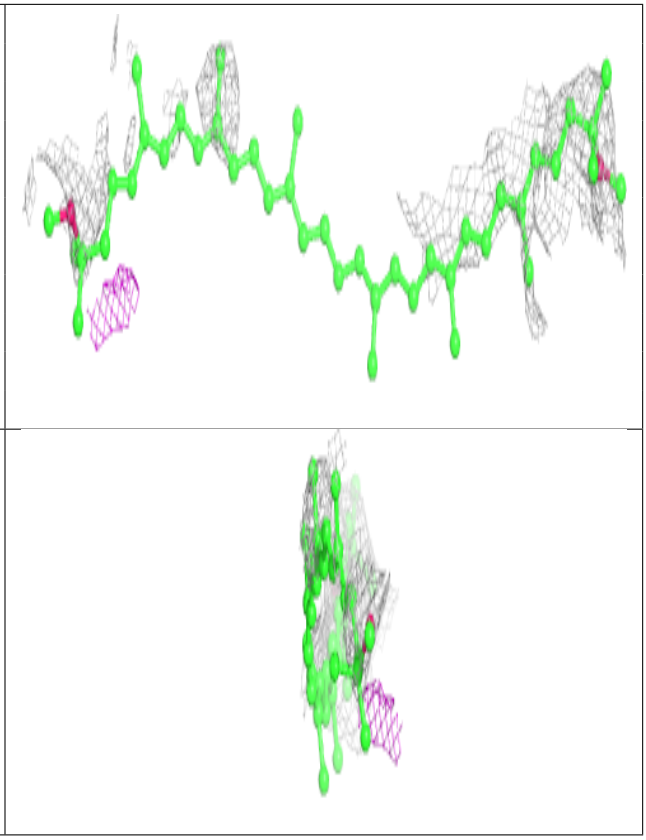
Electron density around CRT BW 103:

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



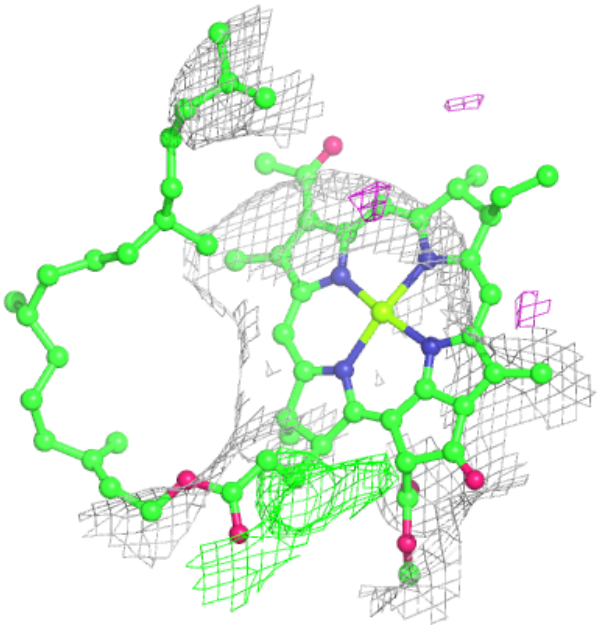
Electron density around CRT AS 104:

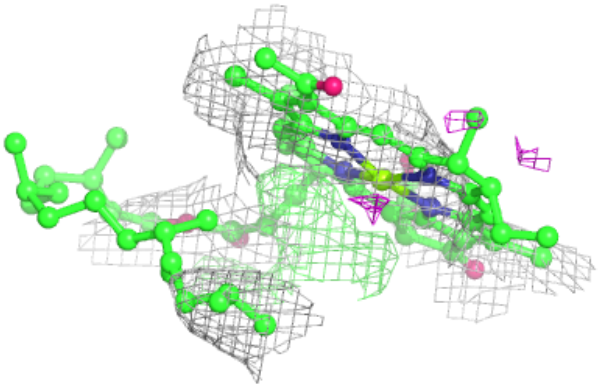
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

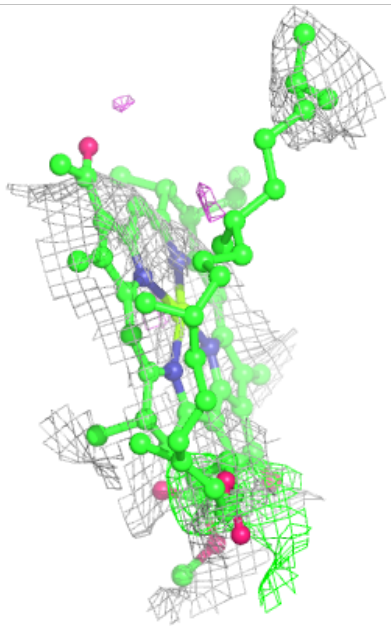


Electron density around BCL BV 101:

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

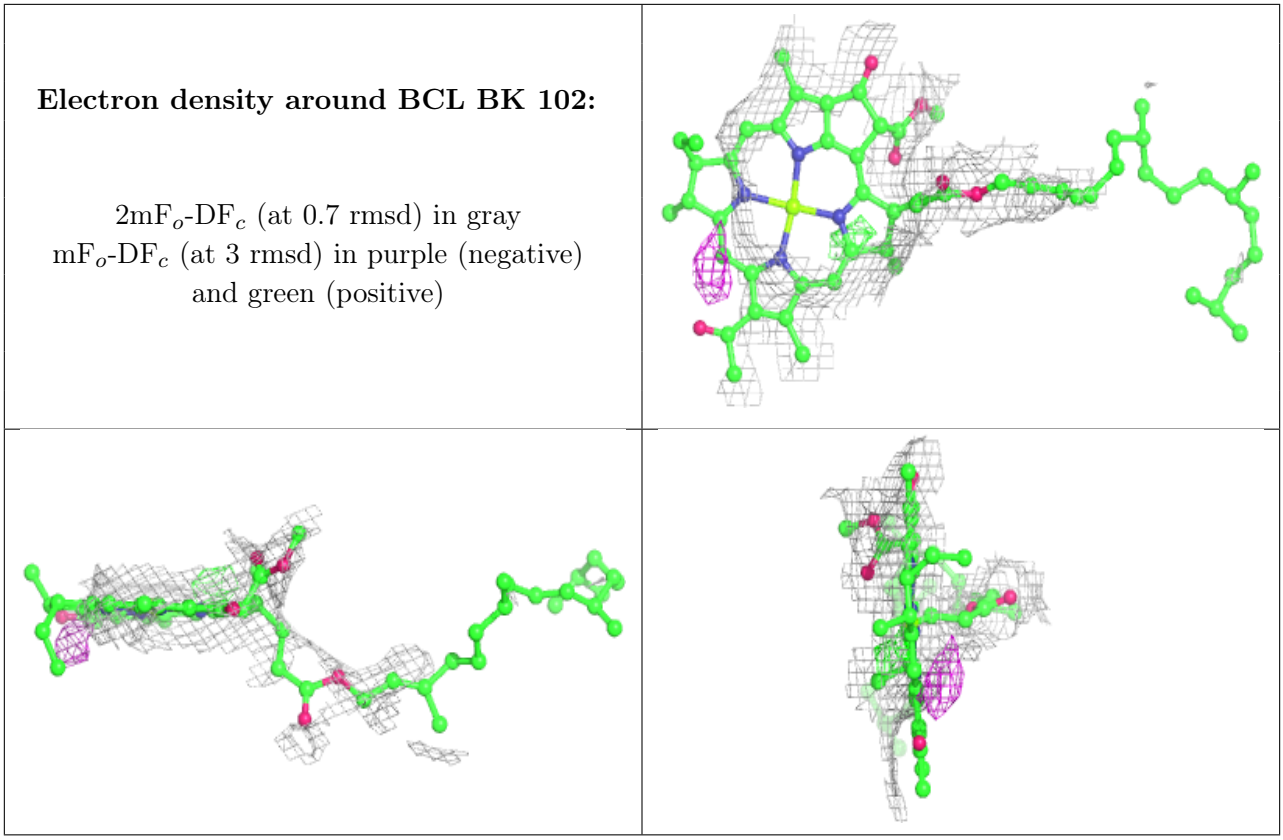






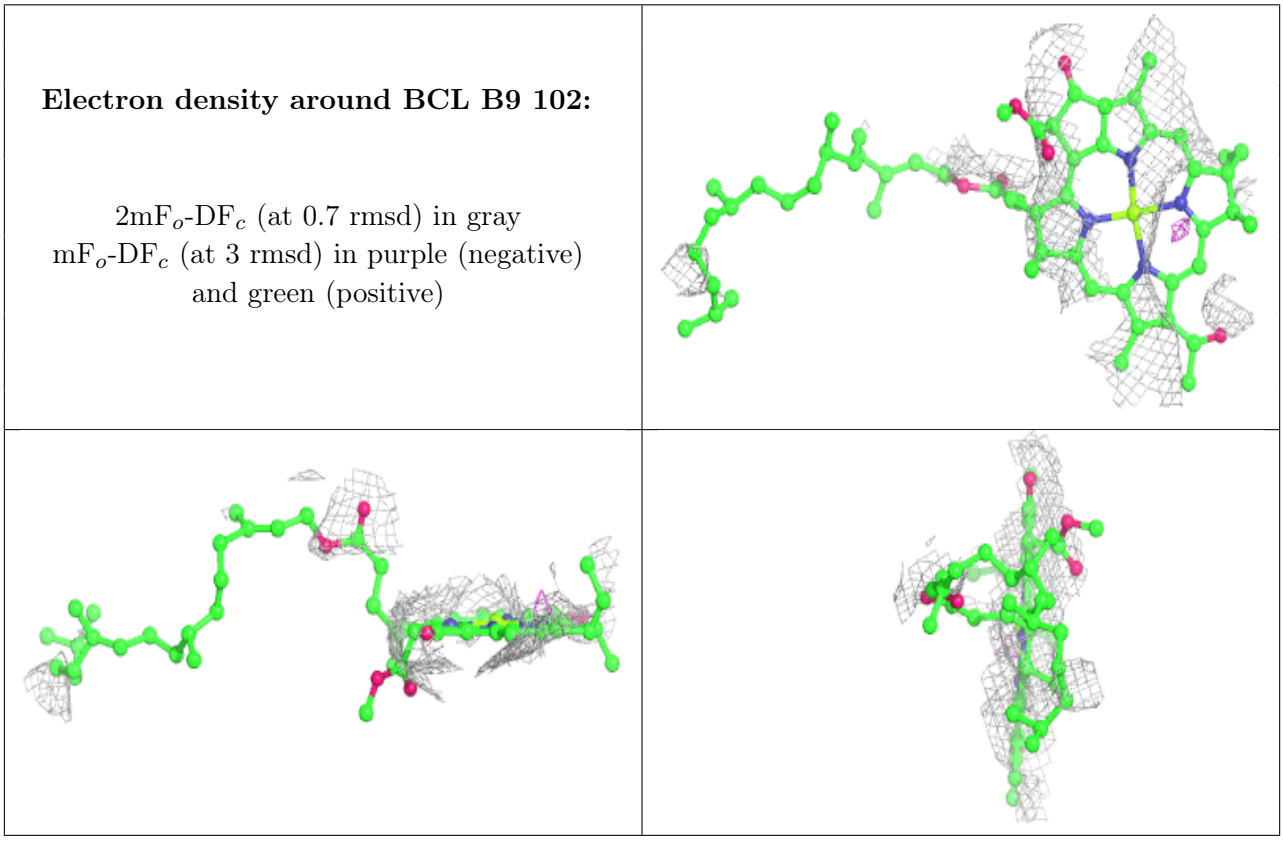
Electron density around BCL BK 102:

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



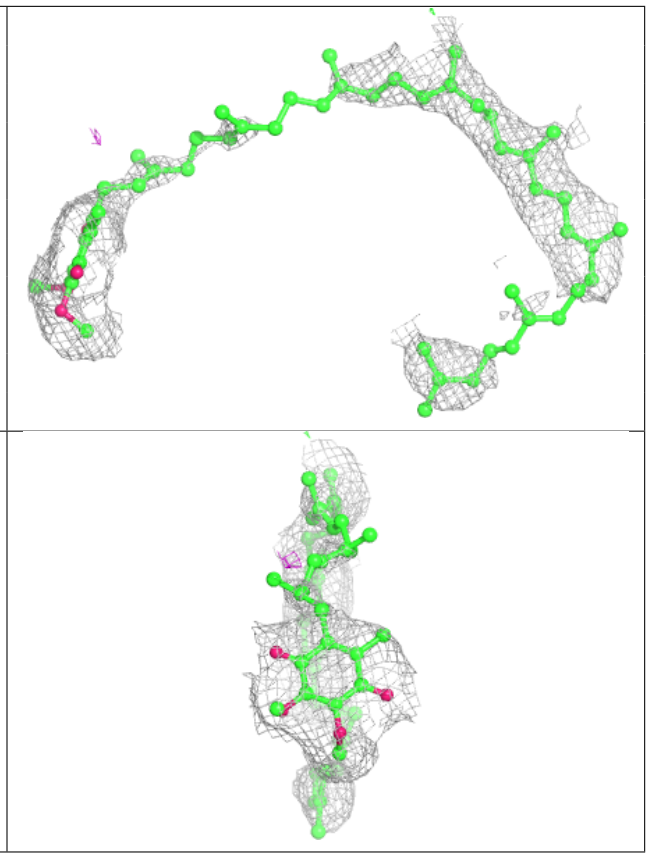
Electron density around BCL B9 102:

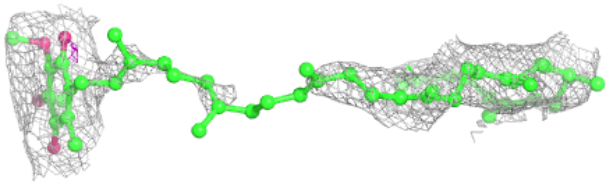
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UQ8 BL 304:

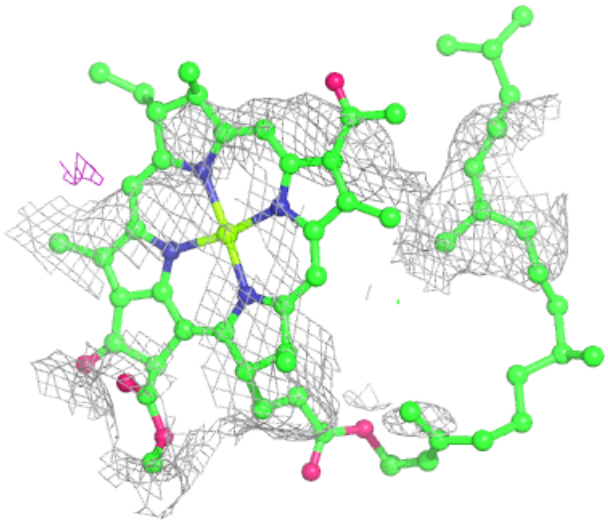
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

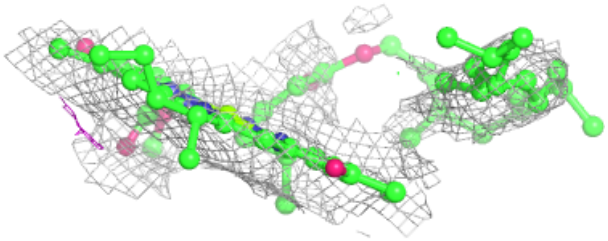


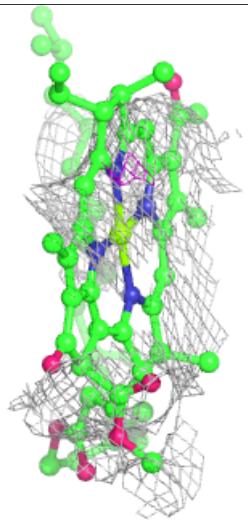


Electron density around BCL BQ 104:

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

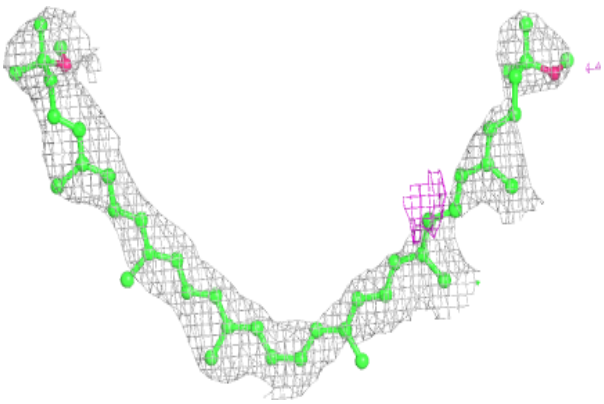


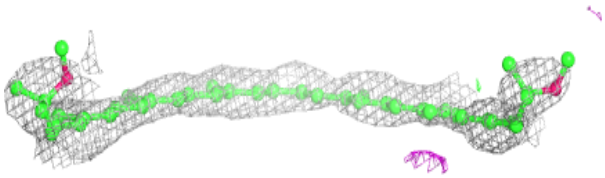


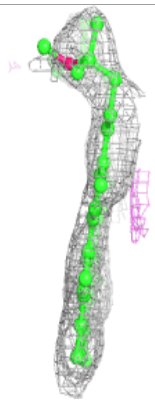


Electron density around CRT BM 406:

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

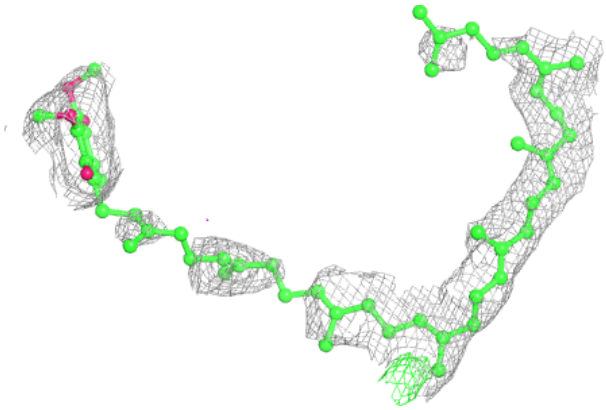


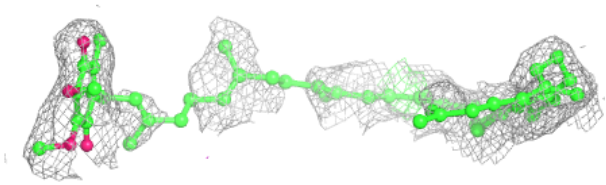


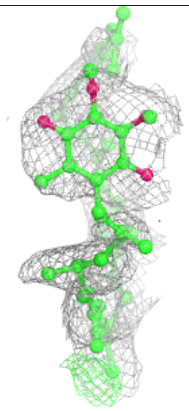


Electron density around UQ8 AL 304:

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

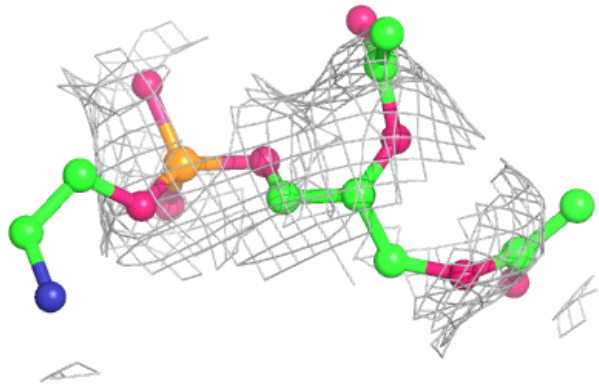


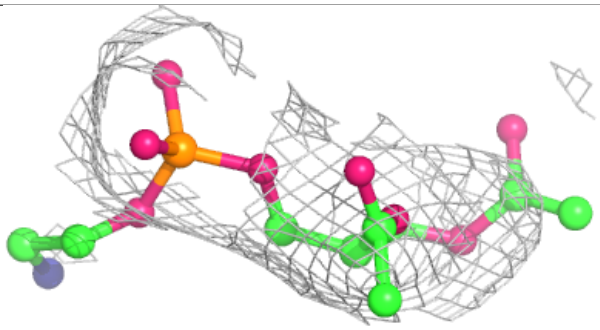


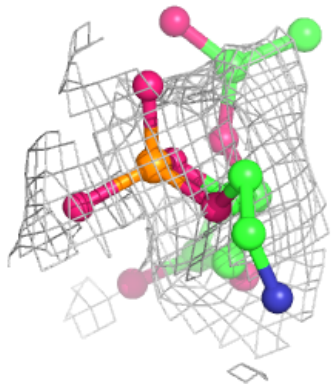


Electron density around PEF AM 407:

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

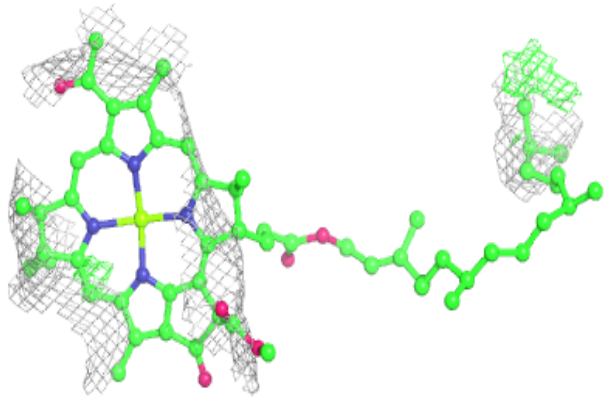


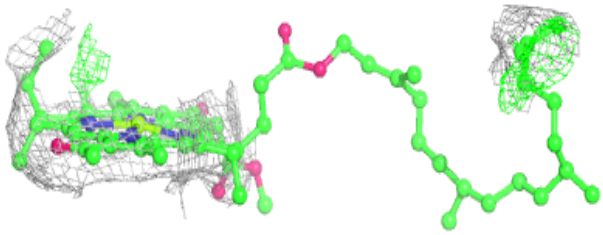


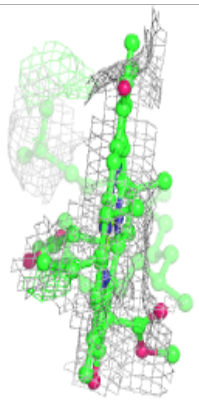


Electron density around BCL BA 101:

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

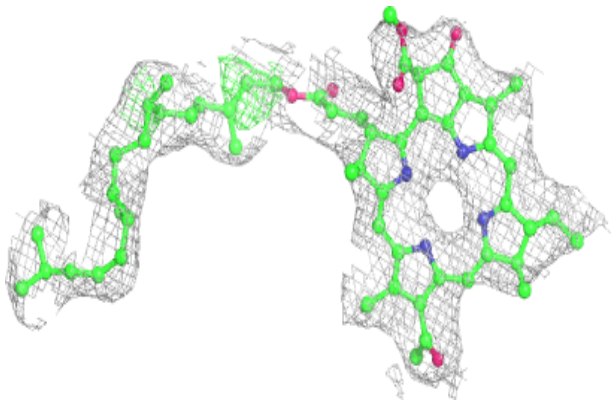


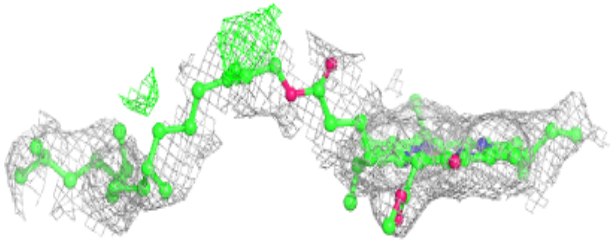


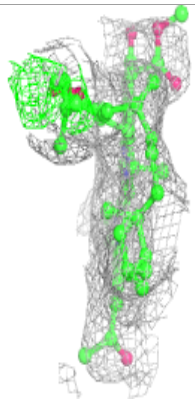


Electron density around BPH BM 403:

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

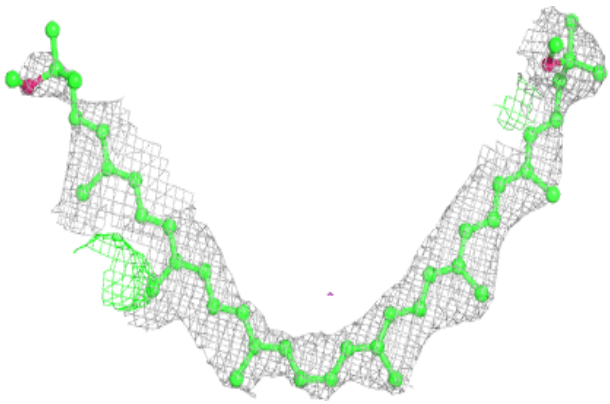


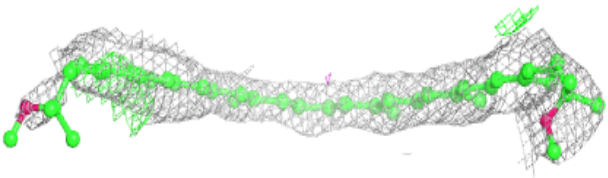


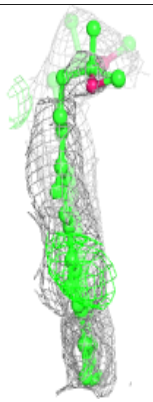


Electron density around CRT AM 406:

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

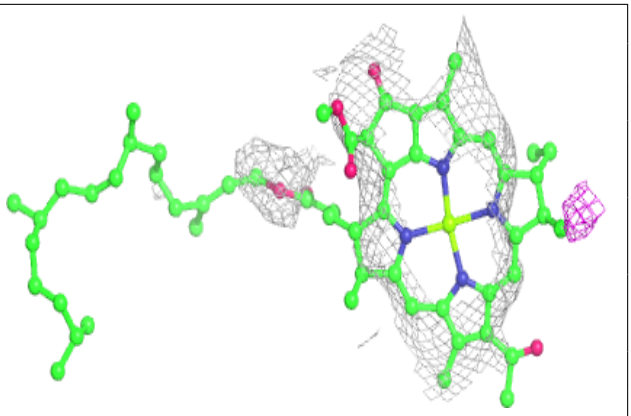


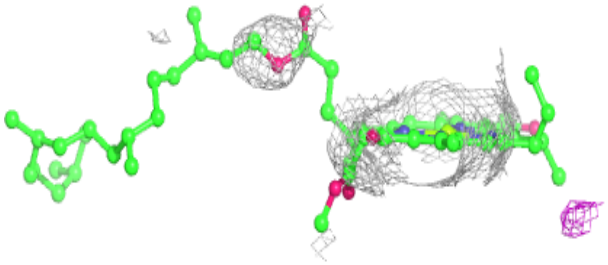


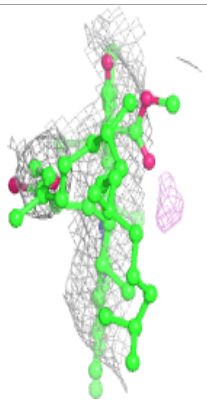


Electron density around BCL AS 103:

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

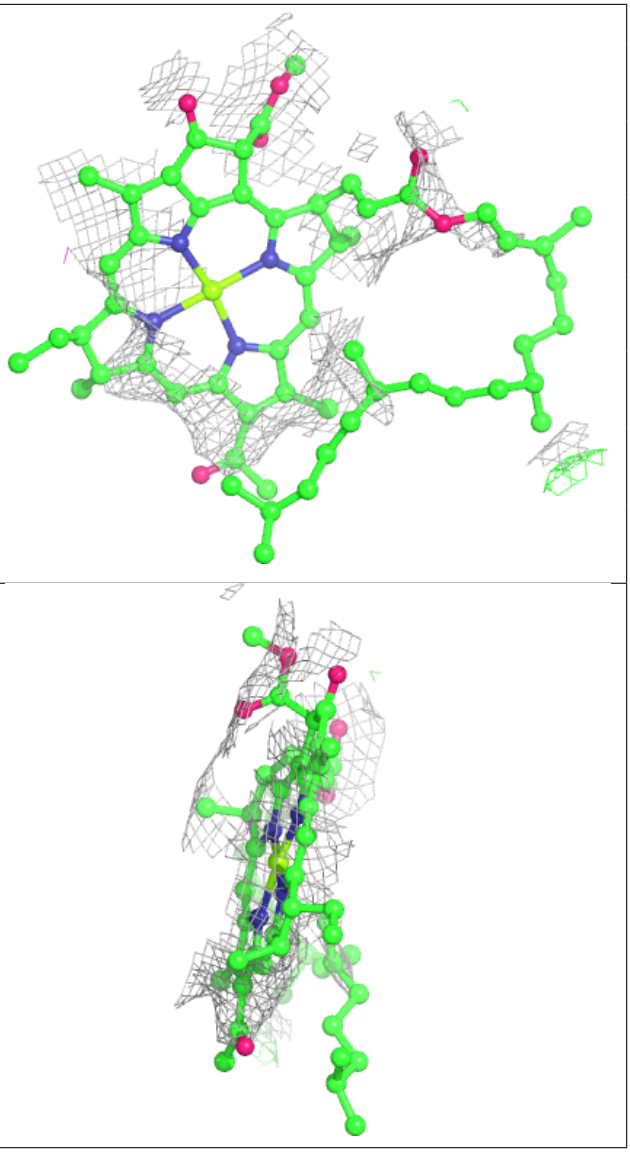






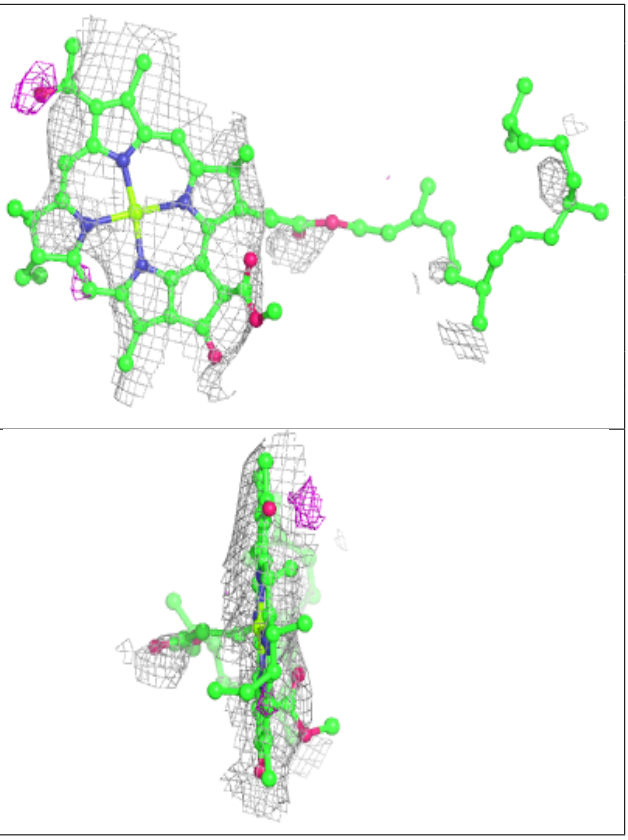
Electron density around BCL BP 101:

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



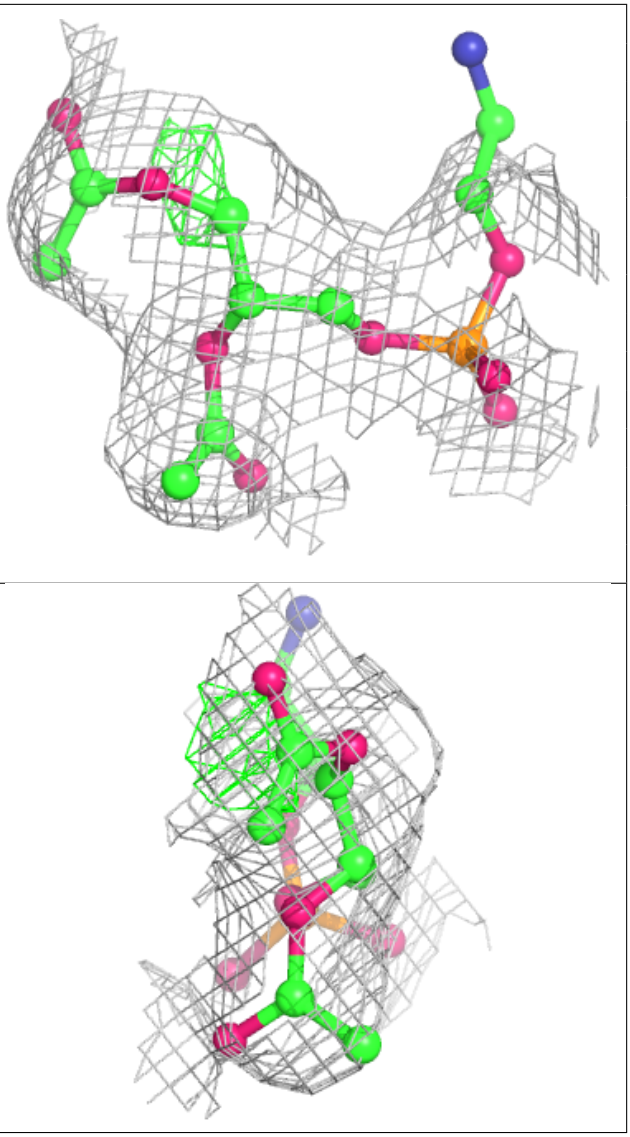
Electron density around BCL A3 103:

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



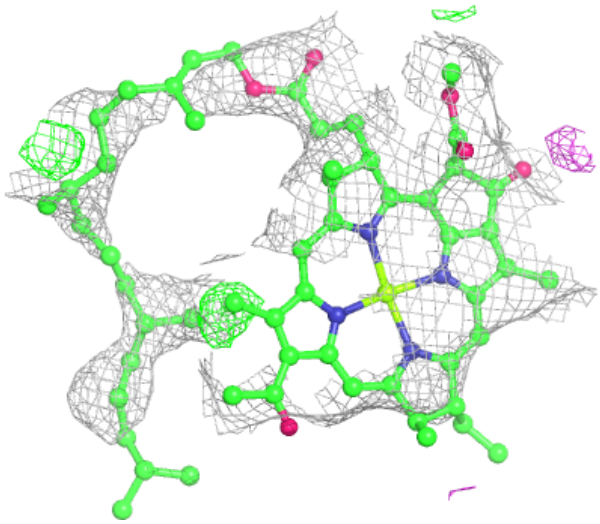
Electron density around PEF AH 301:

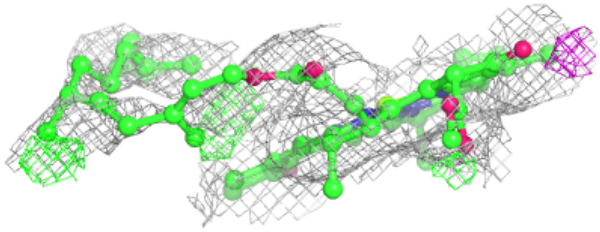
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

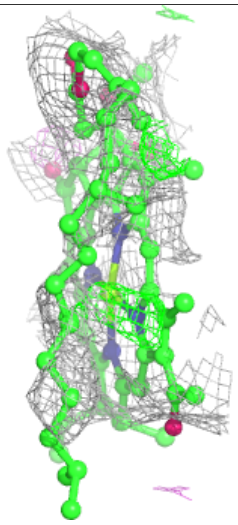


Electron density around BCL BZ 101:

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

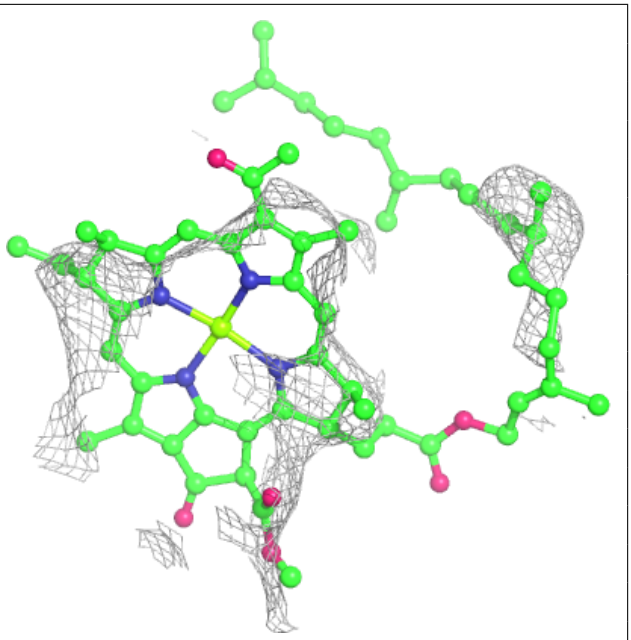


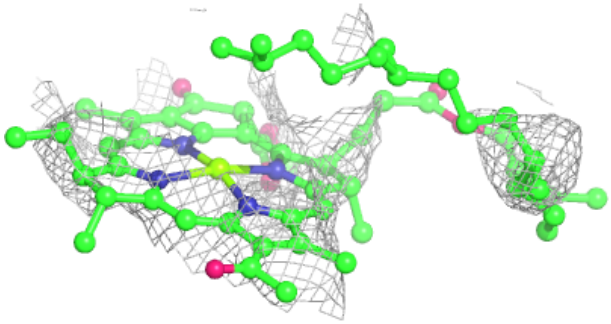


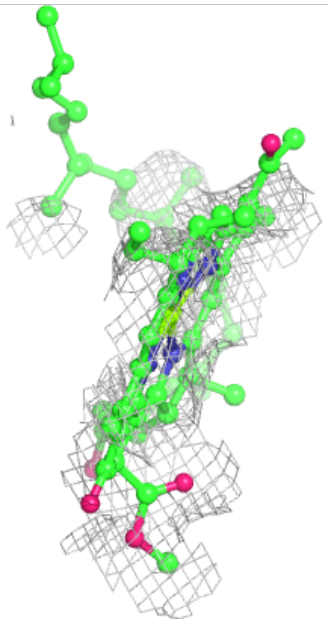


Electron density around BCL B8 101:

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

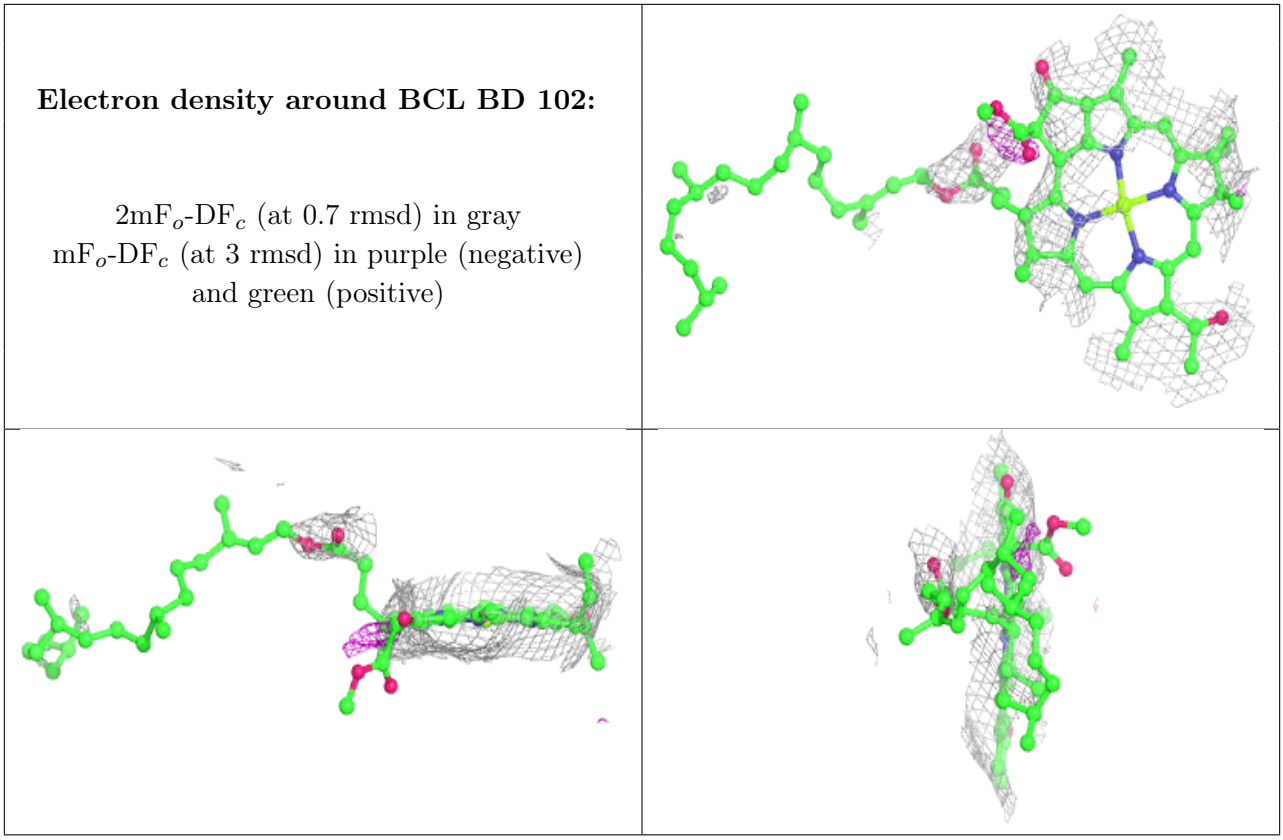






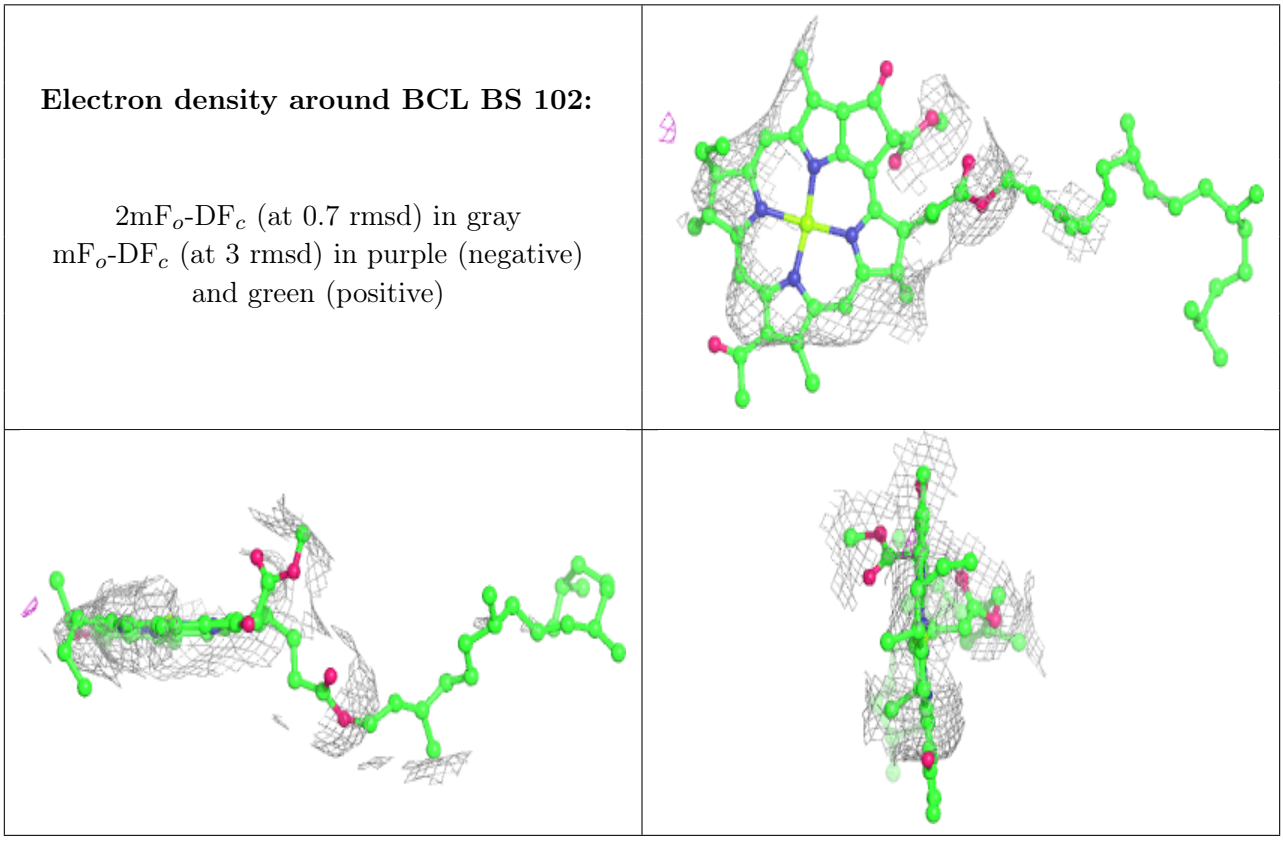
Electron density around BCL BD 102:

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



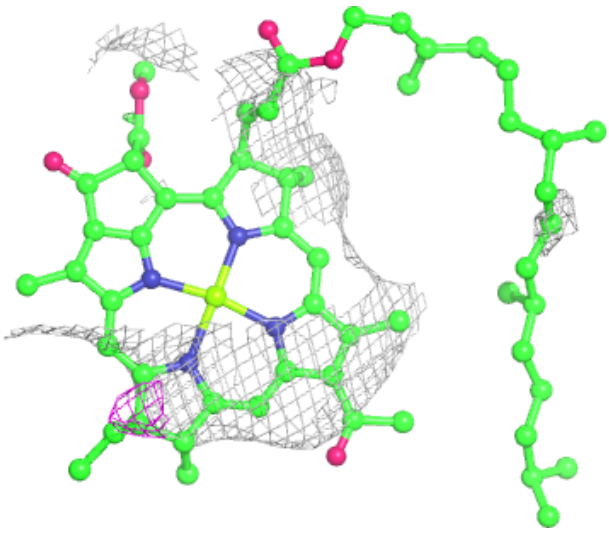
Electron density around BCL BS 102:

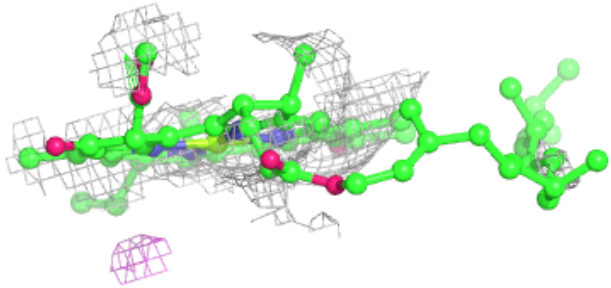
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

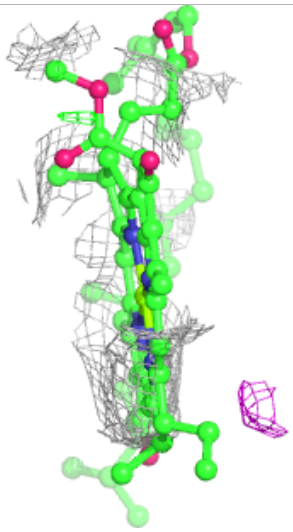


Electron density around BCL BT 101:

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

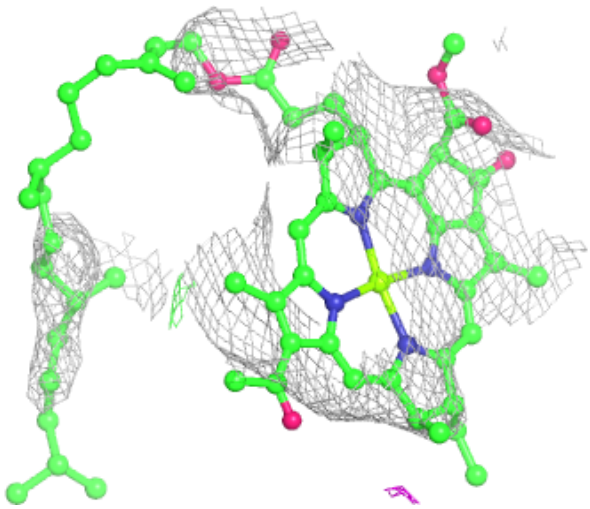


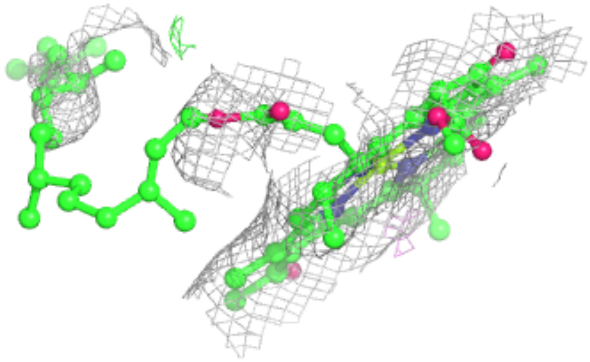


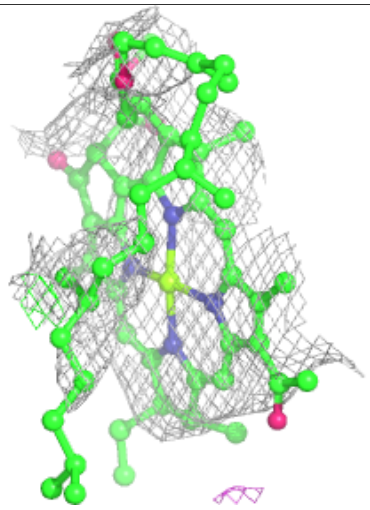


Electron density around BCL AR 101:

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

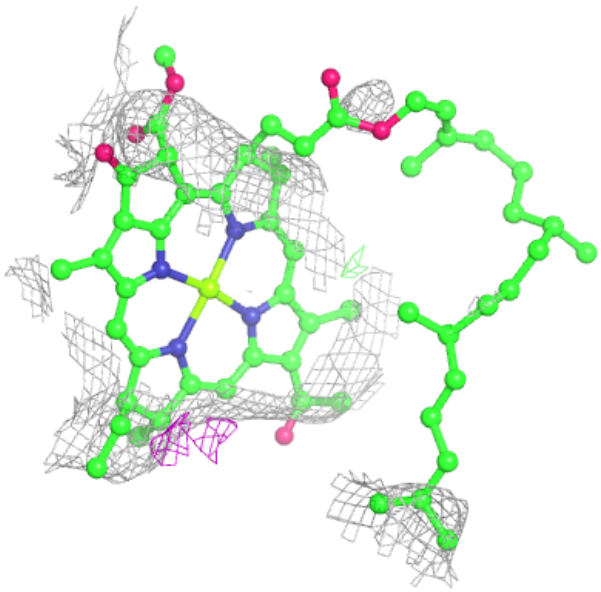


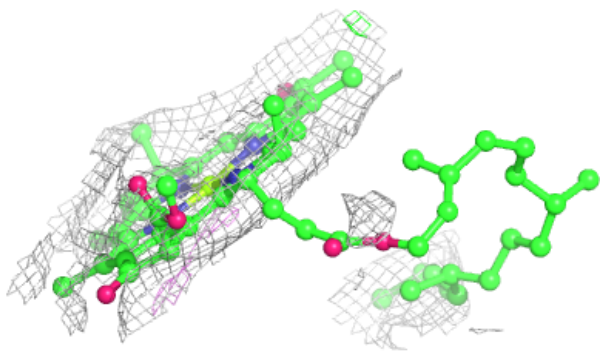


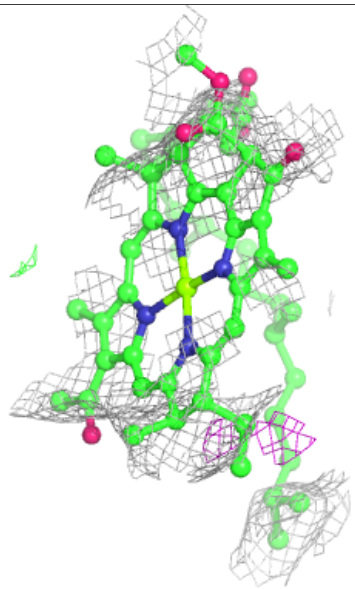


Electron density around BCL BJ 101:

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

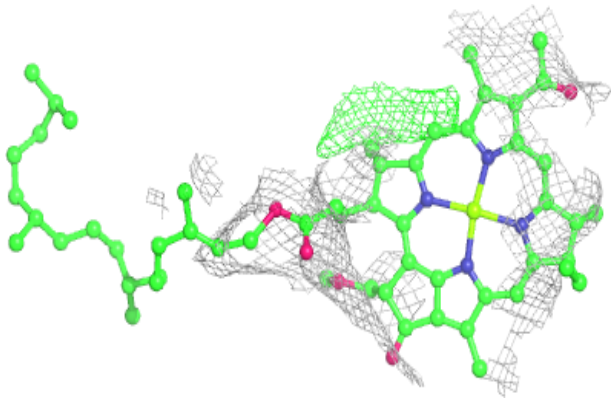


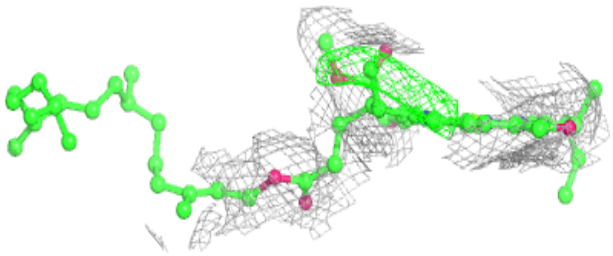


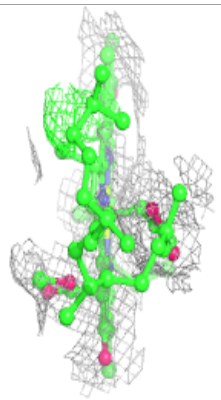


Electron density around BCL A7 103:

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

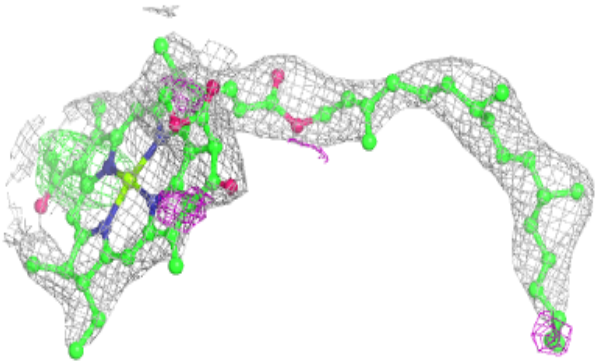


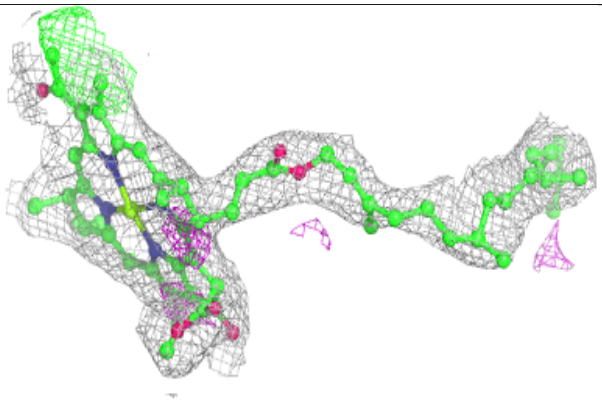


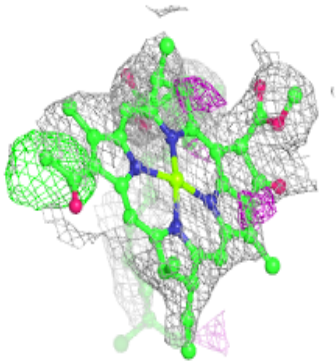


Electron density around BCL BM 402:

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

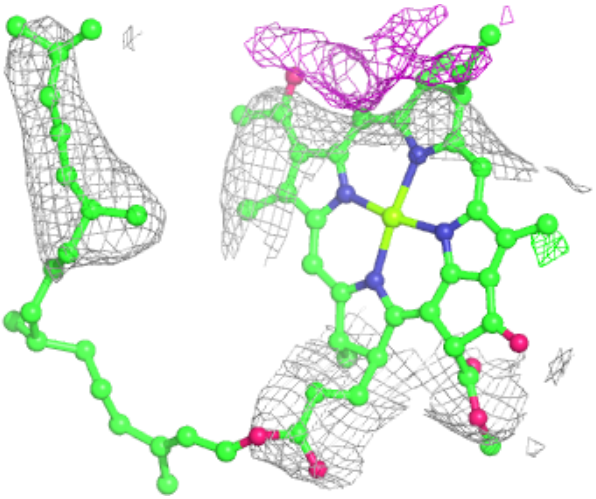


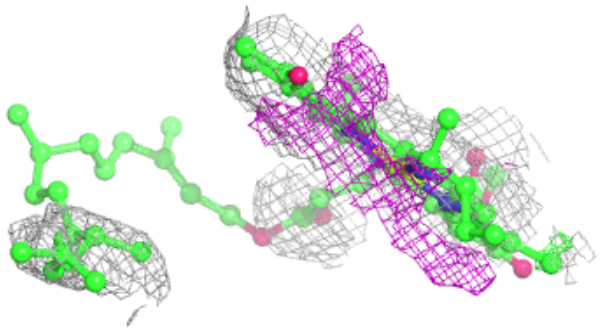


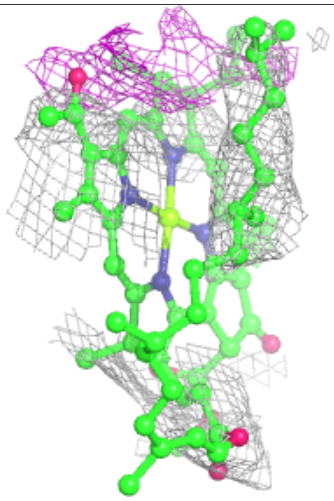


Electron density around BCL A2 101:

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

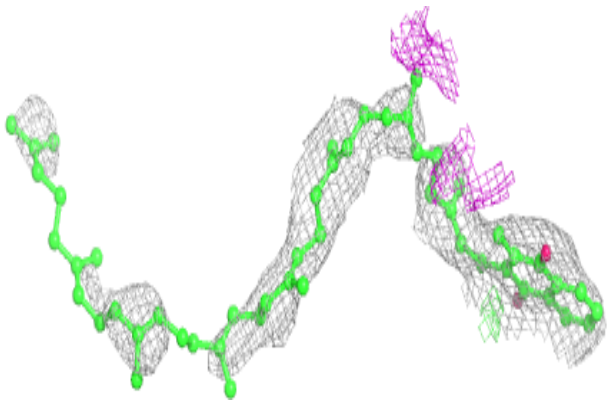


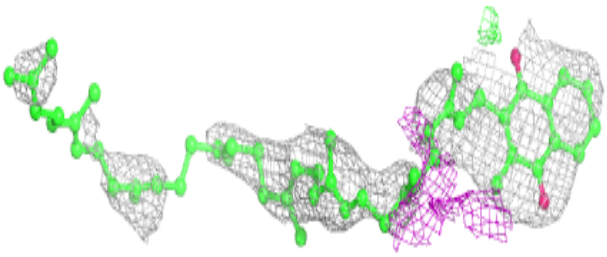


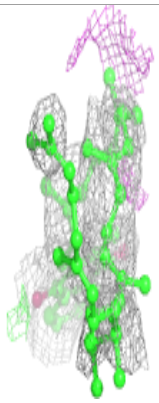


Electron density around MQ8 AM 405:

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

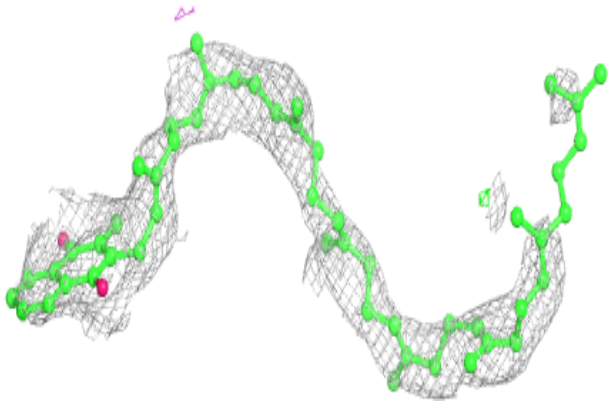


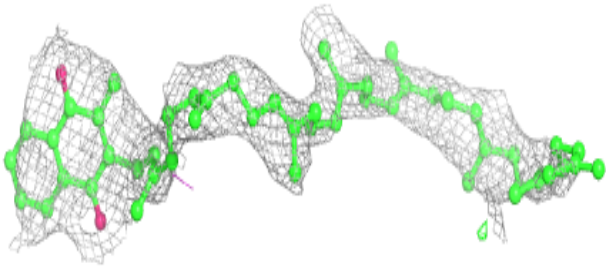


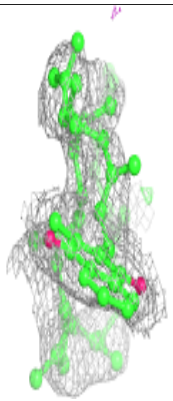


Electron density around MQ8 BM 405:

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

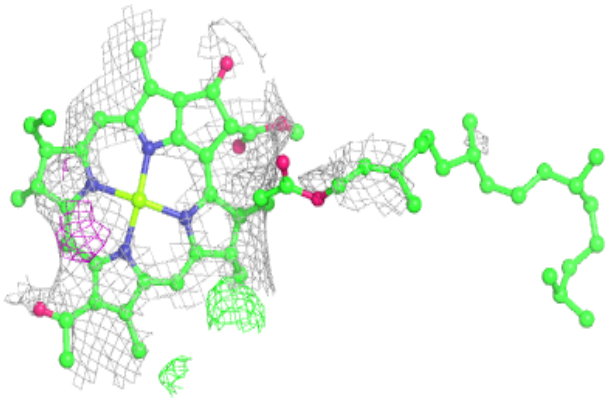


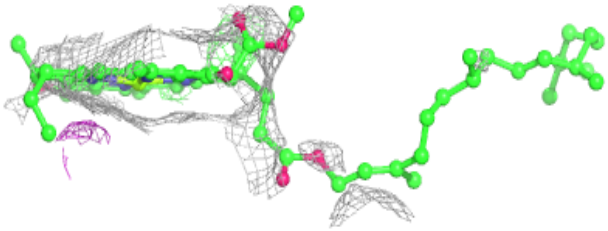


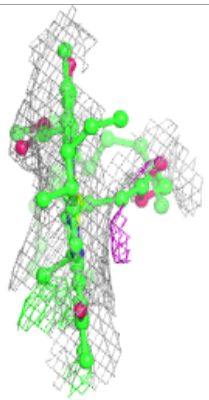


Electron density around BCL BF 102:

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

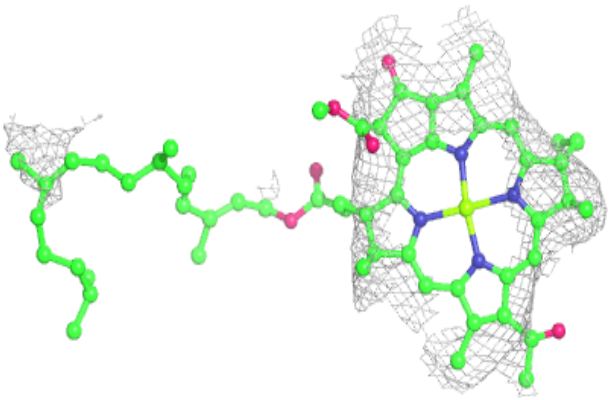


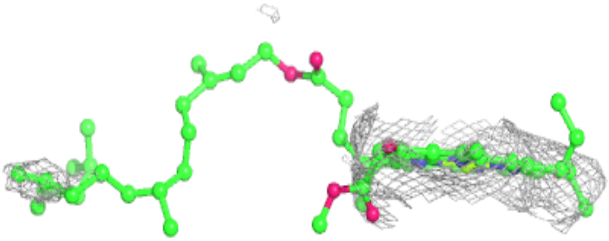


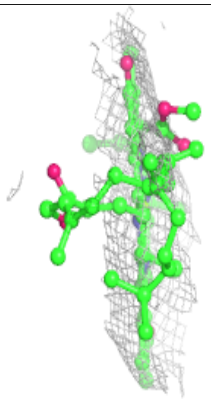


Electron density around BCL AQ 102:

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

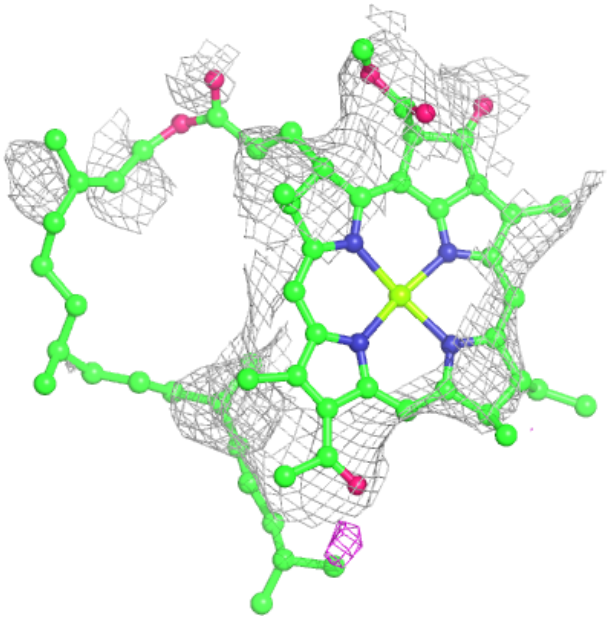


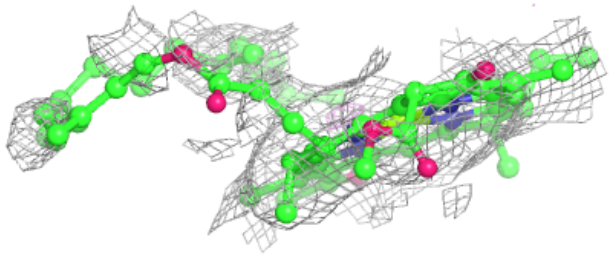


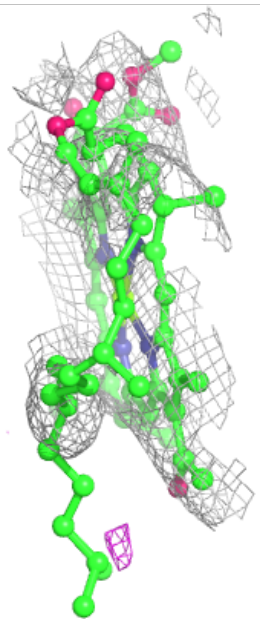


Electron density around BCL A3 104:

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

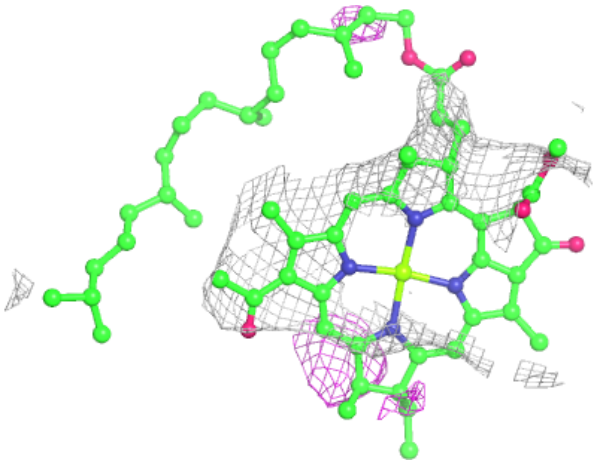


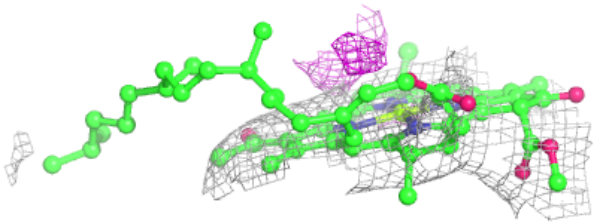


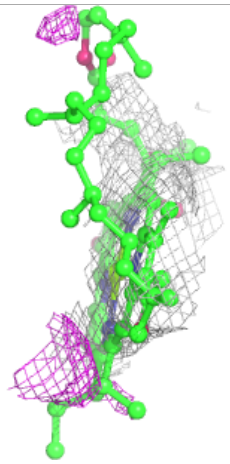


Electron density around BCL BN 101:

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

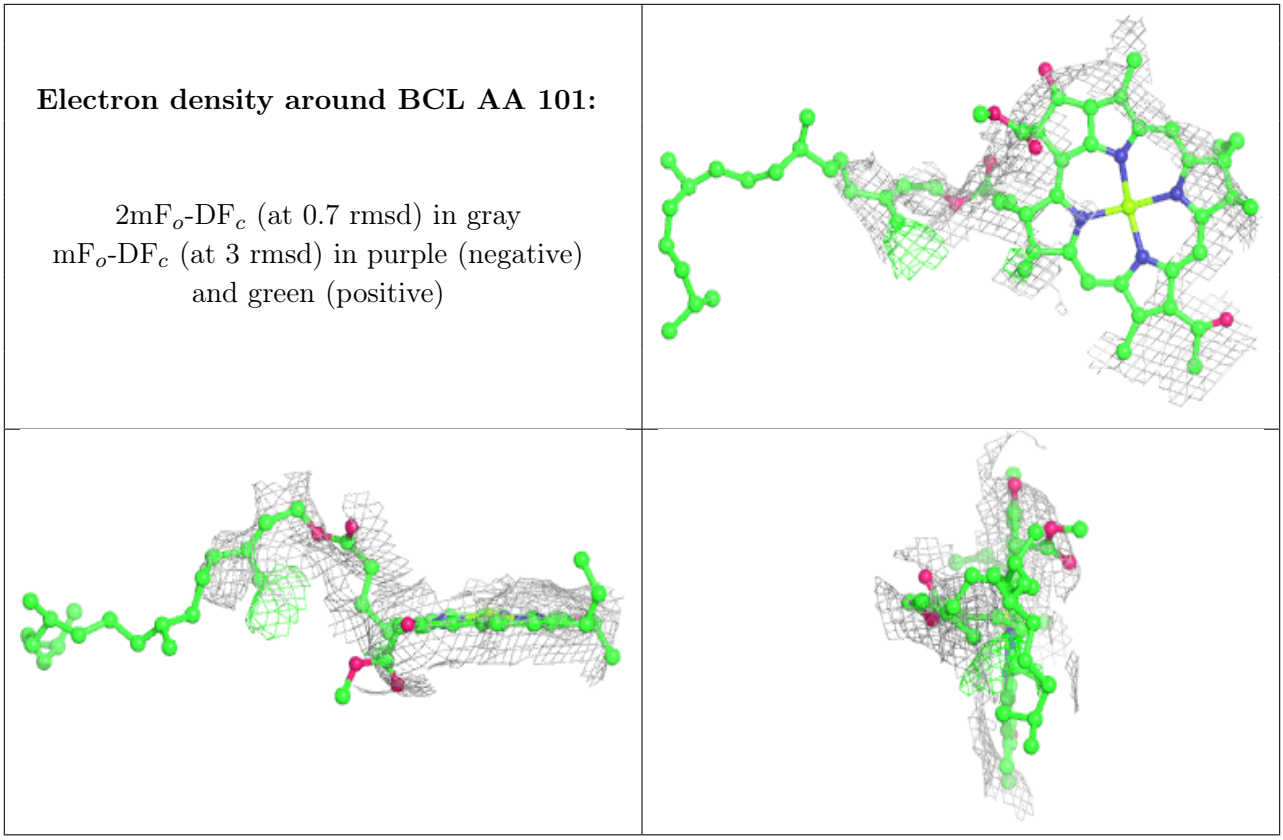






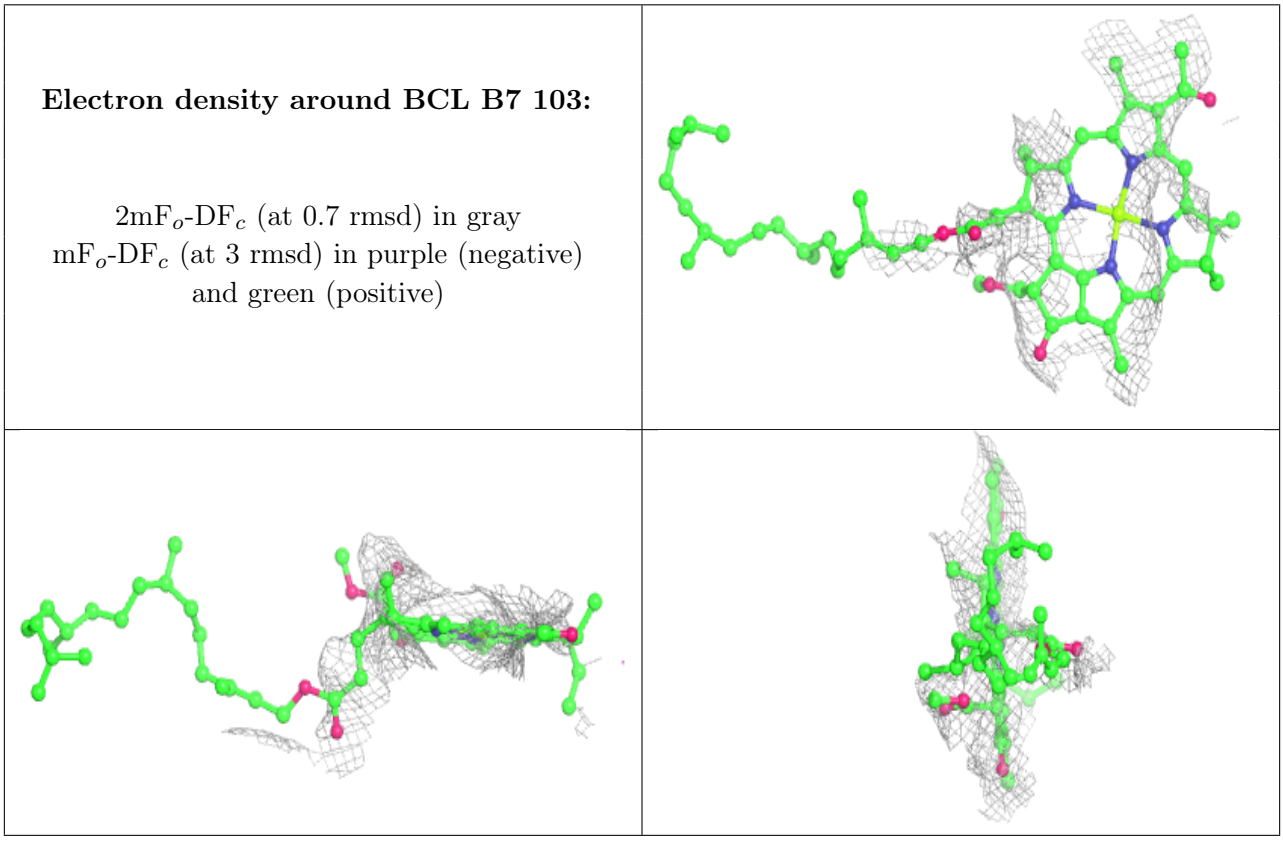
Electron density around BCL AA 101:

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



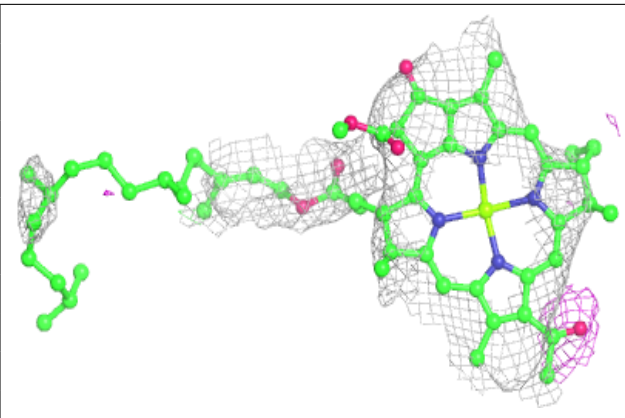
Electron density around BCL B7 103:

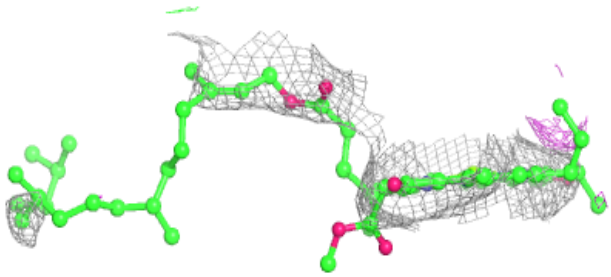
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

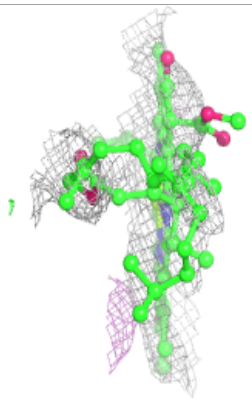


Electron density around BCL AI 102:

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

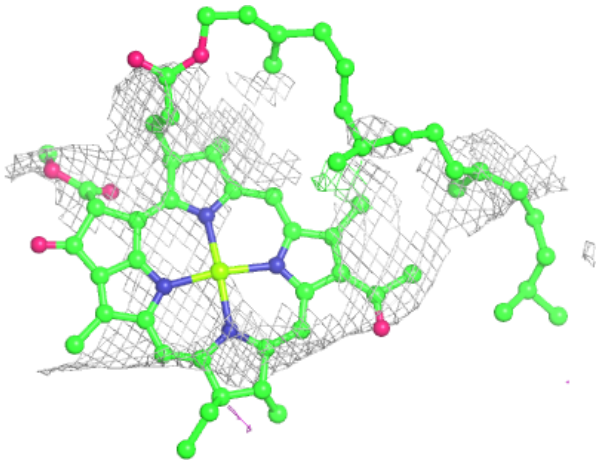


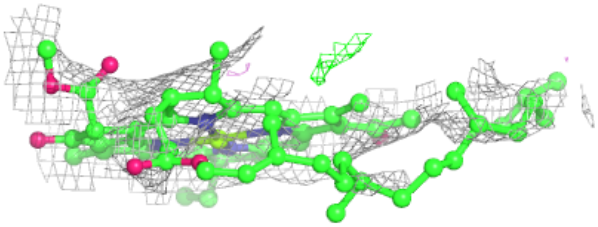


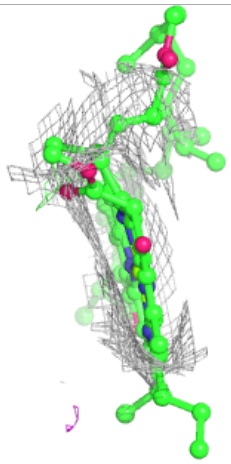


Electron density around BCL AV 102:

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

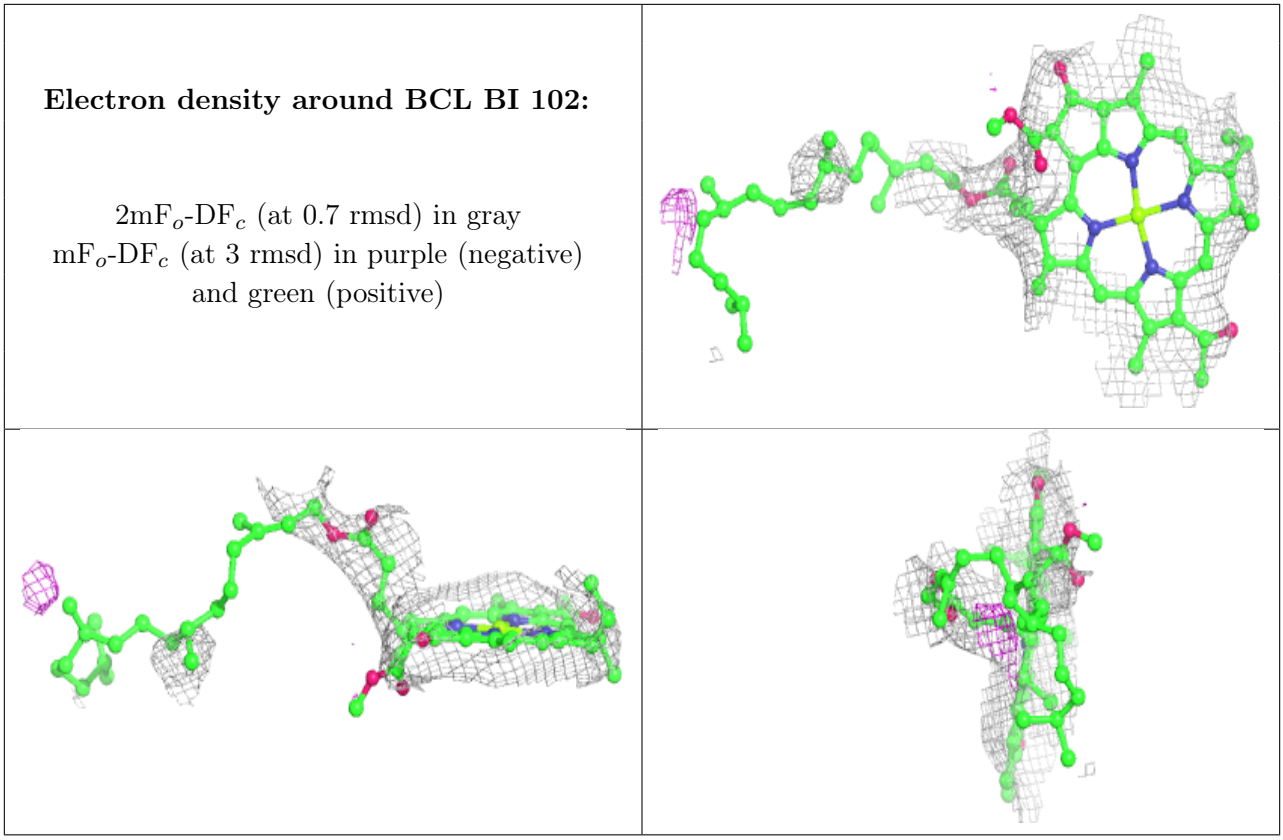






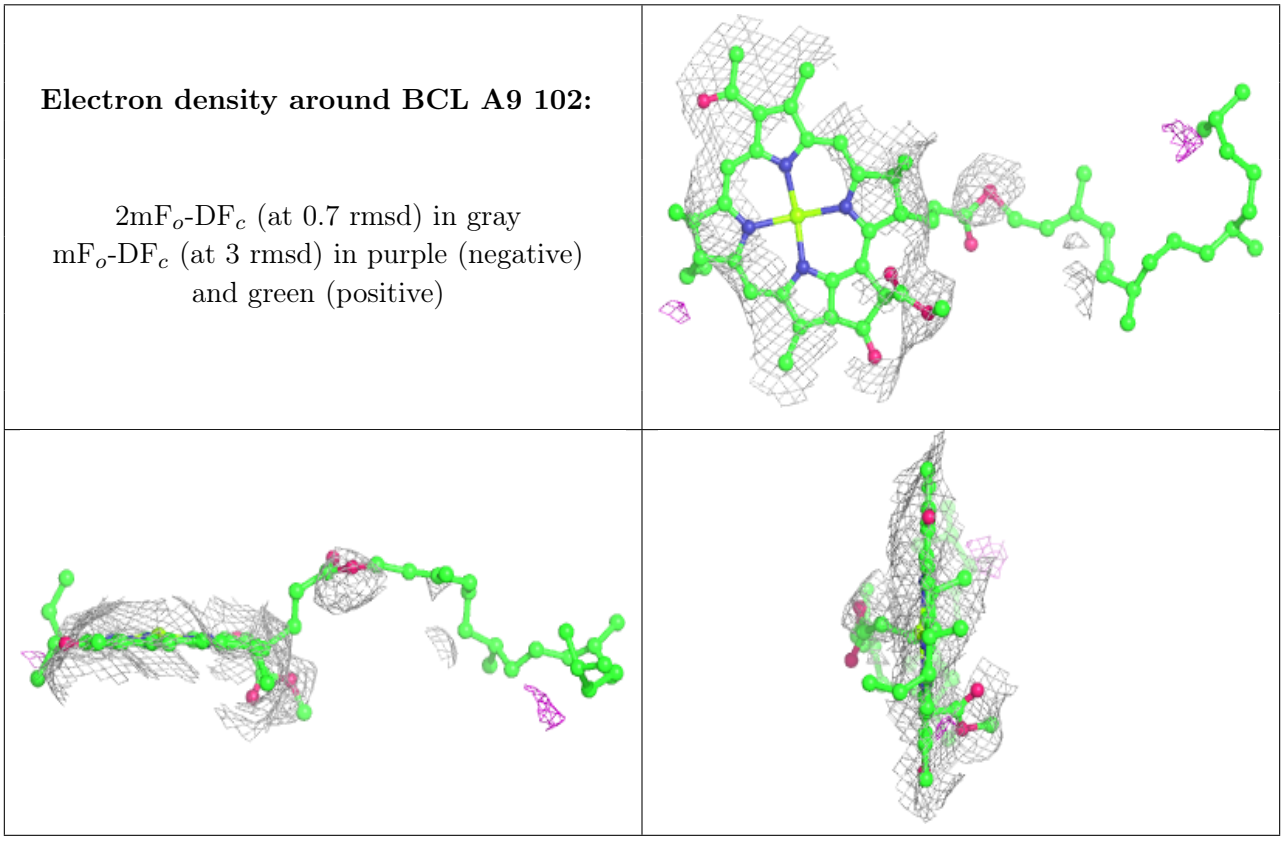
Electron density around BCL BI 102:

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



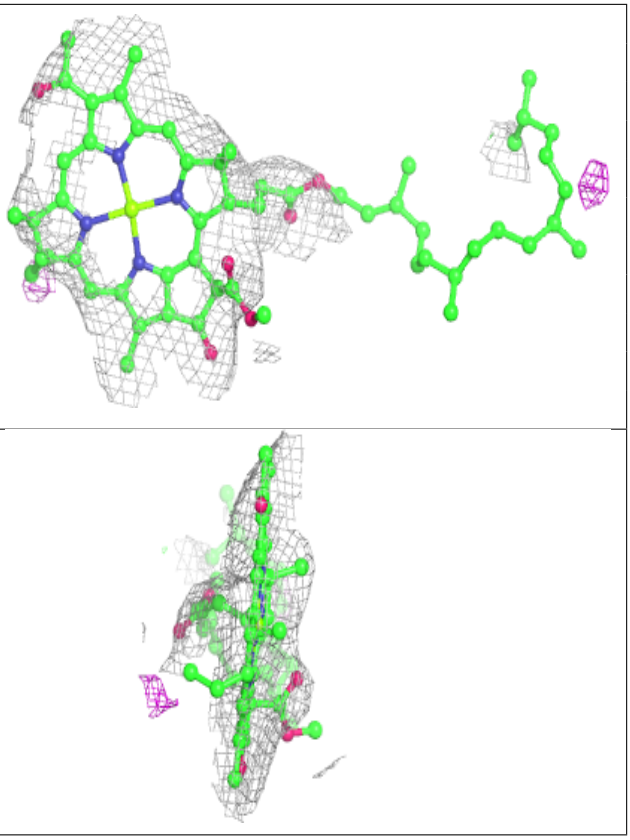
Electron density around BCL A9 102:

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



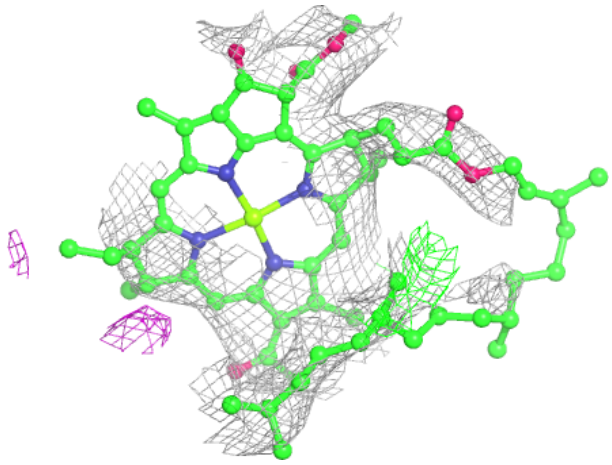
Electron density around BCL A5 102:

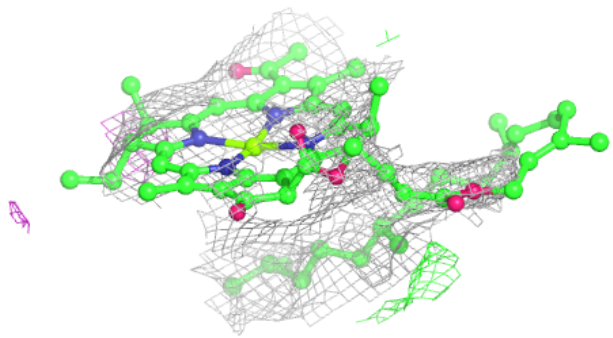
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

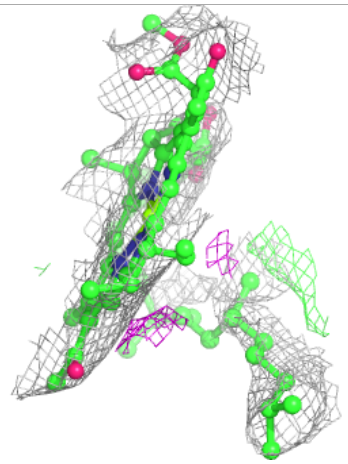


Electron density around BCL AN 101:

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

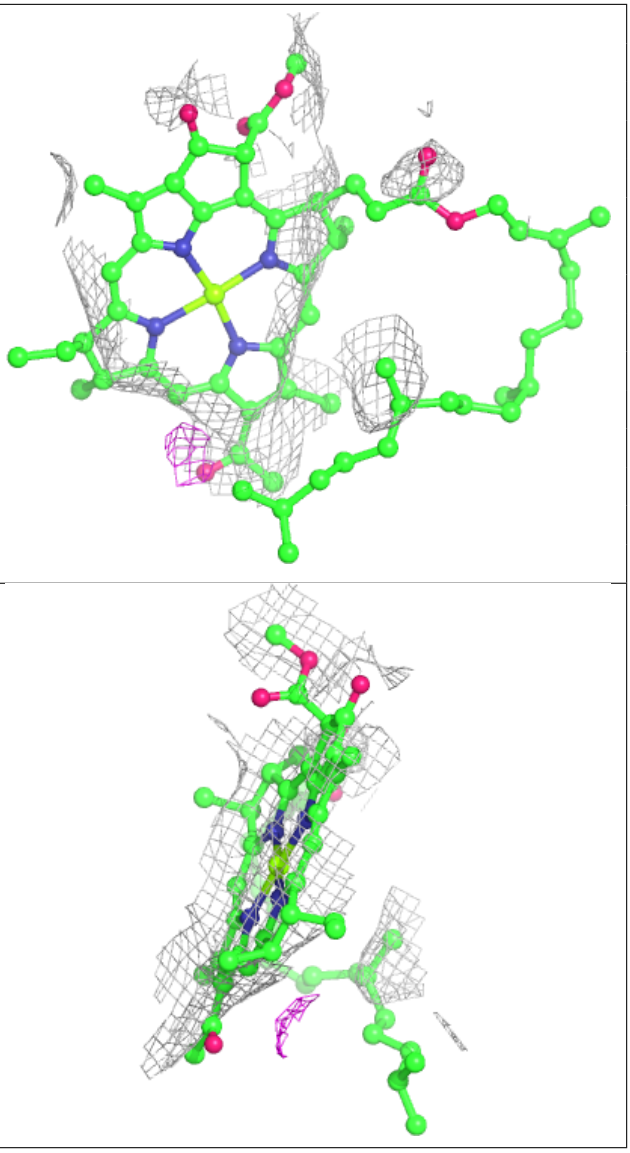






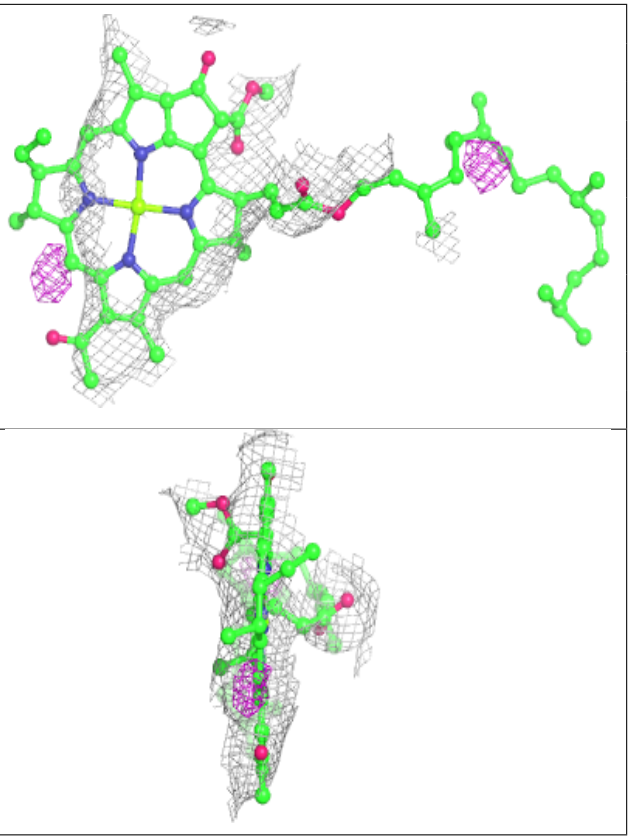
Electron density around BCL B0 102:

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



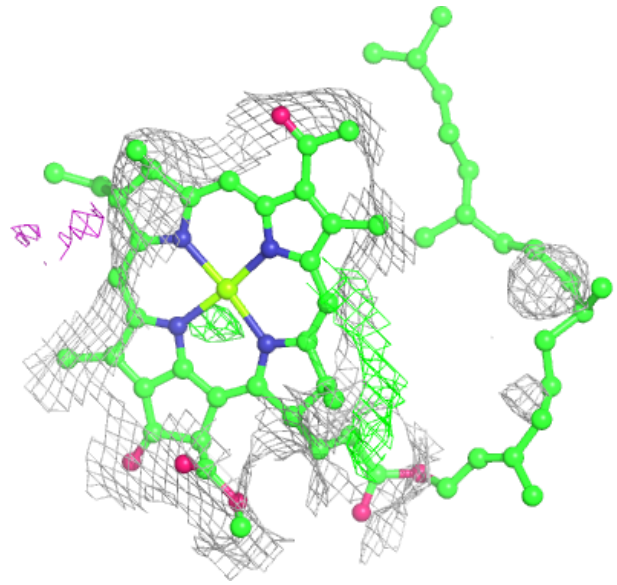
Electron density around BCL AU 102:

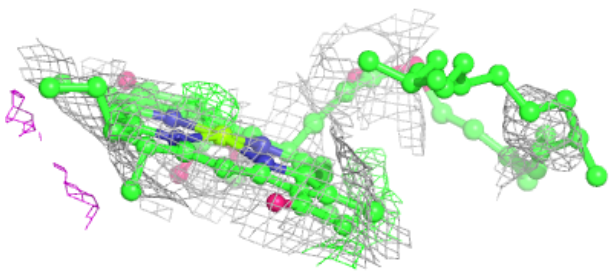
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

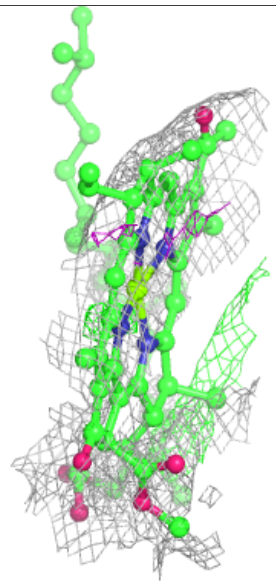


Electron density around BCL A6 101:

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

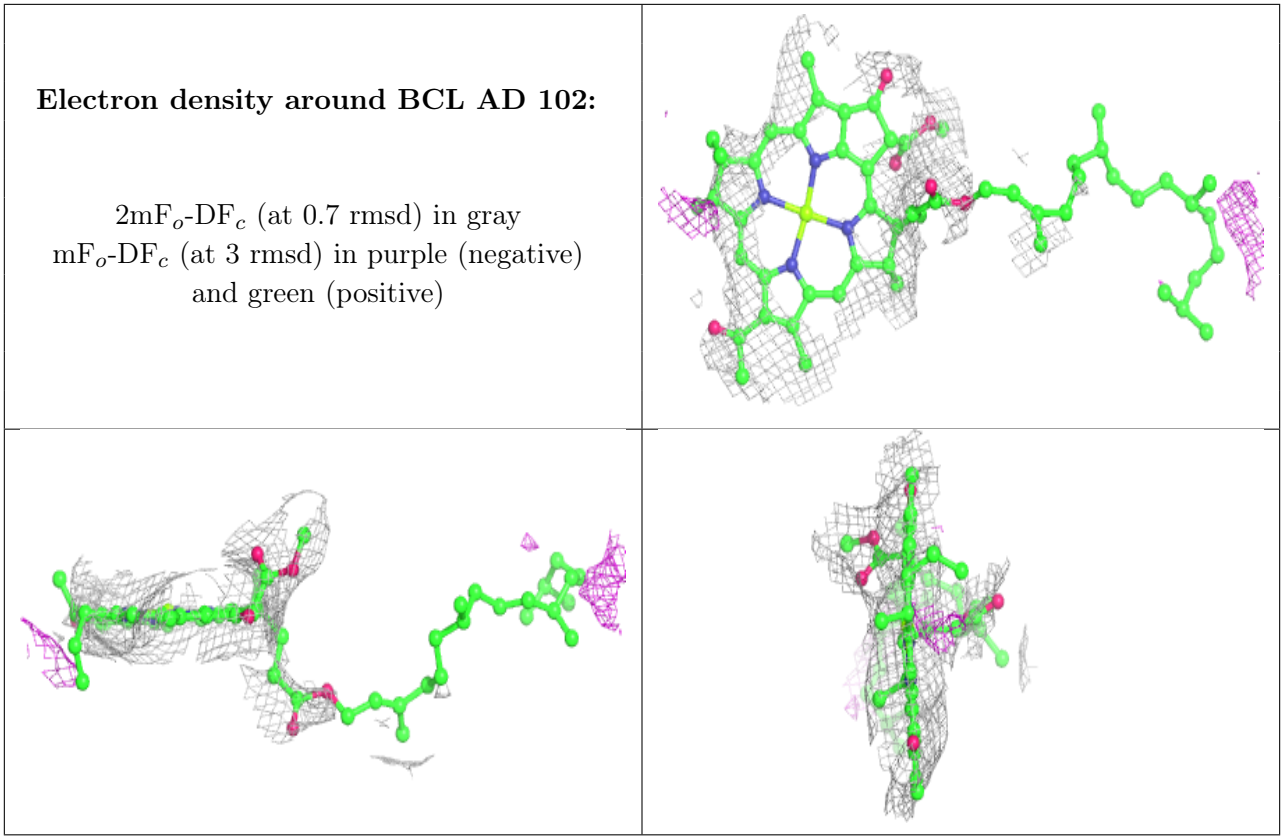






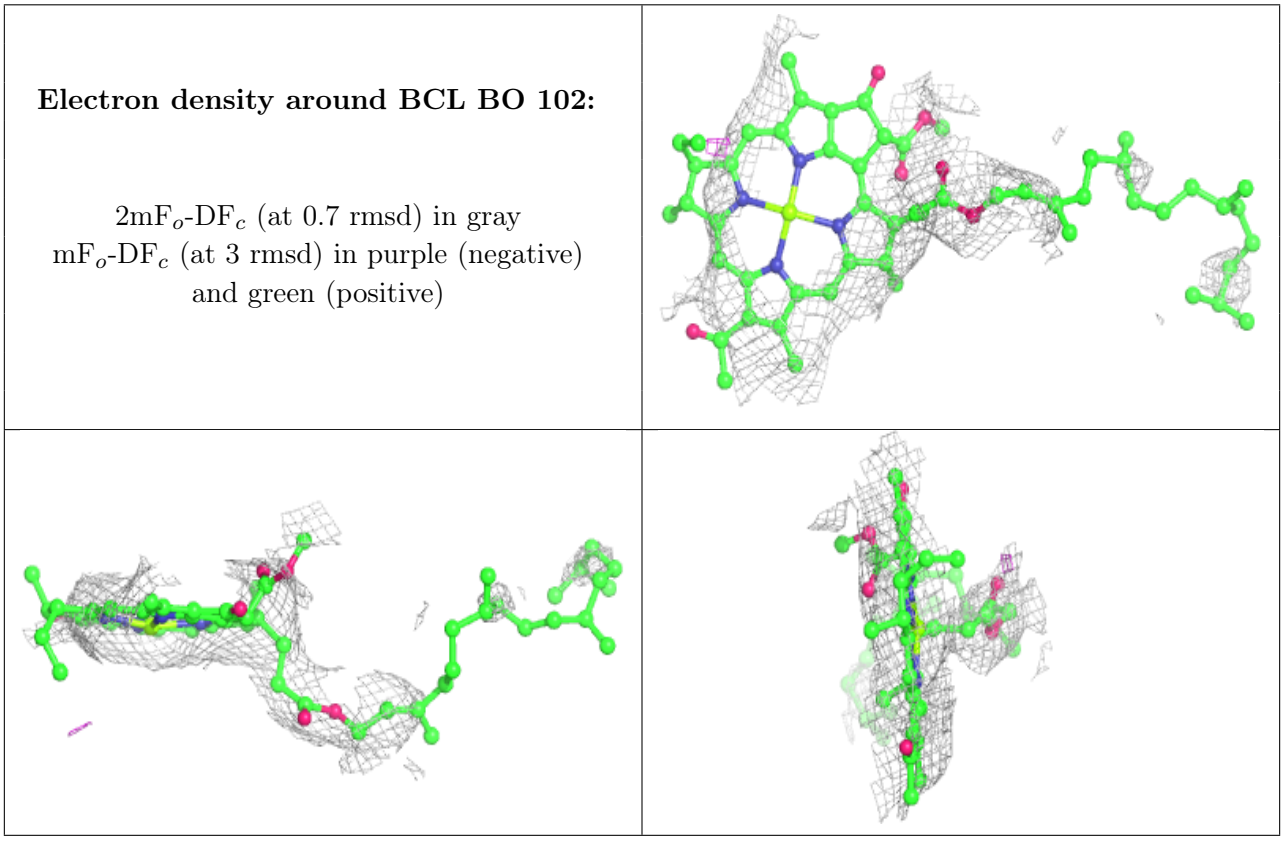
Electron density around BCL AD 102:

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



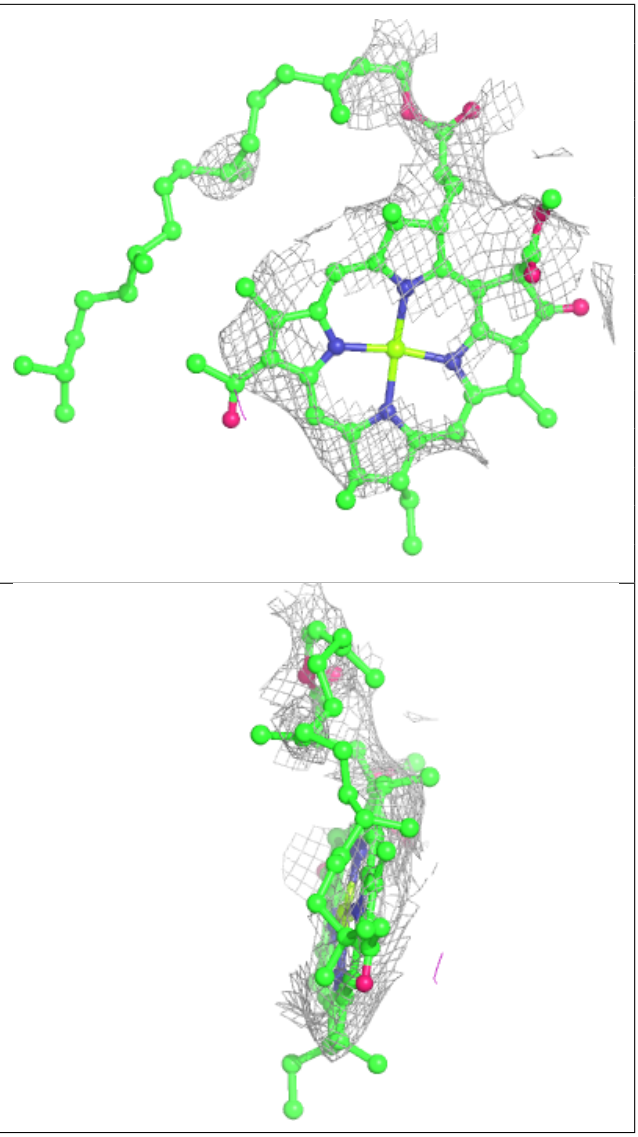
Electron density around BCL BO 102:

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



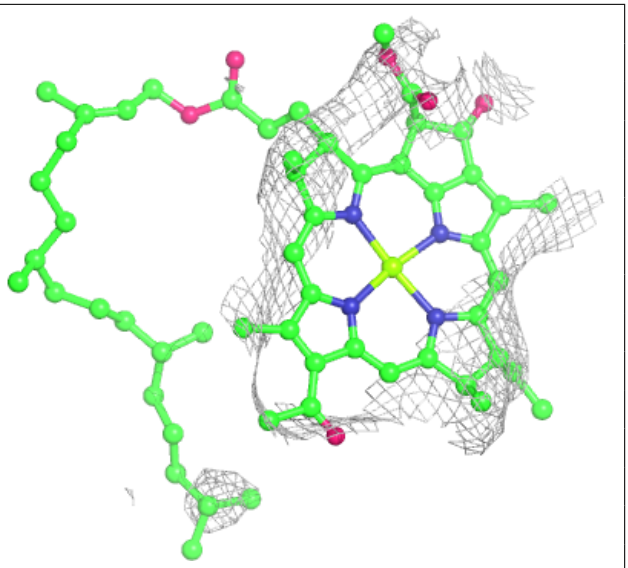
Electron density around BCL AT 101:

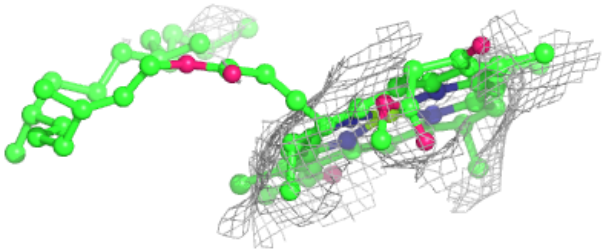
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

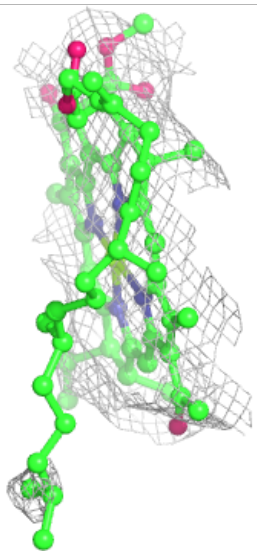


Electron density around BCL B4 101:

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

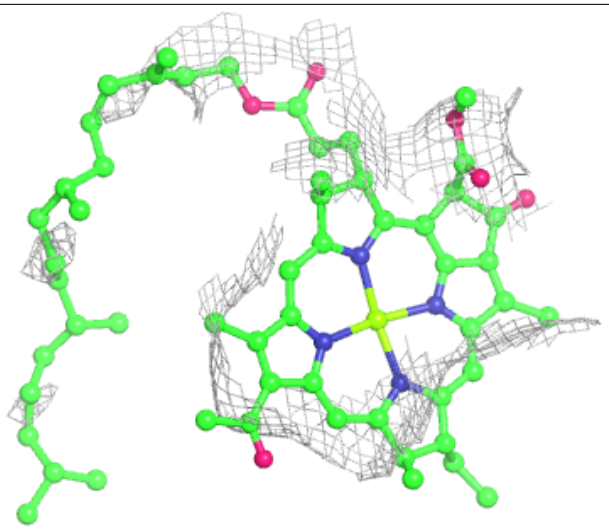


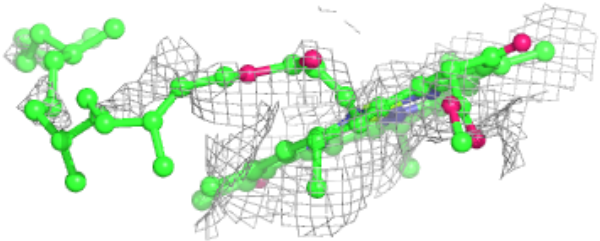


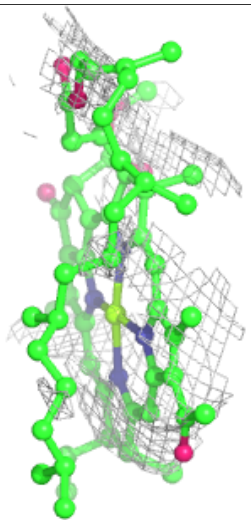


Electron density around BCL B6 101:

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

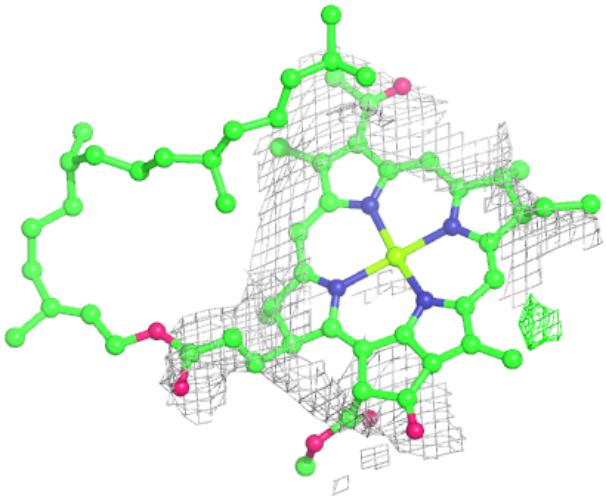


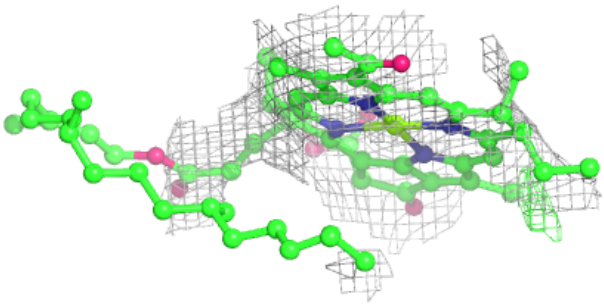


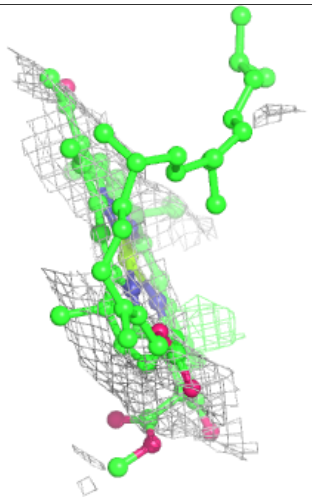


Electron density around BCL BB 101:

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

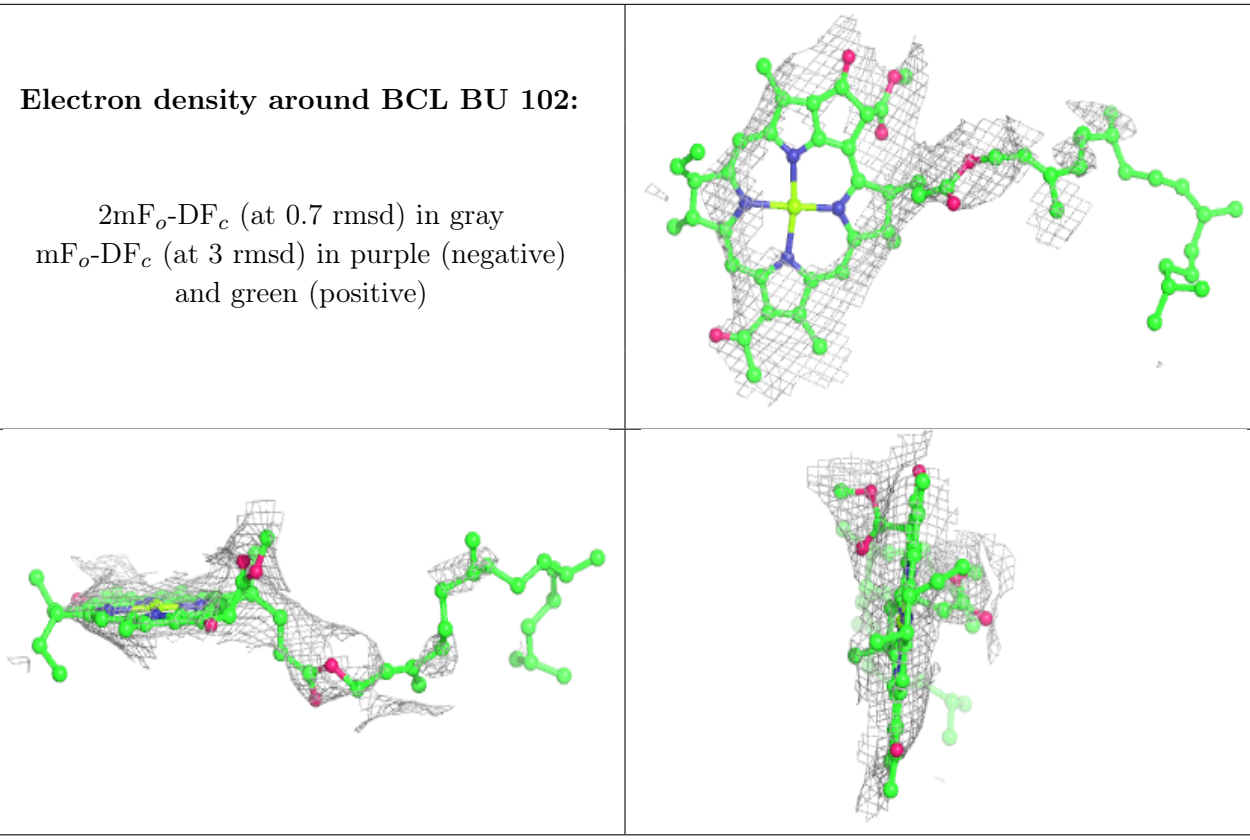






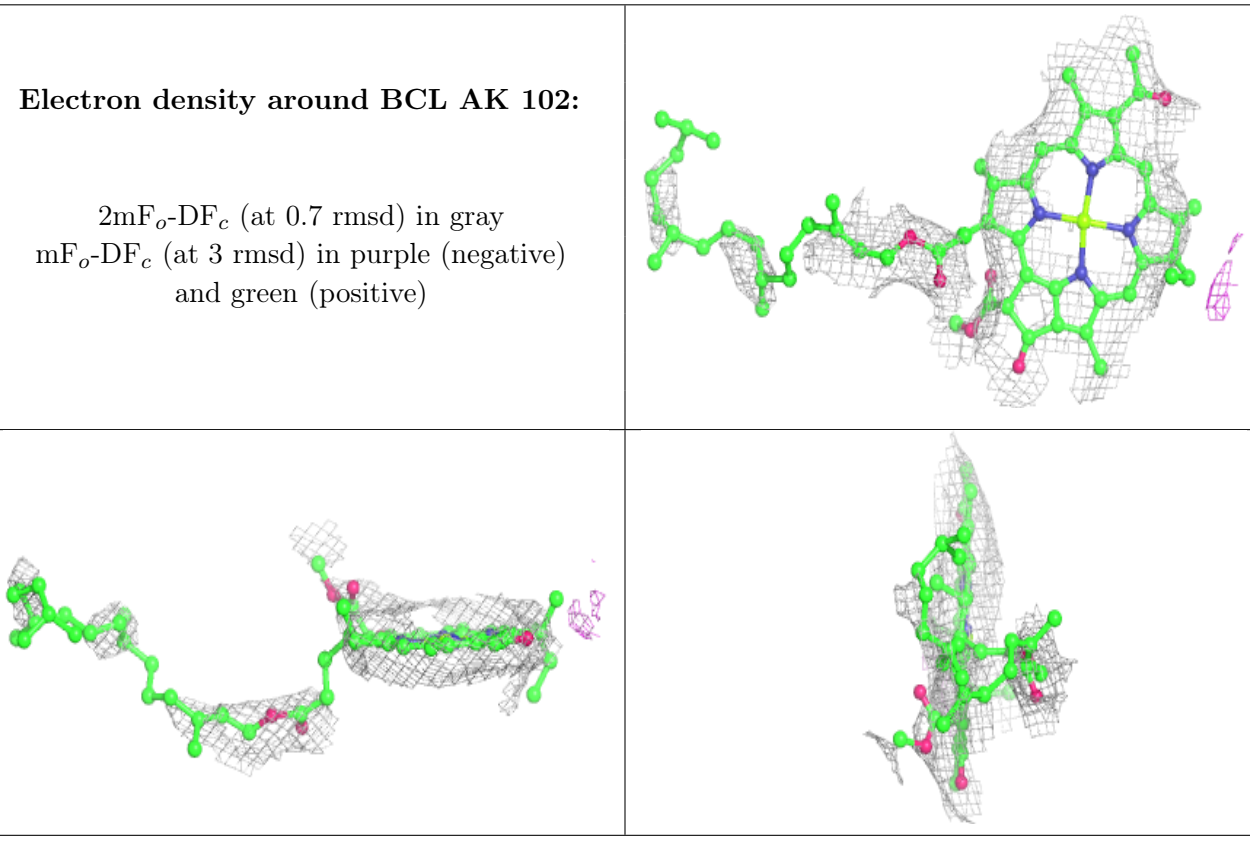
Electron density around BCL BU 102:

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



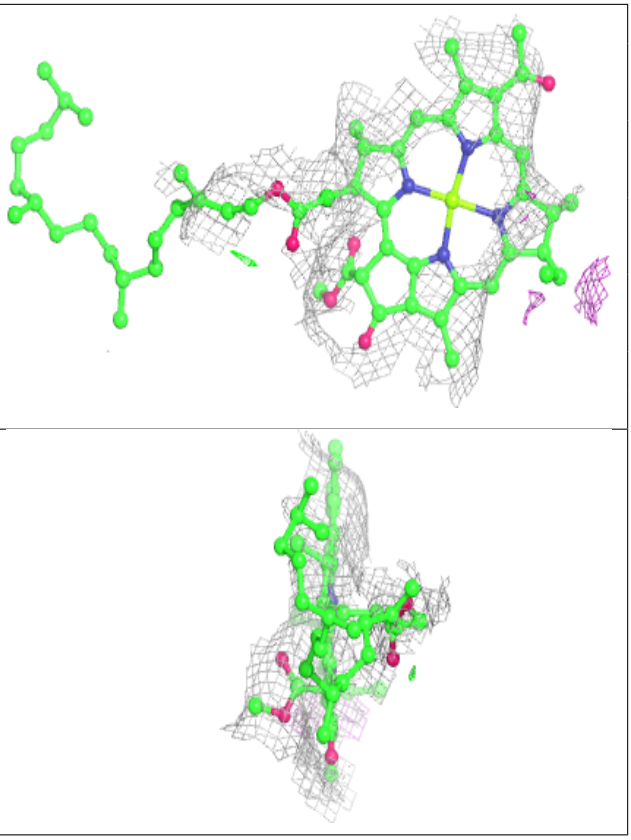
Electron density around BCL AK 102:

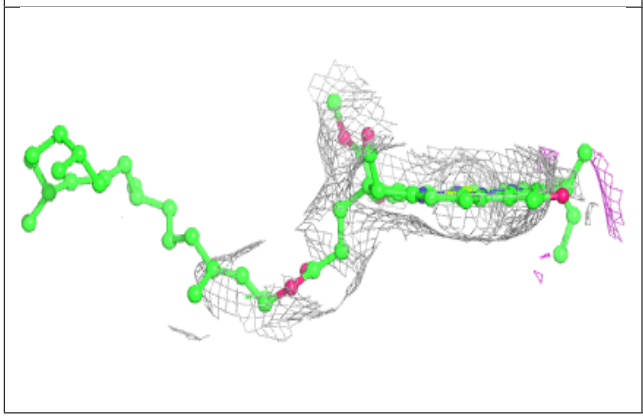
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL BW 102:

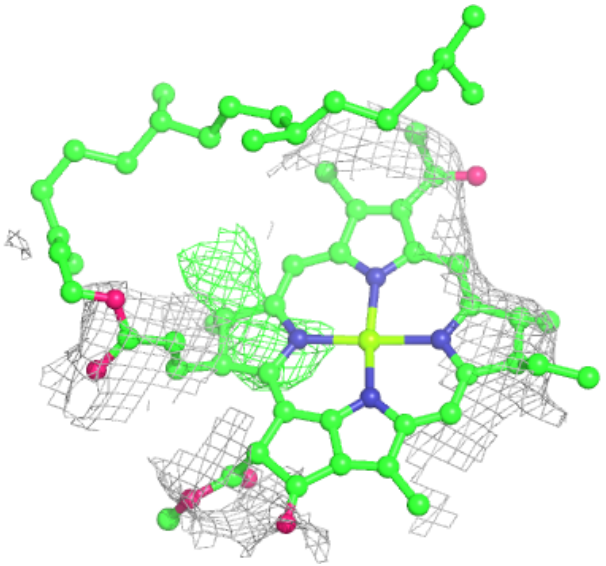
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

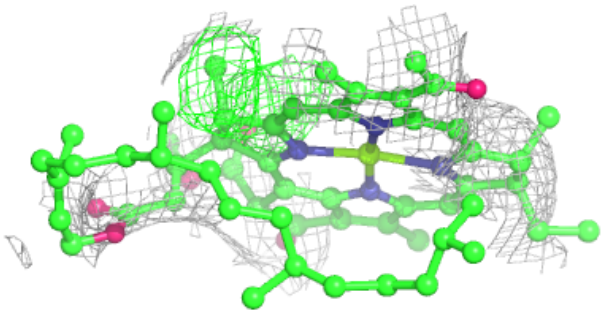


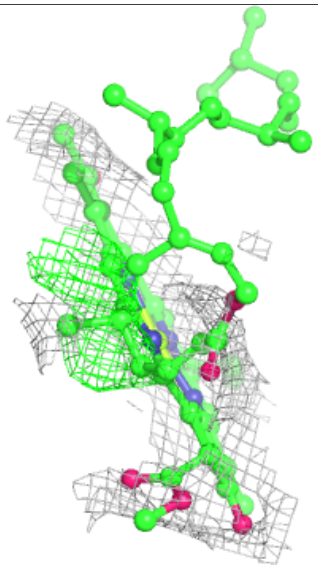


Electron density around BCL BE 101:

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

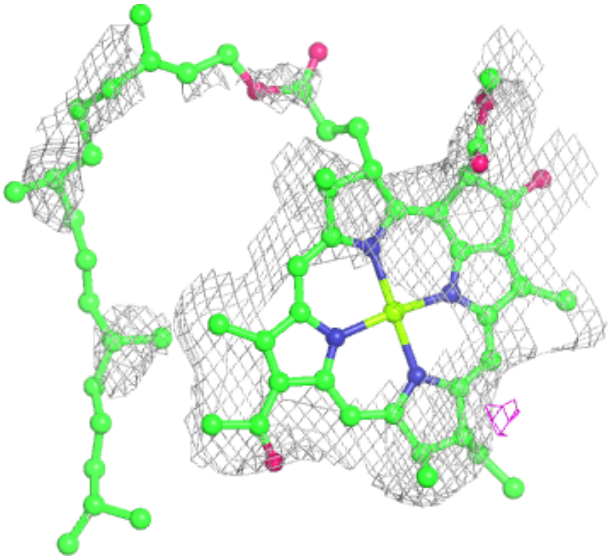


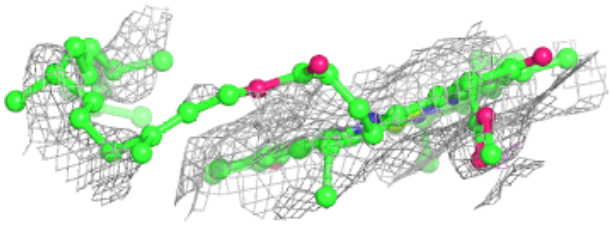


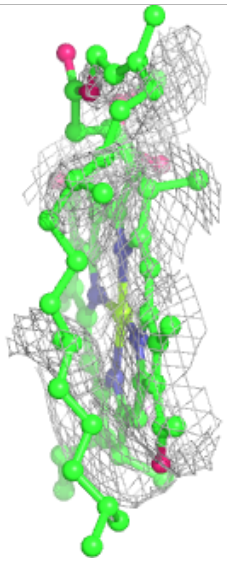


Electron density around BCL AB 101:

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

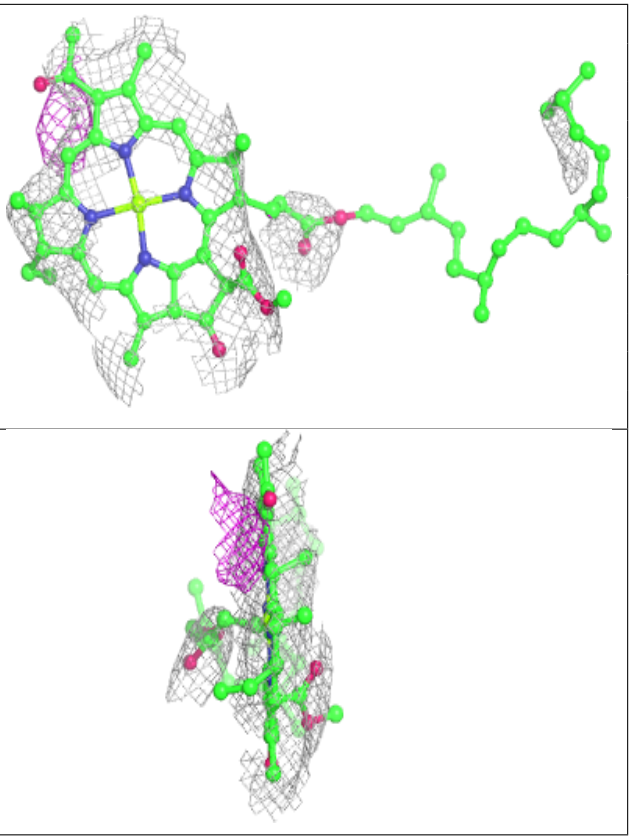


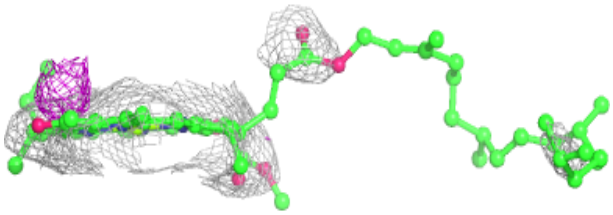




Electron density around BCL AY 102:

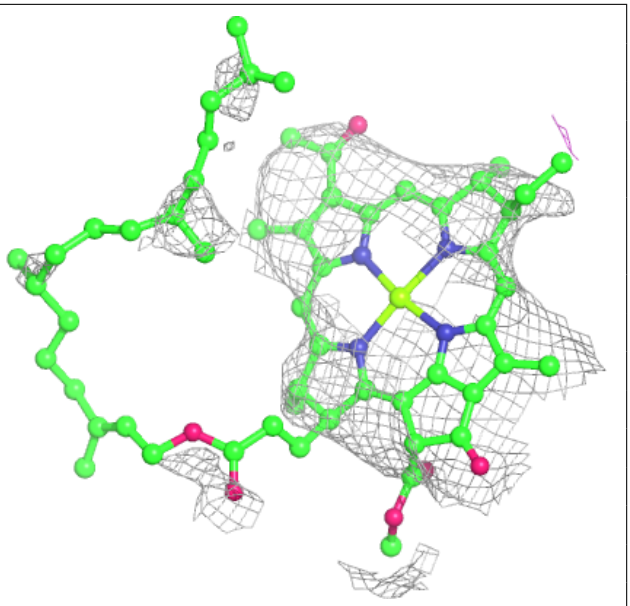
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

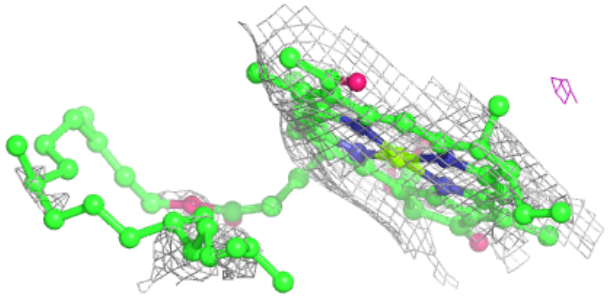


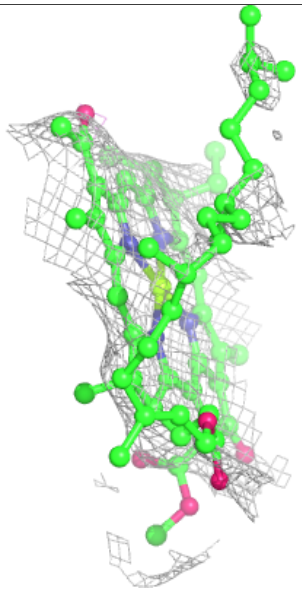


Electron density around BCL AJ 101:

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

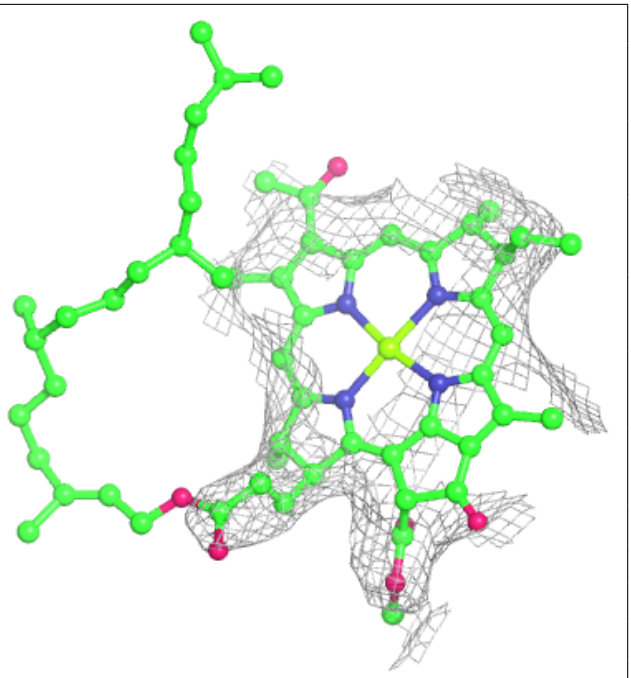


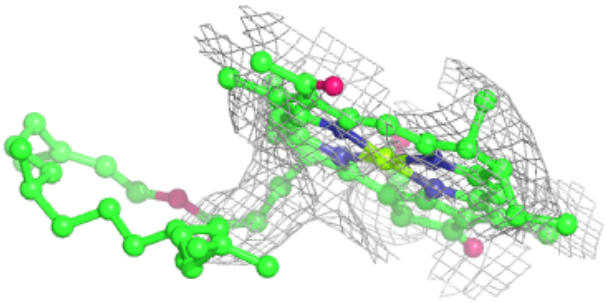


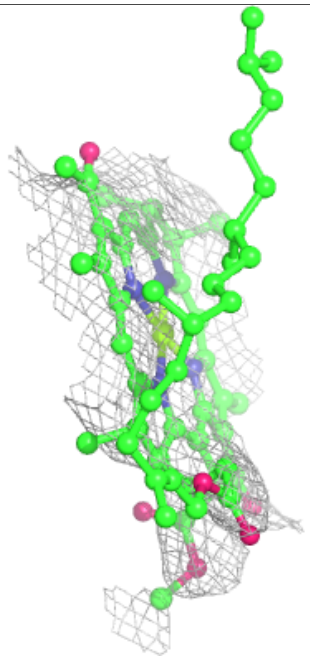


Electron density around BCL B2 101:

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

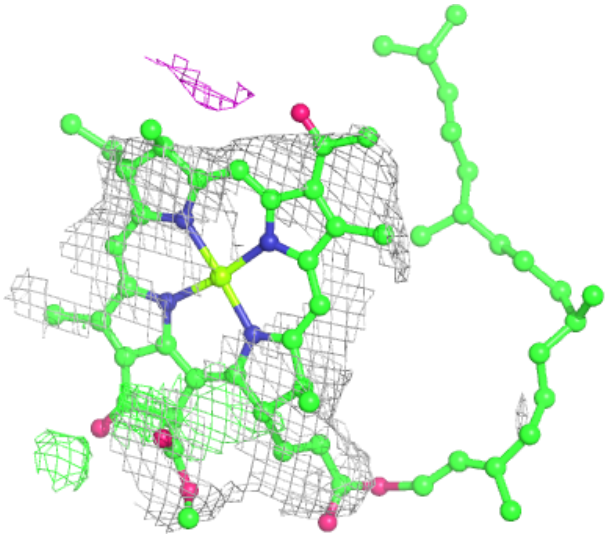


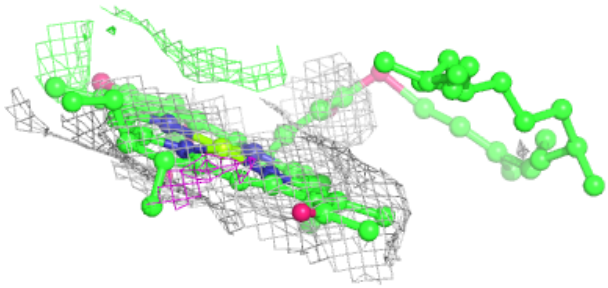


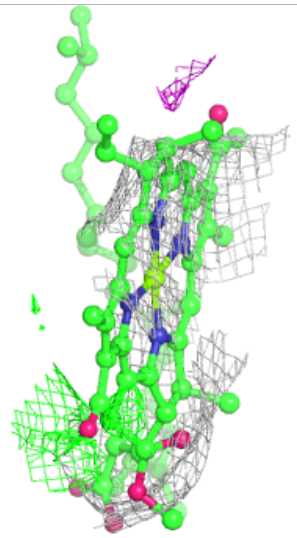


Electron density around BCL AX 101:

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

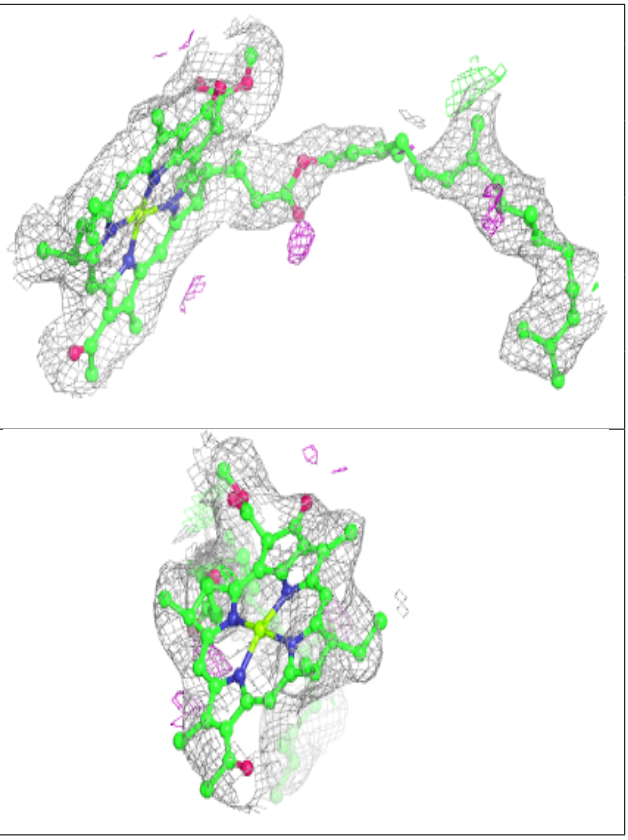






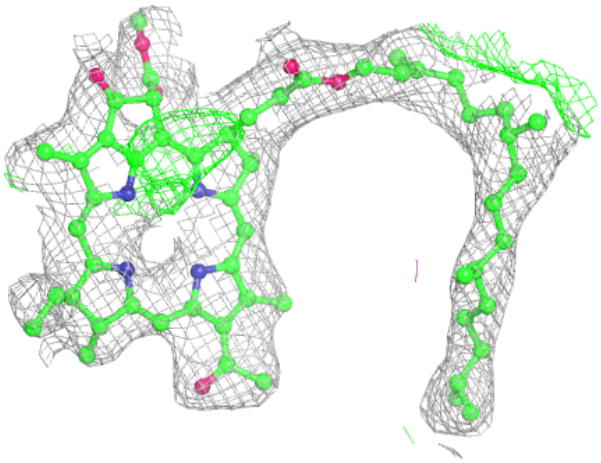
Electron density around BCL AL 301:

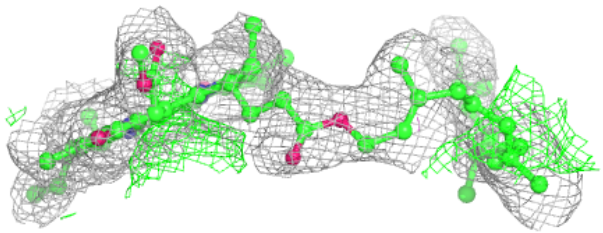
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

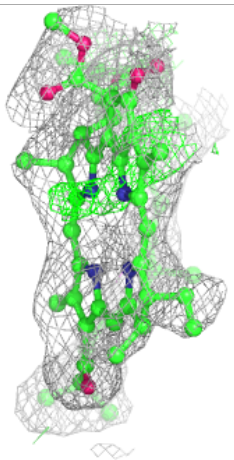


Electron density around BPH AL 302:

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

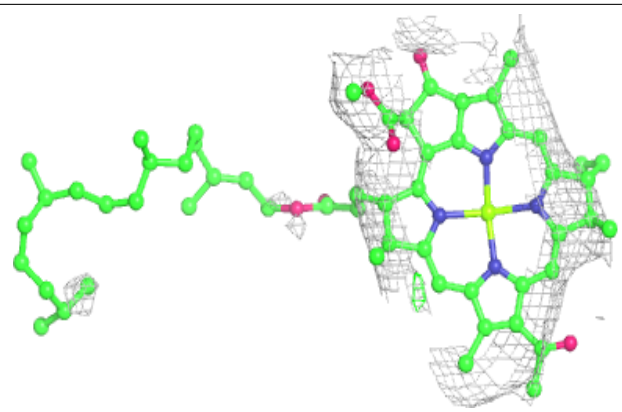


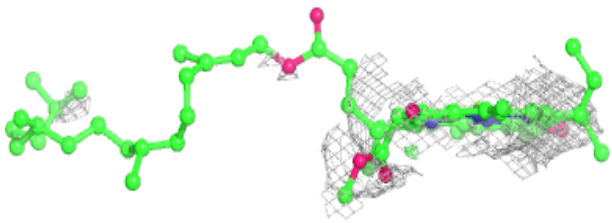


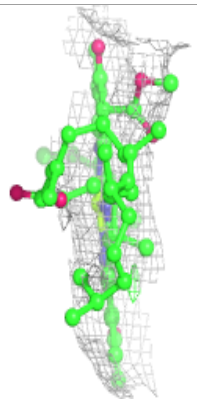


Electron density around BCL AO 102:

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

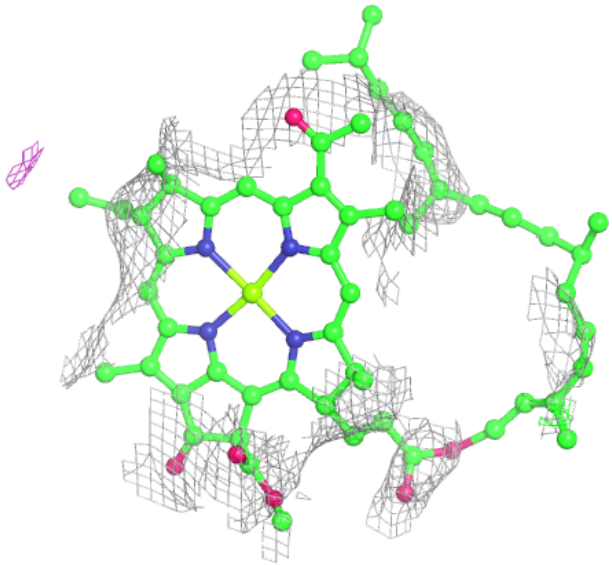


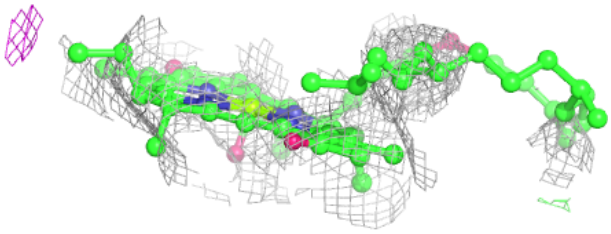


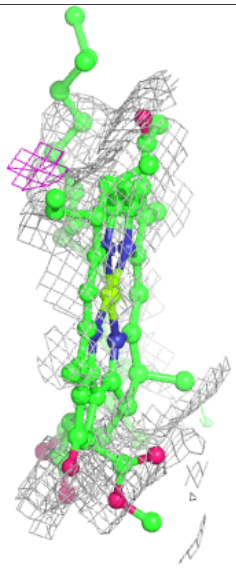


Electron density around BCL A0 102:

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

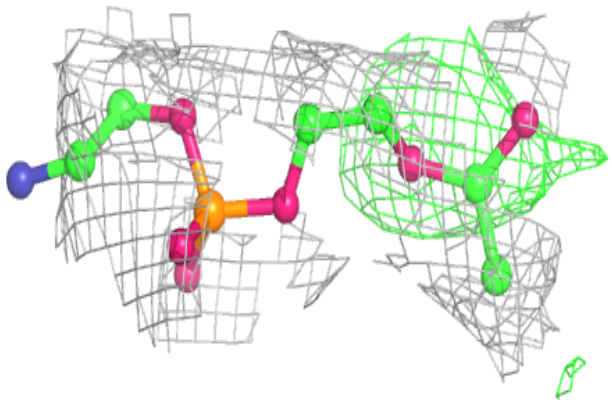


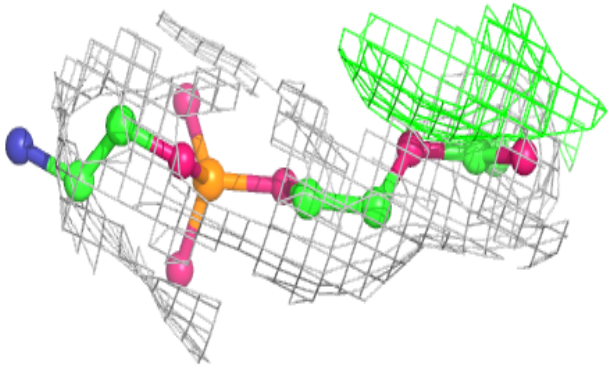


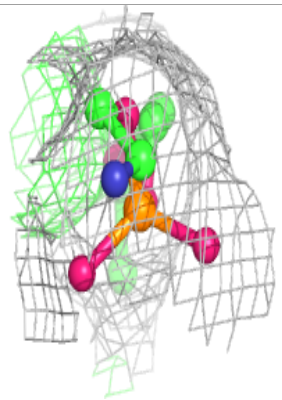


Electron density around PEF AM 408:

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

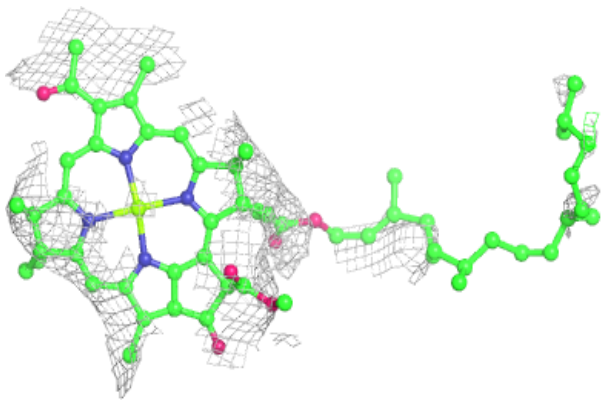


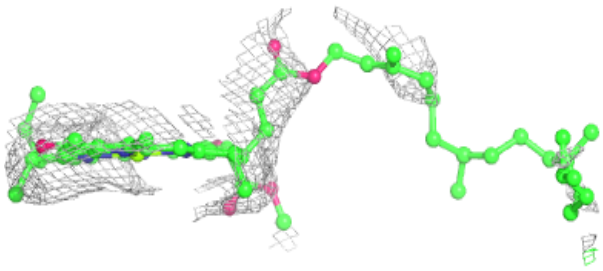


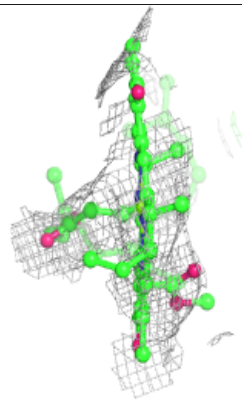


Electron density around BCL B5 102:

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

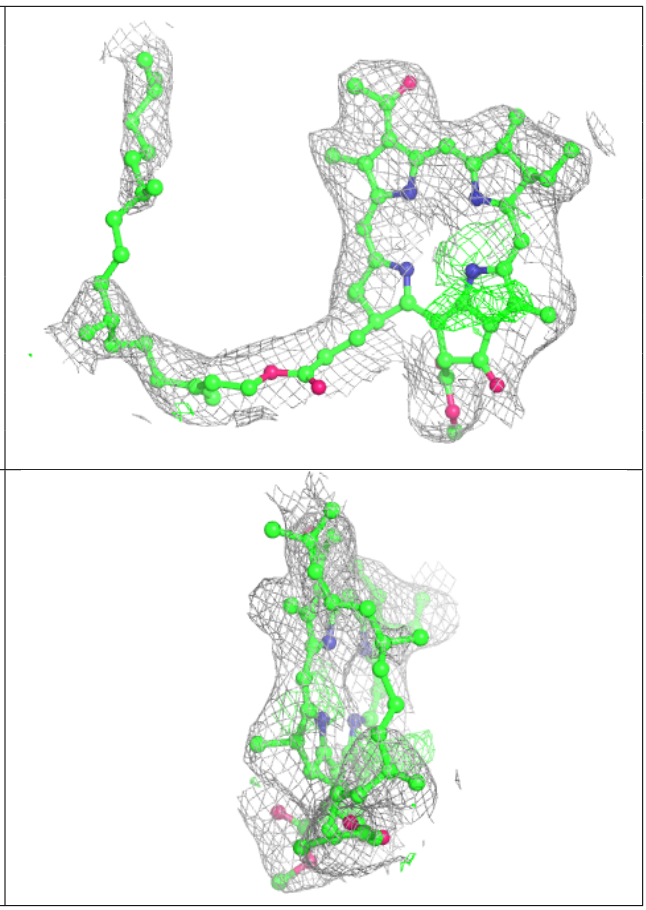






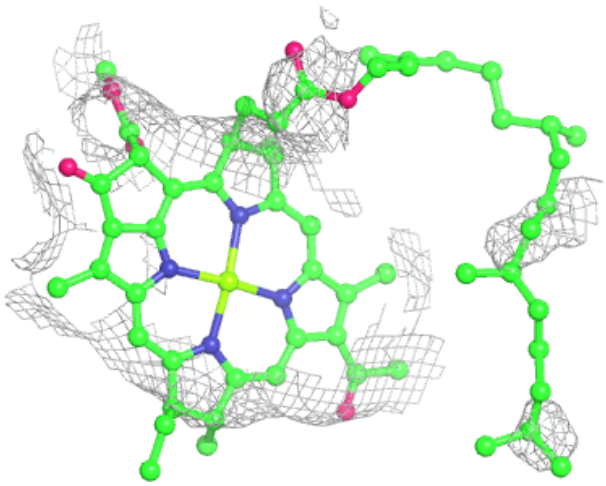
Electron density around BPH BL 302:

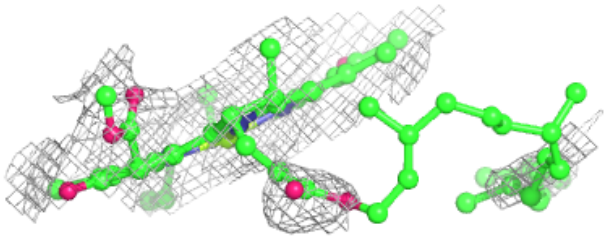
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

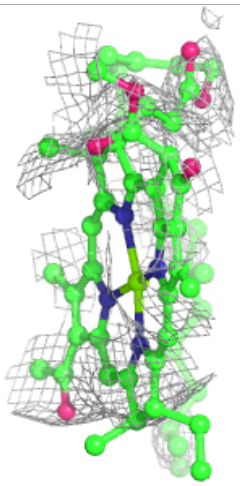


Electron density around BCL BG 101:

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

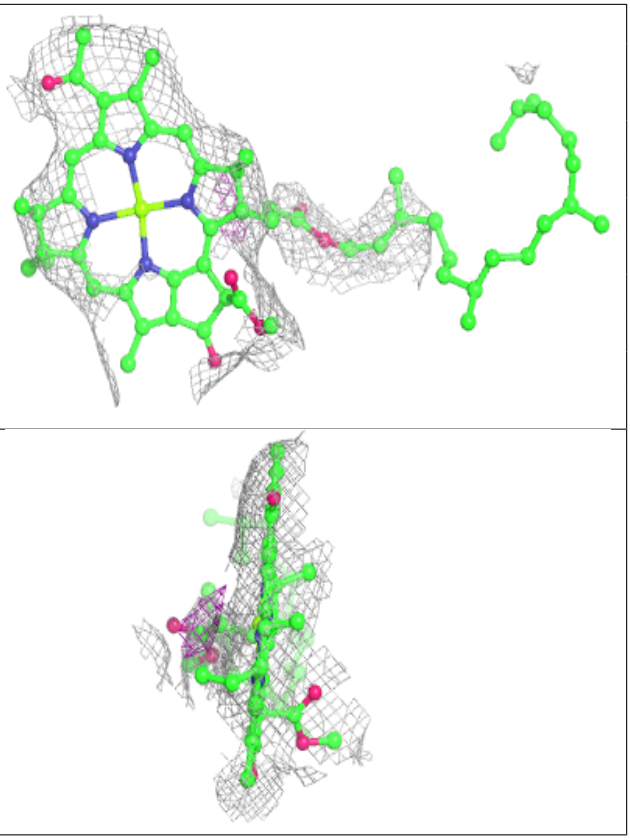


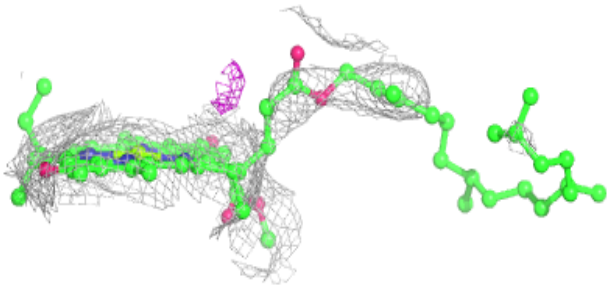




Electron density around BCL BY 102:

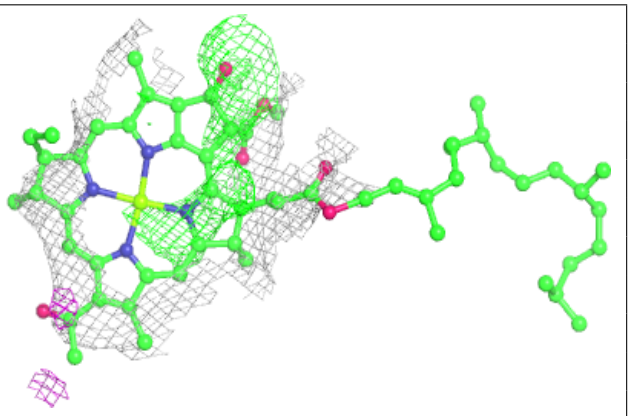
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

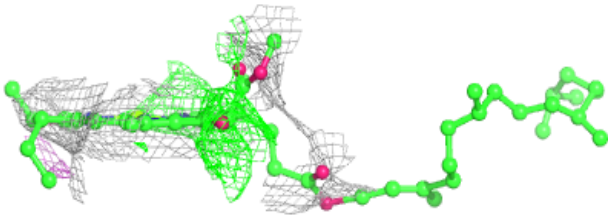


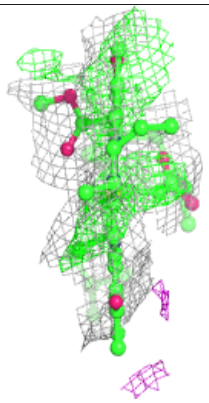


Electron density around BCL AW 101:

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

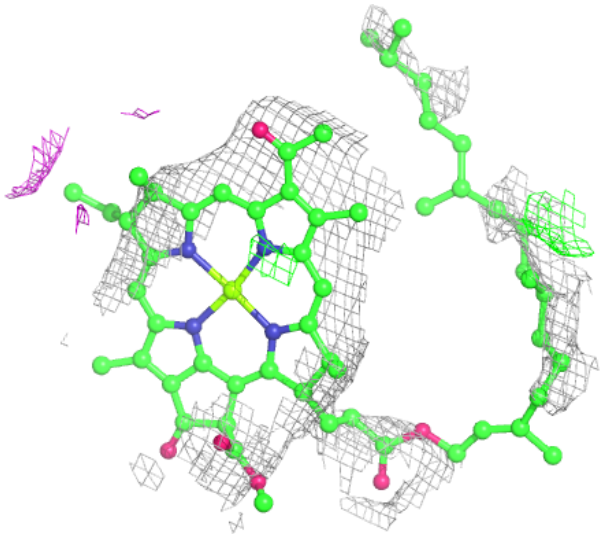


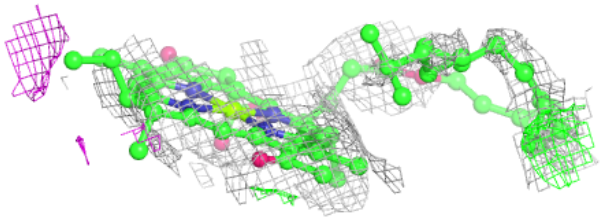


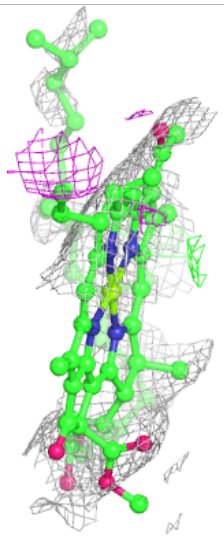


Electron density around BCL AE 101:

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

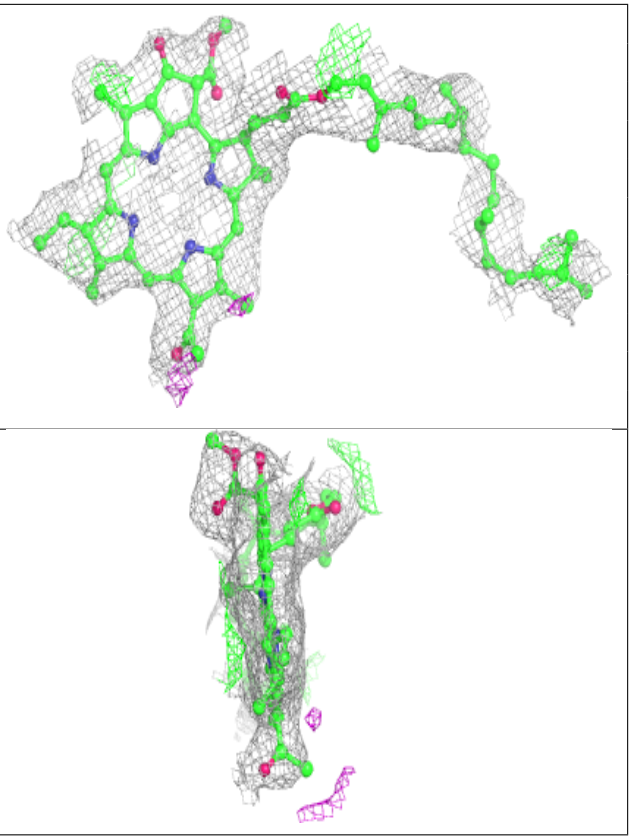






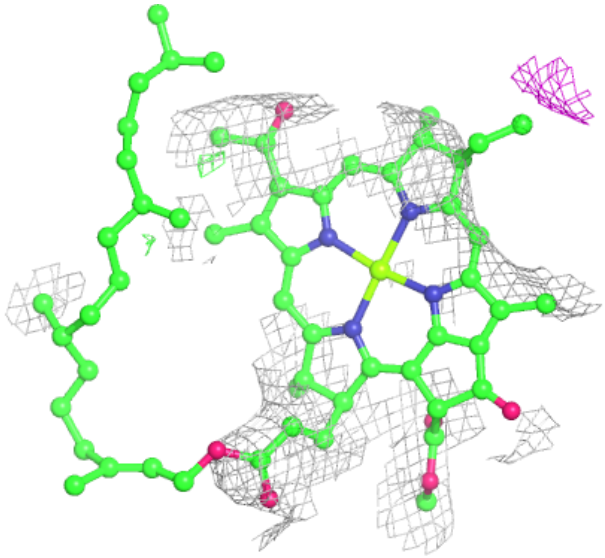
Electron density around BPH AM 403:

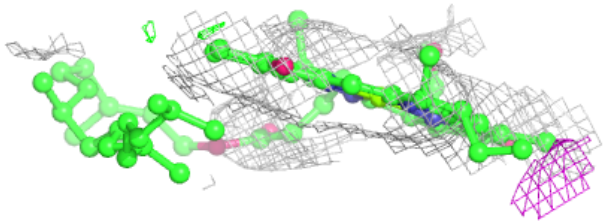
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

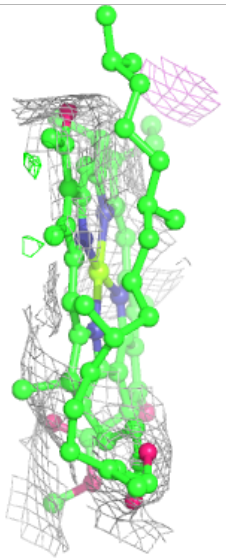


Electron density around BCL BX 101:

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

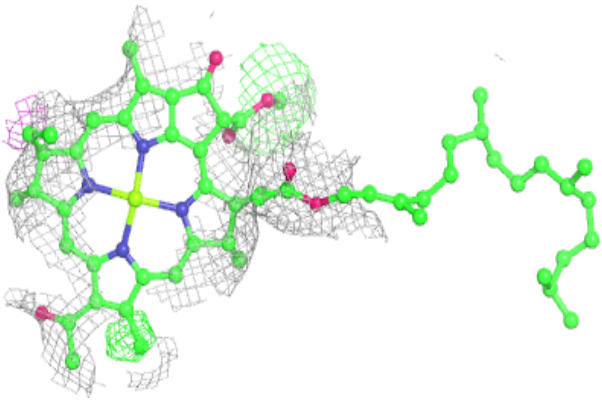


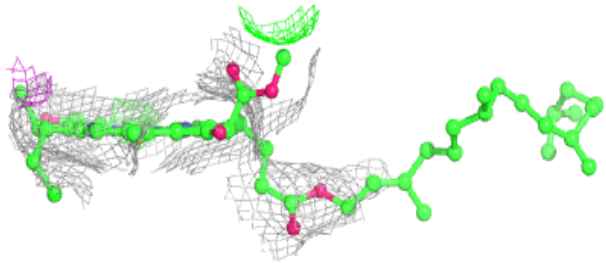


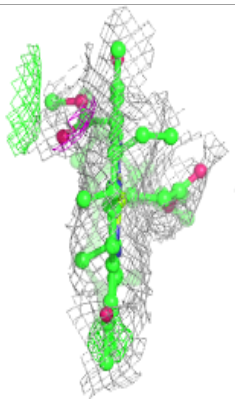


Electron density around BCL AF 102:

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

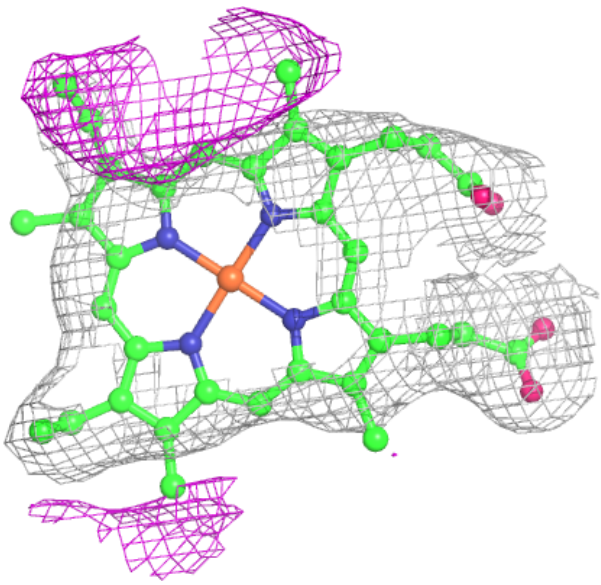


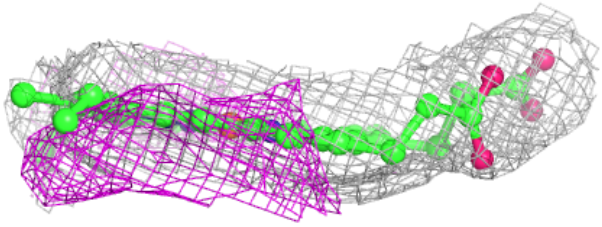


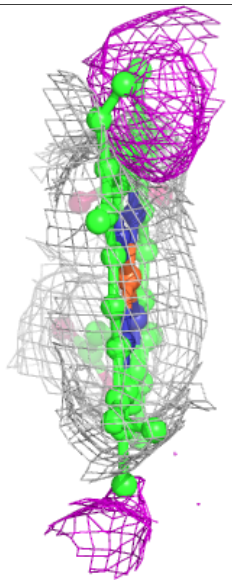


Electron density around HEM BC 502:

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

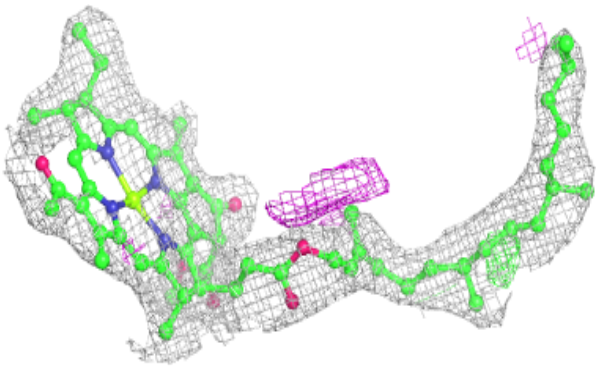


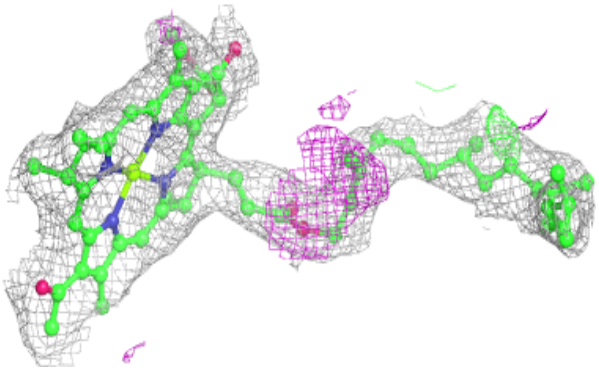


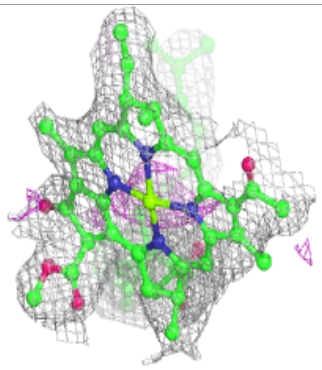


Electron density around BCL AM 402:

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

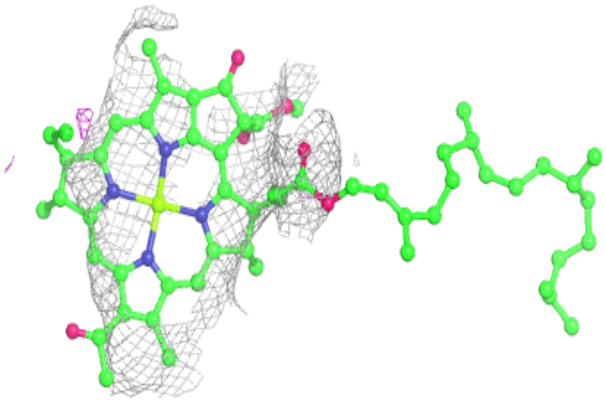


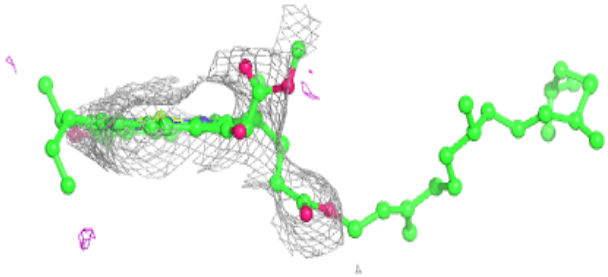


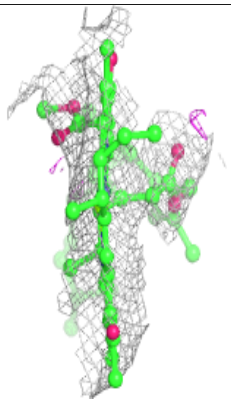


Electron density around BCL BQ 103:

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

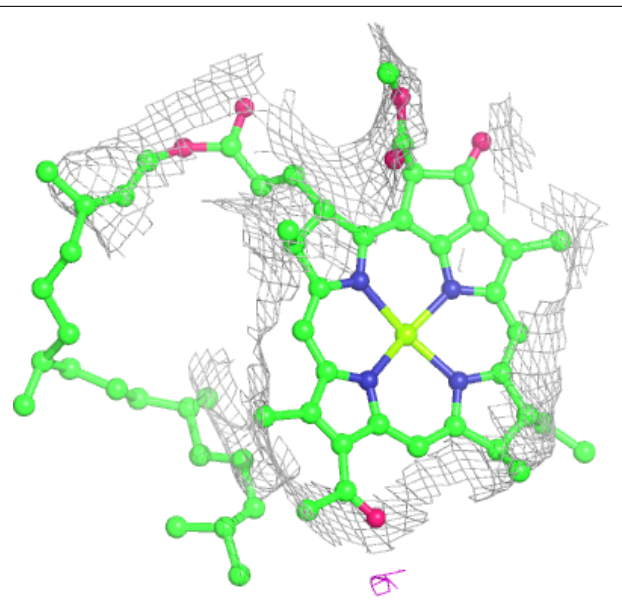


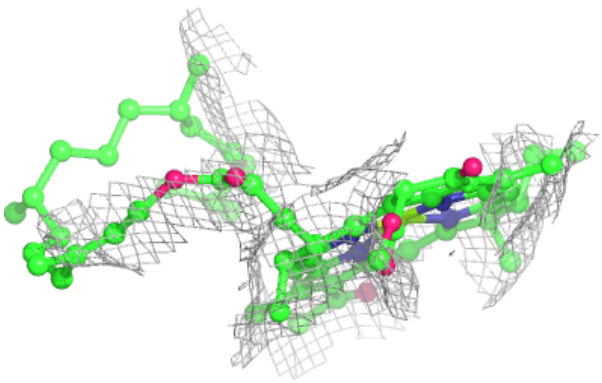


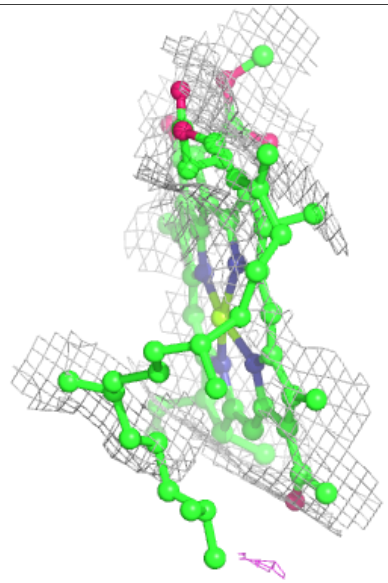


Electron density around BCL A8 101:

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

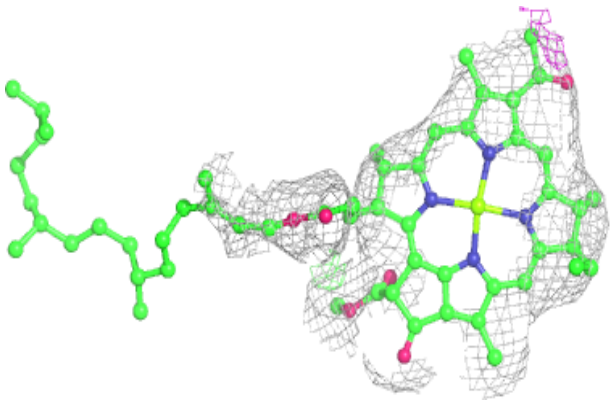


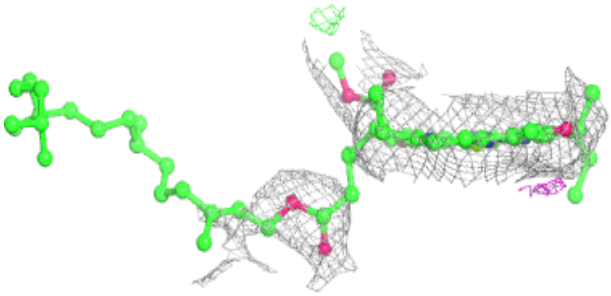


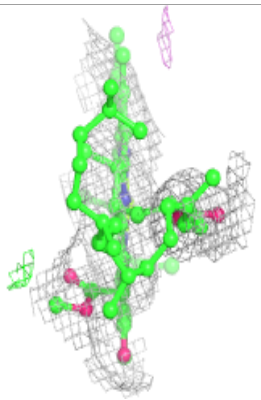


Electron density around BCL B1 102:

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

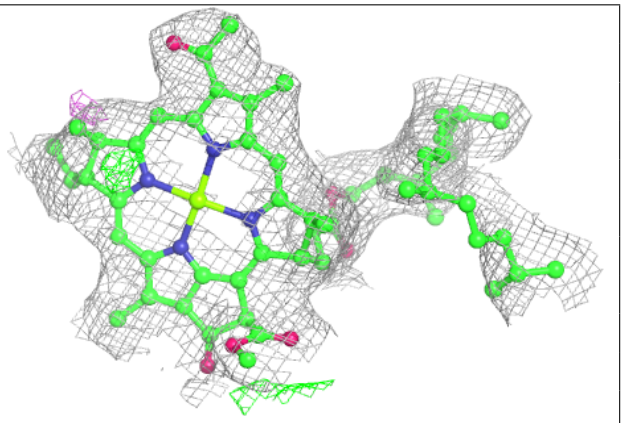


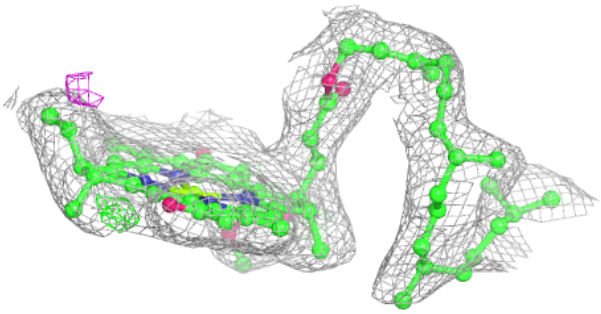


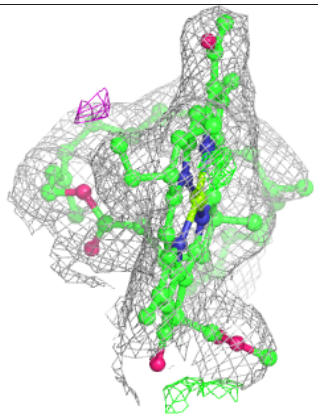


Electron density around BCL BM 401:

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

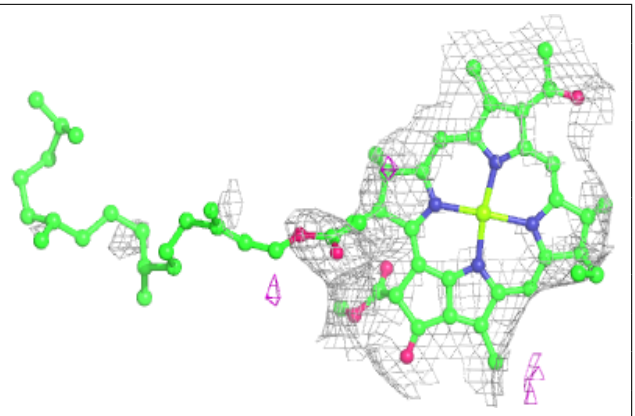


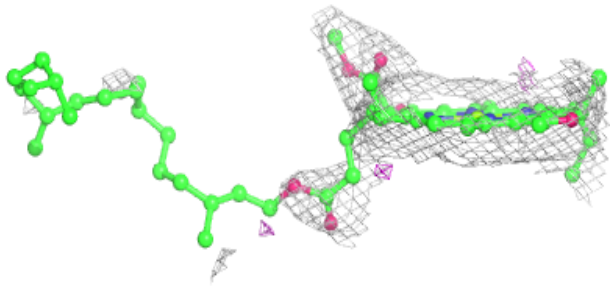


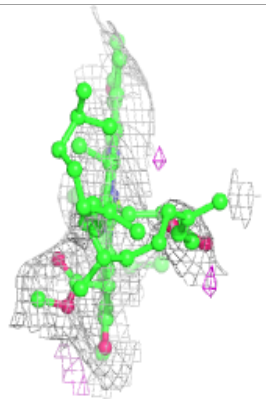


Electron density around BCL B3 102:

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

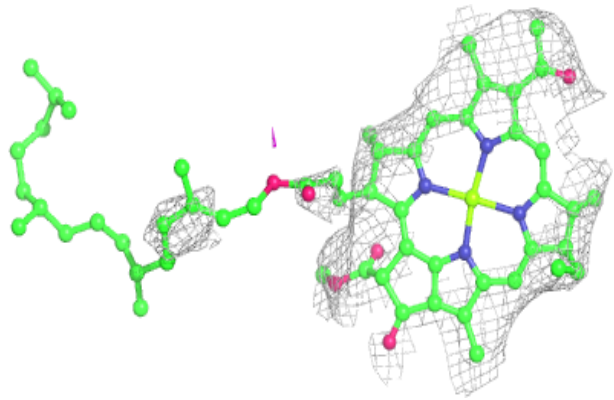


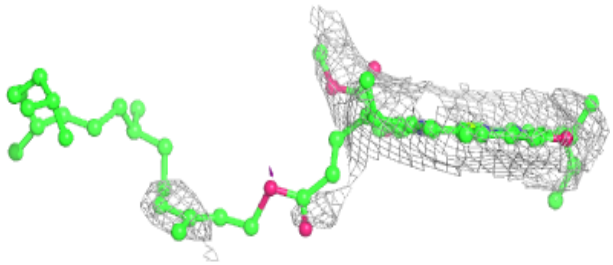


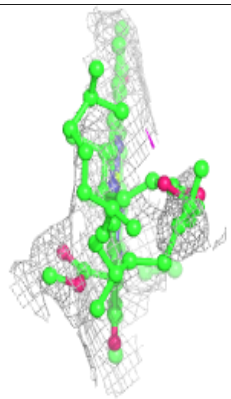


Electron density around BCL A1 102:

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

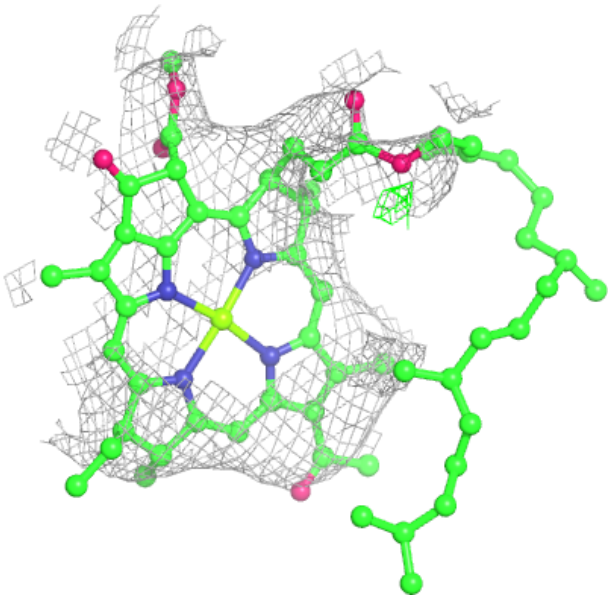


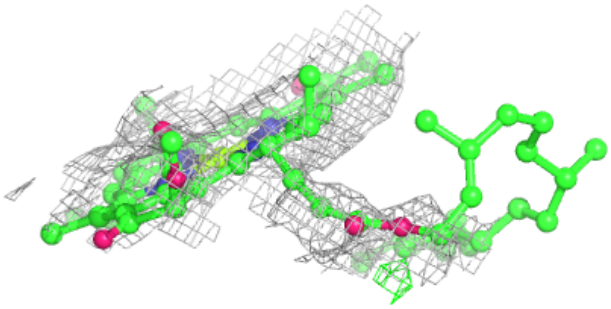


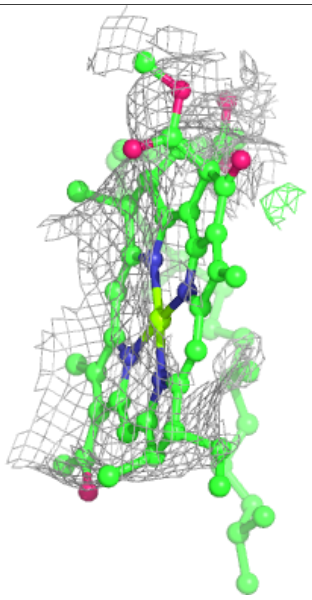


Electron density around BCL AG 101:

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

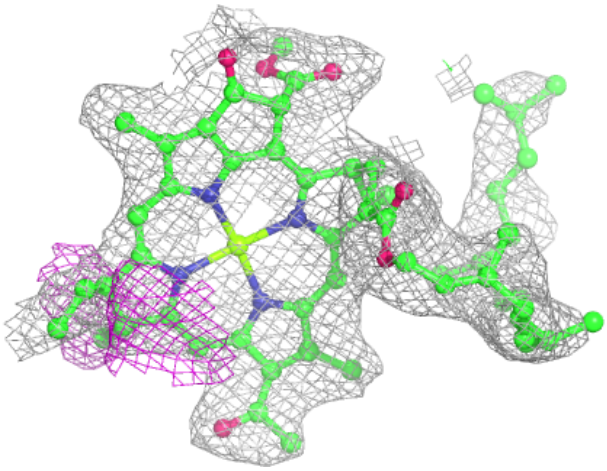


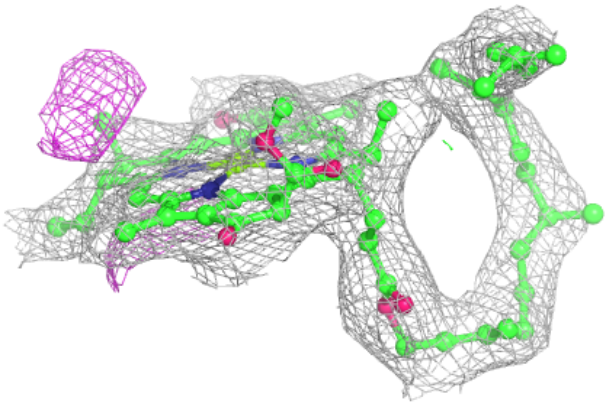


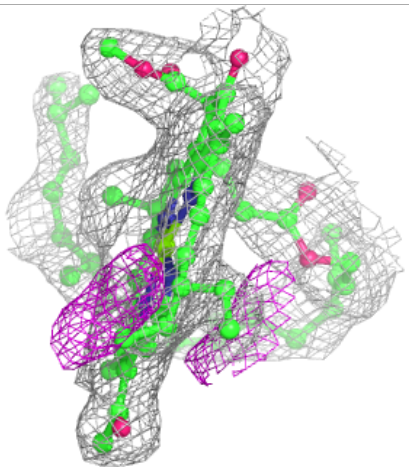


Electron density around BCL AM 401:

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

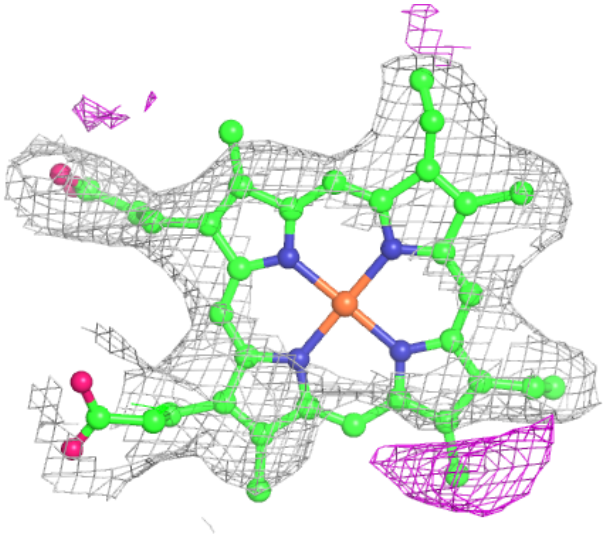


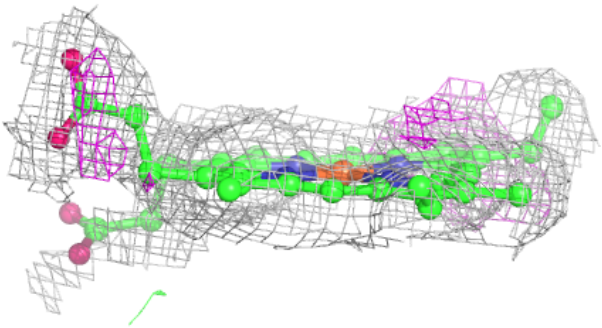


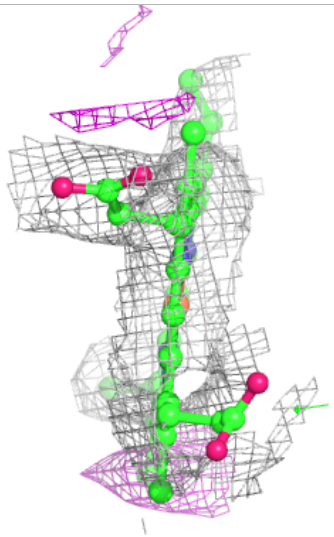


Electron density around HEM BC 501:

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

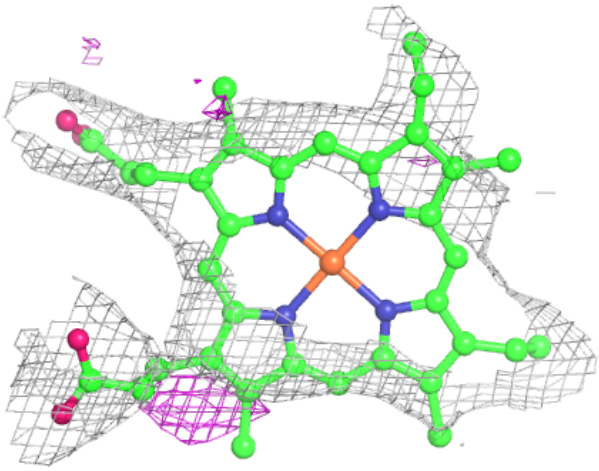


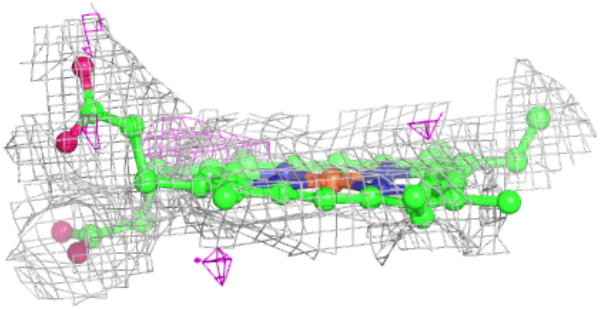


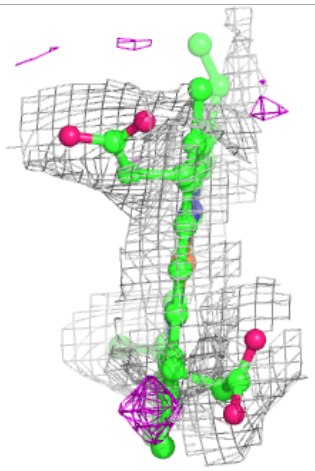


Electron density around HEM AC 501:

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

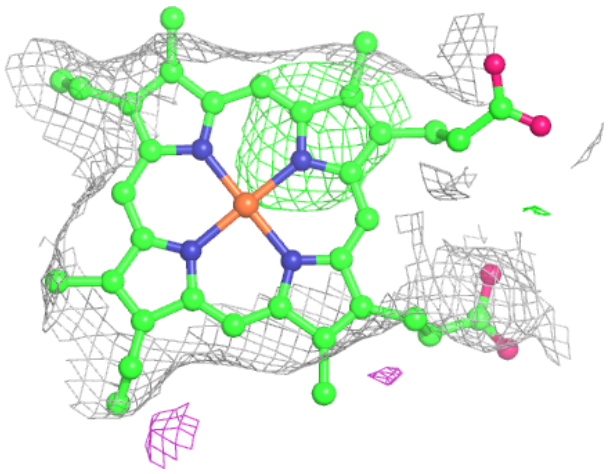


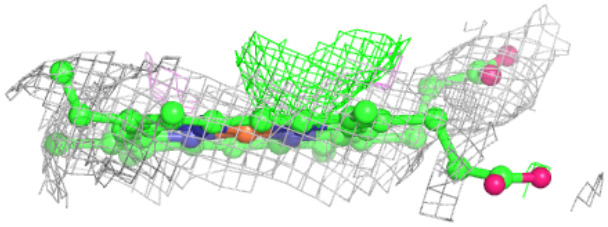




Electron density around HEM BC 503:

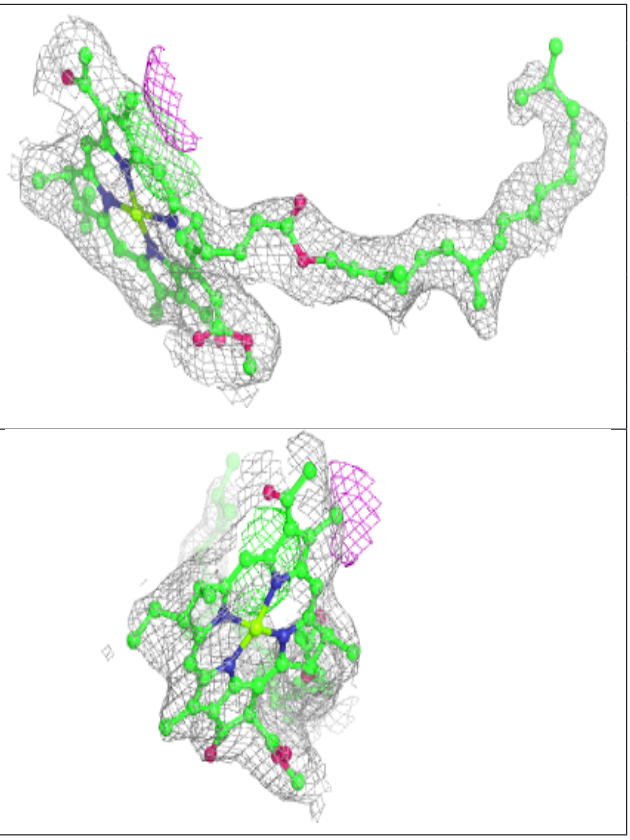
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

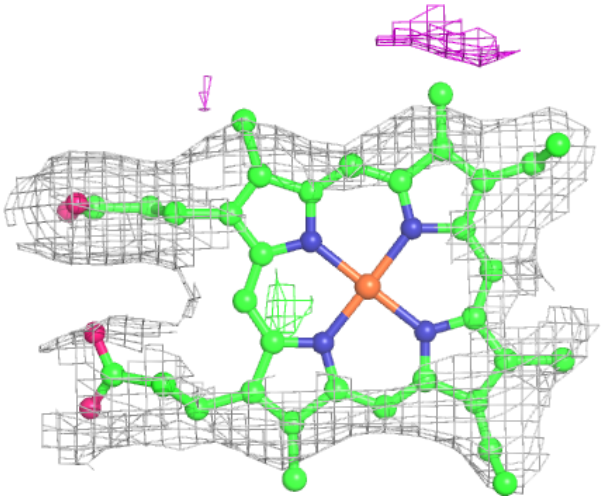
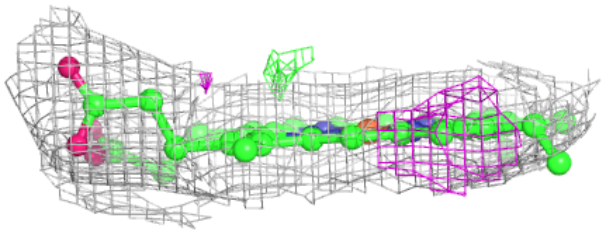
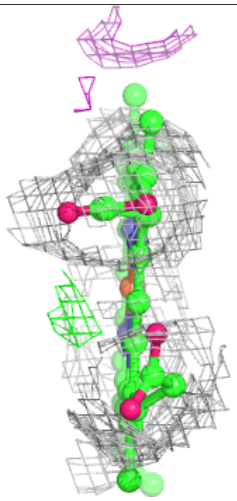




Electron density around BCL BL 301:

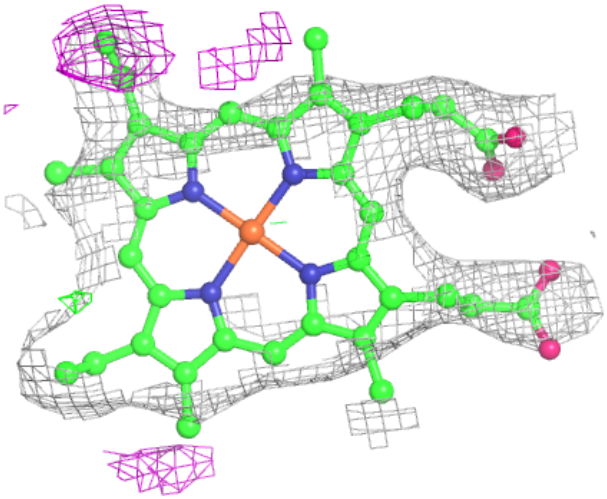
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

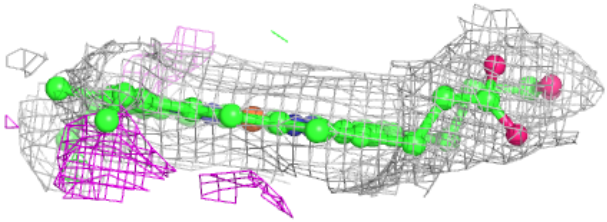


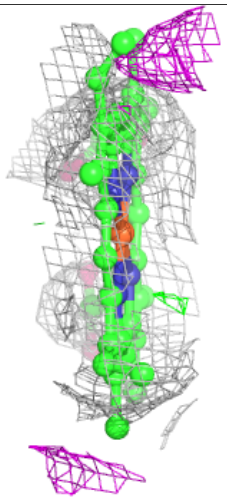
Electron density around HEM BC 504: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around HEM AC 502:

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

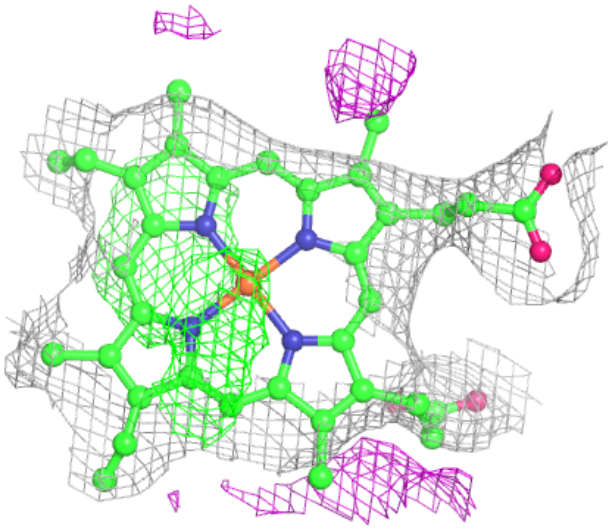


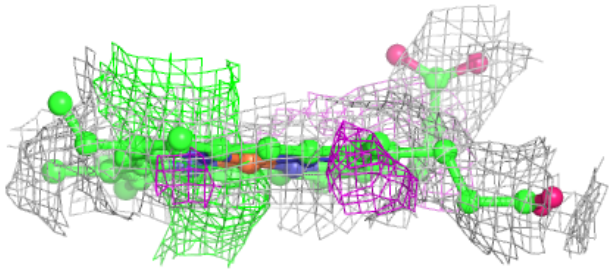


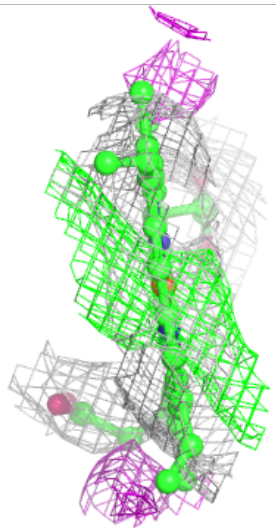


Electron density around HEM AC 503:

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

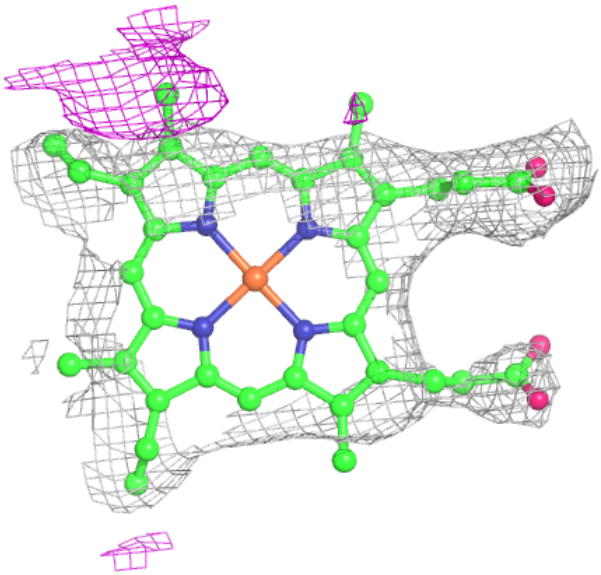


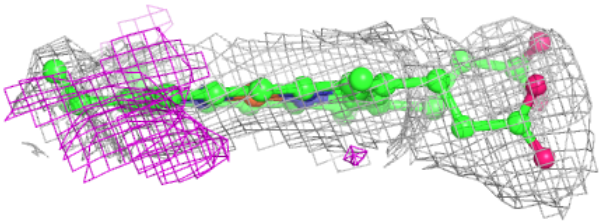


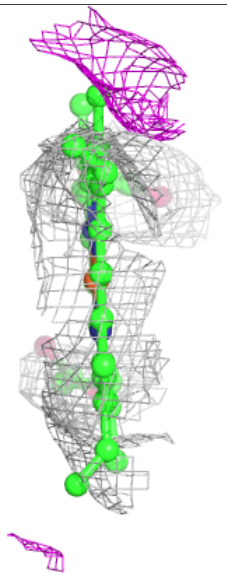


Electron density around HEM AC 504:

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

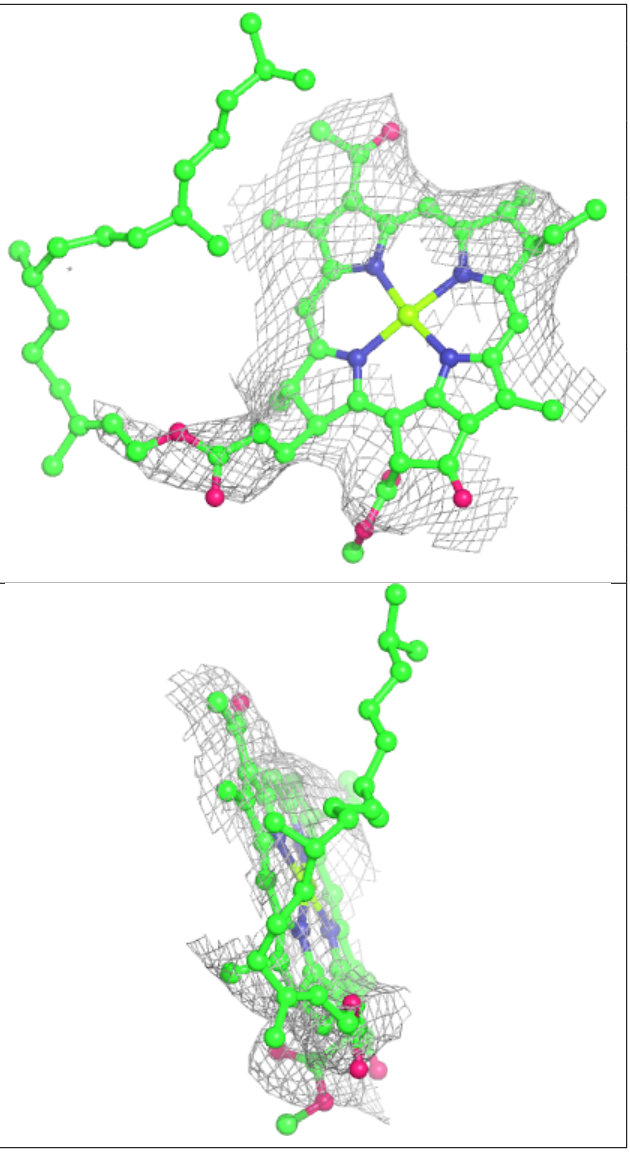






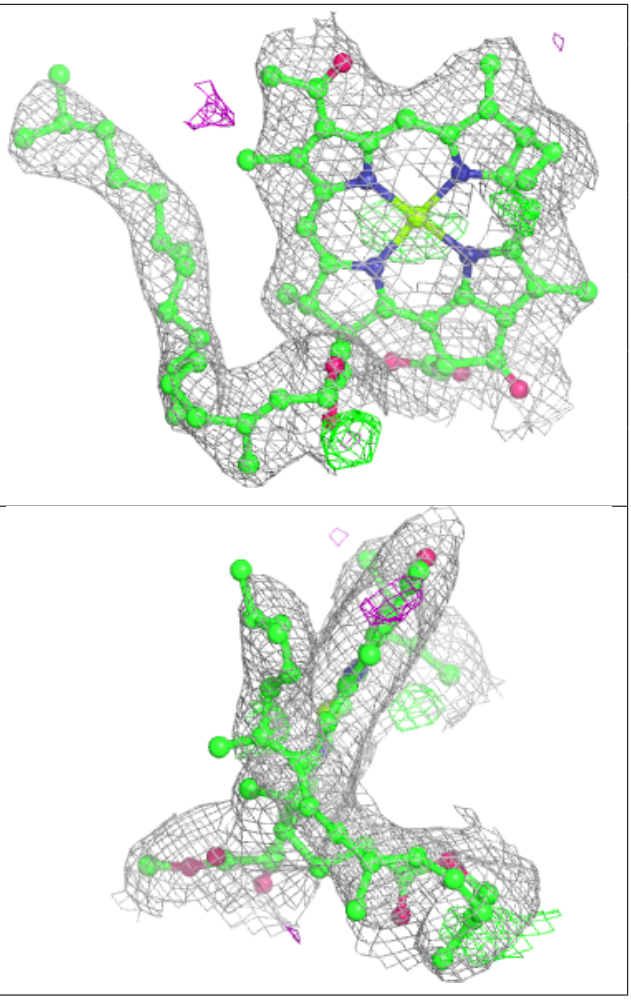
Electron density around BCL AP 101:

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



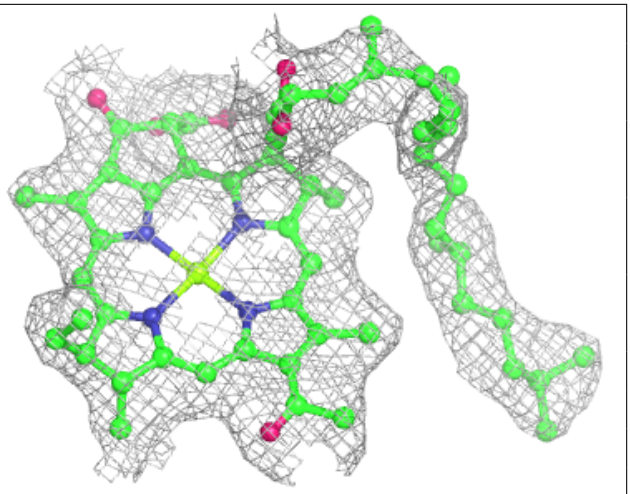
Electron density around BCL AL 303:

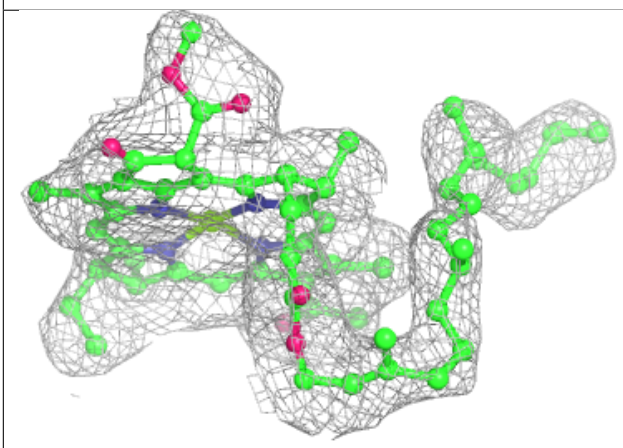
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

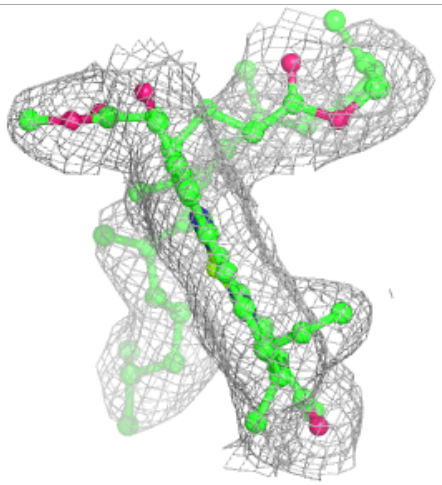


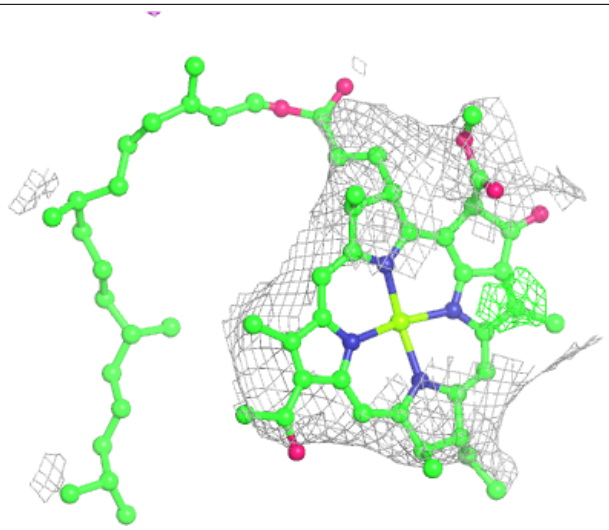
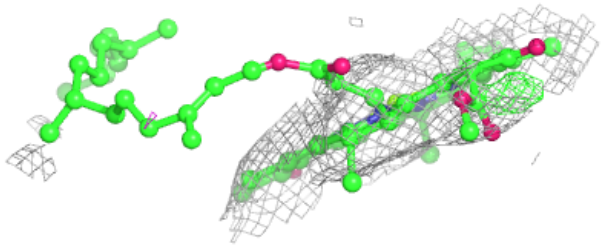
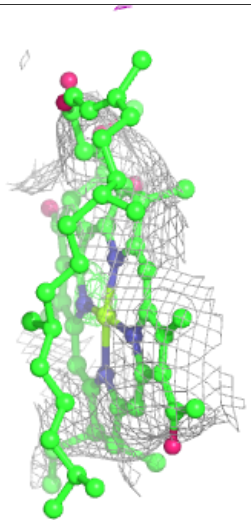
Electron density around BCL BL 303:

$2mF_o$-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 AZ 101: 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.