



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 09:10 PM UTC

PDB ID : 4V8K / pdb_00004v8k
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

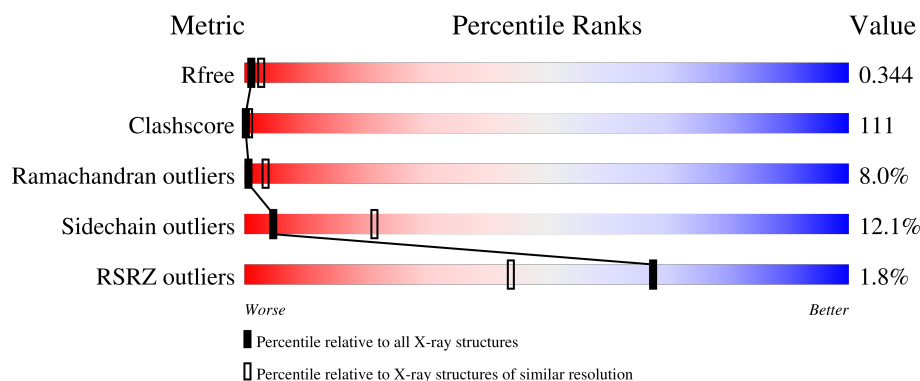
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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.



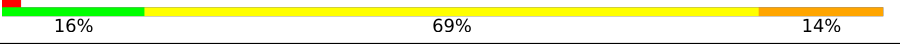
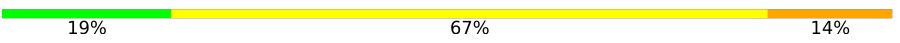
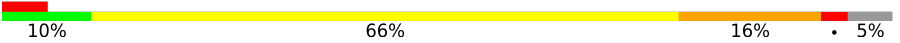
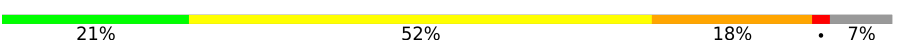
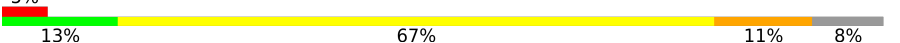
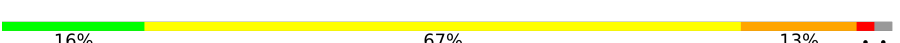
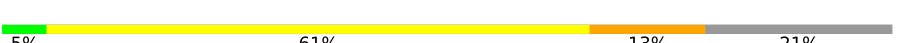
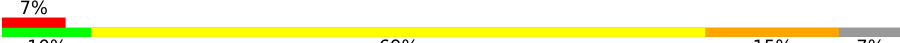
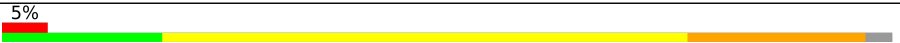
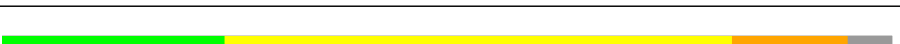
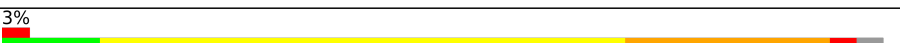
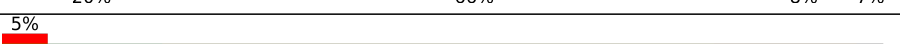
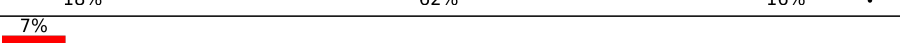
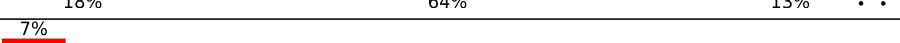
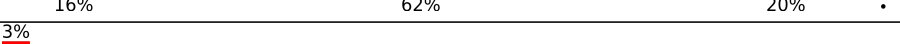
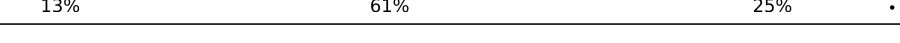
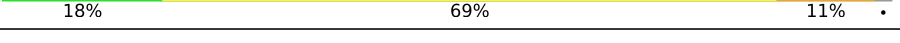
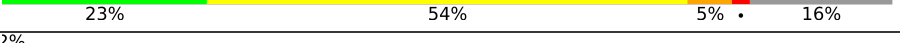
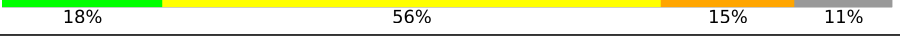
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AC	404	11% 48% 17% 22%
1	BC	404	13% 49% 15% 22%
2	AL	281	8% 63% 26%
2	BL	281	9% 73% 17%
3	AM	325	8% 60% 27%

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Mol	Chain	Length	Quality of chain
3	BM	325	
4	AH	259	
4	BH	259	
5	A1	61	
5	A3	61	
5	A5	61	
5	A7	61	
5	A9	61	
5	AA	61	
5	AD	61	
5	AF	61	
5	AI	61	
5	AK	61	
5	AO	61	
5	AQ	61	
5	AS	61	
5	AU	61	
5	AW	61	
5	AY	61	
5	B1	61	
5	B3	61	
5	B5	61	
5	B7	61	
5	B9	61	
5	BA	61	

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Mol	Chain	Length	Quality of chain
5	BD	61	
5	BF	61	
5	BI	61	
5	BK	61	
5	BO	61	
5	BQ	61	
5	BS	61	
5	BU	61	
5	BW	61	
5	BY	61	
6	A0	47	
6	A2	47	
6	A4	47	
6	A6	47	
6	A8	47	
6	AB	47	
6	AE	47	
6	AG	47	
6	AJ	47	
6	AN	47	
6	AP	47	
6	AR	47	
6	AT	47	
6	AV	47	
6	AX	47	

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Mol	Chain	Length	Quality of chain
6	AZ	47	
6	B0	47	
6	B2	47	
6	B4	47	
6	B6	47	
6	B8	47	
6	BB	47	
6	BE	47	
6	BG	47	
6	BJ	47	
6	BN	47	
6	BP	47	
6	BR	47	
6	BT	47	
6	BV	47	
6	BX	47	
6	BZ	47	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CRT	A0	101	-	-	X	-
14	CRT	A1	103	-	-	X	-
14	CRT	A2	102	-	-	X	-
14	CRT	A5	103	-	-	X	-
14	CRT	A7	102	-	-	X	-
14	CRT	AA	102	-	-	X	-
14	CRT	AB	102	-	-	X	-
14	CRT	AJ	102	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CRT	AP	102	-	-	X	-
14	CRT	AS	104	-	-	X	-
14	CRT	AW	102	-	-	X	-
14	CRT	AX	102	-	-	X	-
14	CRT	B0	101	-	-	X	-
14	CRT	B1	103	-	-	X	-
14	CRT	B2	102	-	-	X	-
14	CRT	B5	103	-	-	X	-
14	CRT	B7	102	-	-	X	-
14	CRT	BA	102	-	-	X	-
14	CRT	BB	102	-	-	X	-
14	CRT	BP	102	-	-	X	-
14	CRT	BU	103	-	-	X	-
14	CRT	BV	102	-	-	X	-
15	PEF	AM	407	-	X	-	-
15	PEF	AS	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	-
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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	B6	101	-	-	X	-
9	BCL	B7	103	-	-	X	-
9	BCL	B8	101	-	-	X	-
9	BCL	B9	102	-	-	X	-
9	BCL	BA	101	-	-	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	-
9	BCL	BJ	101	-	-	X	-
9	BCL	BK	102	-	-	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	BT	101	-	-	X	-
9	BCL	BU	102	-	-	X	-
9	BCL	BV	101	-	-	X	-
9	BCL	BW	102	-	-	X	-
9	BCL	BX	101	-	-	X	-
9	BCL	BY	102	-	-	X	-
9	BCL	BZ	101	-	-	X	-

2 Entry composition

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AM	319	Total	C	N	O	S	0	0	0
			2551	1713	417	410	11			
3	BM	319	Total	C	N	O	S	0	0	0
			2551	1713	417	410	11			

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

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

- Molecule 5 is a protein called LH1 alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AA	48	Total	C	N	O	S	0	0	0
			392	265	62	64	1			
5	AD	57	Total	C	N	O	S	0	0	0
			447	295	74	77	1			
5	AF	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	AI	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	AK	58	Total	C	N	O	S	0	0	0
			455	300	75	78	2			
5	AO	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	AQ	57	Total	C	N	O	S	0	0	0
			447	295	74	77	1			
5	AS	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	AU	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	AW	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	AY	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	A1	58	Total	C	N	O	S	0	0	0
			455	300	75	78	2			
5	A3	57	Total	C	N	O	S	0	0	0
			447	295	74	77	1			
5	A5	56	Total	C	N	O	S	0	0	0
			444	294	73	75	2			
5	A7	51	Total	C	N	O	S	0	0	0
			417	279	67	69	2			
5	A9	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	BA	55	Total	C	N	O	S	0	0	0
			448	299	72	75	2			
5	BD	45	Total	C	N	O	S	0	0	0
			370	250	59	60	1			
5	BF	56	Total	C	N	O	S	0	0	0
			444	294	73	75	2			
5	BI	50	Total	C	N	O	S	0	0	0
			409	274	66	68	1			
5	BK	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	BO	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	BQ	59	Total	C	N	O	S	0	0	0
			467	310	76	79	2			
5	BS	59	Total	C	N	O	S	0	0	0
			462	304	76	80	2			
5	BU	58	Total	C	N	O	S	0	0	0
			462	307	75	78	2			
5	BW	58	Total	C	N	O	S	0	0	0
			455	300	75	78	2			
5	BY	54	Total	C	N	O	S	0	0	0
			426	284	69	72	1			
5	B1	54	Total	C	N	O	S	0	0	0
			426	284	69	72	1			
5	B3	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	B5	51	Total	C	N	O	S	0	0	0
			417	279	67	69	2			
5	B7	54	Total	C	N	O	S	0	0	0
			426	284	69	72	1			
5	B9	51	Total	C	N	O	S	0	0	0
			417	279	67	69	2			

- Molecule 6 is a protein called LH1 beta polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AB	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AE	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AG	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AJ	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AN	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AP	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AR	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AT	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	AV	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

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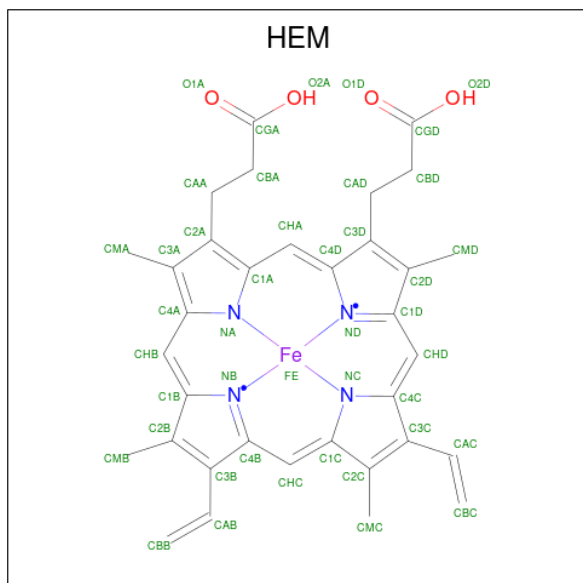
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AX	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	AZ	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A2	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A4	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A6	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A8	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	A0	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BB	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BE	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BG	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BJ	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BN	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BP	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BR	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BT	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BV	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BX	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	BZ	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	B2	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	B4	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	B6	40	Total 337	C 228	N 52	O 55	S 2	0	0	0

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

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



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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

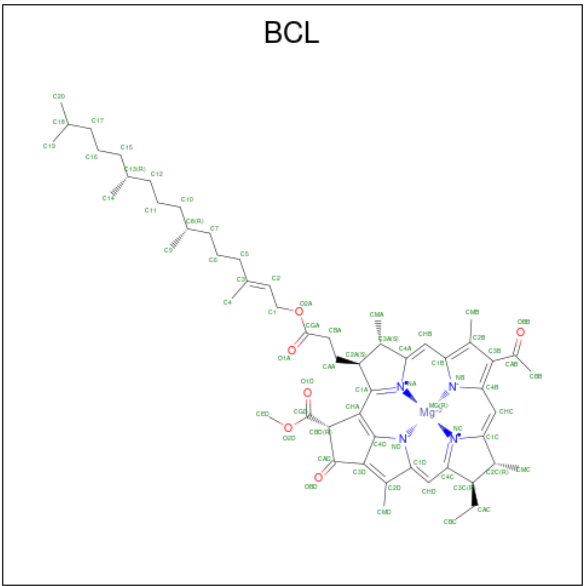
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AC	1	Total Ca 1 1	0	0
8	AA	1	Total Ca 1 1	0	0
8	AD	1	Total Ca 1 1	0	0
8	AF	1	Total Ca 1 1	0	0
8	AI	1	Total Ca 1 1	0	0
8	AK	1	Total Ca 1 1	0	0
8	AO	1	Total Ca 1 1	0	0
8	AQ	1	Total Ca 1 1	0	0
8	AS	1	Total Ca 1 1	0	0
8	AU	1	Total Ca 1 1	0	0
8	AV	1	Total Ca 1 1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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	BK	1	Total	Ca	0	0
			1	1		
8	BO	1	Total	Ca	0	0
			1	1		
8	BQ	1	Total	Ca	0	0
			1	1		
8	BS	1	Total	Ca	0	0
			1	1		
8	BU	1	Total	Ca	0	0
			1	1		
8	BW	1	Total	Ca	0	0
			1	1		
8	BY	1	Total	Ca	0	0
			1	1		
8	B1	1	Total	Ca	0	0
			1	1		
8	B3	1	Total	Ca	0	0
			1	1		
8	B5	1	Total	Ca	0	0
			1	1		
8	B7	1	Total	Ca	0	0
			1	1		
8	B9	1	Total	Ca	0	0
			1	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AL	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AM	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AA	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AB	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AD	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AE	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AF	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AG	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AI	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AJ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AK	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AN	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AO	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AP	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AQ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AR	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AS	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AT	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AU	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	AV	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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

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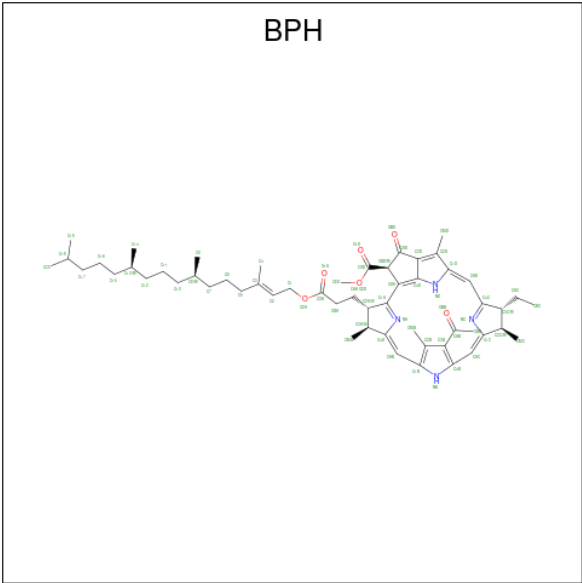
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	BE	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BF	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BG	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BI	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BJ	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BK	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	BN	1	Total 66	C 55	Mg 1	N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

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

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



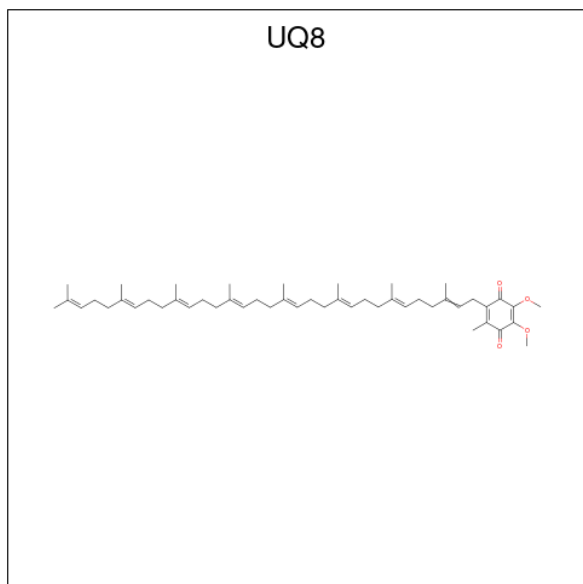
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	AL	1	Total	C	N	O	0	0
			65	55	4	6		
10	AM	1	Total	C	N	O	0	0
			65	55	4	6		
10	BL	1	Total	C	N	O	0	0
			65	55	4	6		

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

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

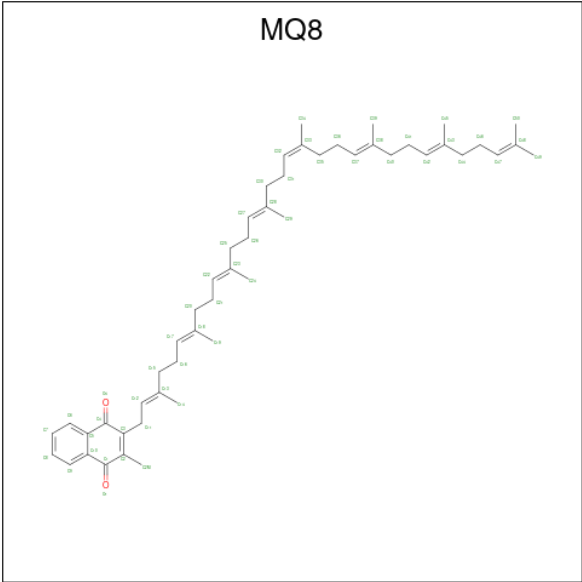


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	AL	1	Total	C	O	0	0
			53	49	4		
11	BL	1	Total	C	O	0	0
			53	49	4		

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

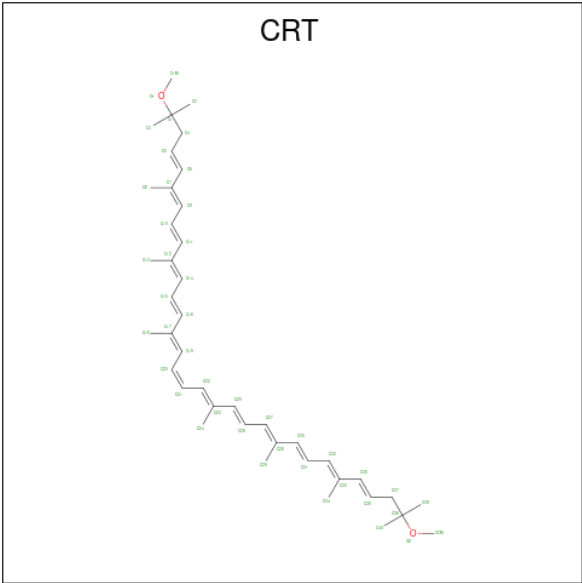
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	AM	1	Total	Fe	0	0
			1	1		
12	BM	1	Total	Fe	0	0
			1	1		

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



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

- Molecule 14 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



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

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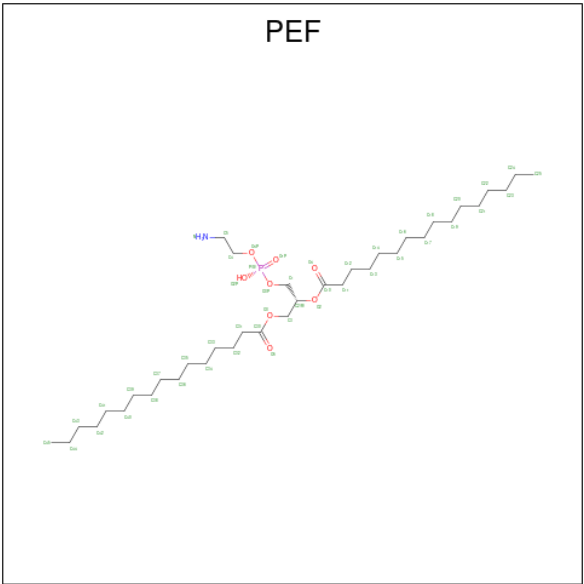
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	AB	1	Total	C	O	0	0
			44	42	2		
14	AG	1	Total	C	O	0	0
			44	42	2		
14	AJ	1	Total	C	O	0	0
			44	42	2		
14	AN	1	Total	C	O	0	0
			44	42	2		
14	AP	1	Total	C	O	0	0
			44	42	2		
14	AR	1	Total	C	O	0	0
			44	42	2		
14	AS	1	Total	C	O	0	0
			44	42	2		
14	AT	1	Total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

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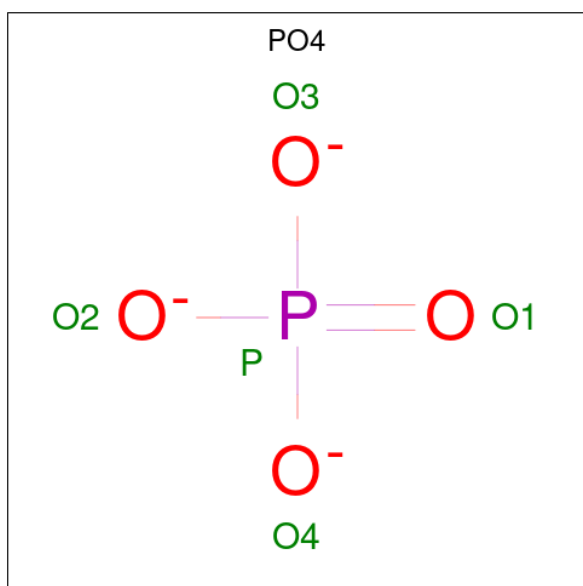
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	BO	1	Total	C	O	0	0
			44	42	2		
14	BP	1	Total	C	O	0	0
			44	42	2		
14	BS	1	Total	C	O	0	0
			44	42	2		
14	BU	1	Total	C	O	0	0
			44	42	2		
14	BV	1	Total	C	O	0	0
			44	42	2		
14	BW	1	Total	C	O	0	0
			44	42	2		
14	B1	1	Total	C	O	0	0
			44	42	2		
14	B2	1	Total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

- Molecule 15 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P).



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

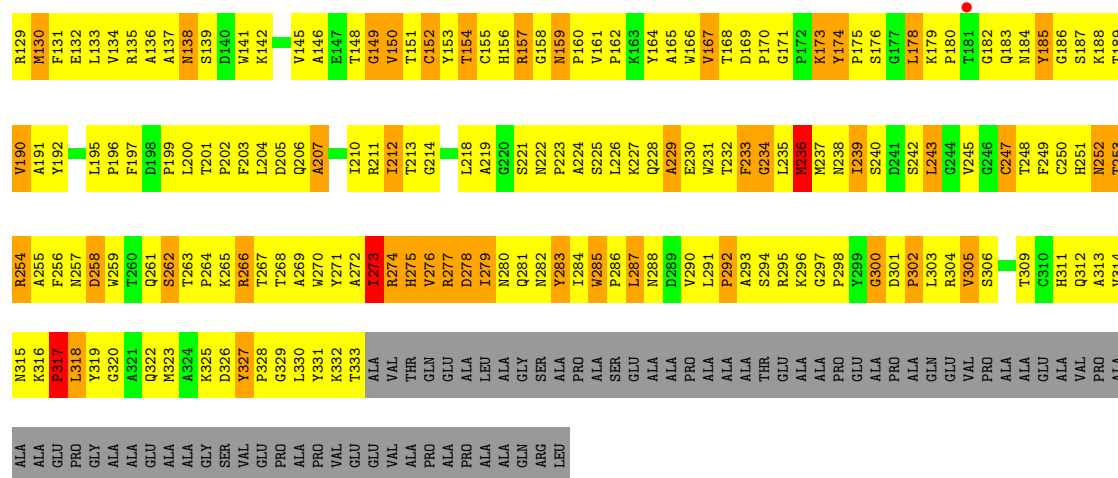
- Molecule 16 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

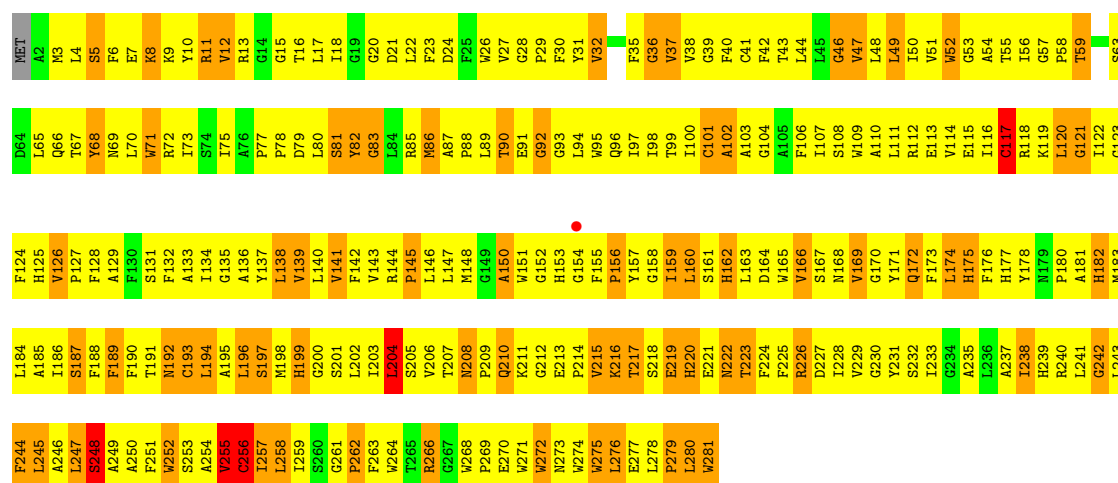
- Molecule 17 is water.

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



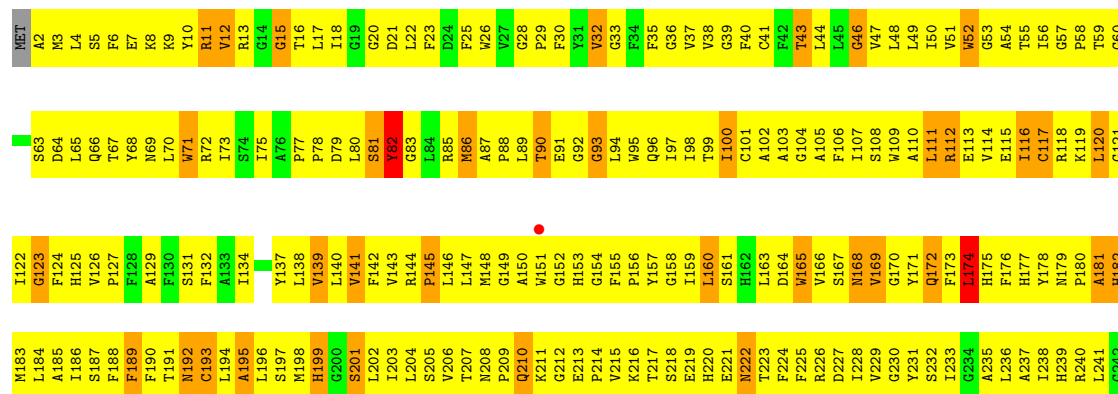
• Molecule 2: Photosynthetic reaction center L subunit

Chain AL: 8% 63% 26%



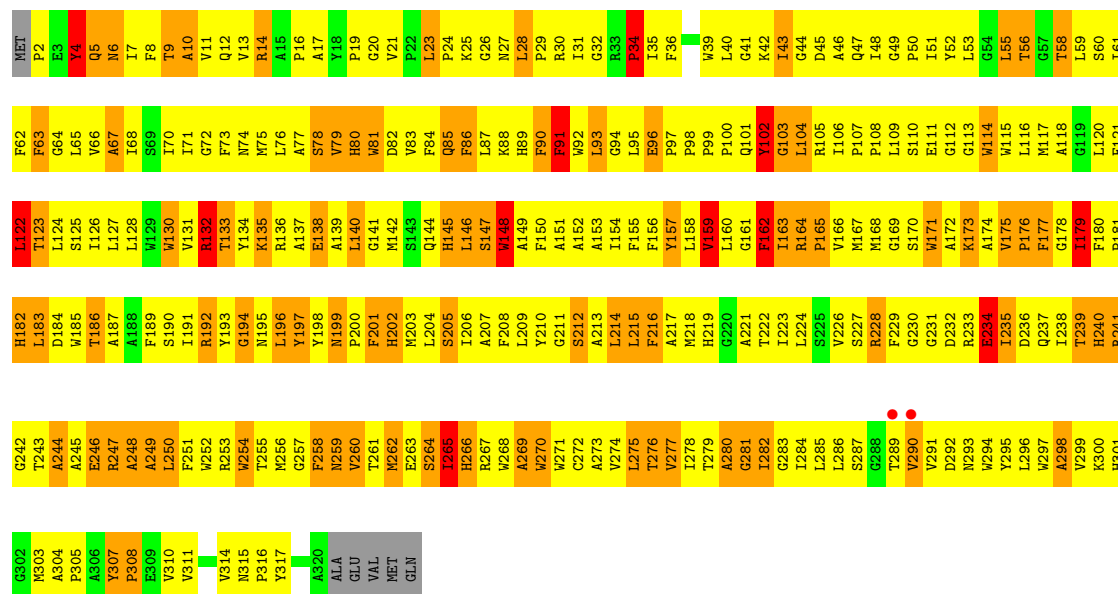
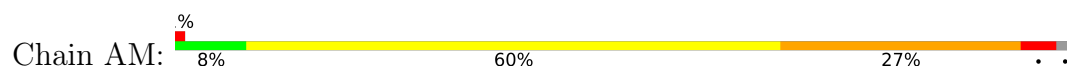
• Molecule 2: Photosynthetic reaction center L subunit

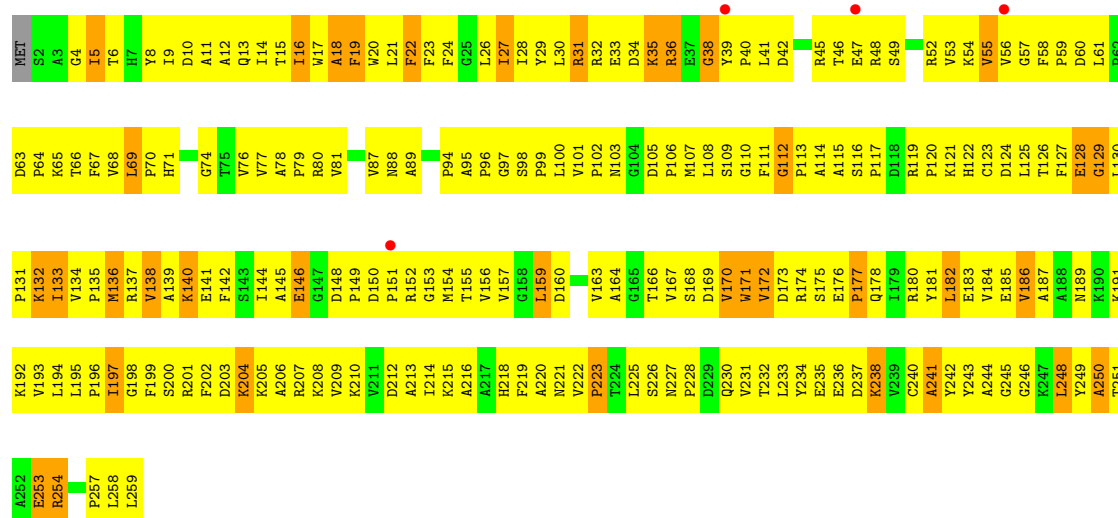
Chain BL: 9% 73% 17%





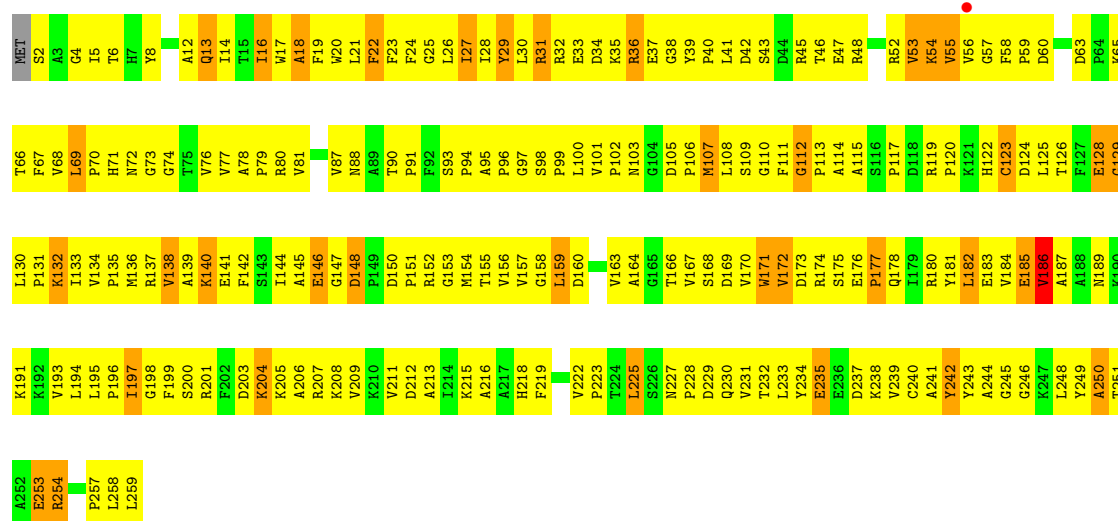
• Molecule 3: Photosynthetic reaction center M subunit





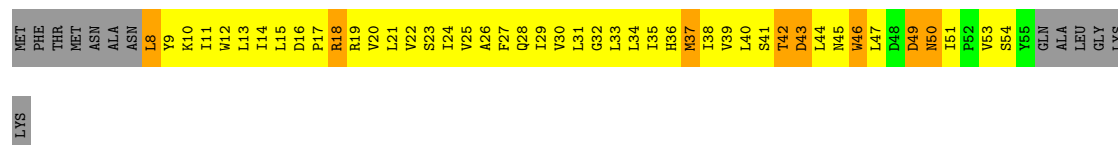
• Molecule 4: Photosynthetic reaction center H subunit

Chain BH: 19% 67% 14%



• Molecule 5: LH1 alpha polypeptide

Chain AA: 5% 61% 13% 21%



• Molecule 5: LH1 alpha polypeptide

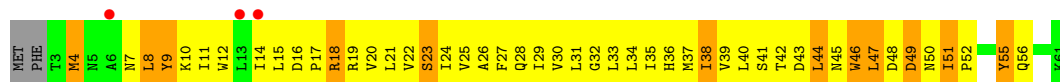
Chain AD: 7% 10% 69% 15% 7%



- Molecule 5: LH1 alpha polypeptide



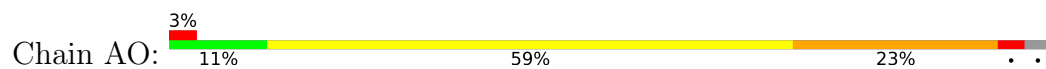
- Molecule 5: LH1 alpha polypeptide



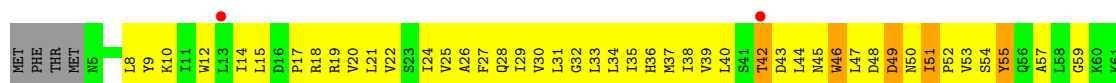
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



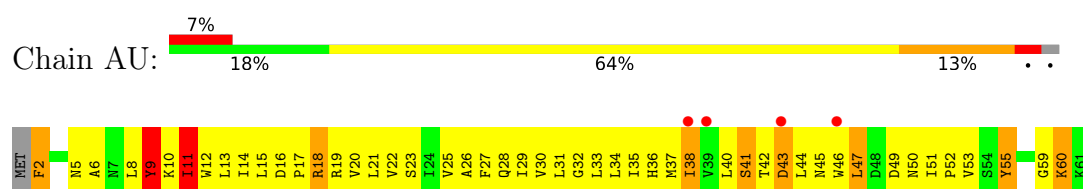
- Molecule 5: LH1 alpha polypeptide



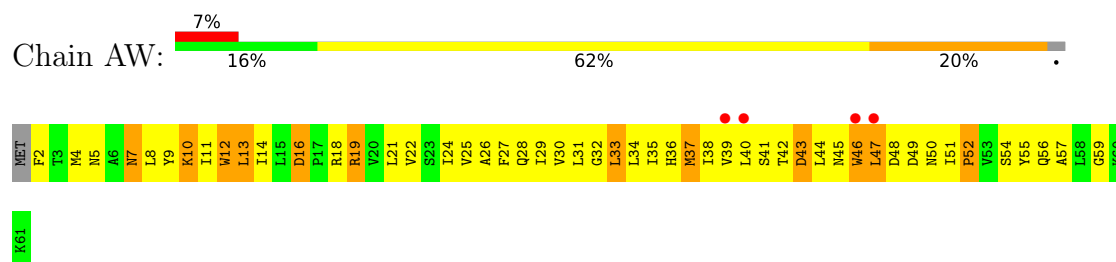
- Molecule 5: LH1 alpha polypeptide



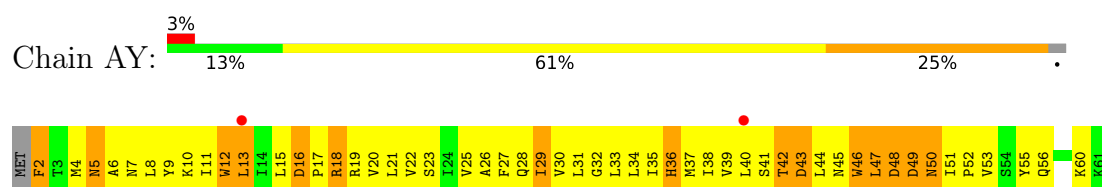
- Molecule 5: LH1 alpha polypeptide



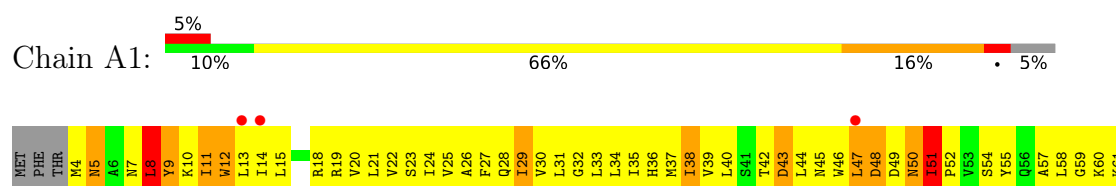
- Molecule 5: LH1 alpha polypeptide



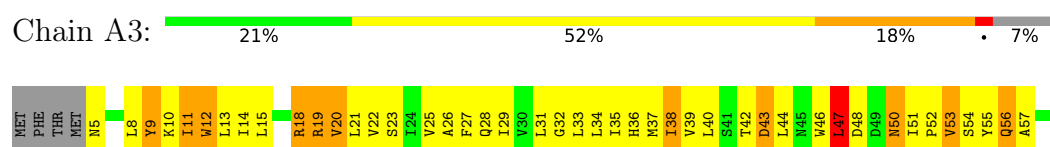
- Molecule 5: LH1 alpha polypeptide



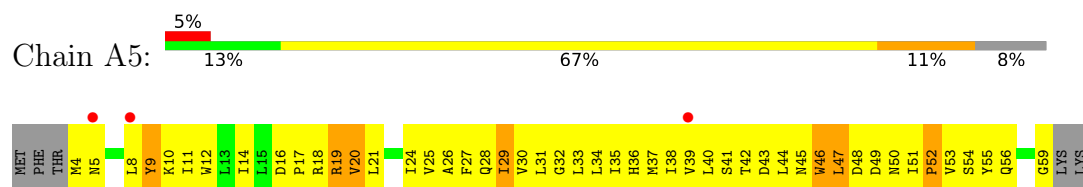
- Molecule 5: LH1 alpha polypeptide



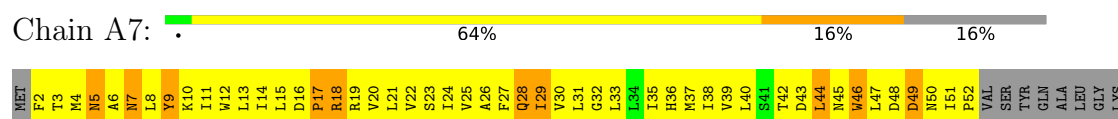
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



LYS

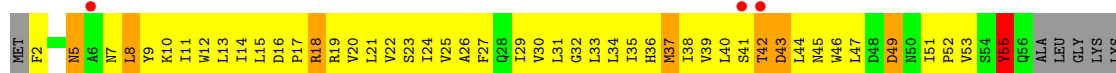
- Molecule 5: LH1 alpha polypeptide

Chain A9: 16% 67% 13% ..



- Molecule 5: LH1 alpha polypeptide

Chain BA: 5% 13% 64% 11% • 10%



- Molecule 5: LH1 alpha polypeptide

Chain BD: 5% 59% 13% 26%



LYS

- Molecule 5: LH1 alpha polypeptide

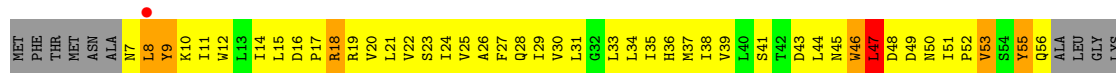
Chain BF: 7% 13% 66% 13% 8%



LYS

- Molecule 5: LH1 alpha polypeptide

Chain BI: 2% 8% 62% 10% • 18%



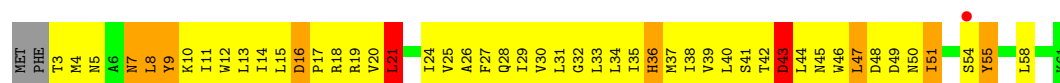
LYS

- Molecule 5: LH1 alpha polypeptide

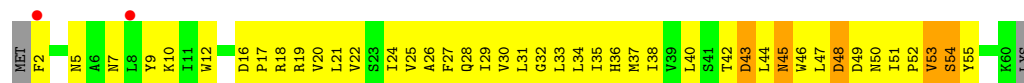
Chain BK: 3% 21% 61% 16% •



- Molecule 5: LH1 alpha polypeptide



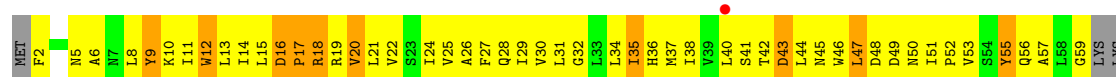
- Molecule 5: LH1 alpha polypeptide



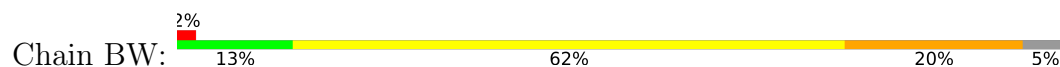
- Molecule 5: LH1 alpha polypeptide



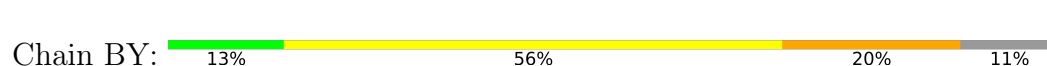
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



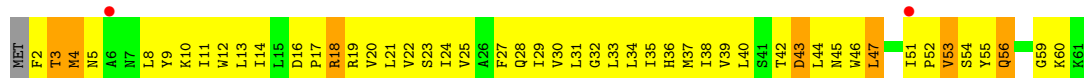
- Molecule 5: LH1 alpha polypeptide

Chain B1: 15% 59% 15% 11%



• Molecule 5: LH1 alpha polypeptide

Chain B3: 3% 18% 69% 11%



• Molecule 5: LH1 alpha polypeptide

Chain B5: 23% 54% 5% 16%



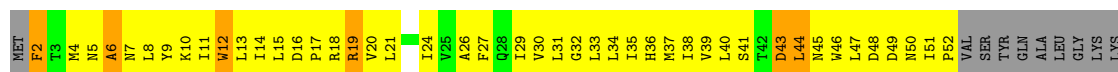
• Molecule 5: LH1 alpha polypeptide

Chain B7: 2% 18% 56% 15% 11%



• Molecule 5: LH1 alpha polypeptide

Chain B9: 10% 64% 10% 16%



• Molecule 6: LH1 beta polypeptide

Chain AB: 2% 17% 55% 13% 15%



• Molecule 6: LH1 beta polypeptide

Chain AE: 4% 23% 57% 15%



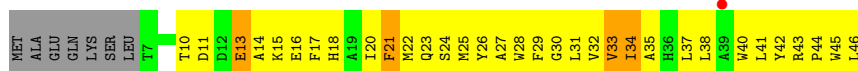
• Molecule 6: LH1 beta polypeptide

Chain AG: 9% 57% 19% 15%



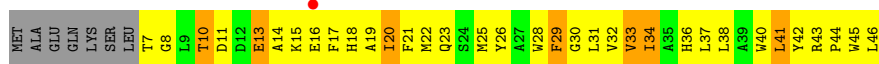
• Molecule 6: LH1 beta polypeptide

Chain AJ: 2% 15% 62% 9% 15%



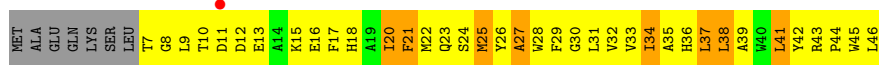
• Molecule 6: LH1 beta polypeptide

Chain AN: 2% 13% 57% 15% 15%



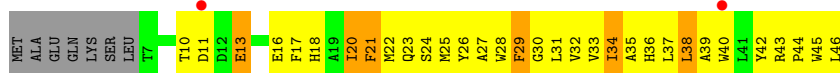
• Molecule 6: LH1 beta polypeptide

Chain AP: 2% 6% 62% 17% 15%



• Molecule 6: LH1 beta polypeptide

Chain AR: 4% 17% 55% 13% 15%



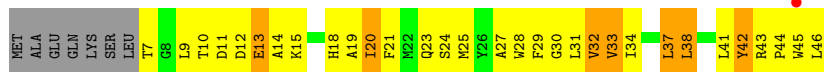
• Molecule 6: LH1 beta polypeptide

Chain AT: 17% 45% 23% 15%



• Molecule 6: LH1 beta polypeptide

Chain AV: 2% 19% 51% 15% 15%



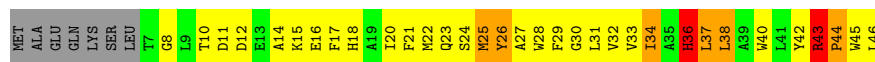
• Molecule 6: LH1 beta polypeptide

Chain AX: 9% 72% 15%



• Molecule 6: LH1 beta polypeptide

Chain AZ: 15% 53% 13% 15%



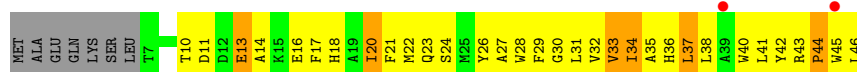
• Molecule 6: LH1 beta polypeptide

Chain A2: 21% 55% 9% 15%



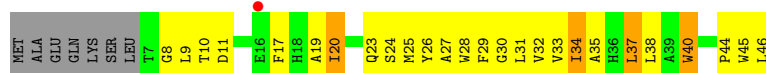
• Molecule 6: LH1 beta polypeptide

Chain A4: 4% 17% 55% 13% 15%



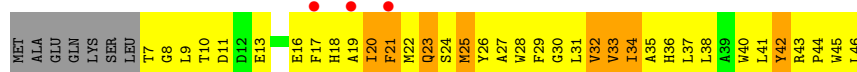
• Molecule 6: LH1 beta polypeptide

Chain A6: 2% 30% 47% 9% 15%



• Molecule 6: LH1 beta polypeptide

Chain A8: 6% 9% 60% 17% 15%



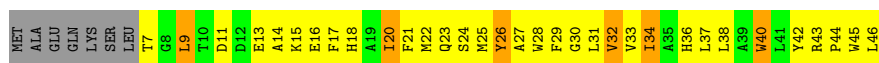
• Molecule 6: LH1 beta polypeptide

Chain A0: 11% 45% 28% 15%



• Molecule 6: LH1 beta polypeptide

Chain BB: 15% 57% 13% 15%



- Molecule 6: LH1 beta polypeptide

Chain BE: 17% 64% 15%



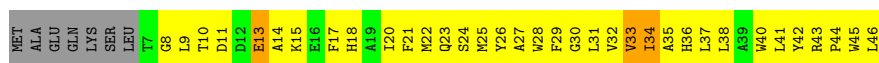
- Molecule 6: LH1 beta polypeptide

Chain BG: 9% 13% 66% 15%



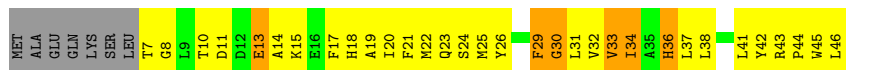
- Molecule 6: LH1 beta polypeptide

Chain BJ: 11% 68% 6% 15%



- Molecule 6: LH1 beta polypeptide

Chain BN: 17% 55% 13% 15%



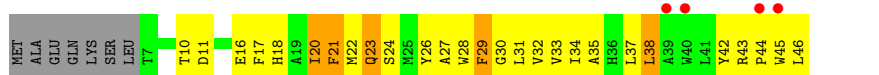
- Molecule 6: LH1 beta polypeptide

Chain BP: 2% 9% 66% 11% 15%



- Molecule 6: LH1 beta polypeptide

Chain BR: 9% 28% 47% 11% 15%

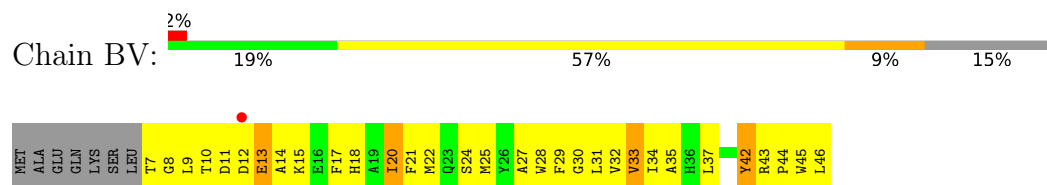


- Molecule 6: LH1 beta polypeptide

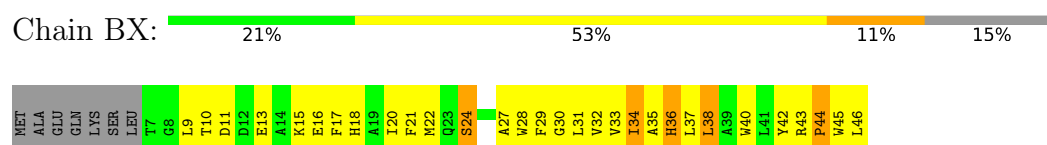
Chain BT: 13% 53% 19% 15%



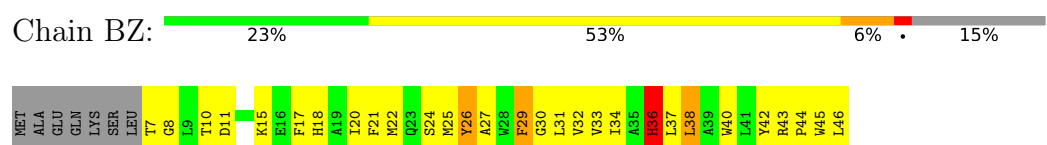
● Molecule 6: LH1 beta polypeptide



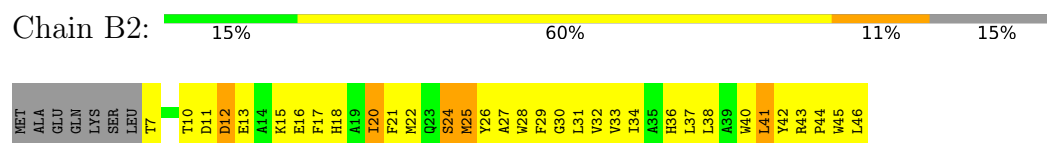
● Molecule 6: LH1 beta polypeptide



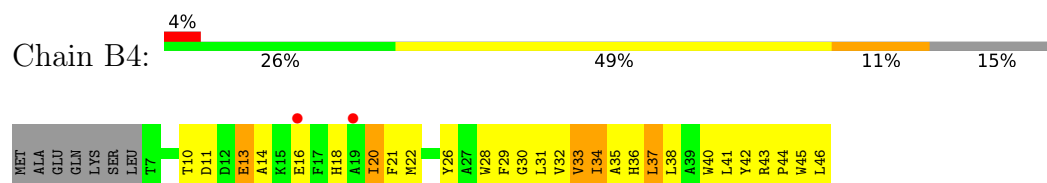
● Molecule 6: LH1 beta polypeptide



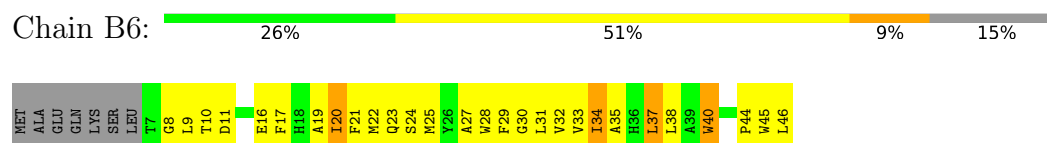
● Molecule 6: LH1 beta polypeptide



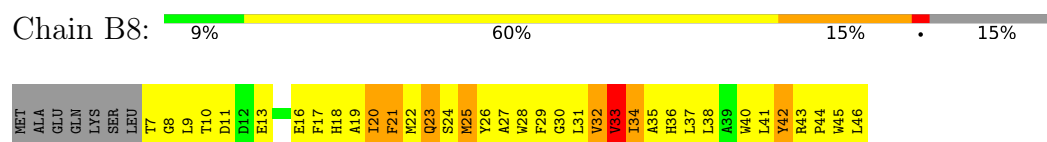
● Molecule 6: LH1 beta polypeptide



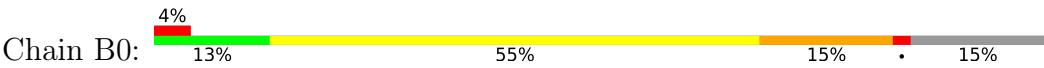
● Molecule 6: LH1 beta polypeptide



● Molecule 6: LH1 beta polypeptide



● Molecule 6: LH1 beta polypeptide



MET	ALA	GLU	GLN	LYS	SER	LEU	T77	G8	L9	T10	D11	D12	E13	A14	K15	E16	F17	H18	A19	I20	F21	M22	Q23	S24	M25	Y26	A27	W28	F29	G30	L31	V32	T33	A34	A35	R36	L37	L38	A39	W40	L41	Y42	R43	P44	W45	L46
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4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.335 , 0.356 0.342 , 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 , 97.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.75	1/2528 (0.0%)	1.20	27/3451 (0.8%)
1	BC	0.74	1/2528 (0.0%)	1.19	23/3451 (0.7%)
2	AL	0.43	0/2318	0.95	10/3167 (0.3%)
2	BL	0.38	0/2318	0.90	9/3167 (0.3%)
3	AM	0.42	0/2651	0.98	22/3628 (0.6%)
3	BM	0.41	0/2651	0.98	18/3628 (0.5%)
4	AH	0.40	0/2037	0.90	6/2776 (0.2%)
4	BH	0.38	0/2037	0.89	5/2776 (0.2%)
5	A1	0.48	0/464	1.21	6/634 (0.9%)
5	A3	0.40	0/456	1.07	5/624 (0.8%)
5	A5	0.47	0/453	0.98	2/620 (0.3%)
5	A7	0.38	0/426	0.89	2/583 (0.3%)
5	A9	0.40	0/483	1.11	7/660 (1.1%)
5	AA	0.41	0/401	0.89	0/550
5	AD	0.39	0/456	0.93	2/624 (0.3%)
5	AF	0.38	0/471	1.01	4/644 (0.6%)
5	AI	0.54	0/471	1.12	3/644 (0.5%)
5	AK	0.36	0/464	0.87	1/634 (0.2%)
5	AO	0.56	0/471	1.33	9/644 (1.4%)
5	AQ	0.38	0/456	0.94	1/624 (0.2%)
5	AS	0.42	0/471	1.06	3/644 (0.5%)
5	AU	0.46	0/483	0.96	3/660 (0.5%)
5	AW	0.41	0/483	0.93	1/660 (0.2%)
5	AY	0.47	0/483	1.06	5/660 (0.8%)
5	B1	0.42	0/435	0.88	0/595
5	B3	0.40	0/483	0.92	1/660 (0.2%)
5	B5	0.38	0/426	0.95	0/583
5	B7	0.41	0/435	0.88	1/595 (0.2%)
5	B9	0.50	0/426	0.94	2/583 (0.3%)
5	BA	0.40	0/458	0.90	1/627 (0.2%)
5	BD	0.63	1/378 (0.3%)	1.13	4/518 (0.8%)
5	BF	0.54	1/453 (0.2%)	1.04	3/620 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	BI	0.44	0/418	0.90	1/573 (0.2%)
5	BK	0.38	0/483	0.82	1/660 (0.2%)
5	BO	0.53	0/471	1.18	6/644 (0.9%)
5	BQ	0.38	0/477	0.89	1/653 (0.2%)
5	BS	0.38	0/471	0.97	2/644 (0.3%)
5	BU	0.53	2/472 (0.4%)	0.94	3/646 (0.5%)
5	BW	0.44	0/464	0.94	2/634 (0.3%)
5	BY	0.42	0/435	0.79	1/595 (0.2%)
6	A0	0.56	0/350	0.86	2/476 (0.4%)
6	A2	0.35	0/350	0.76	0/476
6	A4	0.55	0/350	0.87	0/476
6	A6	0.39	0/350	0.92	0/476
6	A8	0.55	0/350	0.93	0/476
6	AB	0.46	0/350	0.79	0/476
6	AE	0.42	0/350	0.83	0/476
6	AG	0.55	0/350	0.97	0/476
6	AJ	0.46	0/350	0.84	0/476
6	AN	0.48	0/350	0.93	0/476
6	AP	0.51	0/350	0.89	1/476 (0.2%)
6	AR	0.43	0/350	0.85	0/476
6	AT	0.41	0/350	0.94	2/476 (0.4%)
6	AV	0.47	0/350	1.09	2/476 (0.4%)
6	AX	0.43	0/350	0.85	0/476
6	AZ	0.58	1/350 (0.3%)	1.06	6/476 (1.3%)
6	B0	0.55	0/350	0.87	2/476 (0.4%)
6	B2	0.46	0/350	0.90	1/476 (0.2%)
6	B4	0.54	0/350	0.92	0/476
6	B6	0.40	0/350	0.92	0/476
6	B8	0.55	0/350	0.93	1/476 (0.2%)
6	BB	0.49	0/350	0.86	0/476
6	BE	0.42	0/350	0.87	0/476
6	BG	0.54	0/350	1.09	1/476 (0.2%)
6	BJ	0.48	0/350	0.85	0/476
6	BN	0.55	0/350	1.05	2/476 (0.4%)
6	BP	0.50	0/350	0.85	1/476 (0.2%)
6	BR	0.45	0/350	0.87	0/476
6	BT	0.54	0/350	1.02	2/476 (0.4%)
6	BV	0.48	0/350	1.19	4/476 (0.8%)
6	BX	0.39	0/350	0.89	0/476
6	BZ	0.49	0/350	0.90	4/476 (0.8%)
All	All	0.49	7/44845 (0.0%)	0.98	234/61215 (0.4%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BC	236	MET	SD-CE	-7.05	1.61	1.79
5	BD	37	MET	SD-CE	5.62	1.93	1.79
1	AC	40	MET	SD-CE	5.57	1.93	1.79
5	BU	17	PRO	N-CD	5.32	1.55	1.47
5	BF	37	MET	SD-CE	5.25	1.92	1.79

The worst 5 of 234 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AC	301	ASP	N-CA-C	10.60	117.50	108.07
5	BO	21	LEU	N-CA-C	9.99	123.20	111.02
5	AY	49	ASP	N-CA-C	9.36	121.09	111.07
5	A1	8	LEU	N-CA-C	9.18	122.44	111.33
3	AM	122	LEU	N-CA-C	-9.07	99.96	112.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AC	2458	0	2377	508	0
1	BC	2458	0	2377	514	0
2	AL	2231	0	2192	677	0
2	BL	2231	0	2192	598	0
3	AM	2551	0	2526	779	0
3	BM	2551	0	2526	699	0
4	AH	1982	0	1981	421	0
4	BH	1982	0	1981	392	0
5	A1	455	0	460	169	0
5	A3	447	0	451	136	0
5	A5	444	0	456	141	0
5	A7	417	0	441	163	0
5	A9	473	0	476	130	0
5	AA	392	0	412	144	0
5	AD	447	0	451	129	0
5	AF	462	0	467	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AI	462	0	467	154	0
5	AK	455	0	460	94	0
5	AO	462	0	467	160	0
5	AQ	447	0	451	123	0
5	AS	462	0	467	190	0
5	AU	473	0	476	155	0
5	AW	473	0	476	189	0
5	AY	473	0	476	170	0
5	B1	426	0	434	144	0
5	B3	473	0	476	139	0
5	B5	417	0	441	95	0
5	B7	426	0	434	136	0
5	B9	417	0	441	146	0
5	BA	448	0	462	159	0
5	BD	370	0	399	139	0
5	BF	444	0	456	150	0
5	BI	409	0	426	112	0
5	BK	473	0	476	112	0
5	BO	462	0	467	155	0
5	BQ	467	0	474	124	0
5	BS	462	0	467	118	0
5	BU	462	0	472	180	0
5	BW	455	0	460	163	0
5	BY	426	0	434	154	0
6	A0	337	0	323	115	0
6	A2	337	0	323	107	0
6	A4	337	0	323	88	0
6	A6	337	0	323	63	0
6	A8	337	0	323	111	0
6	AB	337	0	321	94	0
6	AE	337	0	323	72	0
6	AG	337	0	323	92	0
6	AJ	337	0	323	97	0
6	AN	337	0	323	87	0
6	AP	337	0	323	110	0
6	AR	337	0	323	78	0
6	AT	337	0	323	81	0
6	AV	337	0	323	101	0
6	AX	337	0	323	88	0
6	AZ	337	0	323	102	0
6	B0	337	0	323	128	0
6	B2	337	0	323	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B4	337	0	323	73	0
6	B6	337	0	323	56	0
6	B8	337	0	323	79	0
6	BB	337	0	323	105	0
6	BE	337	0	323	75	0
6	BG	337	0	323	81	0
6	BJ	337	0	323	97	0
6	BN	337	0	323	70	0
6	BP	337	0	323	97	0
6	BR	337	0	323	73	0
6	BT	337	0	323	66	0
6	BV	337	0	323	110	0
6	BX	337	0	323	76	0
6	BZ	337	0	323	86	0
7	AC	172	0	120	37	0
7	BC	172	0	120	34	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BI	1	0	0	0	0
8	BK	1	0	0	0	0
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	69	0
9	A1	66	0	74	52	0
9	A2	66	0	74	28	0
9	A3	132	0	148	60	0
9	A5	66	0	74	34	0
9	A6	66	0	74	27	0
9	A7	66	0	74	52	0
9	A8	66	0	74	46	0
9	A9	66	0	74	36	0
9	AA	66	0	74	42	0
9	AB	66	0	74	35	0
9	AD	66	0	74	27	0
9	AE	66	0	74	32	0
9	AF	66	0	74	38	0
9	AG	66	0	74	36	0
9	AI	66	0	74	36	0
9	AJ	66	0	74	43	0
9	AK	66	0	74	58	0
9	AL	132	0	148	55	0
9	AM	132	0	148	41	0
9	AN	66	0	74	53	0
9	AO	66	0	74	50	0
9	AP	66	0	74	37	0
9	AQ	66	0	74	25	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	30	0
9	AW	66	0	72	40	0
9	AX	66	0	74	33	0
9	AY	66	0	74	48	0
9	AZ	66	0	72	41	0
9	B0	66	0	74	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B1	66	0	74	37	0
9	B2	66	0	74	43	0
9	B3	66	0	74	47	0
9	B4	66	0	74	20	0
9	B5	66	0	74	20	0
9	B6	66	0	74	24	0
9	B7	66	0	74	39	0
9	B8	66	0	74	36	0
9	B9	66	0	74	38	0
9	BA	66	0	74	38	0
9	BB	66	0	74	47	0
9	BD	66	0	74	34	0
9	BE	66	0	74	46	0
9	BF	66	0	74	39	0
9	BG	66	0	74	46	0
9	BI	66	0	74	50	0
9	BJ	66	0	74	26	0
9	BK	66	0	74	26	0
9	BL	132	0	148	42	0
9	BM	132	0	148	44	0
9	BN	66	0	74	30	0
9	BO	66	0	74	48	0
9	BP	66	0	74	35	0
9	BQ	132	0	148	51	0
9	BS	66	0	74	28	0
9	BT	66	0	74	22	0
9	BU	66	0	74	38	0
9	BV	66	0	74	23	0
9	BW	66	0	74	42	0
9	BX	66	0	74	33	0
9	BY	66	0	74	35	0
9	BZ	66	0	74	31	0
10	AL	65	0	76	17	0
10	AM	65	0	76	12	0
10	BL	65	0	76	11	0
10	BM	65	0	76	7	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	10	0
13	BM	53	0	72	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A0	44	0	60	28	0
14	A1	44	0	60	29	0
14	A2	44	0	60	51	0
14	A5	44	0	60	29	0
14	A7	44	0	60	46	0
14	AA	44	0	60	24	0
14	AB	44	0	60	46	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	15	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	18	0
14	AW	44	0	60	32	0
14	AX	44	0	60	47	0
14	B0	44	0	60	44	0
14	B1	44	0	60	41	0
14	B2	44	0	60	75	0
14	B5	44	0	60	22	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	13	0
14	BM	44	0	60	8	0
14	BN	44	0	60	15	0
14	BO	44	0	60	13	0
14	BP	44	0	60	29	0
14	BS	44	0	60	10	0
14	BU	44	0	60	61	0
14	BV	44	0	60	59	0
14	BW	44	0	60	20	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	BH	5	0	0	1	0
17	AA	1	0	0	0	0
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	11377	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 111.

The worst 5 of 11377 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 ⓘ

5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BI	48/61 (79%)	32 (67%)	13 (27%)	3 (6%)	1	6
5	BK	58/61 (95%)	43 (74%)	12 (21%)	3 (5%)	1	9
5	BO	57/61 (93%)	46 (81%)	11 (19%)	0	100	100
5	BQ	57/61 (93%)	41 (72%)	14 (25%)	2 (4%)	3	16
5	BS	57/61 (93%)	45 (79%)	9 (16%)	3 (5%)	1	9
5	BU	56/61 (92%)	43 (77%)	12 (21%)	1 (2%)	6	31
5	BW	56/61 (92%)	38 (68%)	14 (25%)	4 (7%)	1	4
5	BY	52/61 (85%)	30 (58%)	16 (31%)	6 (12%)	0	1
6	A0	38/47 (81%)	30 (79%)	7 (18%)	1 (3%)	4	23
6	A2	38/47 (81%)	29 (76%)	8 (21%)	1 (3%)	4	23
6	A4	38/47 (81%)	31 (82%)	6 (16%)	1 (3%)	4	23
6	A6	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	A8	38/47 (81%)	27 (71%)	10 (26%)	1 (3%)	4	23
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%)	4	23
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	3
6	AV	38/47 (81%)	35 (92%)	2 (5%)	1 (3%)	4	23
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%)	4	23
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%)	4	23
6	BR	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
6	BT	38/47 (81%)	30 (79%)	5 (13%)	3 (8%)	1	3
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	3

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 ⓘ

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%)	234 (88%)	31 (12%)	5	23
1	BC	265/317 (84%)	240 (91%)	25 (9%)	8	32
2	AL	228/229 (100%)	193 (85%)	35 (15%)	2	13
2	BL	228/229 (100%)	207 (91%)	21 (9%)	8	33
3	AM	256/261 (98%)	214 (84%)	42 (16%)	2	12
3	BM	256/261 (98%)	221 (86%)	35 (14%)	3	17
4	AH	210/211 (100%)	194 (92%)	16 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BH	210/211 (100%)	191 (91%)	19 (9%)	9	34
5	A1	48/56 (86%)	44 (92%)	4 (8%)	10	37
5	A3	47/56 (84%)	41 (87%)	6 (13%)	4	19
5	A5	48/56 (86%)	44 (92%)	4 (8%)	10	37
5	A7	48/56 (86%)	40 (83%)	8 (17%)	2	12
5	A9	50/56 (89%)	45 (90%)	5 (10%)	7	29
5	AA	44/56 (79%)	38 (86%)	6 (14%)	3	17
5	AD	47/56 (84%)	43 (92%)	4 (8%)	10	36
5	AF	49/56 (88%)	44 (90%)	5 (10%)	7	29
5	AI	49/56 (88%)	43 (88%)	6 (12%)	5	21
5	AK	48/56 (86%)	43 (90%)	5 (10%)	7	28
5	AO	49/56 (88%)	43 (88%)	6 (12%)	5	21
5	AQ	47/56 (84%)	44 (94%)	3 (6%)	16	48
5	AS	49/56 (88%)	45 (92%)	4 (8%)	10	37
5	AU	50/56 (89%)	44 (88%)	6 (12%)	5	22
5	AW	50/56 (89%)	44 (88%)	6 (12%)	5	22
5	AY	50/56 (89%)	43 (86%)	7 (14%)	3	16
5	B1	45/56 (80%)	43 (96%)	2 (4%)	25	60
5	B3	50/56 (89%)	47 (94%)	3 (6%)	17	50
5	B5	48/56 (86%)	45 (94%)	3 (6%)	16	48
5	B7	45/56 (80%)	39 (87%)	6 (13%)	4	18
5	B9	48/56 (86%)	46 (96%)	2 (4%)	26	61
5	BA	50/56 (89%)	45 (90%)	5 (10%)	7	29
5	BD	43/56 (77%)	42 (98%)	1 (2%)	44	74
5	BF	48/56 (86%)	45 (94%)	3 (6%)	16	48
5	BI	46/56 (82%)	41 (89%)	5 (11%)	6	26
5	BK	50/56 (89%)	43 (86%)	7 (14%)	3	16
5	BO	49/56 (88%)	42 (86%)	7 (14%)	3	16
5	BQ	50/56 (89%)	46 (92%)	4 (8%)	11	38
5	BS	49/56 (88%)	48 (98%)	1 (2%)	48	76
5	BU	50/56 (89%)	44 (88%)	6 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	BW	48/56 (86%)	42 (88%)	6 (12%)	4	20
5	BY	45/56 (80%)	40 (89%)	5 (11%)	6	25
6	A0	33/39 (85%)	21 (64%)	12 (36%)	0	1
6	A2	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	A4	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	A6	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	A8	33/39 (85%)	25 (76%)	8 (24%)	1	4
6	AB	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	AE	33/39 (85%)	31 (94%)	2 (6%)	17	49
6	AG	33/39 (85%)	24 (73%)	9 (27%)	0	2
6	AJ	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	AN	33/39 (85%)	26 (79%)	7 (21%)	1	6
6	AP	33/39 (85%)	26 (79%)	7 (21%)	1	6
6	AR	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	AT	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	AV	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	AX	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	AZ	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	B0	33/39 (85%)	26 (79%)	7 (21%)	1	6
6	B2	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	B4	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	B6	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	B8	33/39 (85%)	24 (73%)	9 (27%)	0	2
6	BB	33/39 (85%)	25 (76%)	8 (24%)	1	4
6	BE	33/39 (85%)	31 (94%)	2 (6%)	17	49
6	BG	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	BJ	33/39 (85%)	30 (91%)	3 (9%)	9	33
6	BN	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	BP	33/39 (85%)	30 (91%)	3 (9%)	9	33
6	BR	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	BT	33/39 (85%)	28 (85%)	5 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BV	33/39 (85%)	31 (94%)	2 (6%)	17	49
6	BX	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	BZ	33/39 (85%)	31 (94%)	2 (6%)	17	49
All	All	4511/5076 (89%)	3965 (88%)	546 (12%)	5	21

5 of 546 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	BQ	55	TYR
5	BU	12	TRP
5	BQ	45	ASN
6	B6	37	LEU
5	AQ	55	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
5	A3	56	GLN
5	BU	56	GLN
1	BC	159	ASN
5	BU	28	GLN
5	B5	28	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
9	BCL	B9	102	-	69,74,74	1.56	11 (15%)	79,115,115	2.36	24 (30%)
16	PO4	AH	302	-	4,4,4	1.69	0	6,6,6	0.44	0
9	BCL	AD	102	-	69,74,74	1.53	11 (15%)	79,115,115	2.30	23 (29%)
9	BCL	BQ	103	-	69,74,74	1.67	17 (24%)	79,115,115	2.19	18 (22%)
14	CRT	A5	103	-	43,43,43	1.23	5 (11%)	48,54,54	1.80	17 (35%)
14	CRT	BG	102	-	43,43,43	1.25	3 (6%)	48,54,54	1.82	16 (33%)
15	PEF	BM	407	-	18,18,46	3.17	7 (38%)	21,23,51	2.02	6 (28%)
7	HEM	AC	504	1	50,50,50	1.90	14 (28%)	67,82,82	1.47	9 (13%)
7	HEM	AC	503	1	50,50,50	1.84	14 (28%)	67,82,82	1.37	9 (13%)
13	MQ8	AM	405	-	54,54,54	1.14	5 (9%)	67,69,69	1.55	12 (17%)
7	HEM	BC	502	1	50,50,50	1.88	17 (34%)	67,82,82	1.46	11 (16%)
9	BCL	AM	401	-	69,74,74	1.32	8 (11%)	79,115,115	2.25	23 (29%)
14	CRT	AB	102	-	43,43,43	1.25	4 (9%)	48,54,54	1.99	17 (35%)
9	BCL	BX	101	-	69,74,74	1.83	20 (28%)	79,115,115	2.41	23 (29%)
16	PO4	BH	301	-	4,4,4	1.68	0	6,6,6	0.44	0
9	BCL	BT	101	-	69,74,74	1.64	14 (20%)	79,115,115	2.26	28 (35%)
7	HEM	AC	501	1	50,50,50	1.87	13 (26%)	67,82,82	1.49	7 (10%)
11	UQ8	BL	304	-	53,53,53	1.44	3 (5%)	66,67,67	1.63	14 (21%)
9	BCL	AM	402	-	69,74,74	1.32	9 (13%)	79,115,115	2.33	23 (29%)
9	BCL	AW	101	-	69,74,74	1.83	14 (20%)	79,115,115	3.10	28 (35%)
9	BCL	BJ	101	-	69,74,74	1.70	16 (23%)	79,115,115	2.16	24 (30%)
9	BCL	BY	102	-	69,74,74	1.51	12 (17%)	79,115,115	2.27	21 (26%)
14	CRT	B2	102	-	43,43,43	1.94	9 (20%)	48,54,54	2.14	17 (35%)
16	PO4	AM	410	-	4,4,4	1.73	0	6,6,6	0.47	0
9	BCL	A8	101	-	69,74,74	1.91	19 (27%)	79,115,115	2.87	28 (35%)
9	BCL	BF	102	-	69,74,74	1.77	14 (20%)	79,115,115	2.39	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	A0	102	-	69,74,74	2.04	15 (21%)	79,115,115	2.93	26 (32%)
9	BCL	AV	102	-	69,74,74	1.79	16 (23%)	79,115,115	2.16	26 (32%)
9	BCL	AL	301	-	69,74,74	1.52	15 (21%)	79,115,115	2.18	23 (29%)
14	CRT	BV	102	-	43,43,43	1.54	10 (23%)	48,54,54	1.87	13 (27%)
9	BCL	AF	102	-	69,74,74	1.57	13 (18%)	79,115,115	2.24	24 (30%)
14	CRT	AW	102	-	43,43,43	1.54	6 (13%)	48,54,54	1.85	20 (41%)
9	BCL	BI	102	-	69,74,74	1.60	13 (18%)	79,115,115	2.30	22 (27%)
9	BCL	BL	303	-	69,74,74	1.33	10 (14%)	79,115,115	2.28	22 (27%)
9	BCL	BG	101	-	69,74,74	1.67	13 (18%)	79,115,115	2.35	23 (29%)
9	BCL	A5	102	-	69,74,74	1.88	17 (24%)	79,115,115	2.58	26 (32%)
14	CRT	AJ	102	-	43,43,43	1.28	4 (9%)	48,54,54	2.07	16 (33%)
14	CRT	BN	102	-	43,43,43	1.32	7 (16%)	48,54,54	1.97	16 (33%)
9	BCL	BK	102	-	69,74,74	1.57	12 (17%)	79,115,115	2.25	23 (29%)
14	CRT	AM	406	-	43,43,43	1.38	3 (6%)	48,54,54	1.64	10 (20%)
14	CRT	AT	102	-	43,43,43	1.28	4 (9%)	48,54,54	1.90	14 (29%)
14	CRT	BU	103	-	43,43,43	1.60	6 (13%)	48,54,54	2.38	16 (33%)
9	BCL	BD	102	-	69,74,74	1.83	17 (24%)	79,115,115	2.32	23 (29%)
14	CRT	BF	103	-	43,43,43	1.28	4 (9%)	48,54,54	2.38	17 (35%)
7	HEM	AC	502	1	50,50,50	1.93	16 (32%)	67,82,82	1.43	9 (13%)
9	BCL	AL	303	-	69,74,74	1.35	10 (14%)	79,115,115	2.28	20 (25%)
15	PEF	AH	301	-	18,18,46	3.17	7 (38%)	21,23,51	2.02	6 (28%)
9	BCL	BL	301	-	69,74,74	1.53	13 (18%)	79,115,115	2.18	23 (29%)
14	CRT	AX	102	-	43,43,43	1.60	9 (20%)	48,54,54	2.27	14 (29%)
14	CRT	AG	102	-	43,43,43	1.25	4 (9%)	48,54,54	1.87	17 (35%)
9	BCL	A9	102	-	69,74,74	1.64	15 (21%)	79,115,115	2.80	28 (35%)
9	BCL	AK	102	-	69,74,74	1.53	13 (18%)	79,115,115	2.34	24 (30%)
15	PEF	AM	408	-	13,13,46	2.98	5 (38%)	15,16,51	1.18	1 (6%)
15	PEF	BQ	101	-	46,46,46	2.19	7 (15%)	49,51,51	1.40	6 (12%)
9	BCL	AO	102	-	69,74,74	1.56	14 (20%)	79,115,115	2.24	26 (32%)
9	BCL	BM	402	-	69,74,74	1.42	13 (18%)	79,115,115	2.44	23 (29%)
9	BCL	AA	101	-	69,74,74	1.54	14 (20%)	79,115,115	2.21	21 (26%)
10	BPH	AL	302	-	59,70,70	1.58	6 (10%)	59,101,101	1.67	10 (16%)
9	BCL	AR	101	-	69,74,74	1.66	16 (23%)	79,115,115	2.31	24 (30%)
9	BCL	AS	103	-	69,74,74	1.66	14 (20%)	79,115,115	2.32	25 (31%)
9	BCL	A6	101	-	69,74,74	2.13	13 (18%)	79,115,115	2.45	27 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	PO4	A3	101	-	4,4,4	1.73	1 (25%)	6,6,6	0.46	0
10	BPH	AM	403	-	59,70,70	1.65	7 (11%)	59,101,101	1.88	9 (15%)
9	BCL	BB	101	-	69,74,74	1.85	14 (20%)	79,115,115	2.51	25 (31%)
14	CRT	BO	103	-	43,43,43	1.24	3 (6%)	48,54,54	1.89	15 (31%)
9	BCL	AG	101	-	69,74,74	1.63	13 (18%)	79,115,115	2.24	24 (30%)
9	BCL	B8	101	-	69,74,74	1.64	15 (21%)	79,115,115	2.57	27 (34%)
14	CRT	AP	102	-	43,43,43	1.49	7 (16%)	48,54,54	1.87	16 (33%)
9	BCL	B2	101	-	69,74,74	1.66	13 (18%)	79,115,115	2.30	25 (31%)
9	BCL	AP	101	-	69,74,74	1.70	13 (18%)	79,115,115	2.42	26 (32%)
9	BCL	AE	101	-	69,74,74	1.75	14 (20%)	79,115,115	2.45	26 (32%)
7	HEM	BC	504	1	50,50,50	1.97	15 (30%)	67,82,82	1.44	8 (11%)
14	CRT	BP	102	-	43,43,43	1.60	7 (16%)	48,54,54	1.75	15 (31%)
9	BCL	AI	102	-	69,74,74	1.59	12 (17%)	79,115,115	2.25	23 (29%)
9	BCL	A3	104	-	69,74,74	1.66	15 (21%)	79,115,115	2.80	26 (32%)
7	HEM	BC	501	1	50,50,50	1.95	14 (28%)	67,82,82	1.43	8 (11%)
9	BCL	B0	102	-	69,74,74	1.49	14 (20%)	79,115,115	2.36	27 (34%)
13	MQ8	BM	405	-	54,54,54	1.19	7 (12%)	67,69,69	1.37	11 (16%)
9	BCL	BA	101	-	69,74,74	1.47	11 (15%)	79,115,115	2.21	21 (26%)
9	BCL	B1	102	-	69,74,74	1.49	14 (20%)	79,115,115	2.24	20 (25%)
9	BCL	BU	102	-	69,74,74	1.67	10 (14%)	79,115,115	2.29	21 (26%)
9	BCL	AT	101	-	69,74,74	1.78	18 (26%)	79,115,115	2.26	25 (31%)
9	BCL	BE	101	-	69,74,74	1.98	18 (26%)	79,115,115	2.14	23 (29%)
14	CRT	BW	103	-	43,43,43	1.50	7 (16%)	48,54,54	1.75	16 (33%)
9	BCL	A3	103	-	69,74,74	1.84	14 (20%)	79,115,115	2.29	23 (29%)
14	CRT	A0	101	-	43,43,43	1.36	6 (13%)	48,54,54	2.01	13 (27%)
9	BCL	AQ	102	-	69,74,74	1.56	15 (21%)	79,115,115	2.26	20 (25%)
9	BCL	BM	401	-	69,74,74	1.30	9 (13%)	79,115,115	2.26	25 (31%)
9	BCL	BN	101	-	69,74,74	1.57	13 (18%)	79,115,115	2.17	25 (31%)
9	BCL	A1	102	-	69,74,74	2.61	20 (28%)	79,115,115	2.53	24 (30%)
14	CRT	B1	103	-	43,43,43	1.23	3 (6%)	48,54,54	2.07	18 (37%)
11	UQ8	AL	304	-	53,53,53	1.49	3 (5%)	66,67,67	1.74	14 (21%)
9	BCL	B5	102	-	69,74,74	1.58	12 (17%)	79,115,115	2.27	24 (30%)
14	CRT	AS	104	-	43,43,43	1.26	2 (4%)	48,54,54	2.23	15 (31%)
9	BCL	BZ	101	-	69,74,74	1.60	12 (17%)	79,115,115	2.27	27 (34%)
9	BCL	B6	101	-	69,74,74	1.66	13 (18%)	79,115,115	2.33	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	AN	101	-	69,74,74	1.67	14 (20%)	79,115,115	2.38	25 (31%)
9	BCL	AU	102	-	69,74,74	1.83	17 (24%)	79,115,115	2.73	30 (37%)
9	BCL	BO	102	-	69,74,74	1.53	13 (18%)	79,115,115	2.31	21 (26%)
14	CRT	BA	102	-	43,43,43	1.25	2 (4%)	48,54,54	1.73	14 (29%)
10	BPH	BM	403	-	59,70,70	1.68	5 (8%)	59,101,101	1.94	9 (15%)
9	BCL	B7	103	-	69,74,74	1.62	13 (18%)	79,115,115	2.37	24 (30%)
14	CRT	AN	102	-	43,43,43	1.25	4 (9%)	48,54,54	1.93	18 (37%)
9	BCL	BV	101	-	69,74,74	1.58	12 (17%)	79,115,115	2.28	29 (36%)
14	CRT	B5	103	-	43,43,43	1.26	4 (9%)	48,54,54	1.74	14 (29%)
9	BCL	BW	102	-	69,74,74	1.54	13 (18%)	79,115,115	2.29	23 (29%)
14	CRT	BB	102	-	43,43,43	1.34	4 (9%)	48,54,54	2.01	18 (37%)
15	PEF	AM	407	-	18,18,46	3.17	7 (38%)	21,23,51	2.02	6 (28%)
15	PEF	AS	101	-	46,46,46	2.20	7 (15%)	49,51,51	1.40	6 (12%)
14	CRT	A7	102	-	43,43,43	3.02	6 (13%)	48,54,54	3.75	14 (29%)
14	CRT	A2	102	-	43,43,43	1.50	8 (18%)	48,54,54	1.86	14 (29%)
14	CRT	AR	102	-	43,43,43	1.22	3 (6%)	48,54,54	1.89	15 (31%)
9	BCL	A7	103	-	69,74,74	2.12	16 (23%)	79,115,115	2.42	25 (31%)
14	CRT	A1	103	-	43,43,43	1.37	6 (13%)	48,54,54	2.46	17 (35%)
14	CRT	BS	103	-	43,43,43	1.24	2 (4%)	48,54,54	1.84	16 (33%)
7	HEM	BC	503	1	50,50,50	1.88	15 (30%)	67,82,82	1.38	10 (14%)
14	CRT	B7	102	-	43,43,43	1.57	6 (13%)	48,54,54	2.06	13 (27%)
14	CRT	AA	102	-	43,43,43	1.26	2 (4%)	48,54,54	1.73	12 (25%)
14	CRT	B0	101	-	43,43,43	1.59	10 (23%)	48,54,54	1.99	15 (31%)
9	BCL	AX	101	-	69,74,74	2.16	15 (21%)	79,115,115	2.63	24 (30%)
9	BCL	BS	102	-	69,74,74	1.38	10 (14%)	79,115,115	2.35	22 (27%)
9	BCL	A2	101	-	69,74,74	1.68	16 (23%)	79,115,115	2.48	22 (27%)
9	BCL	BP	101	-	69,74,74	1.77	19 (27%)	79,115,115	2.47	27 (34%)
9	BCL	B4	101	-	69,74,74	1.65	17 (24%)	79,115,115	2.40	26 (32%)
9	BCL	AB	101	-	69,74,74	1.63	15 (21%)	79,115,115	2.39	24 (30%)
9	BCL	AJ	101	-	69,74,74	1.56	13 (18%)	79,115,115	2.35	23 (29%)
10	BPH	BL	302	-	59,70,70	1.56	8 (13%)	59,101,101	1.65	9 (15%)
9	BCL	BQ	104	-	69,74,74	1.61	13 (18%)	79,115,115	2.20	25 (31%)
9	BCL	AZ	101	-	69,74,74	2.70	19 (27%)	79,115,115	3.07	24 (30%)
9	BCL	AY	102	-	69,74,74	1.85	15 (21%)	79,115,115	2.37	23 (29%)
9	BCL	B3	102	-	69,74,74	1.45	10 (14%)	79,115,115	2.27	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PEF	AM	409	-	46,46,46	2.20	7 (15%)	49,51,51	1.33	6 (12%)
14	CRT	BM	406	-	43,43,43	1.30	4 (9%)	48,54,54	1.68	13 (27%)

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
9	BCL	B9	102	-	-	14/41/137/137	-
9	BCL	AD	102	-	-	17/41/137/137	-
9	BCL	BQ	103	-	-	15/41/137/137	-
14	CRT	A5	103	-	-	1/51/51/51	-
14	CRT	BG	102	-	-	2/51/51/51	-
15	PEF	BM	407	-	-	11/20/20/50	-
7	HEM	AC	504	1	-	6/14/54/54	-
7	HEM	AC	503	1	-	9/14/54/54	-
13	MQ8	AM	405	-	-	10/47/67/67	0/2/2/2
7	HEM	BC	502	1	-	5/14/54/54	-
9	BCL	AM	401	-	-	12/41/137/137	-
14	CRT	AB	102	-	-	5/51/51/51	-
9	BCL	BX	101	-	-	12/41/137/137	-
9	BCL	BT	101	-	-	6/41/137/137	-
7	HEM	AC	501	1	-	7/14/54/54	-
11	UQ8	BL	304	-	-	4/51/75/75	0/1/1/1
9	BCL	AM	402	-	-	13/41/137/137	-
9	BCL	AW	101	-	-	16/41/137/137	-
9	BCL	BJ	101	-	-	7/41/137/137	-
9	BCL	BY	102	-	-	15/41/137/137	-
14	CRT	B2	102	-	-	2/51/51/51	-
9	BCL	A8	101	-	-	8/41/137/137	-
9	BCL	BF	102	-	-	13/41/137/137	-
9	BCL	A0	102	-	-	15/41/137/137	-
9	BCL	AV	102	-	-	13/41/137/137	-
9	BCL	AL	301	-	-	9/41/137/137	-
14	CRT	BV	102	-	-	2/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	AF	102	-	-	9/41/137/137	-
14	CRT	AW	102	-	-	0/51/51/51	-
9	BCL	BI	102	-	-	14/41/137/137	-
9	BCL	BL	303	-	-	11/41/137/137	-
9	BCL	BG	101	-	-	11/41/137/137	-
9	BCL	A5	102	-	-	14/41/137/137	-
14	CRT	AJ	102	-	-	1/51/51/51	-
14	CRT	BN	102	-	-	1/51/51/51	-
9	BCL	BK	102	-	-	12/41/137/137	-
14	CRT	AM	406	-	-	0/51/51/51	-
14	CRT	AT	102	-	-	2/51/51/51	-
14	CRT	BU	103	-	-	2/51/51/51	-
9	BCL	BD	102	-	-	13/41/137/137	-
14	CRT	BF	103	-	-	1/51/51/51	-
7	HEM	AC	502	1	-	9/14/54/54	-
9	BCL	AL	303	-	-	12/41/137/137	-
15	PEF	AH	301	-	-	9/20/20/50	-
9	BCL	BL	301	-	-	11/41/137/137	-
14	CRT	AX	102	-	-	1/51/51/51	-
14	CRT	AG	102	-	-	1/51/51/51	-
9	BCL	A9	102	-	-	19/41/137/137	-
9	BCL	AK	102	-	-	15/41/137/137	-
15	PEF	AM	408	-	-	8/13/13/50	-
15	PEF	BQ	101	-	-	22/50/50/50	-
9	BCL	AO	102	-	-	17/41/137/137	-
9	BCL	BM	402	-	-	13/41/137/137	-
9	BCL	AA	101	-	-	17/41/137/137	-
10	BPH	AL	302	-	-	12/37/105/105	0/5/6/6
9	BCL	AR	101	-	-	14/41/137/137	-
9	BCL	AS	103	-	-	17/41/137/137	-
9	BCL	A6	101	-	-	18/41/137/137	-
10	BPH	AM	403	-	-	9/37/105/105	0/5/6/6
9	BCL	BB	101	-	-	9/41/137/137	-
14	CRT	BO	103	-	-	1/51/51/51	-
9	BCL	AG	101	-	-	12/41/137/137	-
9	BCL	B8	101	-	-	11/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CRT	AP	102	-	-	2/51/51/51	-
9	BCL	B2	101	-	-	11/41/137/137	-
9	BCL	AP	101	-	-	8/41/137/137	-
9	BCL	AE	101	-	-	9/41/137/137	-
7	HEM	BC	504	1	-	9/14/54/54	-
14	CRT	BP	102	-	-	2/51/51/51	-
9	BCL	AI	102	-	-	13/41/137/137	-
9	BCL	A3	104	-	-	16/41/137/137	-
7	HEM	BC	501	1	-	6/14/54/54	-
9	BCL	B0	102	-	-	12/41/137/137	-
13	MQ8	BM	405	-	-	14/47/67/67	0/2/2/2
9	BCL	BA	101	-	-	12/41/137/137	-
9	BCL	B1	102	-	-	14/41/137/137	-
9	BCL	BU	102	-	-	15/41/137/137	-
9	BCL	AT	101	-	-	9/41/137/137	-
9	BCL	BE	101	-	-	14/41/137/137	-
14	CRT	BW	103	-	-	0/51/51/51	-
9	BCL	A3	103	-	-	17/41/137/137	-
14	CRT	A0	101	-	-	2/51/51/51	-
9	BCL	AQ	102	-	-	17/41/137/137	-
9	BCL	BM	401	-	-	12/41/137/137	-
9	BCL	BN	101	-	-	12/41/137/137	-
9	BCL	A1	102	-	-	16/41/137/137	-
14	CRT	B1	103	-	-	2/51/51/51	-
11	UQ8	AL	304	-	-	9/51/75/75	0/1/1/1
9	BCL	B5	102	-	-	13/41/137/137	-
14	CRT	AS	104	-	-	2/51/51/51	-
9	BCL	BZ	101	-	-	13/41/137/137	-
9	BCL	B6	101	-	-	17/41/137/137	-
9	BCL	AN	101	-	-	13/41/137/137	-
9	BCL	AU	102	-	-	18/41/137/137	-
9	BCL	BO	102	-	-	15/41/137/137	-
14	CRT	BA	102	-	-	1/51/51/51	-
10	BPH	BM	403	-	-	9/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	B7	103	-	-	11/41/137/137	-
14	CRT	AN	102	-	-	1/51/51/51	-
9	BCL	BV	101	-	-	15/41/137/137	-
14	CRT	B5	103	-	-	1/51/51/51	-
9	BCL	BW	102	-	-	15/41/137/137	-
14	CRT	BB	102	-	-	2/51/51/51	-
15	PEF	AM	407	-	-	14/20/20/50	-
15	PEF	AS	101	-	-	27/50/50/50	-
14	CRT	A7	102	-	-	4/51/51/51	-
14	CRT	A2	102	-	-	1/51/51/51	-
14	CRT	AR	102	-	-	1/51/51/51	-
9	BCL	A7	103	-	-	13/41/137/137	-
14	CRT	A1	103	-	-	2/51/51/51	-
14	CRT	BS	103	-	-	2/51/51/51	-
7	HEM	BC	503	1	-	10/14/54/54	-
14	CRT	B7	102	-	-	2/51/51/51	-
14	CRT	AA	102	-	-	1/51/51/51	-
14	CRT	B0	101	-	-	5/51/51/51	-
9	BCL	AX	101	-	-	18/41/137/137	-
9	BCL	BS	102	-	-	15/41/137/137	-
9	BCL	A2	101	-	-	15/41/137/137	-
9	BCL	BP	101	-	-	6/41/137/137	-
9	BCL	B4	101	-	-	7/41/137/137	-
9	BCL	AB	101	-	-	10/41/137/137	-
9	BCL	AJ	101	-	-	11/41/137/137	-
10	BPH	BL	302	-	-	12/37/105/105	0/5/6/6
9	BCL	BQ	104	-	-	10/41/137/137	-
9	BCL	AZ	101	-	-	18/41/137/137	-
9	BCL	AY	102	-	-	17/41/137/137	-
9	BCL	B3	102	-	-	14/41/137/137	-
15	PEF	AM	409	-	-	19/50/50/50	-
14	CRT	BM	406	-	-	0/51/51/51	-

The worst 5 of 1387 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AZ	101	BCL	O2A-C1	-18.12	0.97	1.46
9	A1	102	BCL	O2A-C1	15.94	1.89	1.46
14	A7	102	CRT	C21-C20	12.93	1.71	1.36
14	A7	102	CRT	C21-C22	12.54	1.82	1.43
9	A6	101	BCL	O2A-C1	12.28	1.79	1.46

The worst 5 of 2456 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A7	102	CRT	C20-C21-C22	-18.13	86.41	123.52
9	AW	101	BCL	O2A-C1-C2	17.78	176.53	108.11
9	A0	102	BCL	O2A-C1-C2	15.01	165.88	108.11
9	AZ	101	BCL	C1-O2A-CGA	14.84	152.58	116.65
9	A3	104	BCL	O2A-C1-C2	13.20	158.90	108.11

There are no chirality outliers.

5 of 1250 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	501	HEM	C2C-C3C-CAC-CBC
7	AC	502	HEM	C2B-C3B-CAB-CBB
7	AC	502	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

131 monomers are involved in 3136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B9	102	BCL	38	0
16	AH	302	PO4	1	0
9	AD	102	BCL	27	0
9	BQ	103	BCL	30	0
14	A5	103	CRT	29	0
14	BG	102	CRT	13	0
15	BM	407	PEF	2	0
7	AC	504	HEM	5	0
7	AC	503	HEM	13	0
13	AM	405	MQ8	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	BC	502	HEM	7	0
9	AM	401	BCL	15	0
14	AB	102	CRT	46	0
9	BX	101	BCL	33	0
16	BH	301	PO4	1	0
9	BT	101	BCL	22	0
7	AC	501	HEM	9	0
11	BL	304	UQ8	12	0
9	AM	402	BCL	31	0
9	AW	101	BCL	40	0
9	BJ	101	BCL	26	0
9	BY	102	BCL	35	0
14	B2	102	CRT	75	0
9	A8	101	BCL	46	0
9	BF	102	BCL	39	0
9	A0	102	BCL	69	0
9	AV	102	BCL	30	0
9	AL	301	BCL	40	0
14	BV	102	CRT	59	0
9	AF	102	BCL	38	0
14	AW	102	CRT	32	0
9	BI	102	BCL	50	0
9	BL	303	BCL	13	0
9	BG	101	BCL	46	0
9	A5	102	BCL	34	0
14	AJ	102	CRT	21	0
14	BN	102	CRT	15	0
9	BK	102	BCL	26	0
14	AM	406	CRT	13	0
14	AT	102	CRT	18	0
14	BU	103	CRT	61	0
9	BD	102	BCL	34	0
14	BF	103	CRT	19	0
7	AC	502	HEM	11	0
9	AL	303	BCL	21	0
15	AH	301	PEF	8	0
9	BL	301	BCL	33	0
14	AX	102	CRT	47	0
14	AG	102	CRT	11	0
9	A9	102	BCL	36	0
9	AK	102	BCL	58	0
15	AM	408	PEF	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	BQ	101	PEF	12	0
9	AO	102	BCL	50	0
9	BM	402	BCL	35	0
9	AA	101	BCL	42	0
10	AL	302	BPH	17	0
9	AR	101	BCL	34	0
9	AS	103	BCL	32	0
9	A6	101	BCL	27	0
10	AM	403	BPH	12	0
9	BB	101	BCL	47	0
14	BO	103	CRT	13	0
9	AG	101	BCL	36	0
9	B8	101	BCL	36	0
14	AP	102	CRT	24	0
9	B2	101	BCL	43	0
9	AP	101	BCL	37	0
9	AE	101	BCL	32	0
7	BC	504	HEM	9	0
14	BP	102	CRT	29	0
9	AI	102	BCL	36	0
9	A3	104	BCL	25	0
7	BC	501	HEM	7	0
9	B0	102	BCL	57	0
13	BM	405	MQ8	8	0
9	BA	101	BCL	38	0
9	B1	102	BCL	37	0
9	BU	102	BCL	38	0
9	AT	101	BCL	25	0
9	BE	101	BCL	46	0
14	BW	103	CRT	20	0
9	A3	103	BCL	42	0
14	A0	101	CRT	28	0
9	AQ	102	BCL	25	0
9	BM	401	BCL	14	0
9	BN	101	BCL	30	0
9	A1	102	BCL	52	0
14	B1	103	CRT	41	0
11	AL	304	UQ8	8	0
9	B5	102	BCL	20	0
14	AS	104	CRT	77	0
9	BZ	101	BCL	31	0
9	B6	101	BCL	24	0

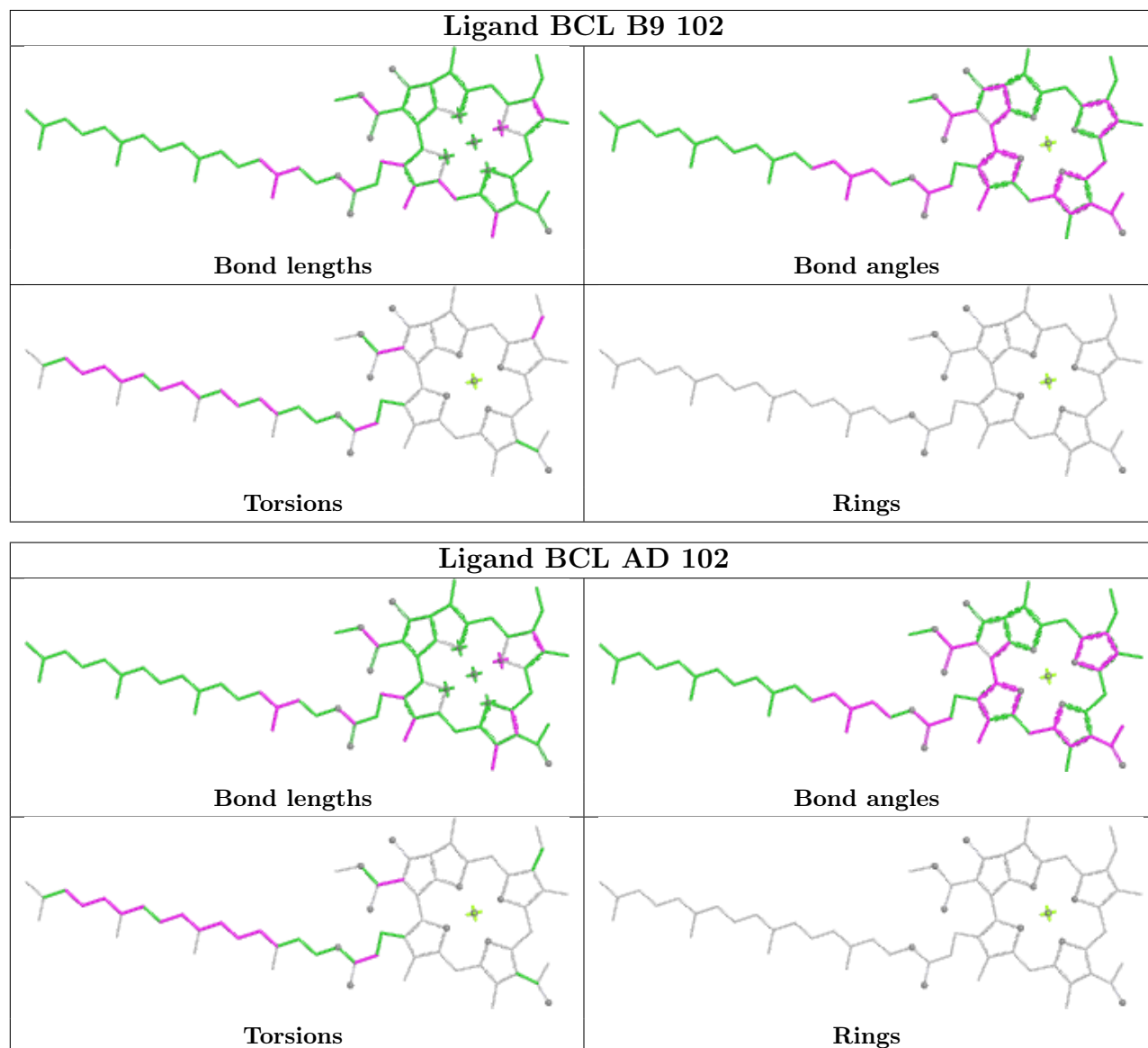
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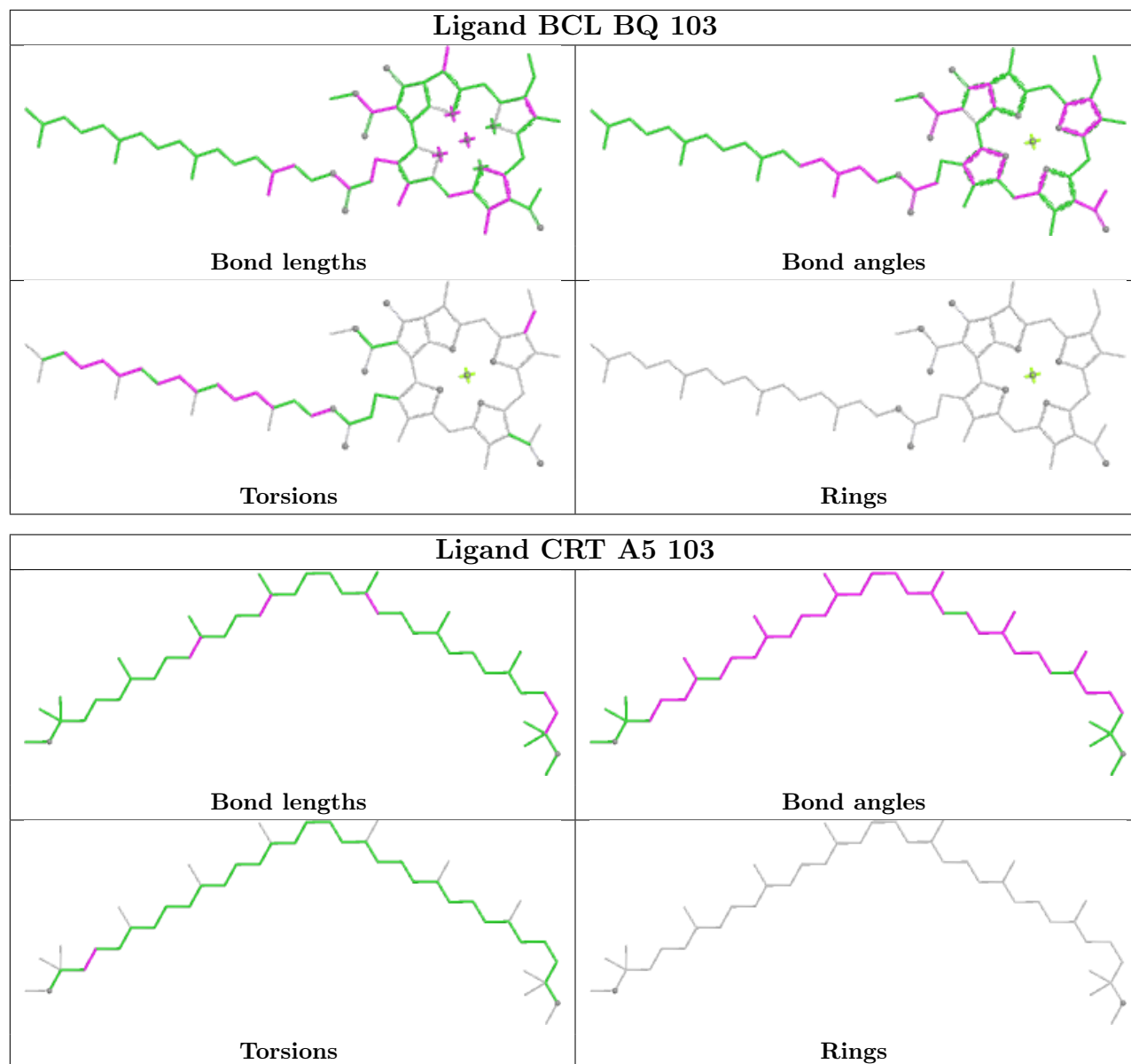
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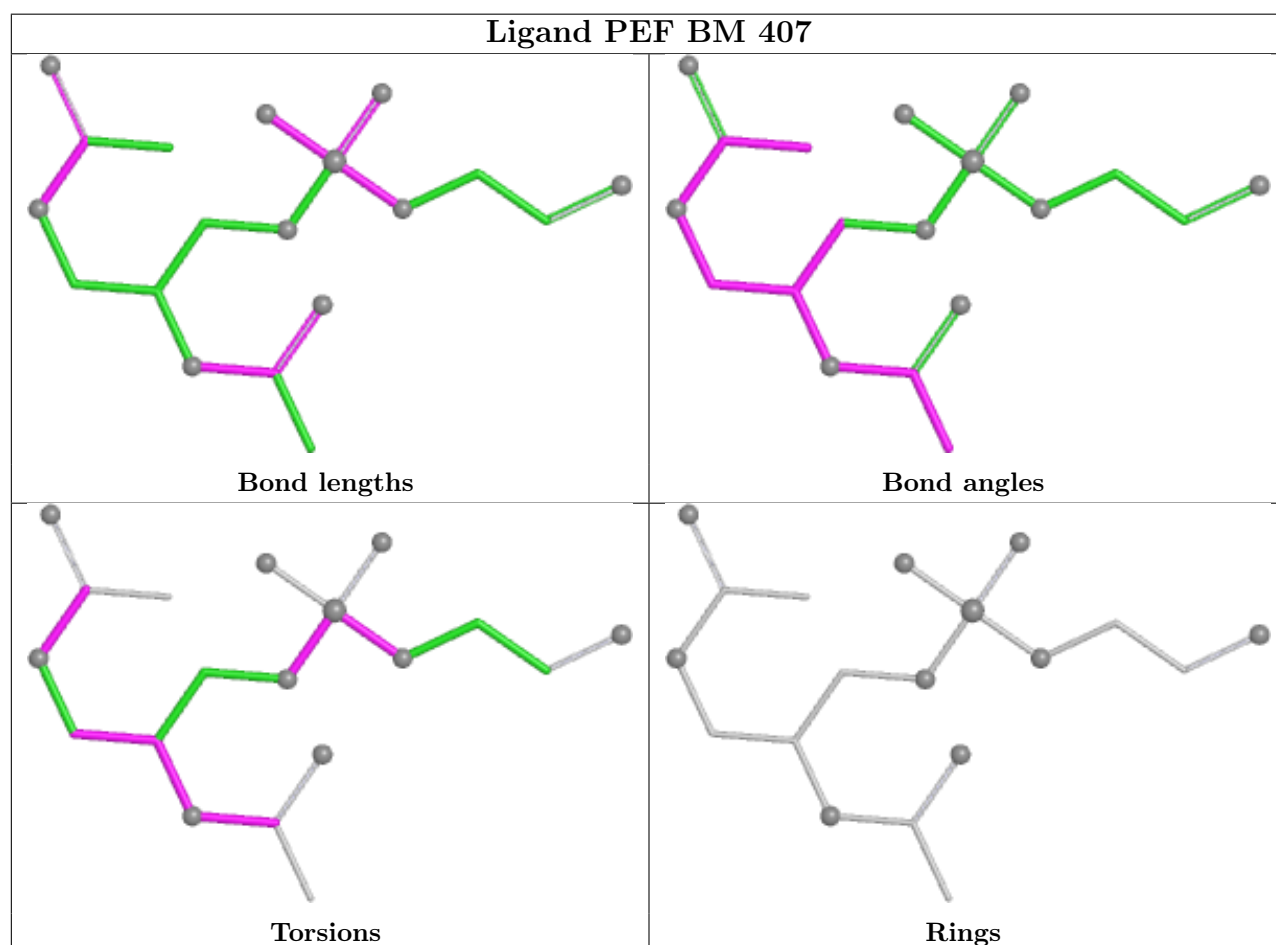
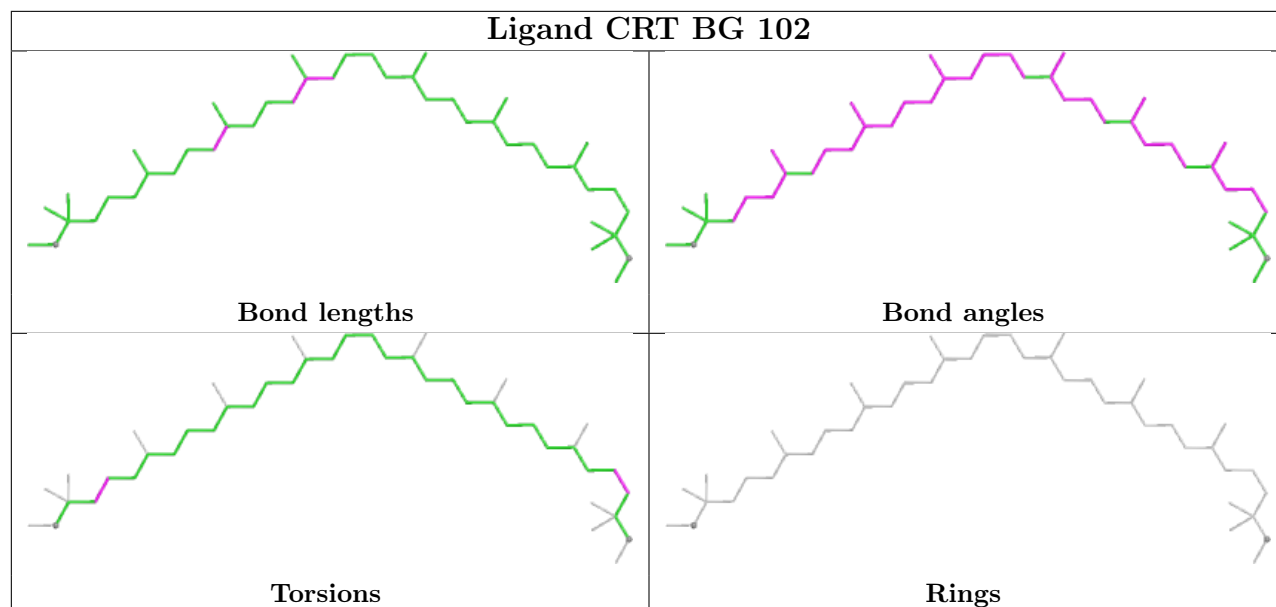
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AN	101	BCL	53	0
9	AU	102	BCL	46	0
9	BO	102	BCL	48	0
14	BA	102	CRT	26	0
10	BM	403	BPH	7	0
9	B7	103	BCL	39	0
14	AN	102	CRT	15	0
9	BV	101	BCL	23	0
14	B5	103	CRT	22	0
9	BW	102	BCL	42	0
14	BB	102	CRT	27	0
15	AM	407	PEF	3	0
15	AS	101	PEF	37	0
14	A7	102	CRT	46	0
14	A2	102	CRT	51	0
14	AR	102	CRT	20	0
9	A7	103	BCL	52	0
14	A1	103	CRT	29	0
14	BS	103	CRT	10	0
7	BC	503	HEM	11	0
14	B7	102	CRT	39	0
14	AA	102	CRT	24	0
14	B0	101	CRT	44	0
9	AX	101	BCL	33	0
9	BS	102	BCL	28	0
9	A2	101	BCL	28	0
9	BP	101	BCL	35	0
9	B4	101	BCL	20	0
9	AB	101	BCL	35	0
9	AJ	101	BCL	43	0
10	BL	302	BPH	11	0
9	BQ	104	BCL	34	0
9	AZ	101	BCL	41	0
9	AY	102	BCL	48	0
9	B3	102	BCL	47	0
15	AM	409	PEF	14	0
14	BM	406	CRT	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

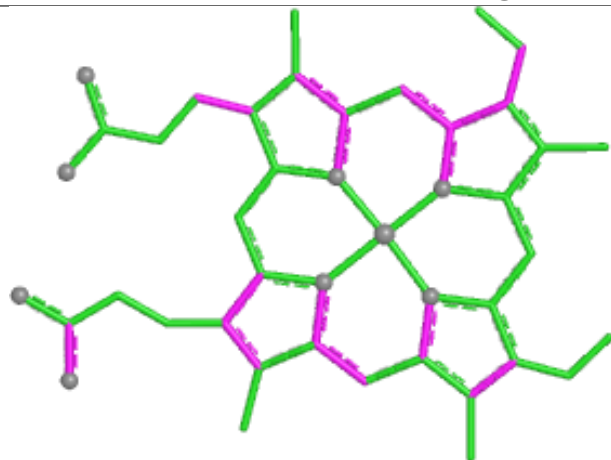
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



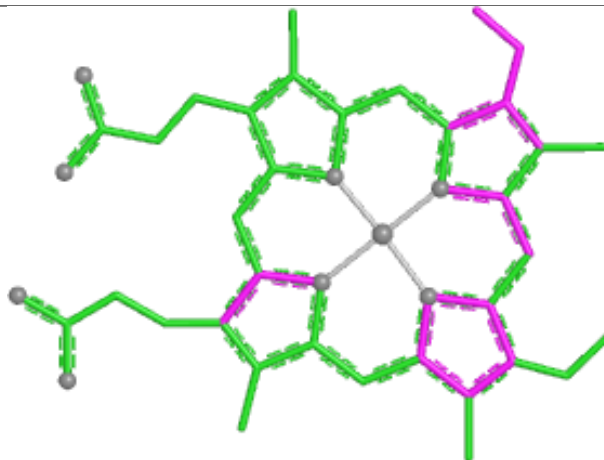




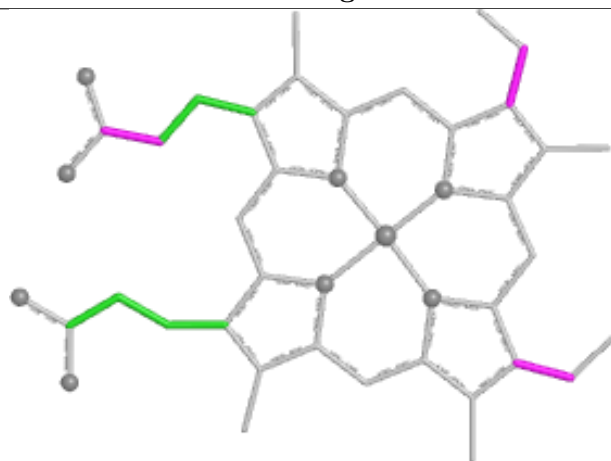
Ligand HEM AC 504



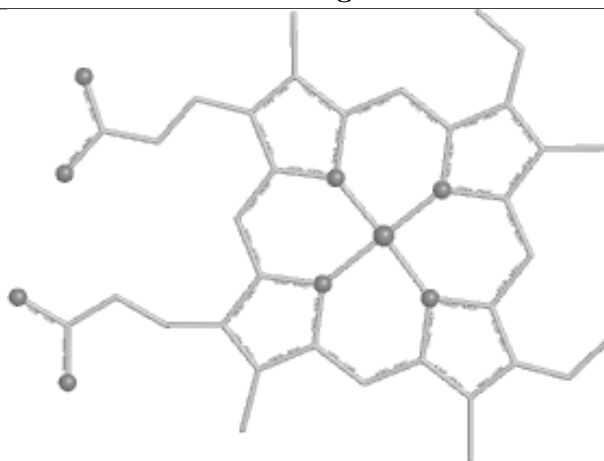
Bond lengths



Bond angles

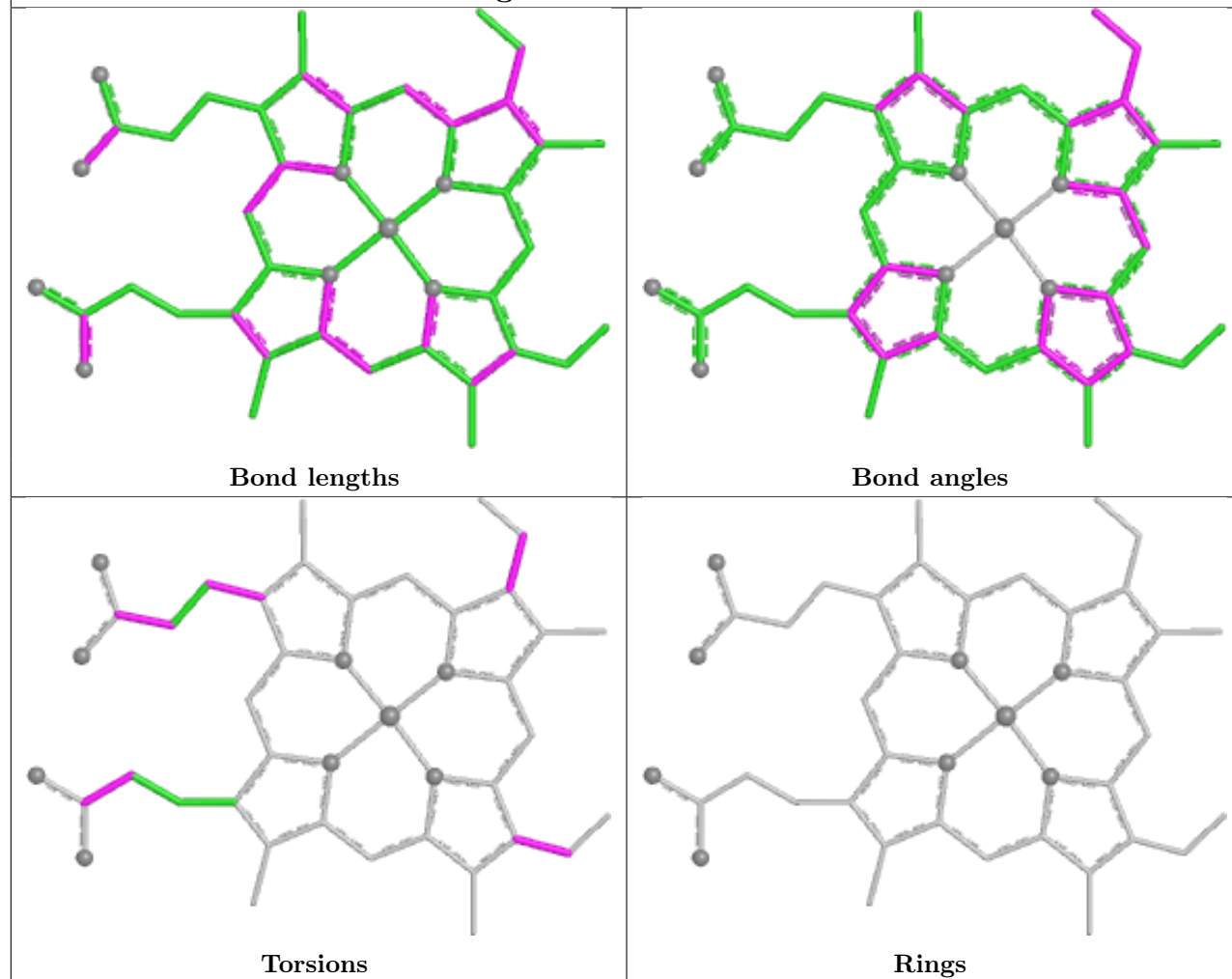


Torsions

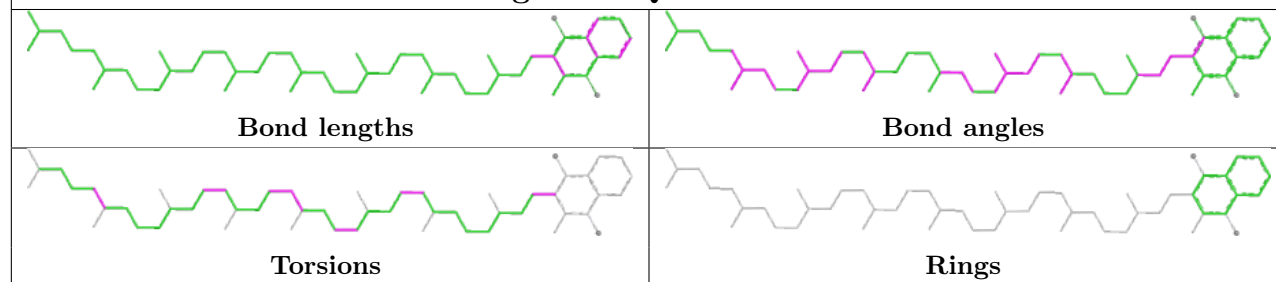


Rings

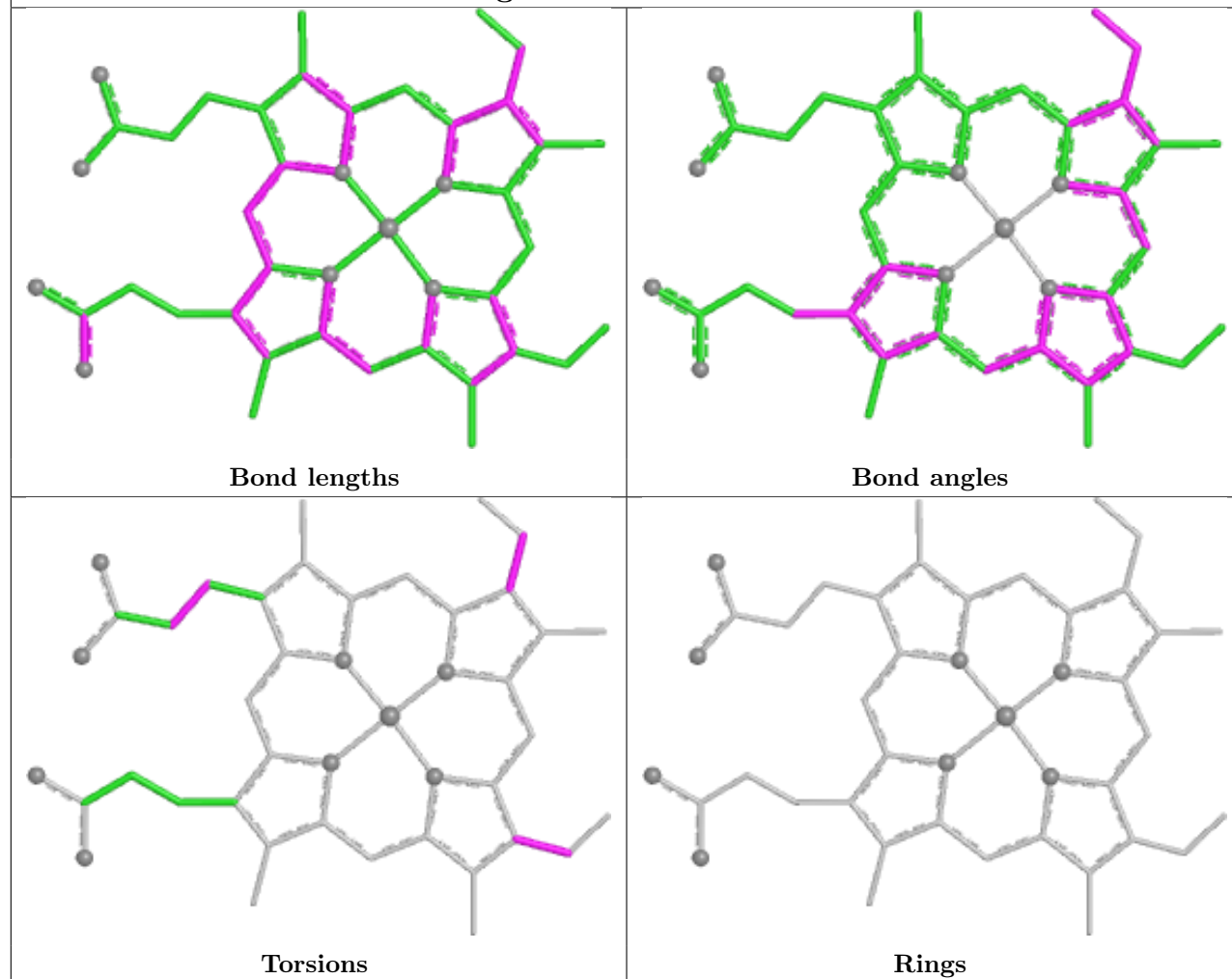
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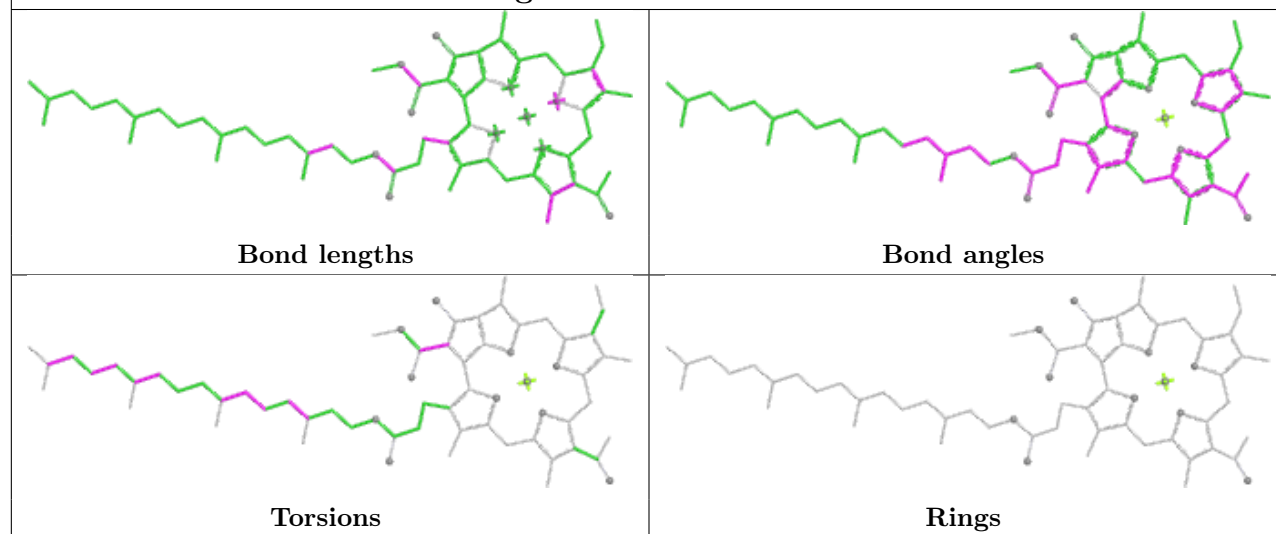
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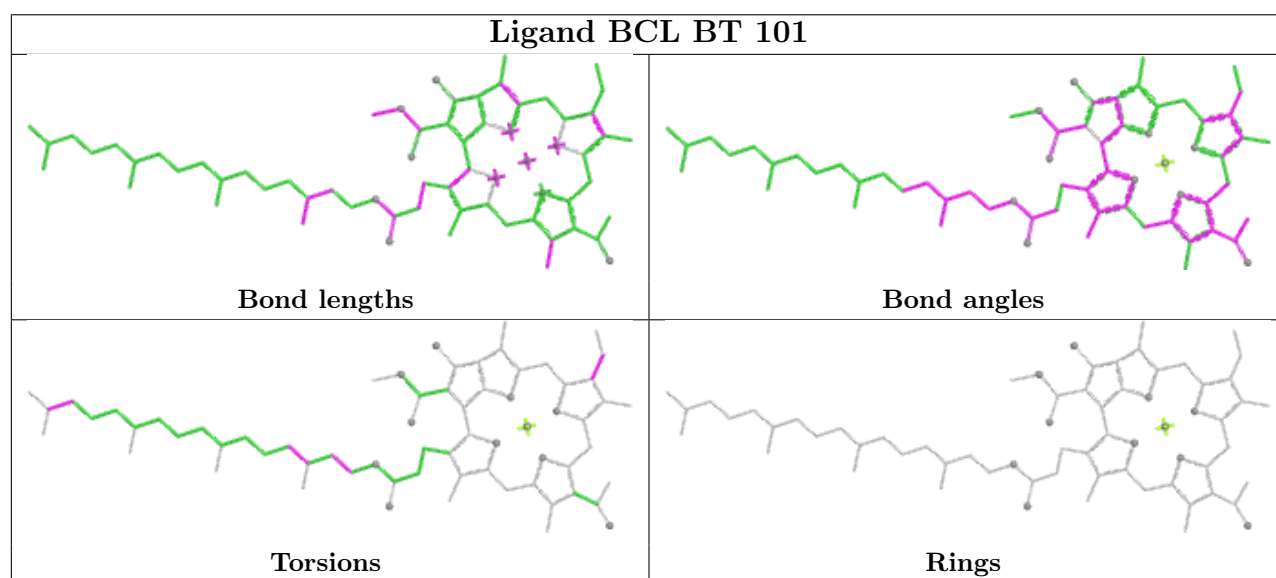
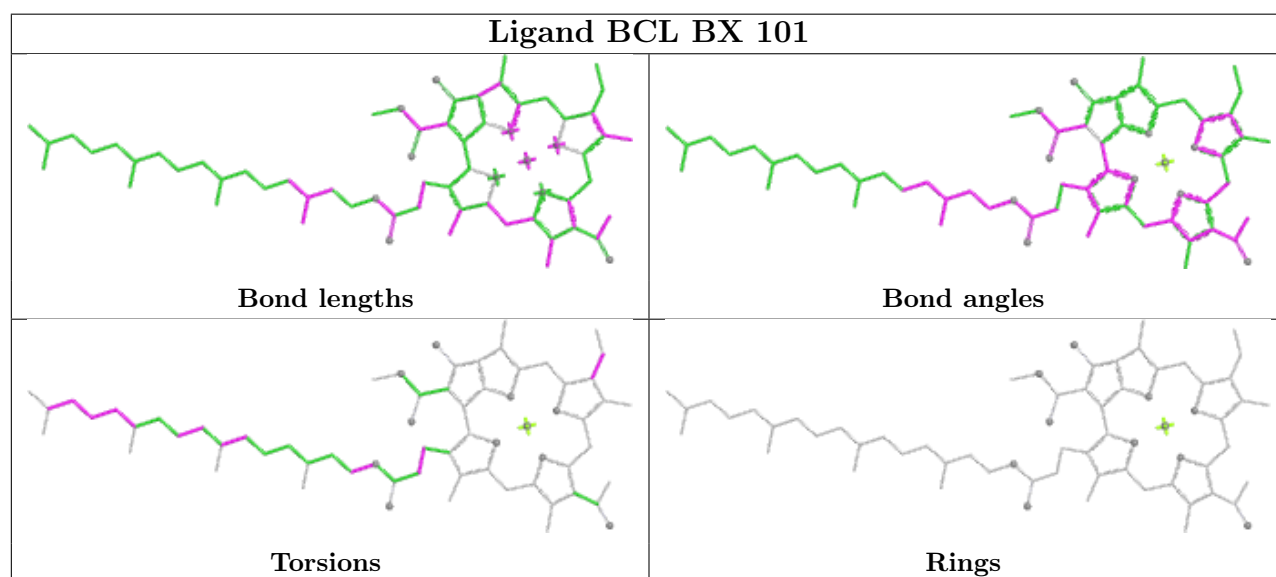
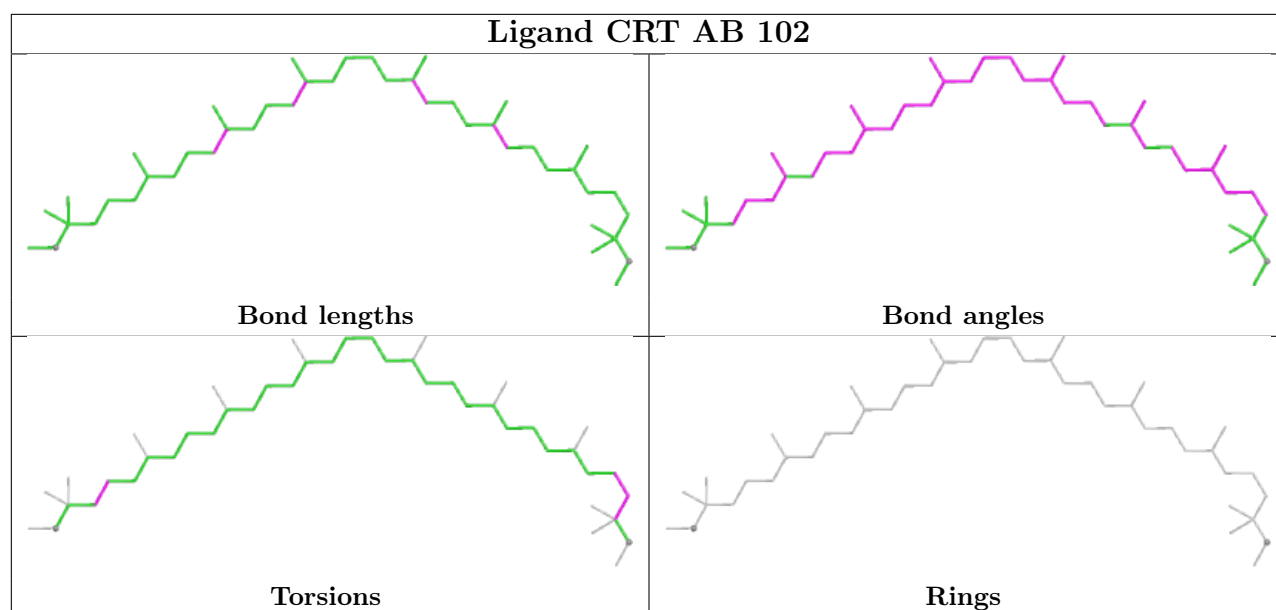


Ligand HEM BC 502

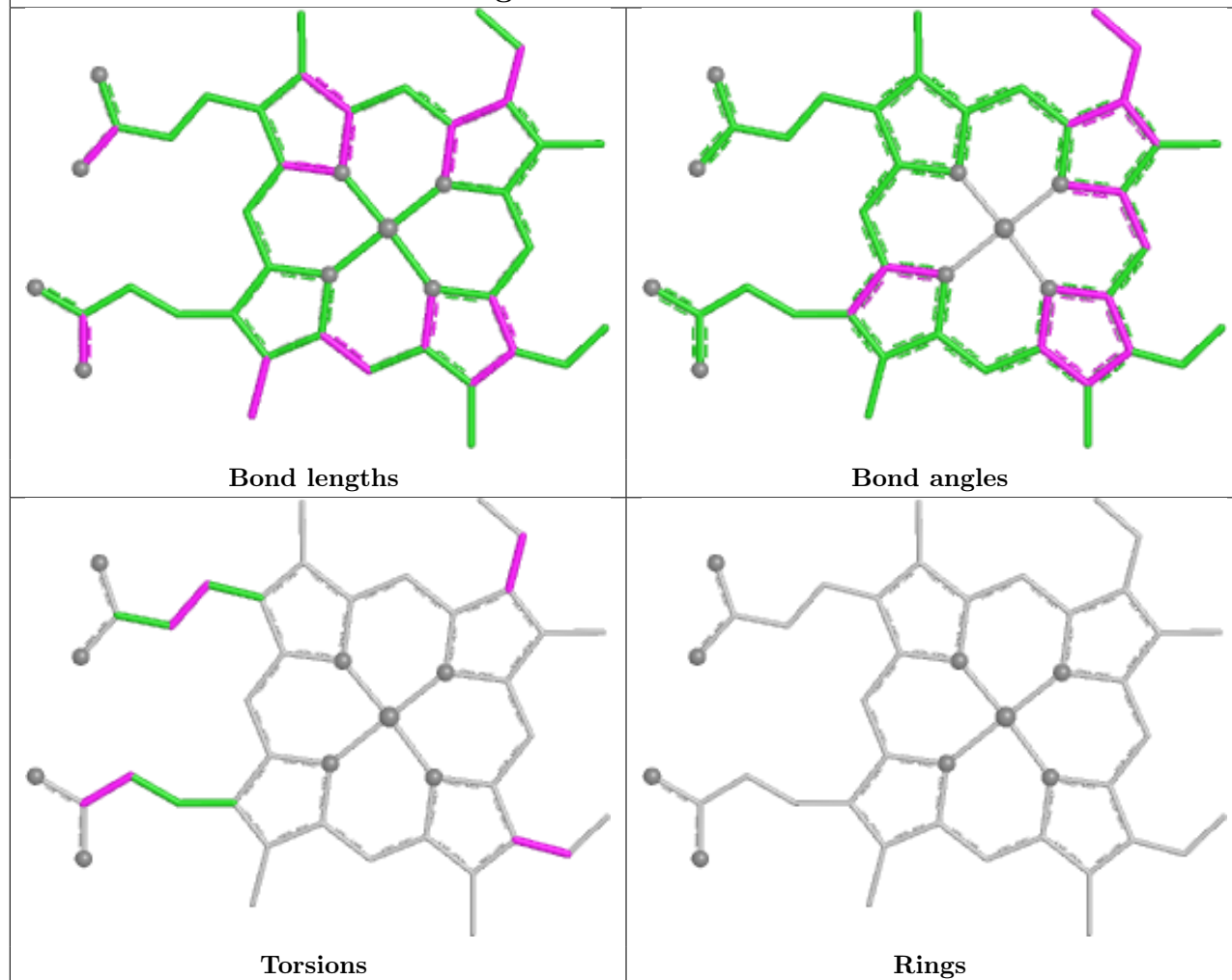


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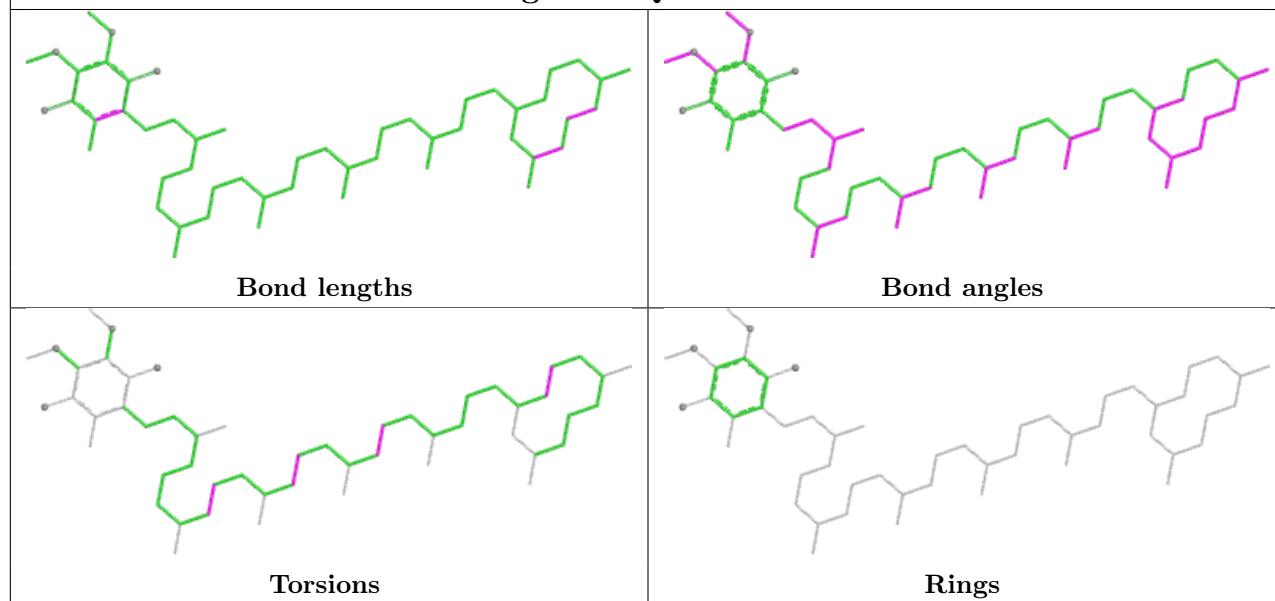




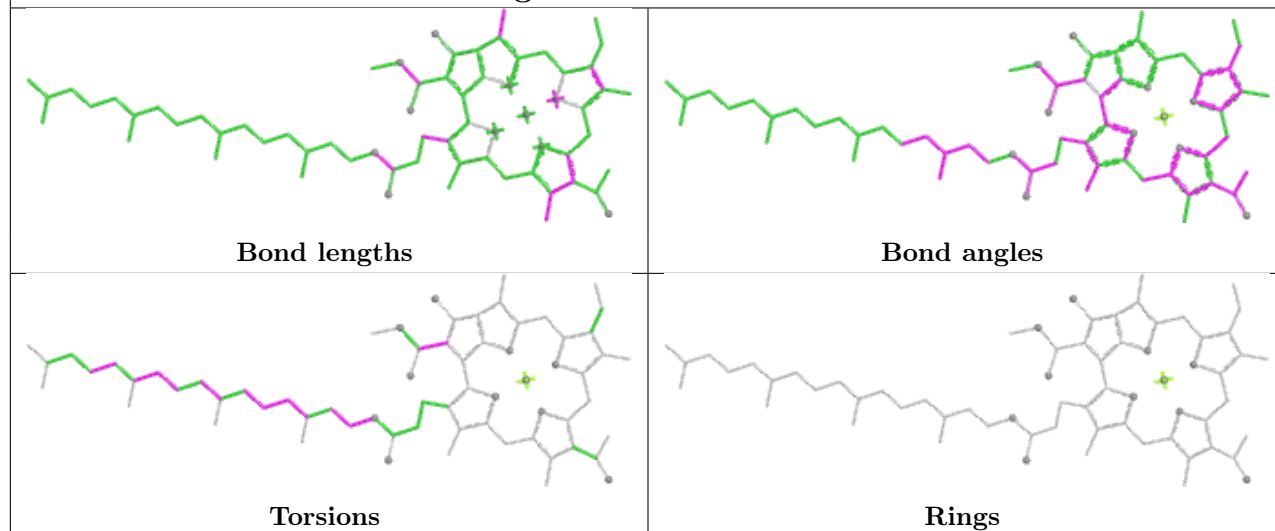
Ligand HEM AC 501



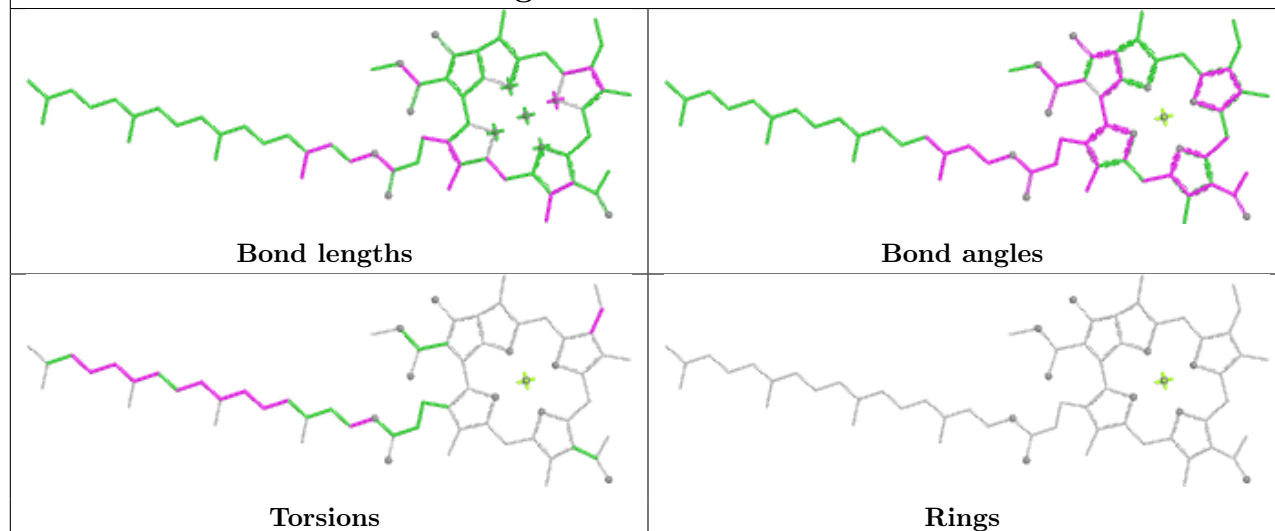
Ligand UQ8 BL 304



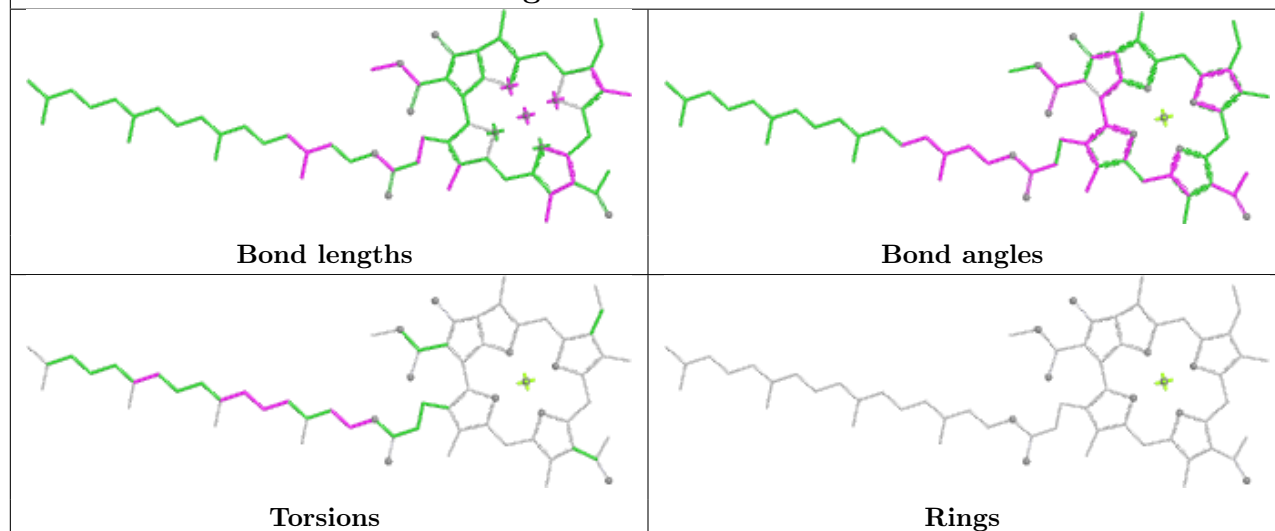
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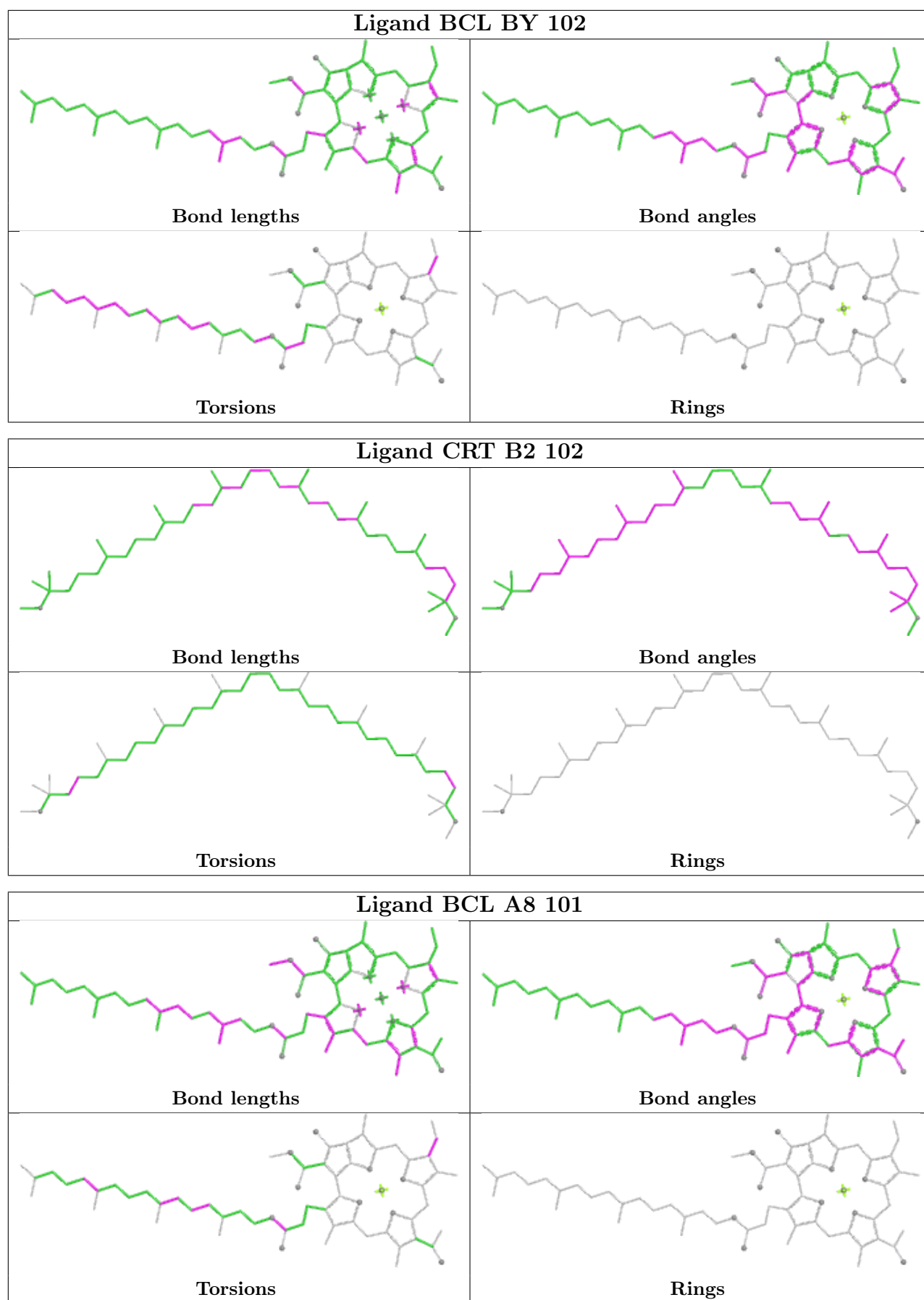


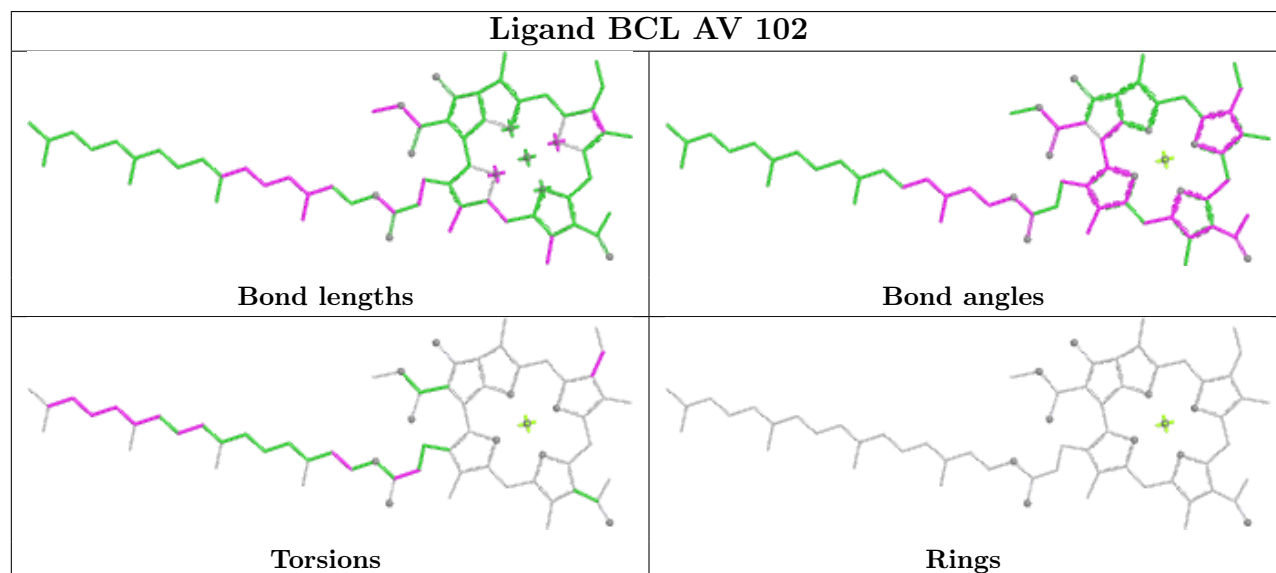
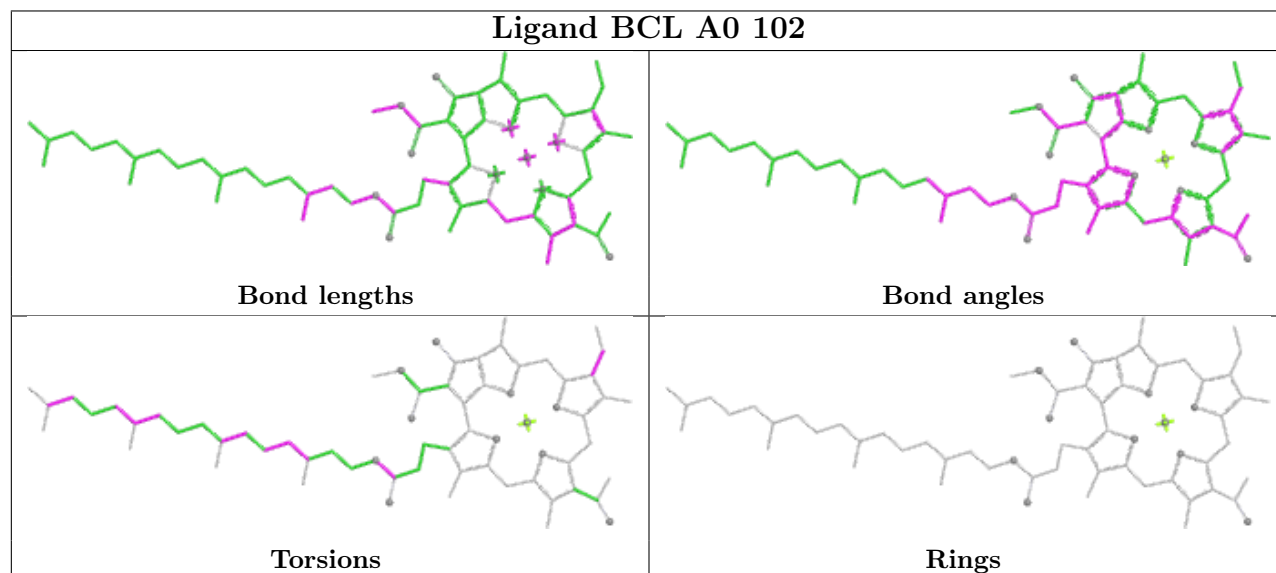
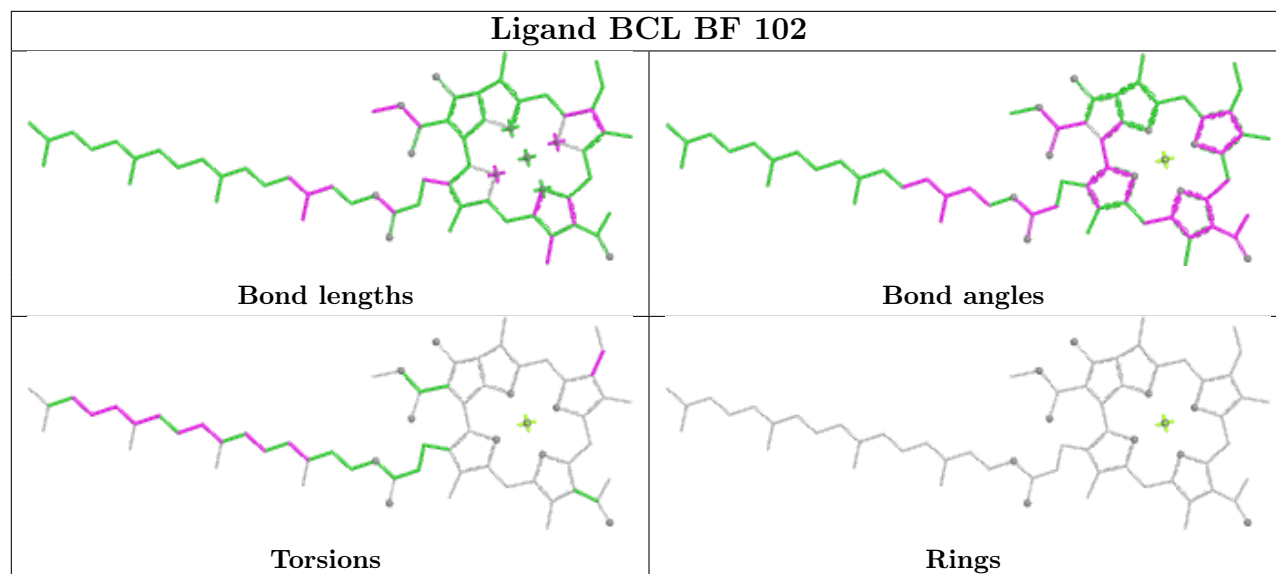
Ligand BCL AW 101

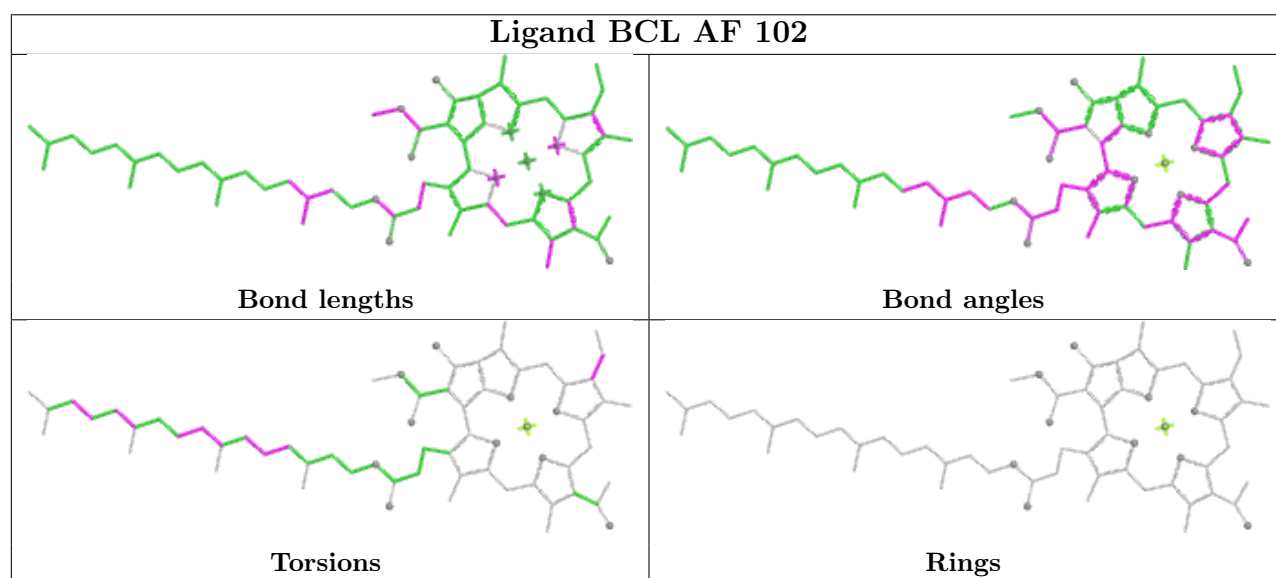
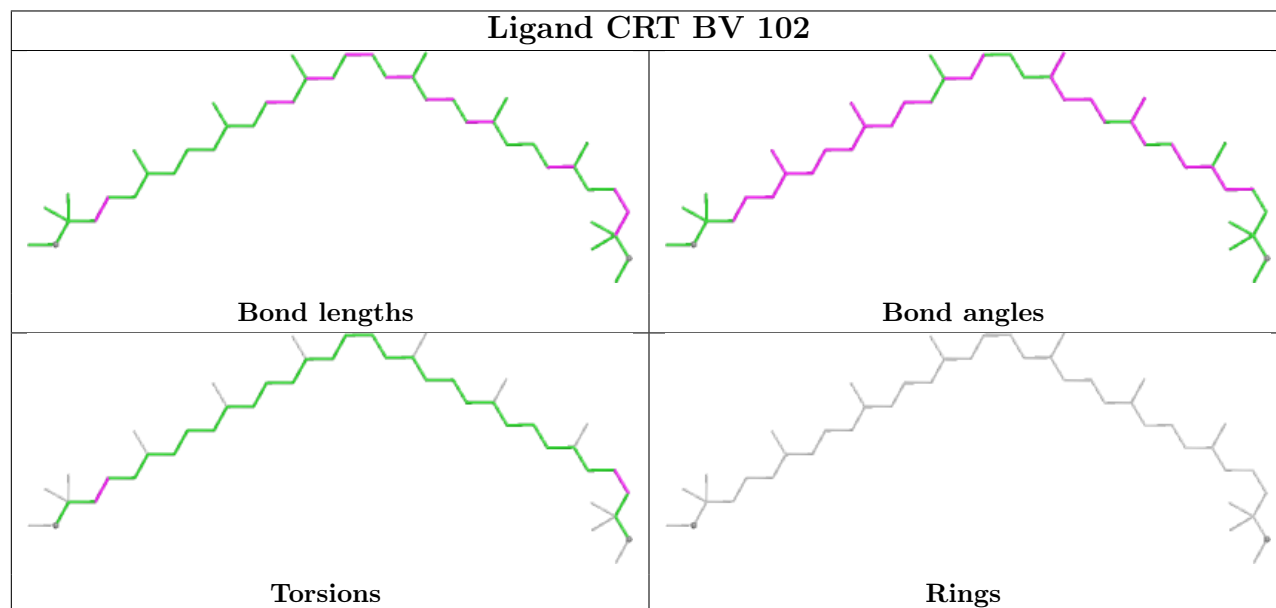
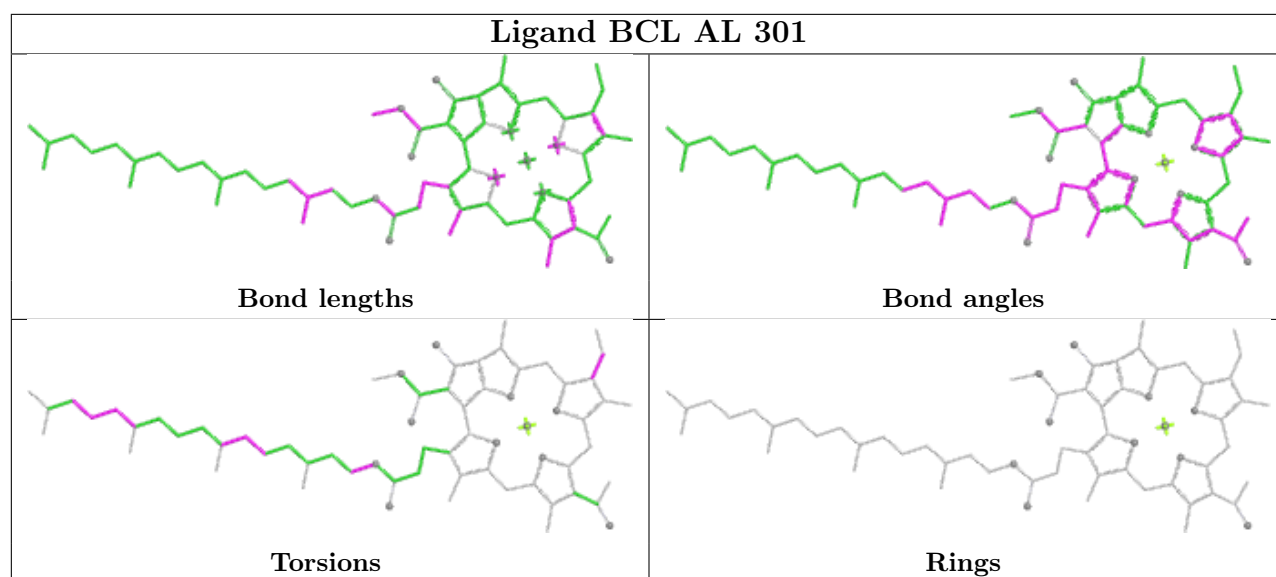


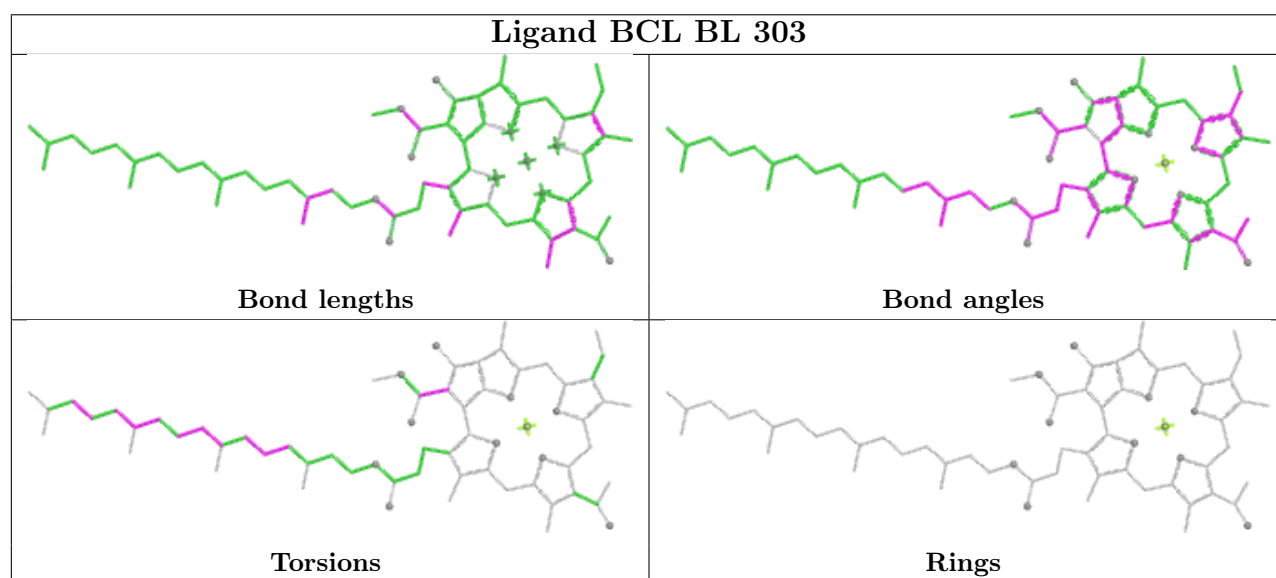
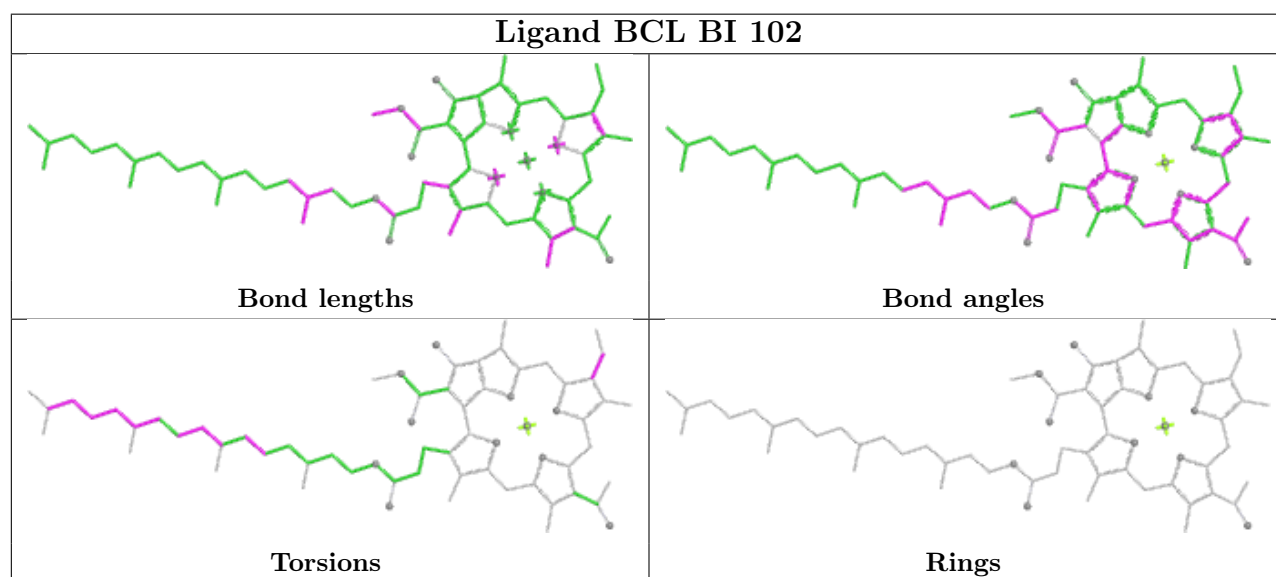
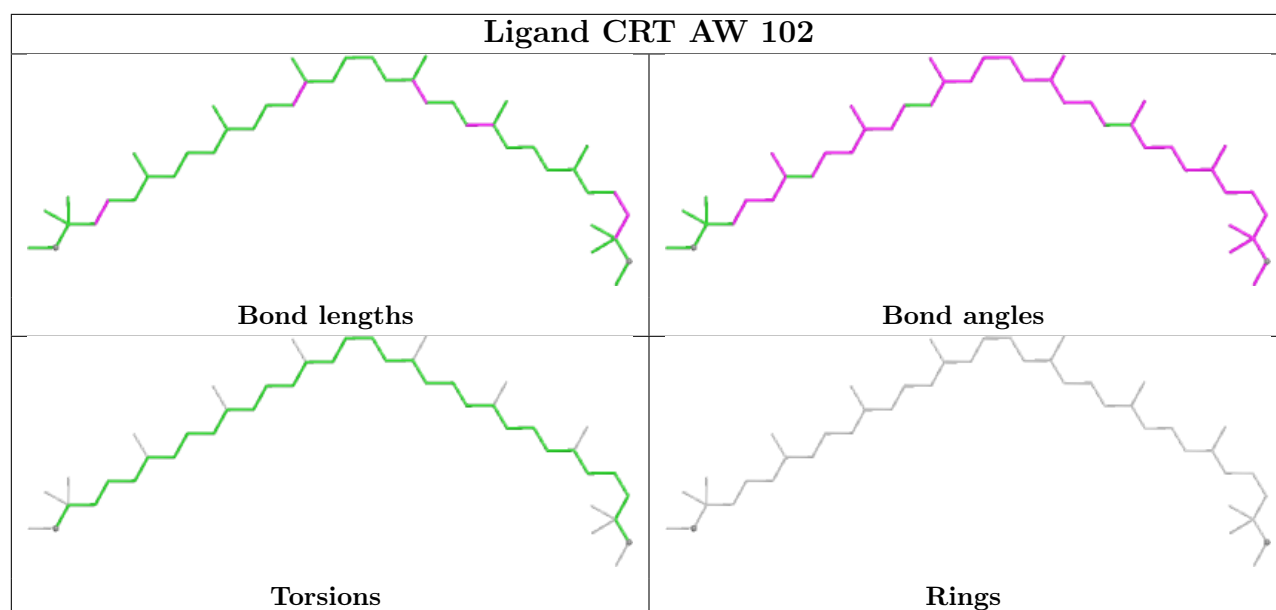
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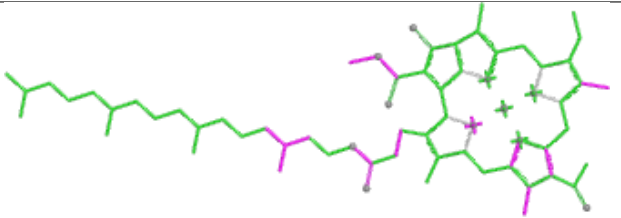
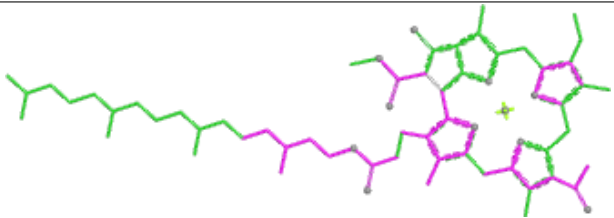
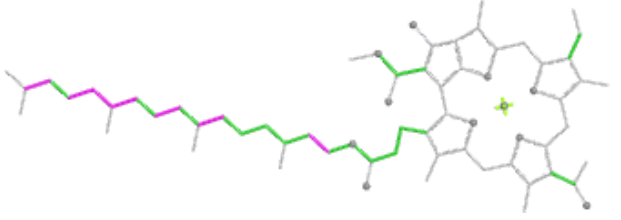
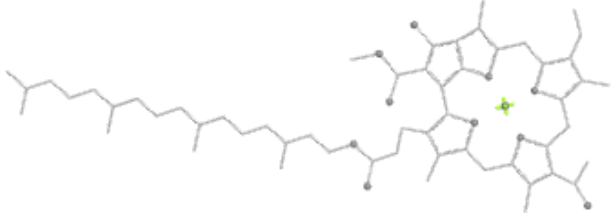


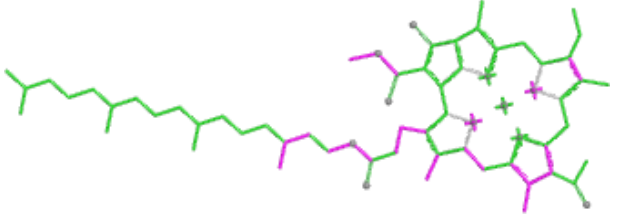
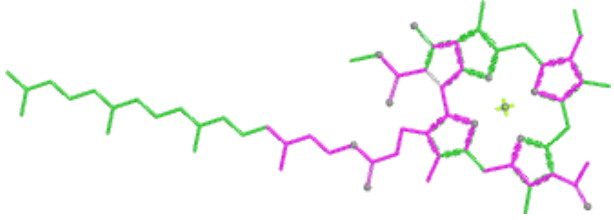
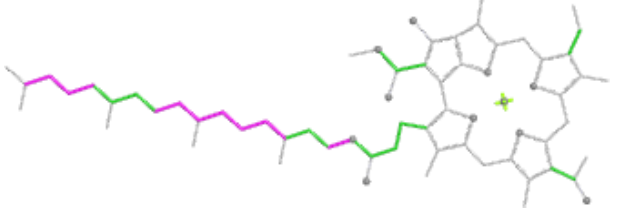
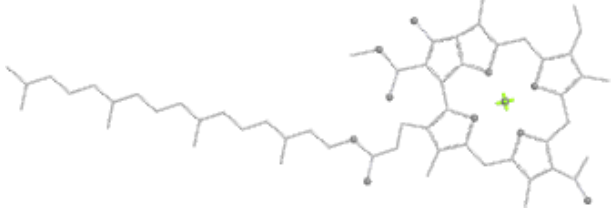


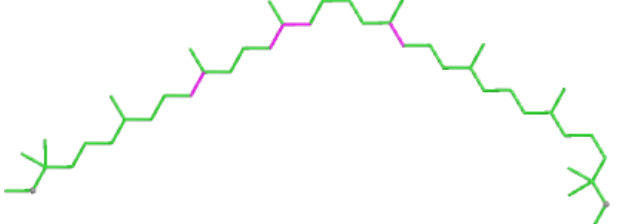
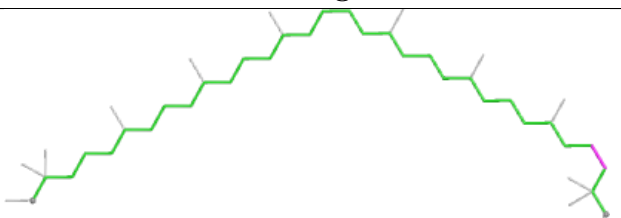
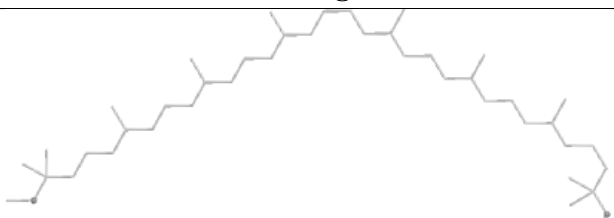


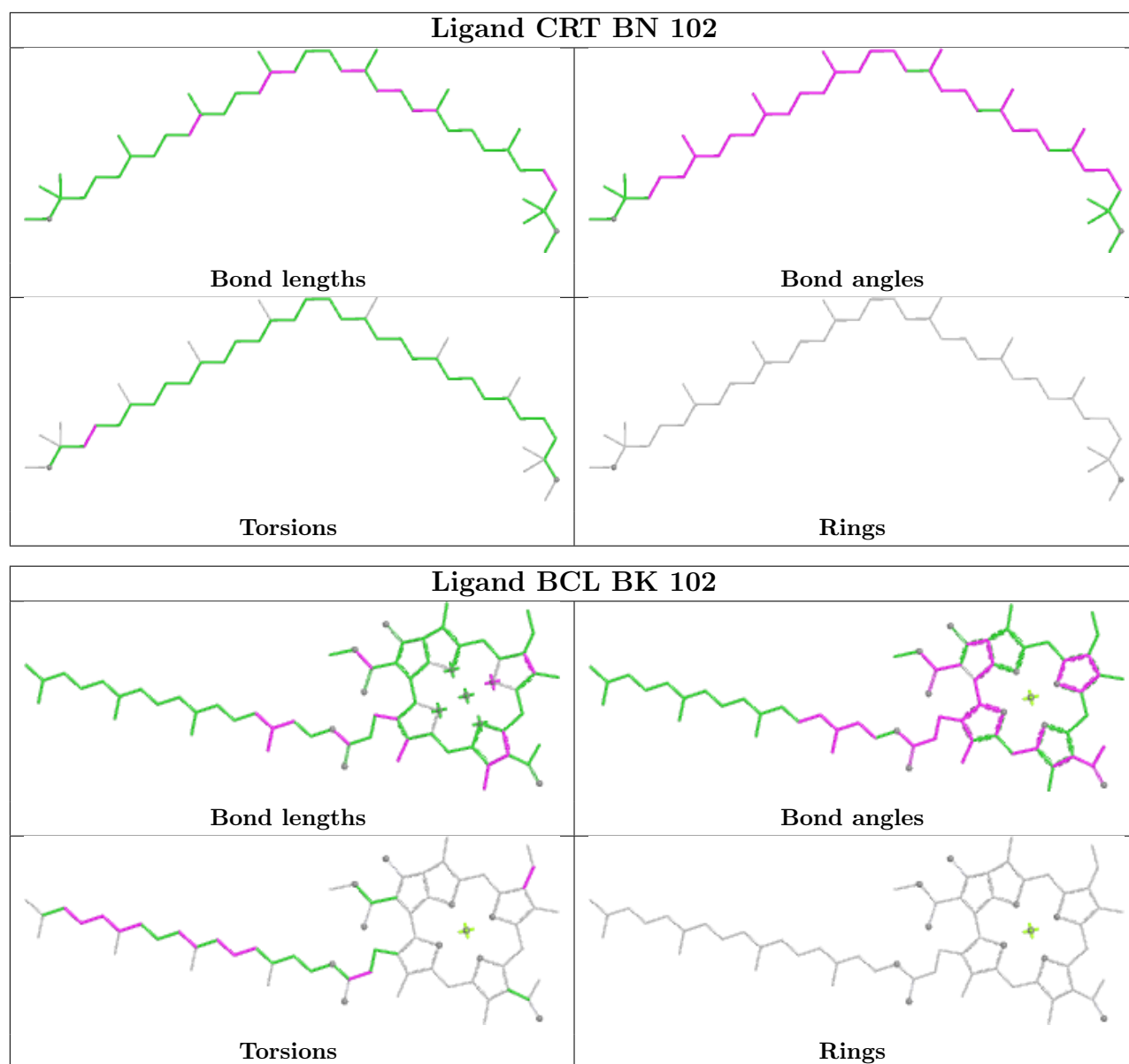


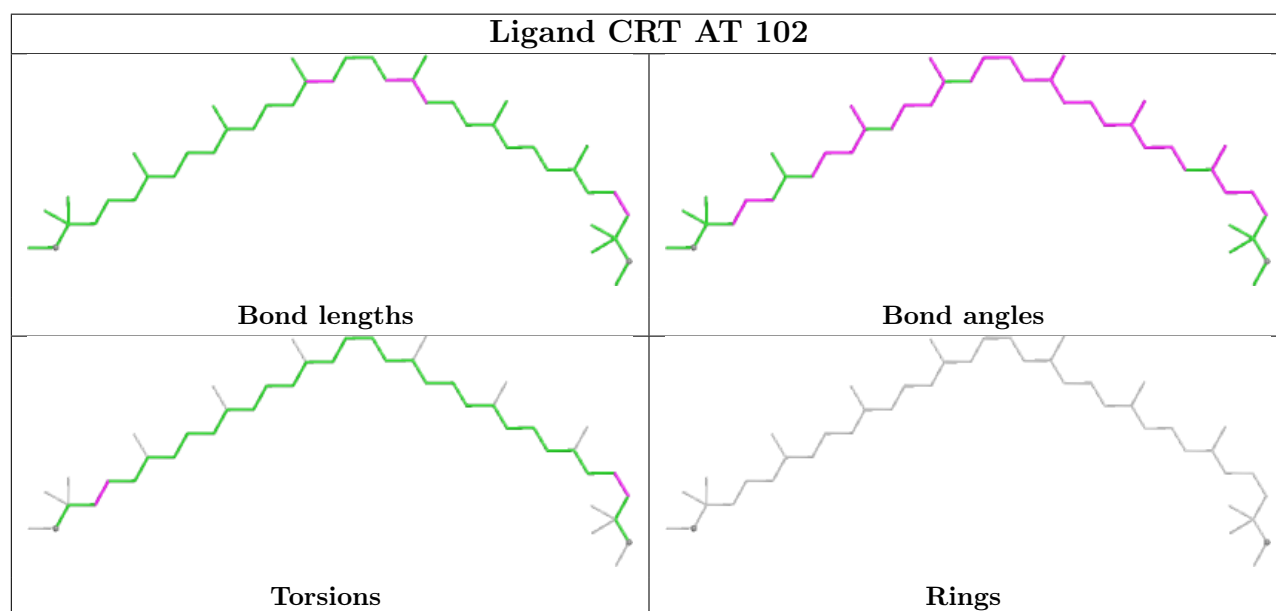
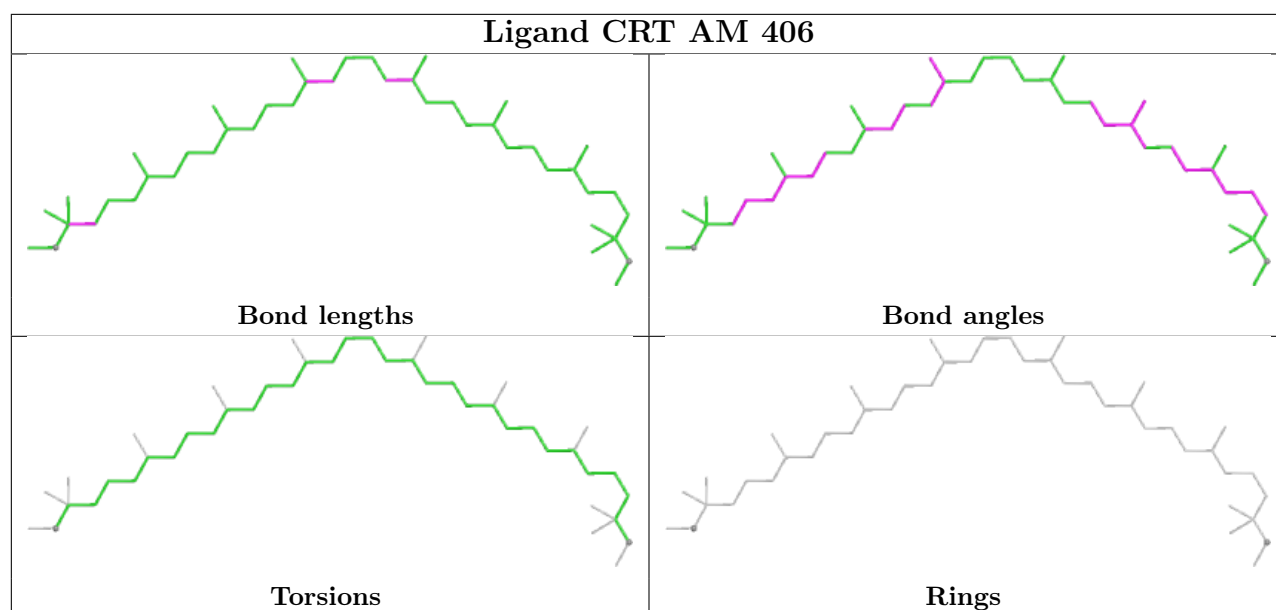


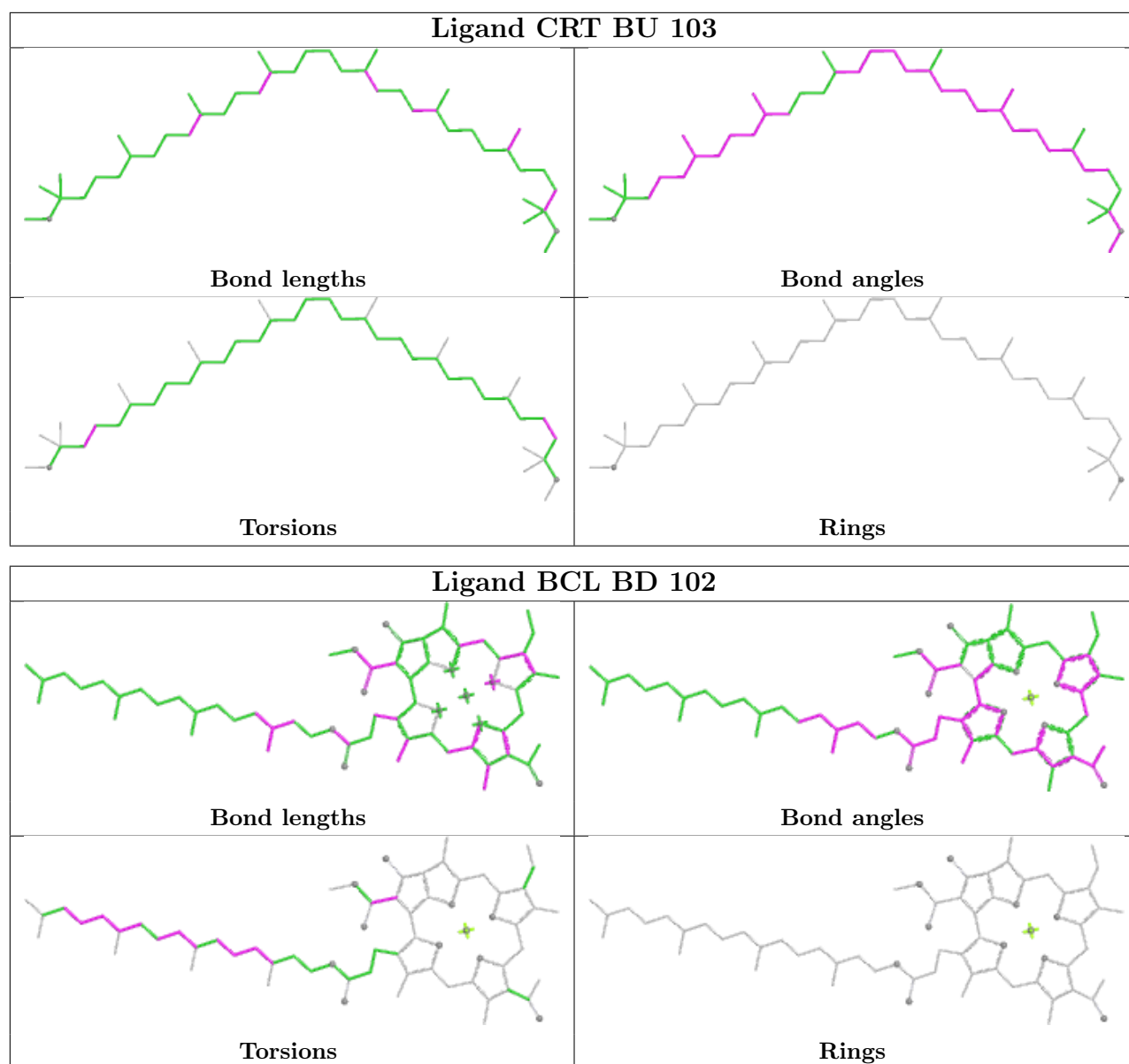
Ligand BCL BG 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

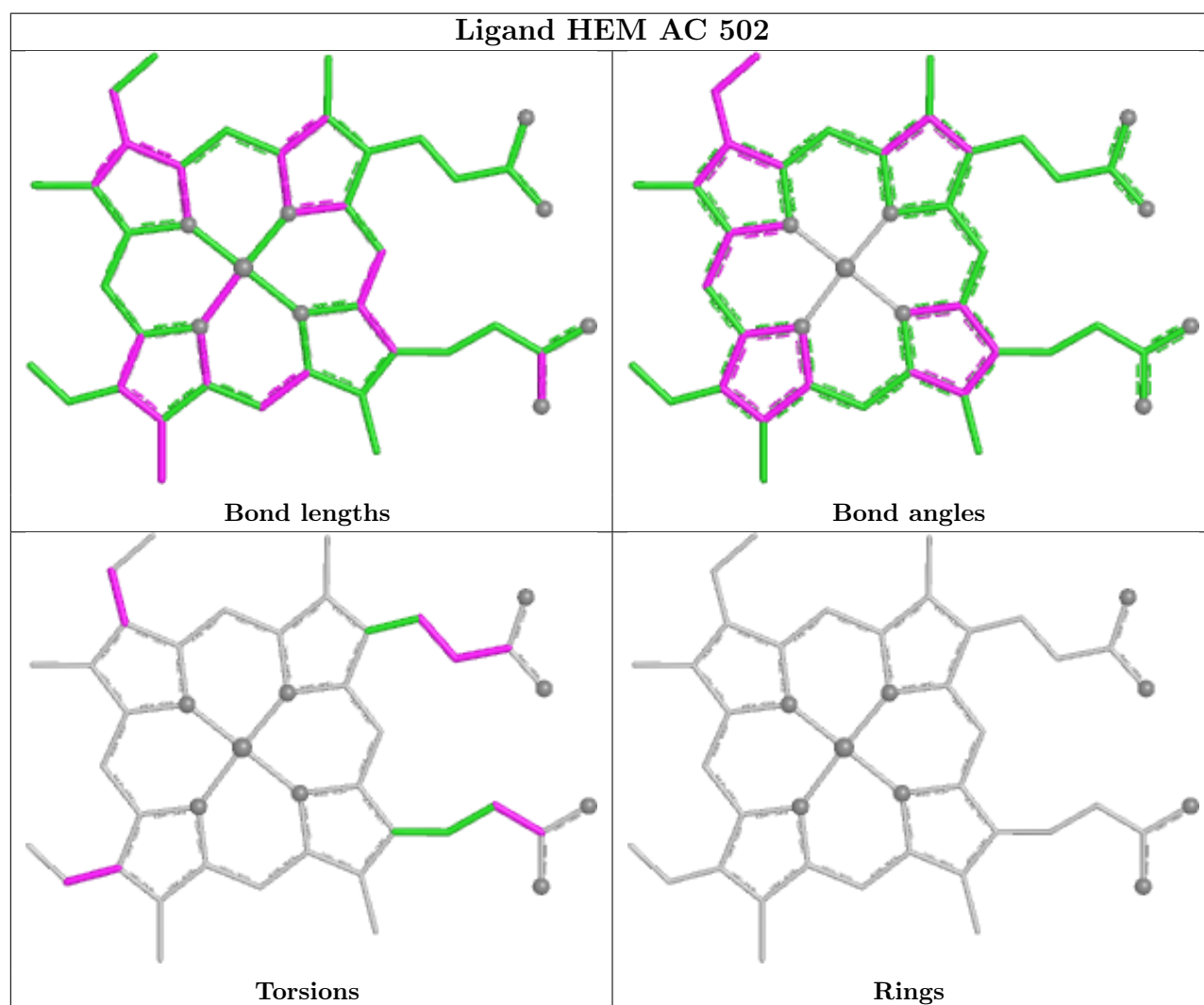
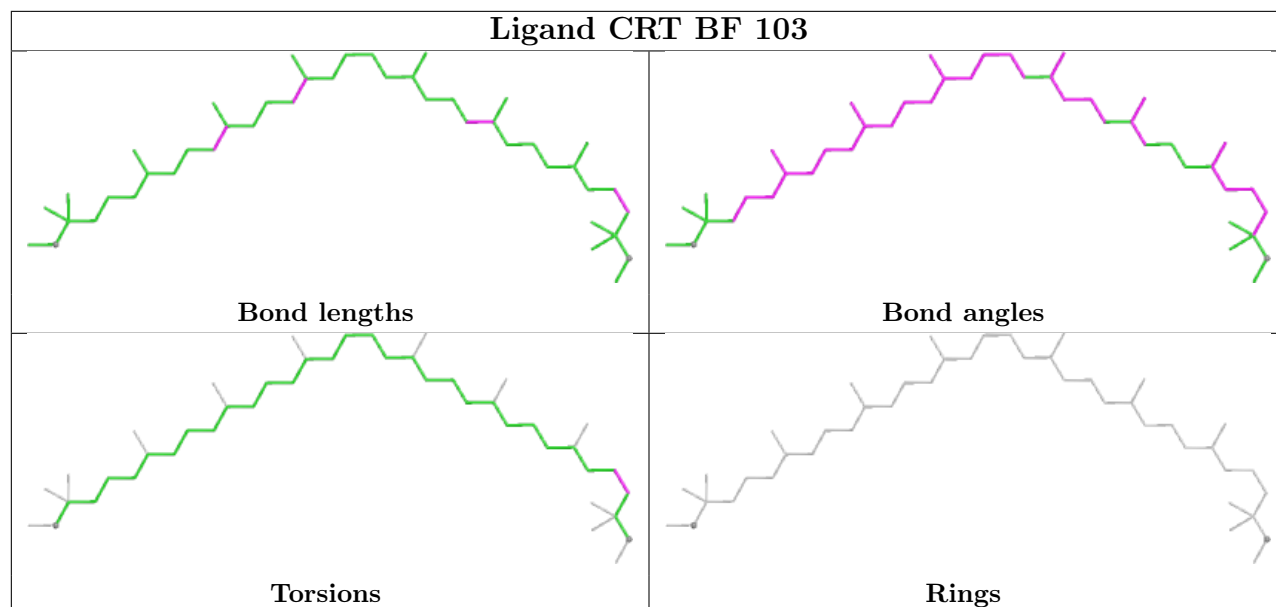
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Bond lengths	Bond angles
	
Torsions	Rings

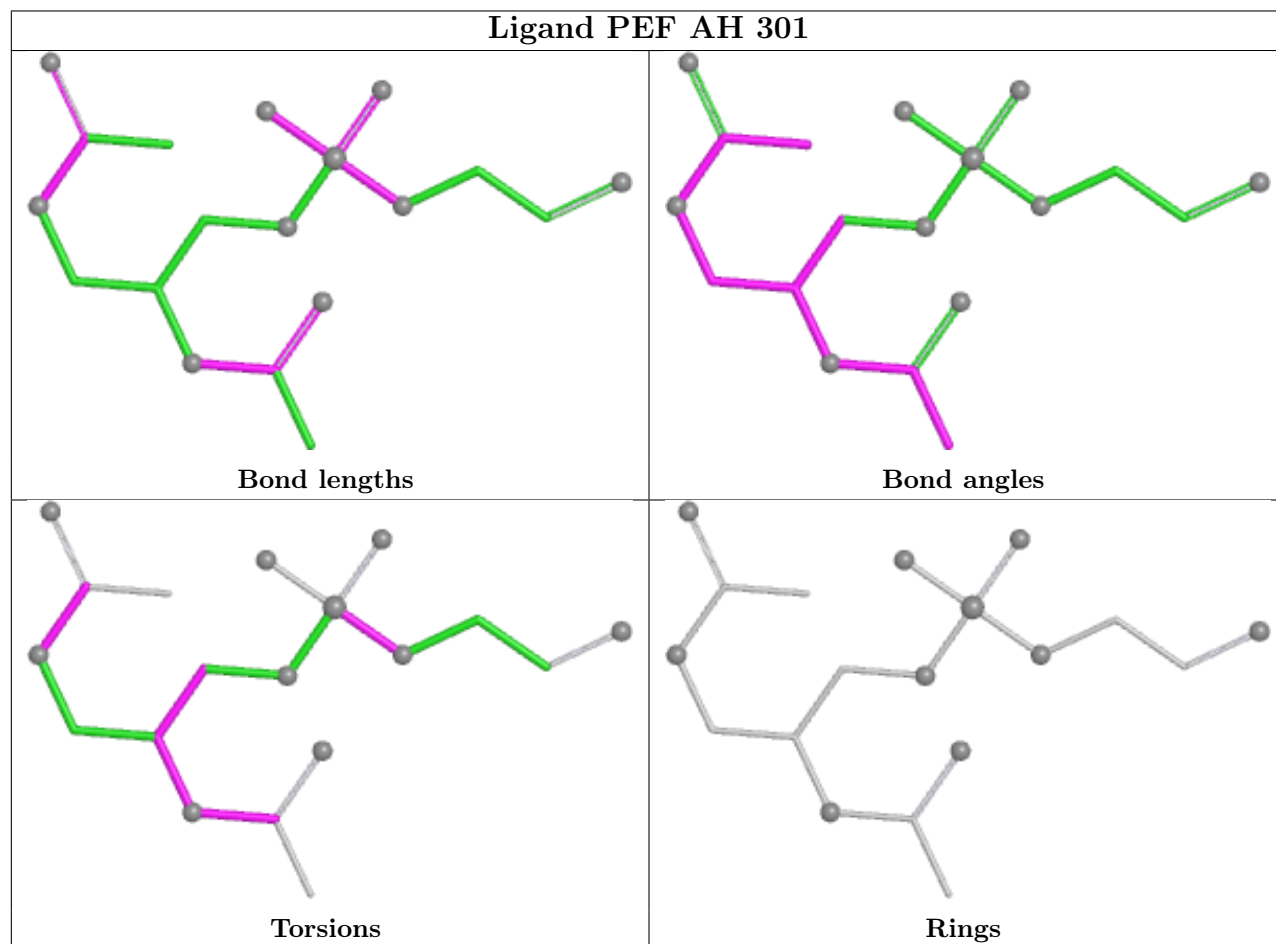
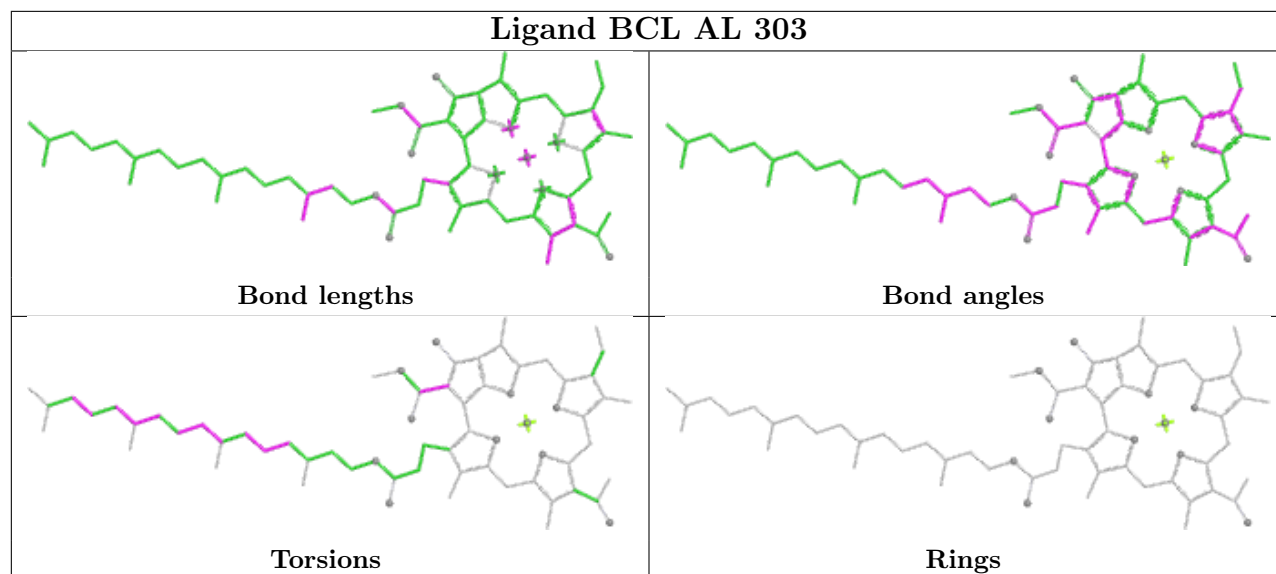
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Bond lengths	Bond angles
	
Torsions	Rings

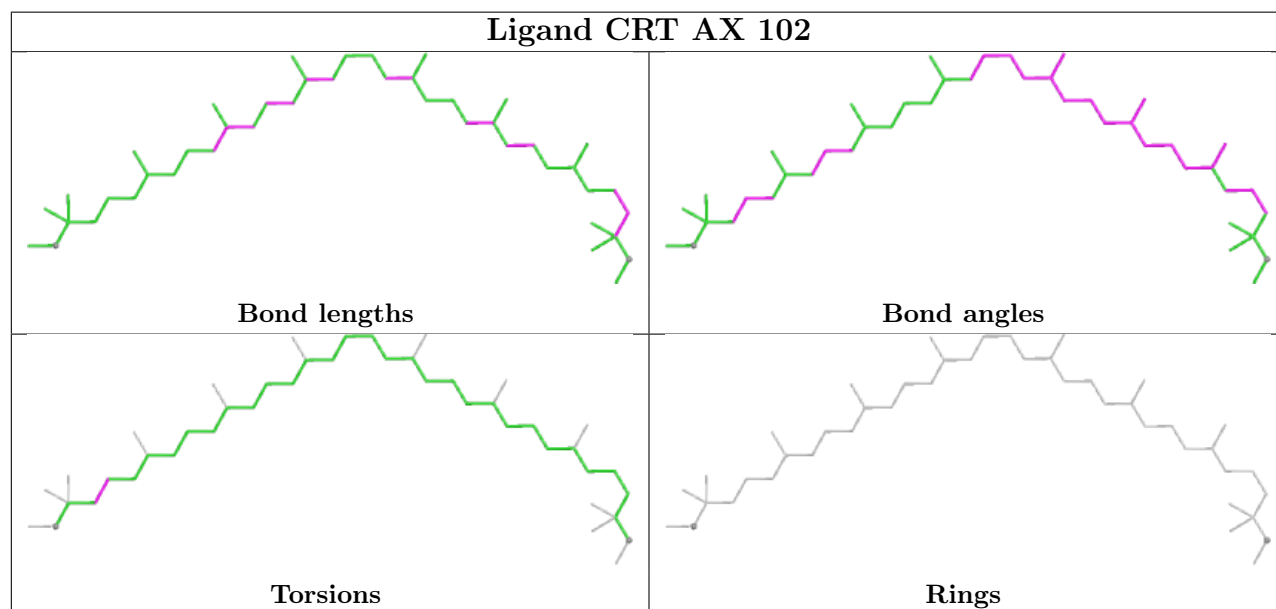
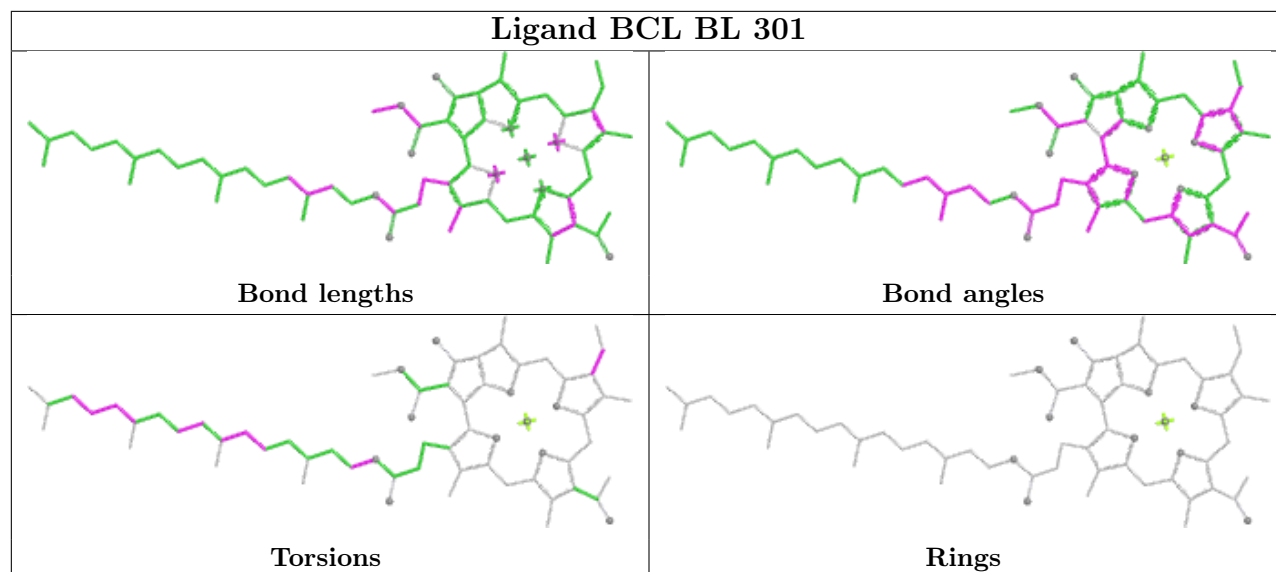


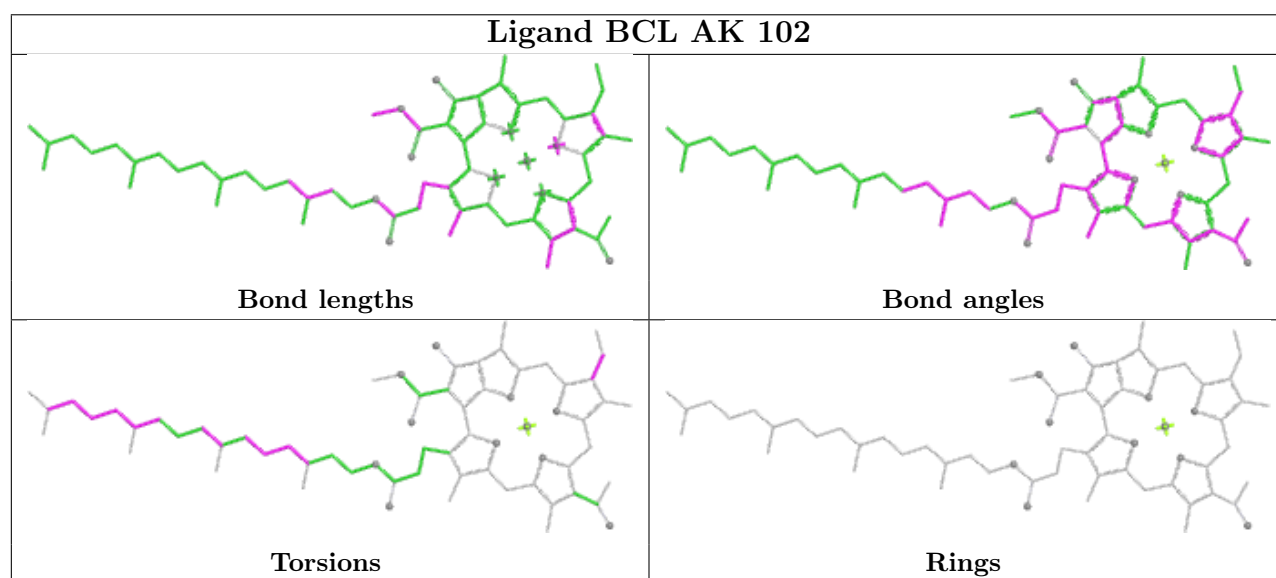
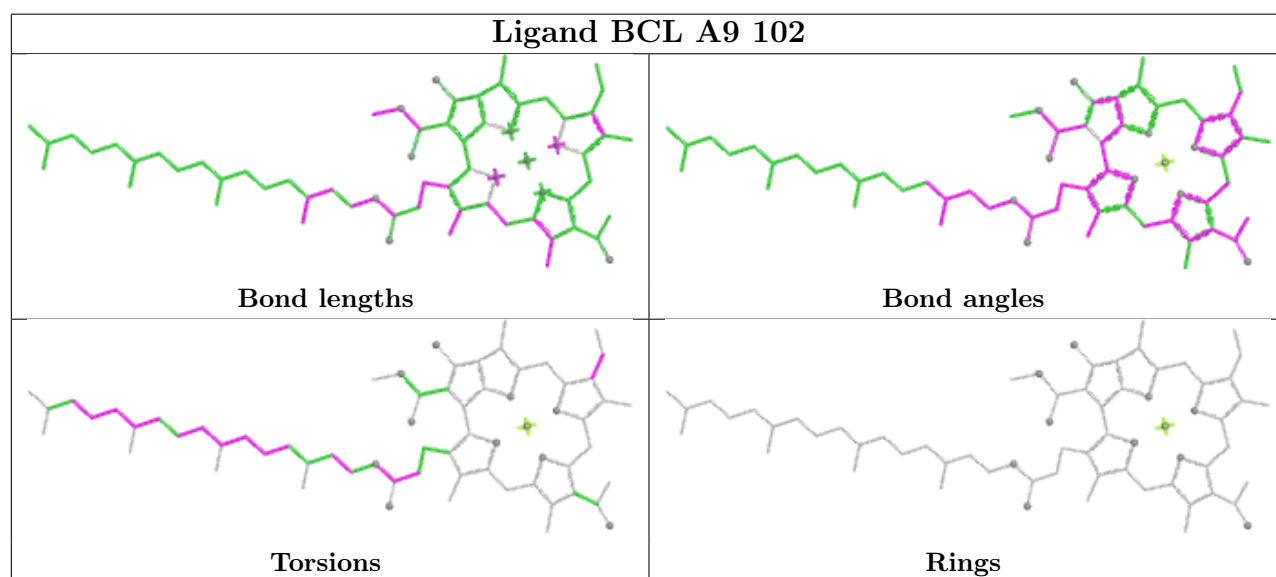
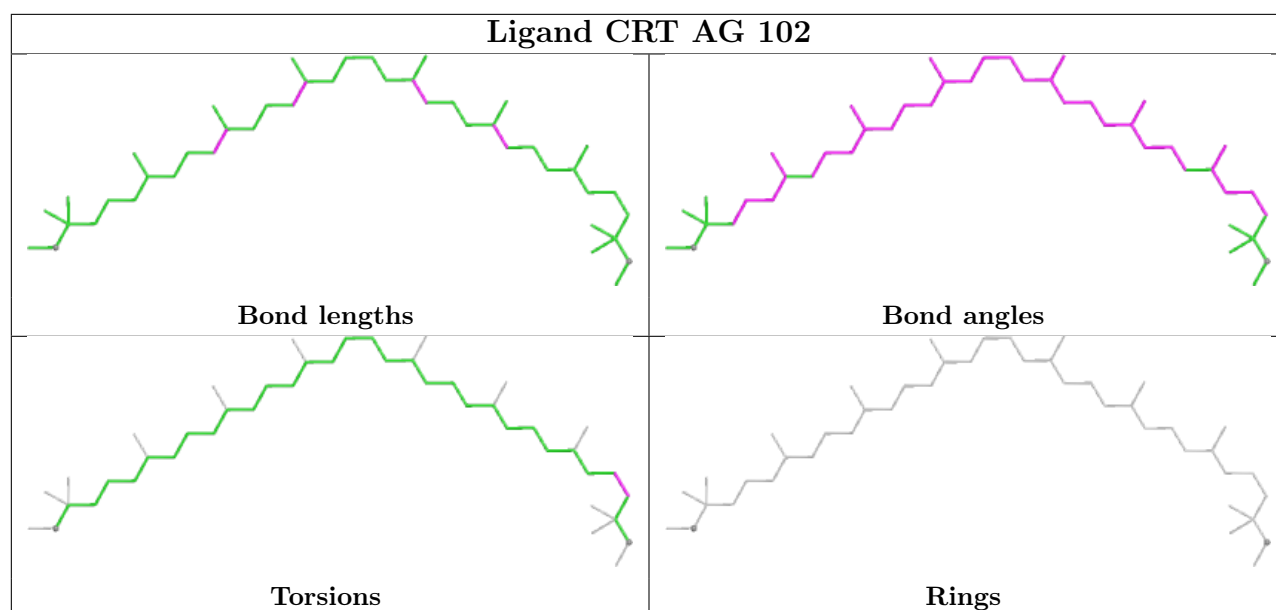




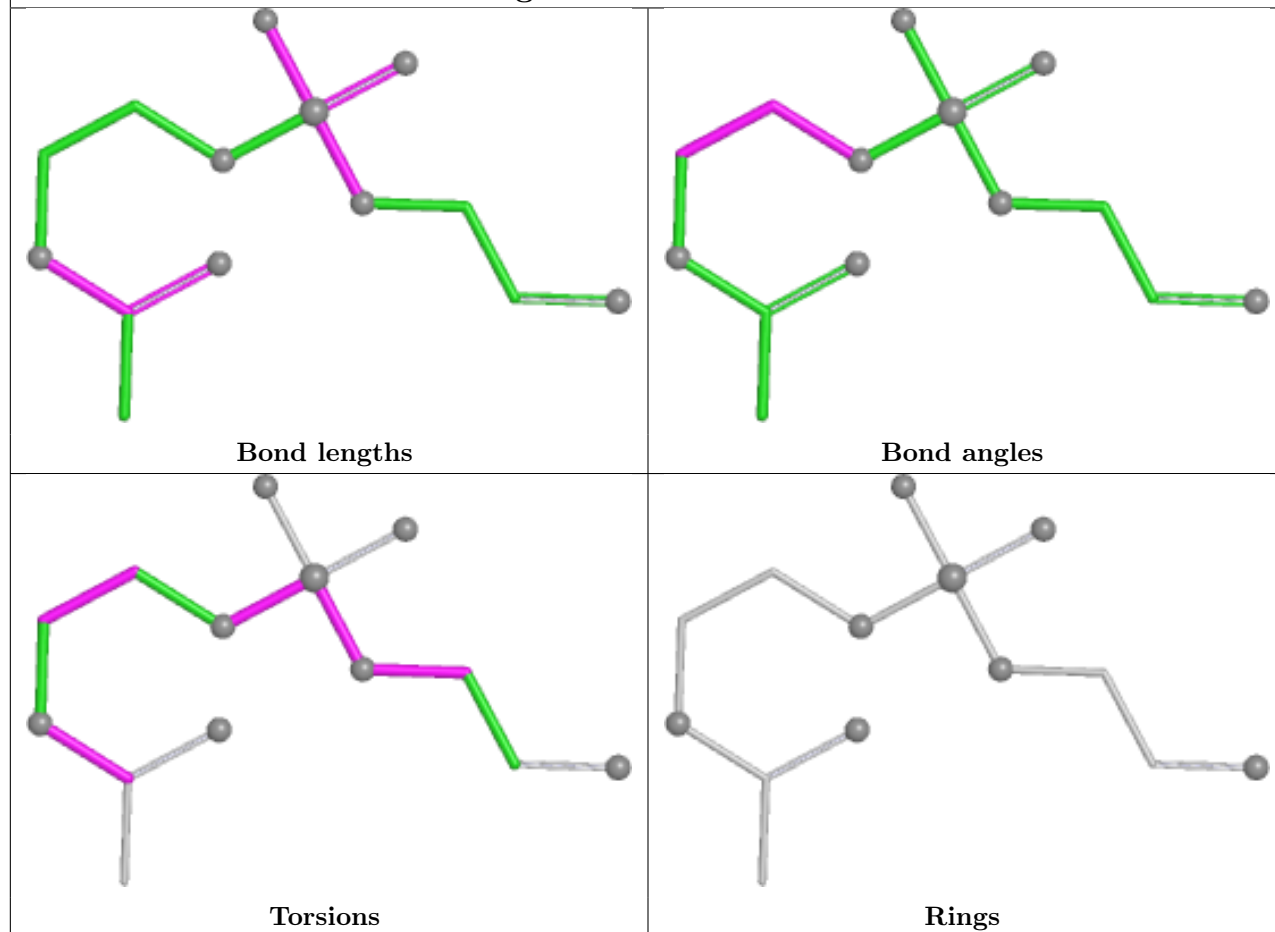




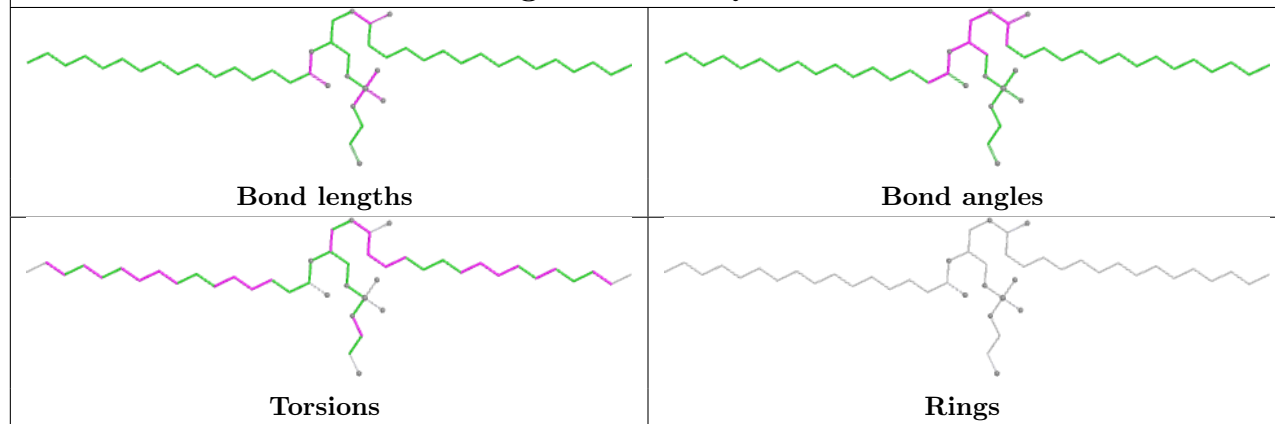


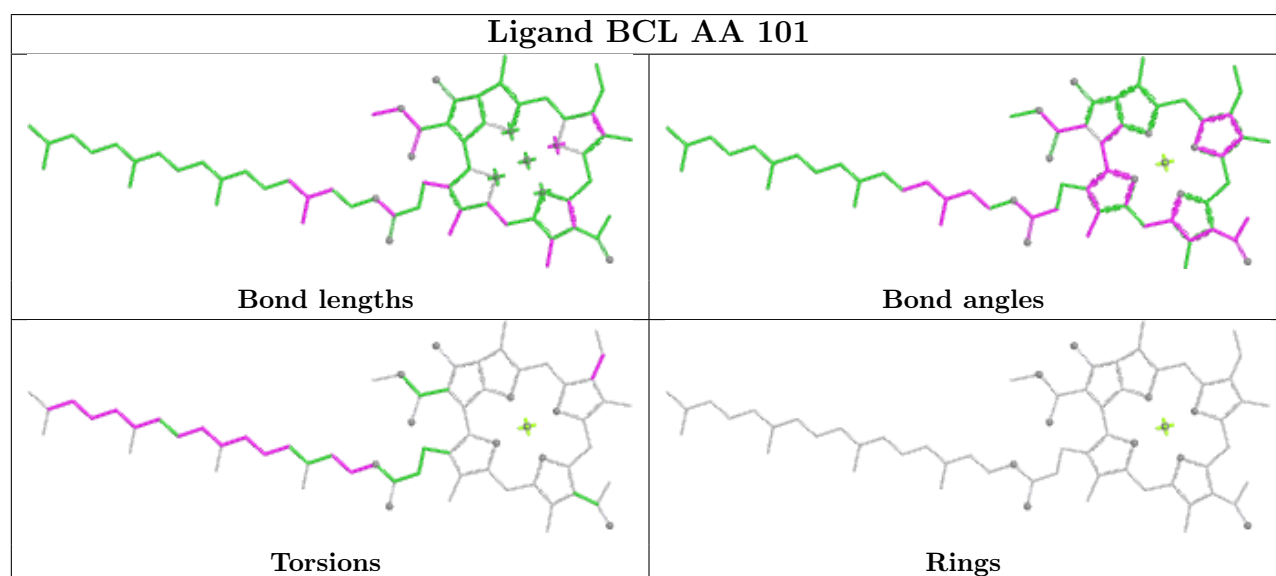
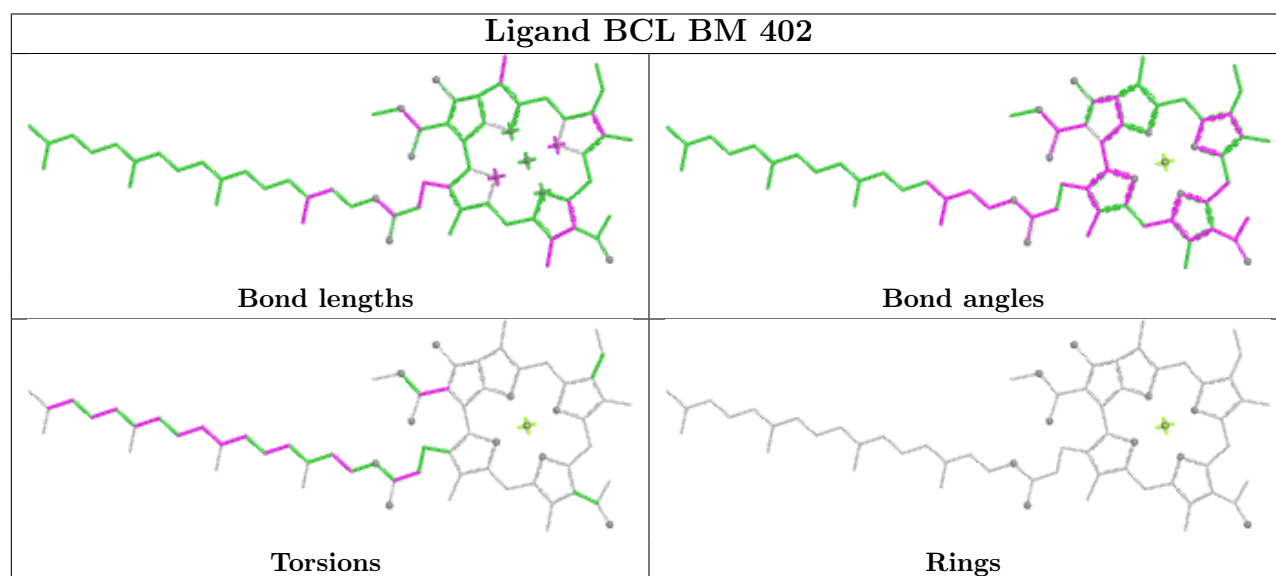
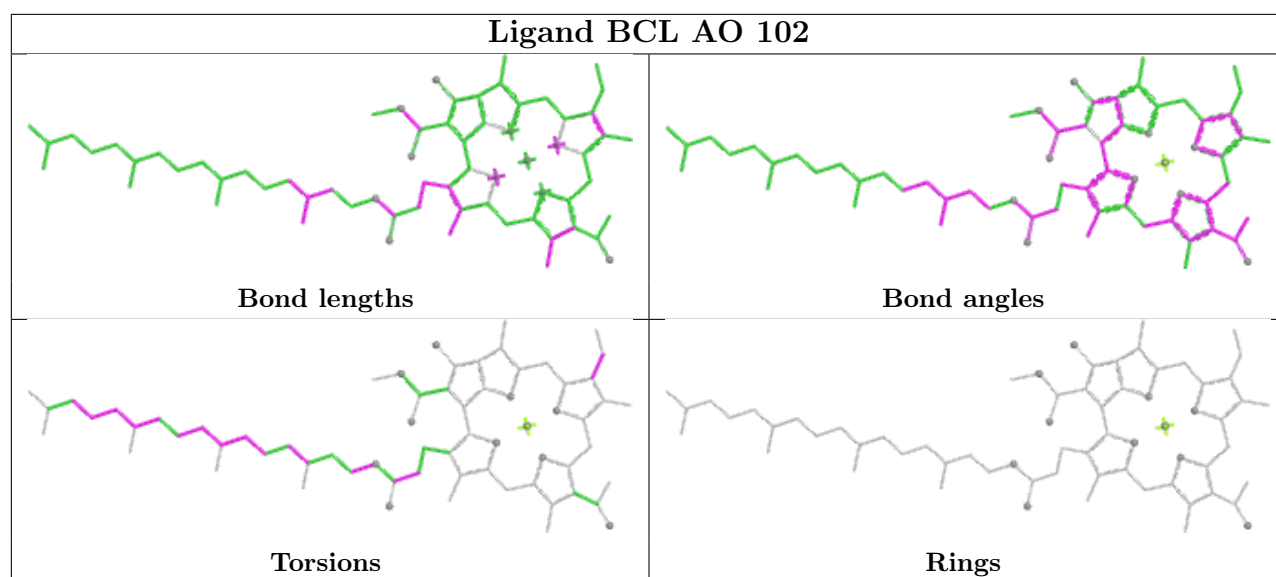


Ligand PEF AM 408

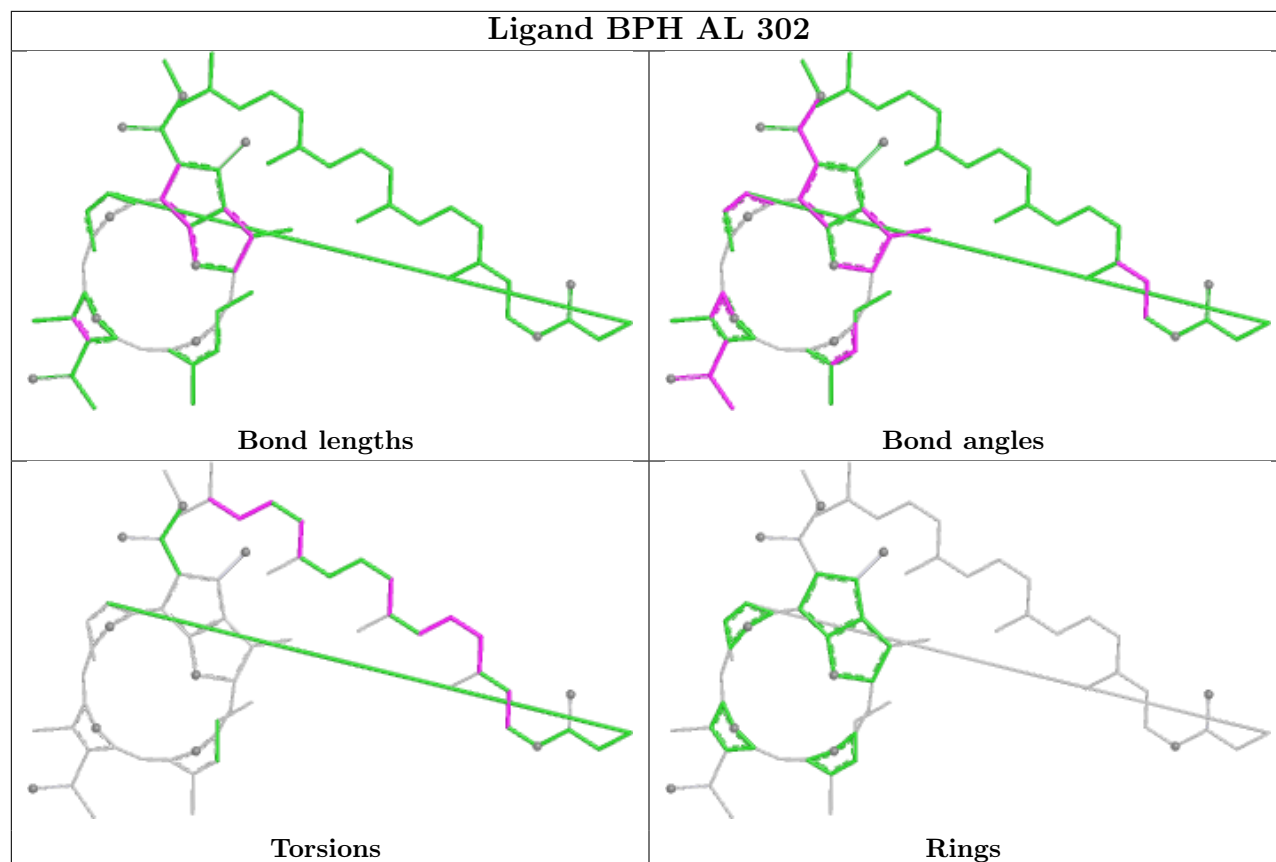


Ligand PEF BQ 101

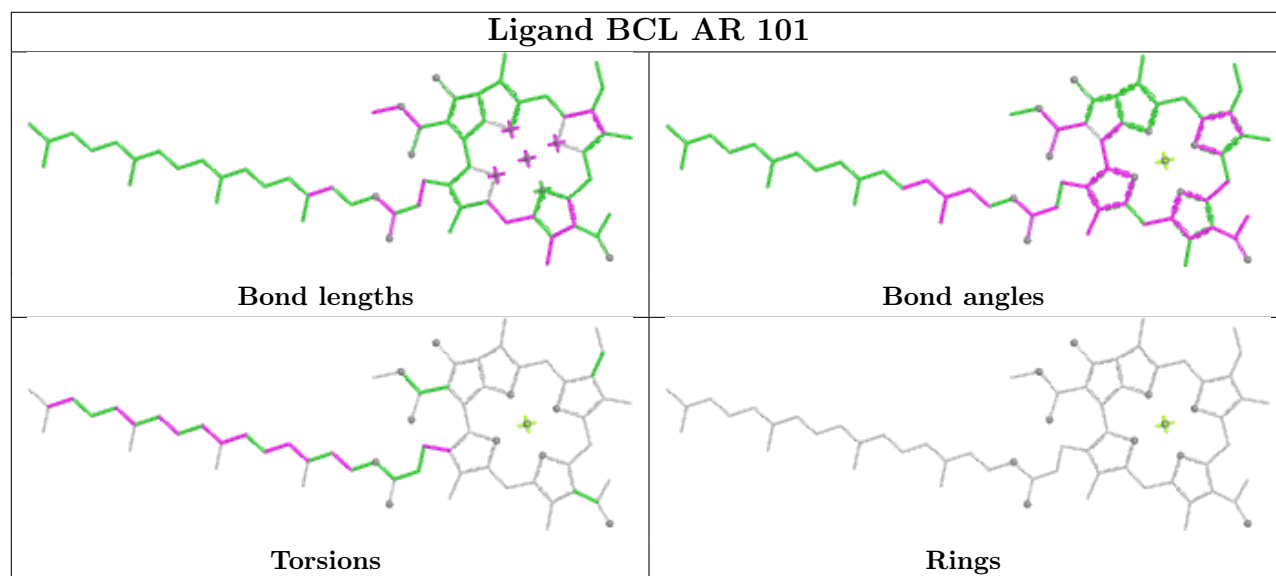


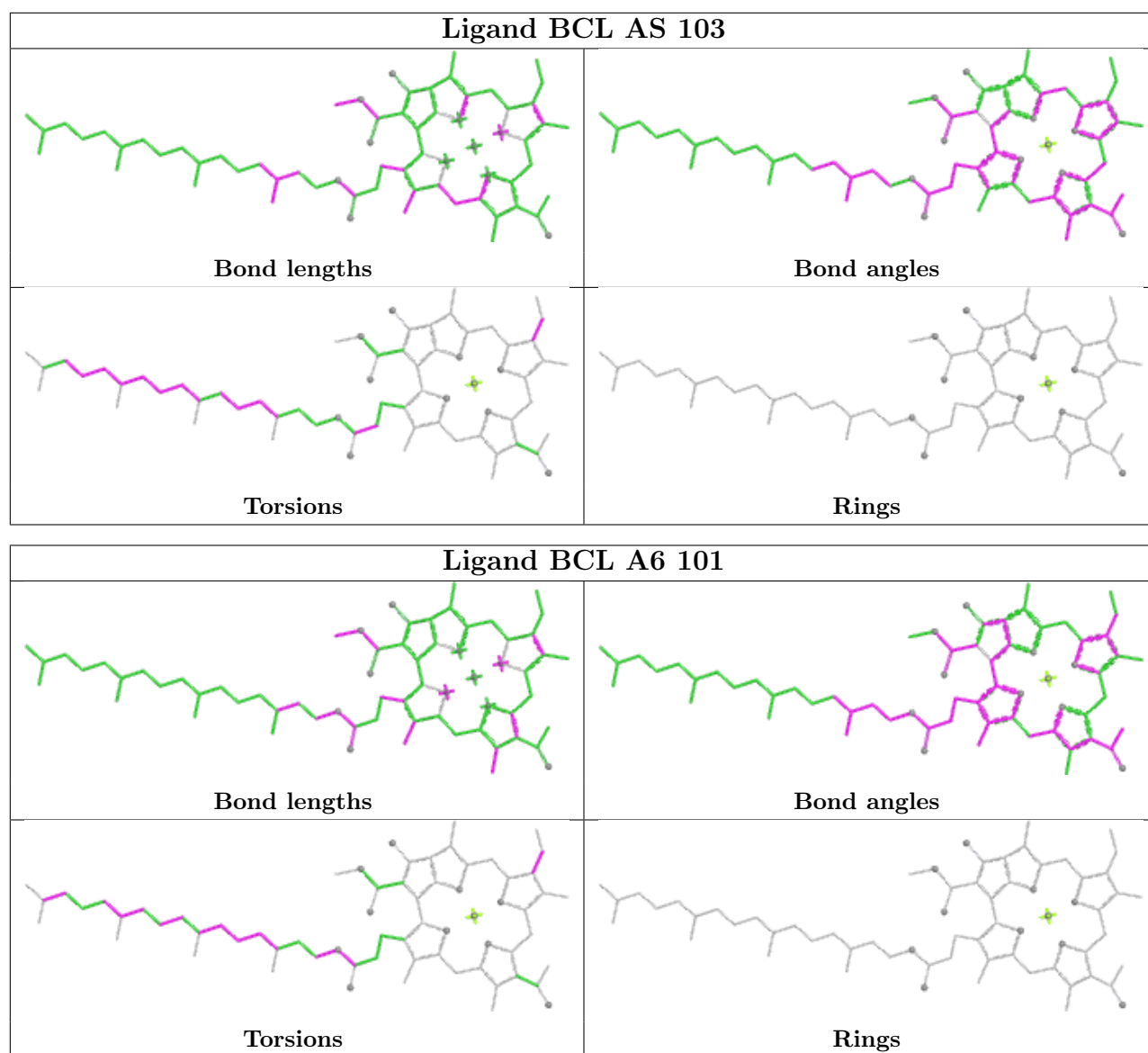


Ligand BPH AL 302

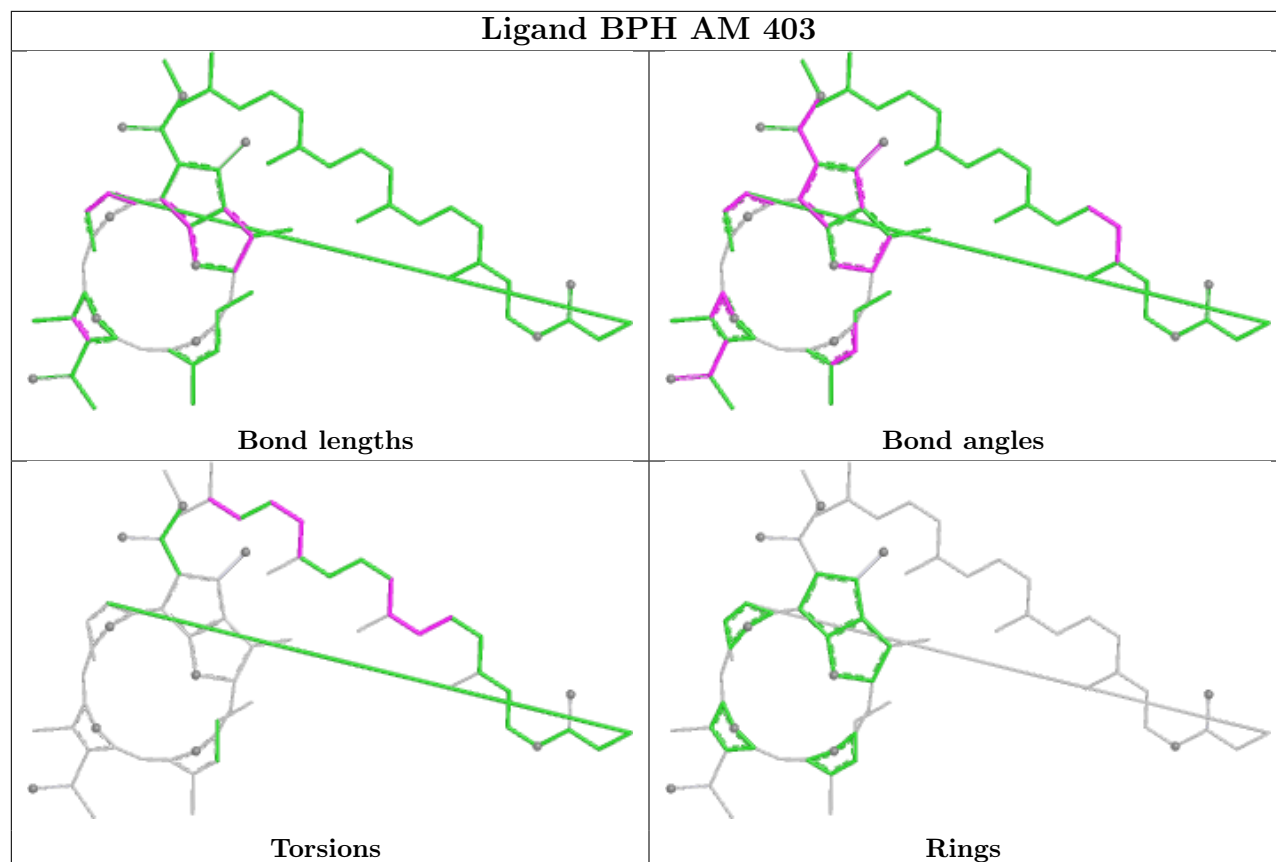


Ligand BCL AR 101

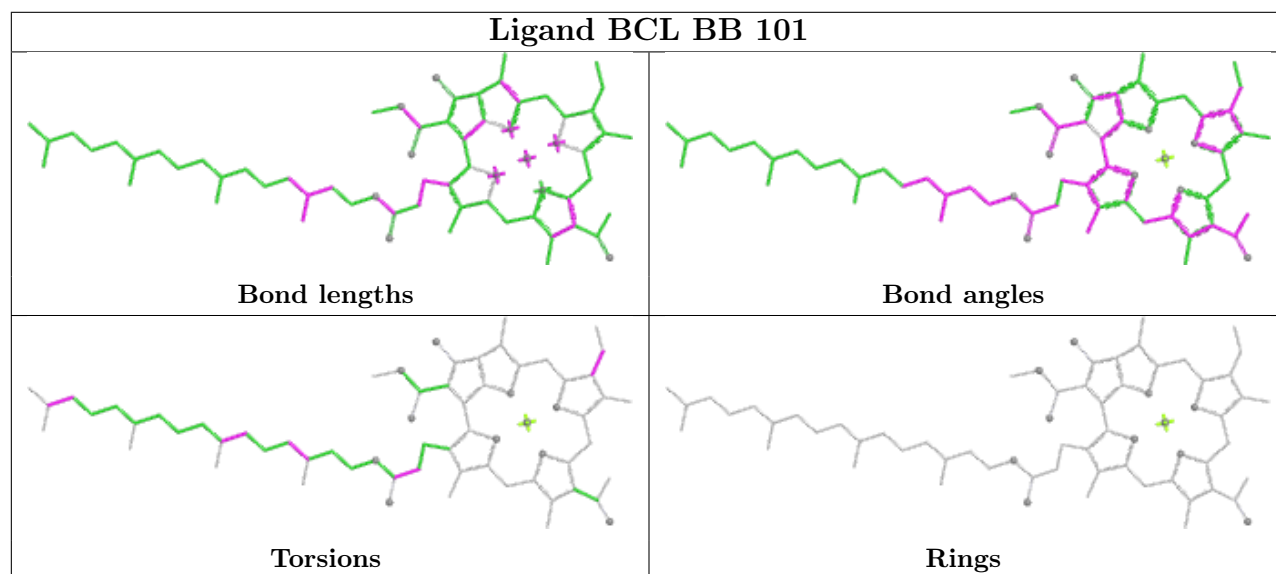


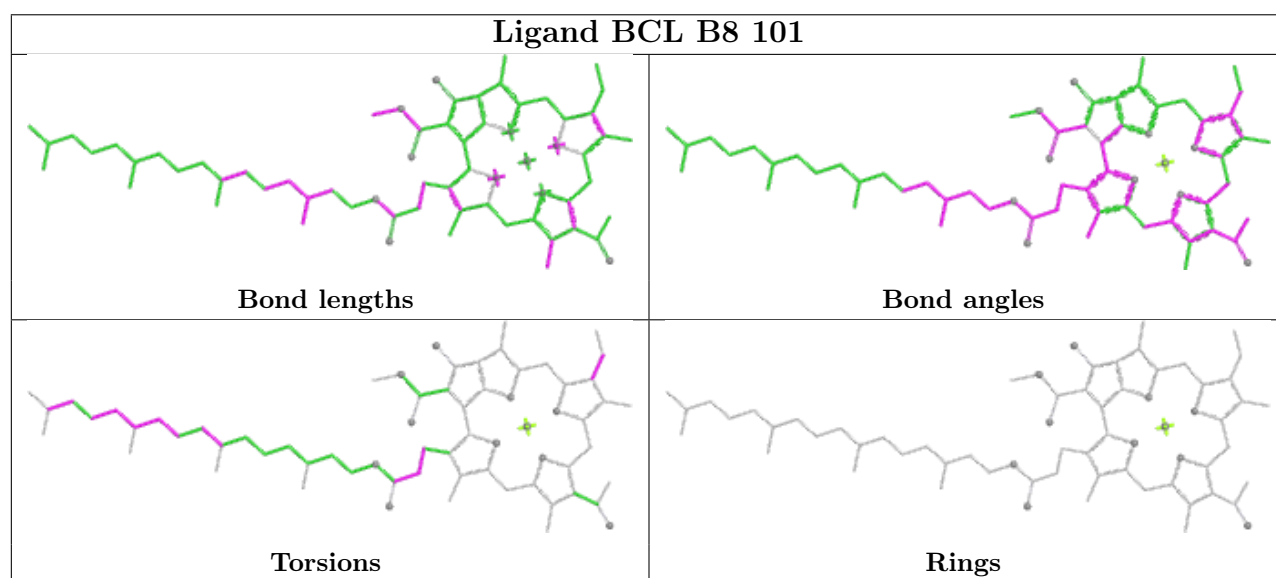
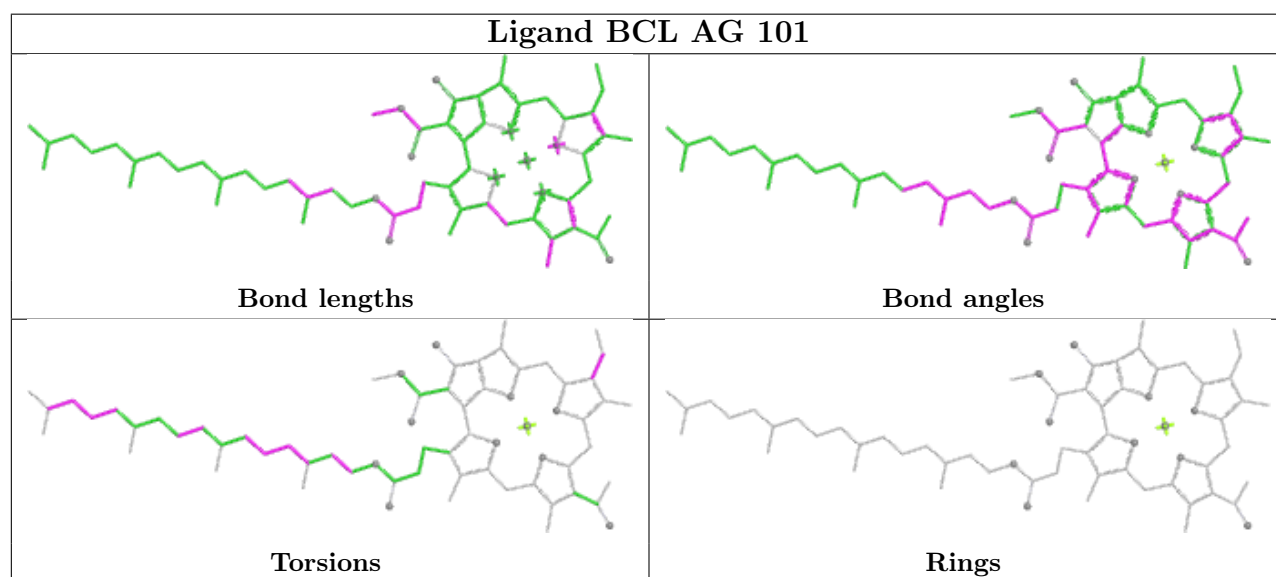
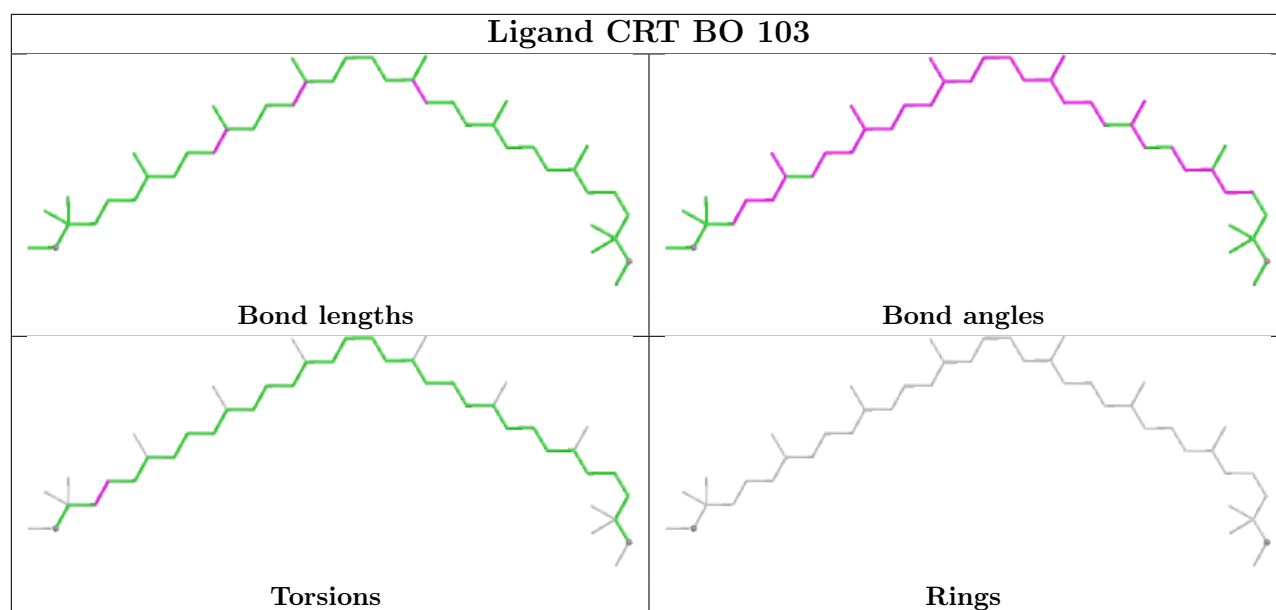


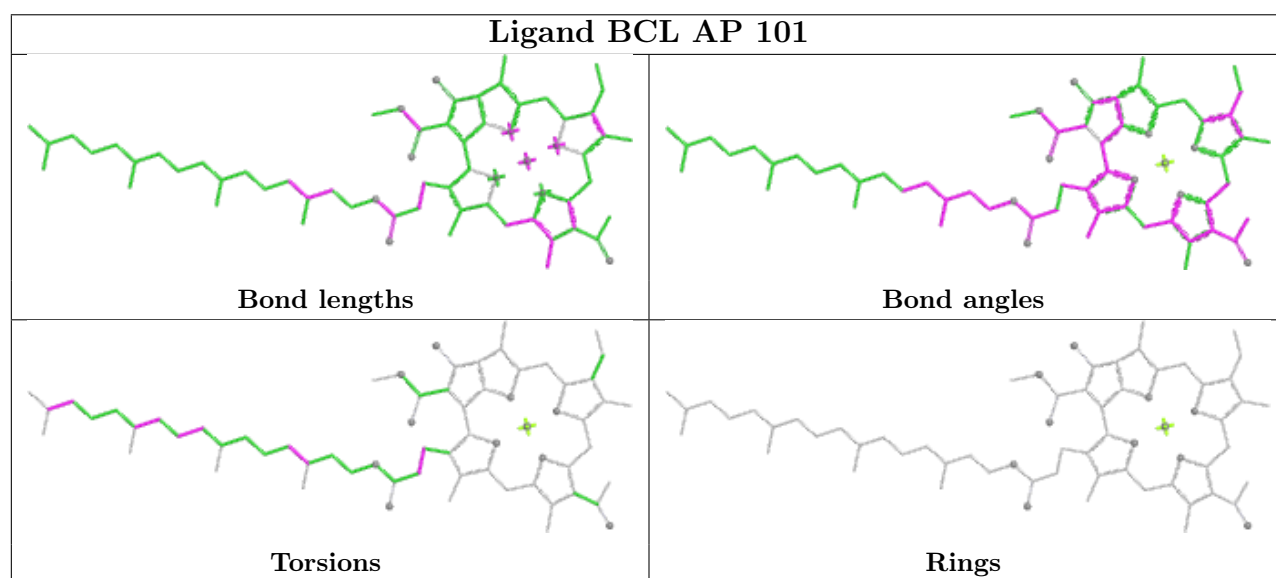
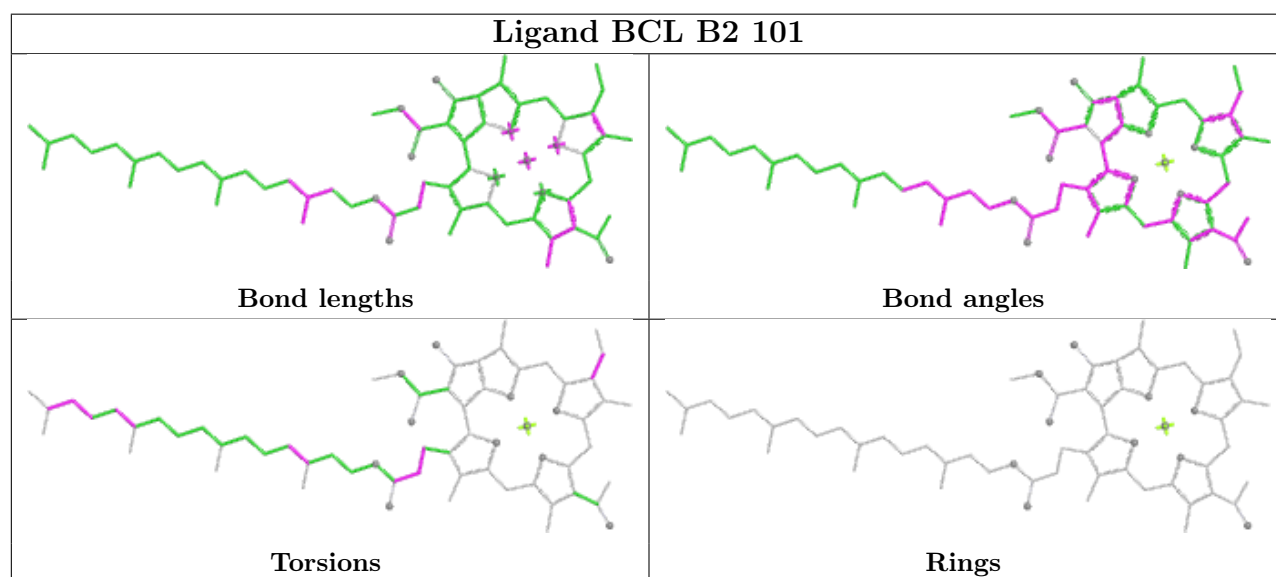
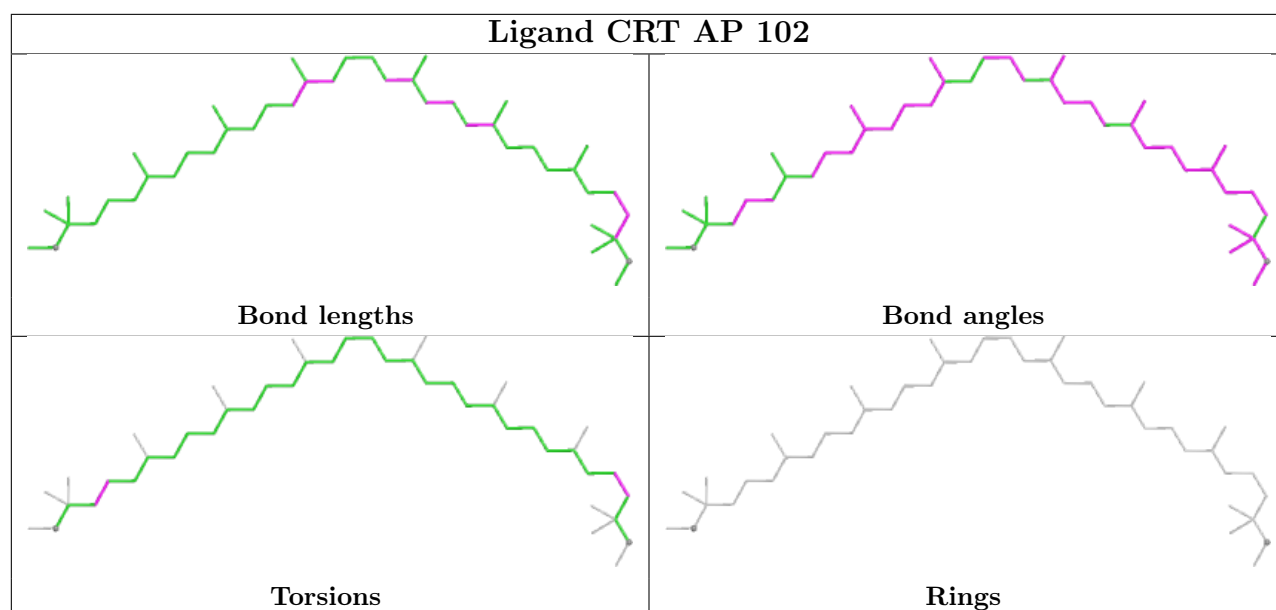
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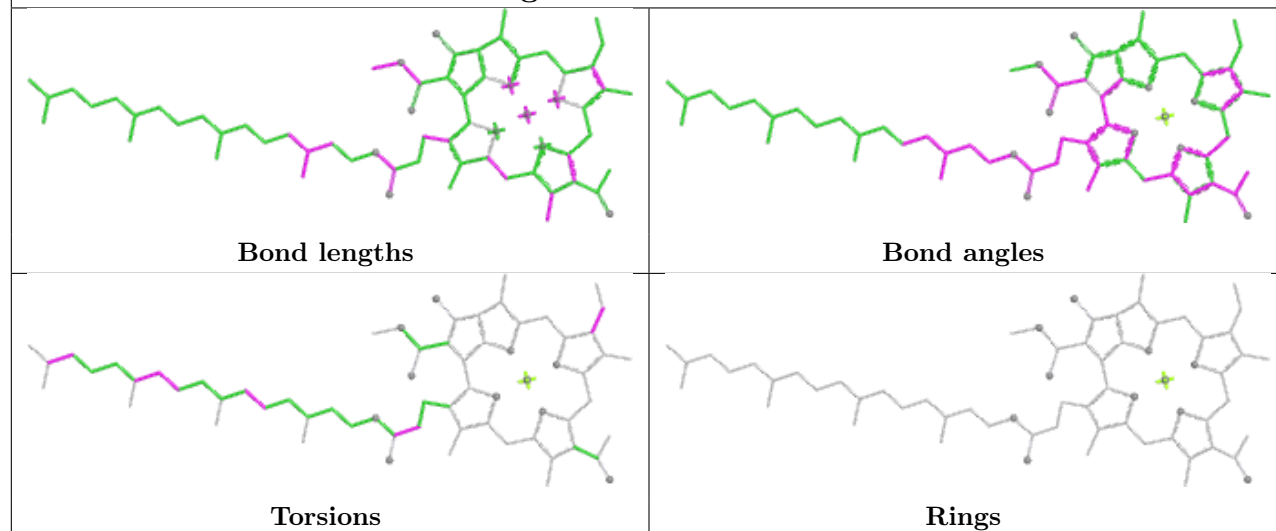
Ligand BCL BB 101



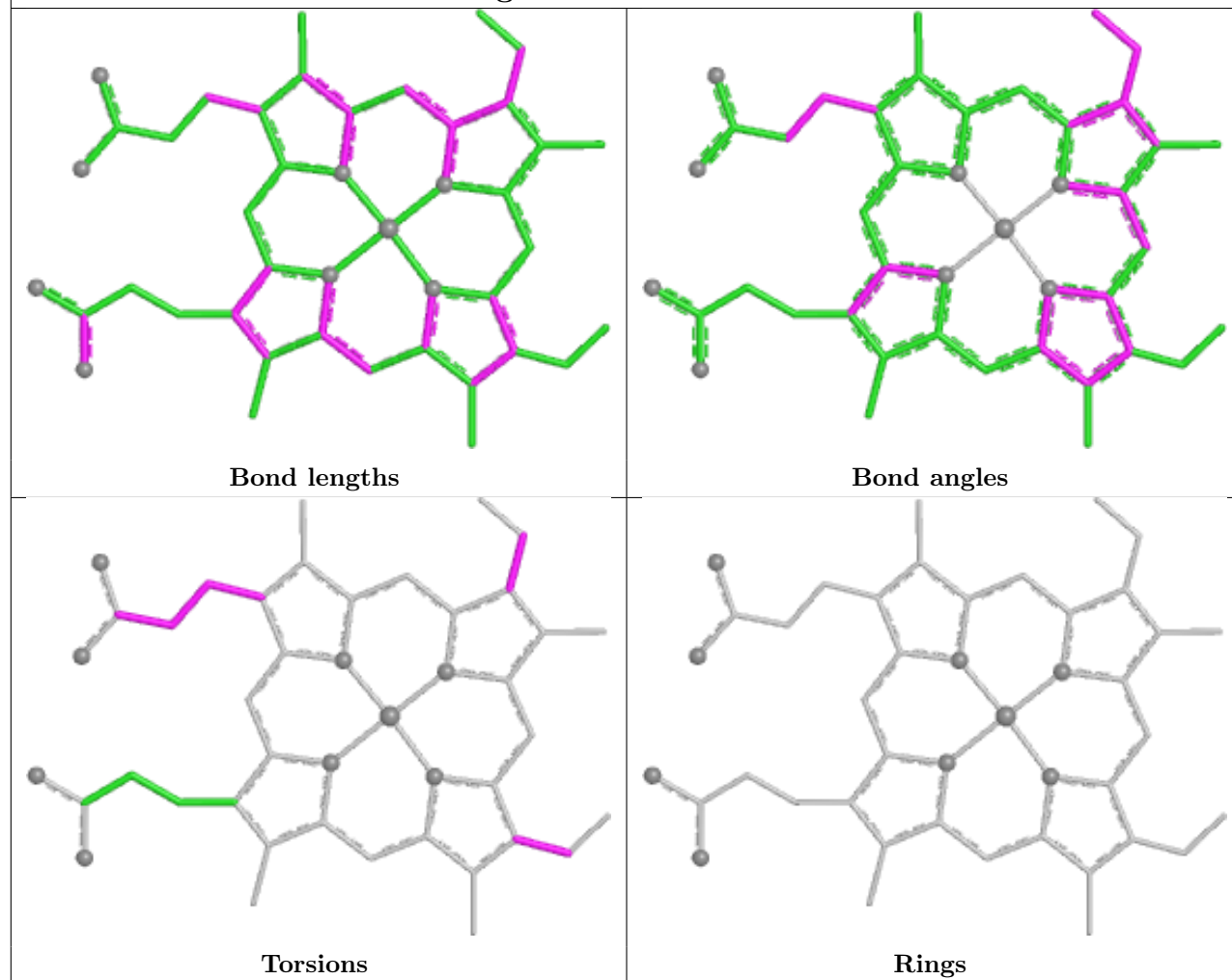


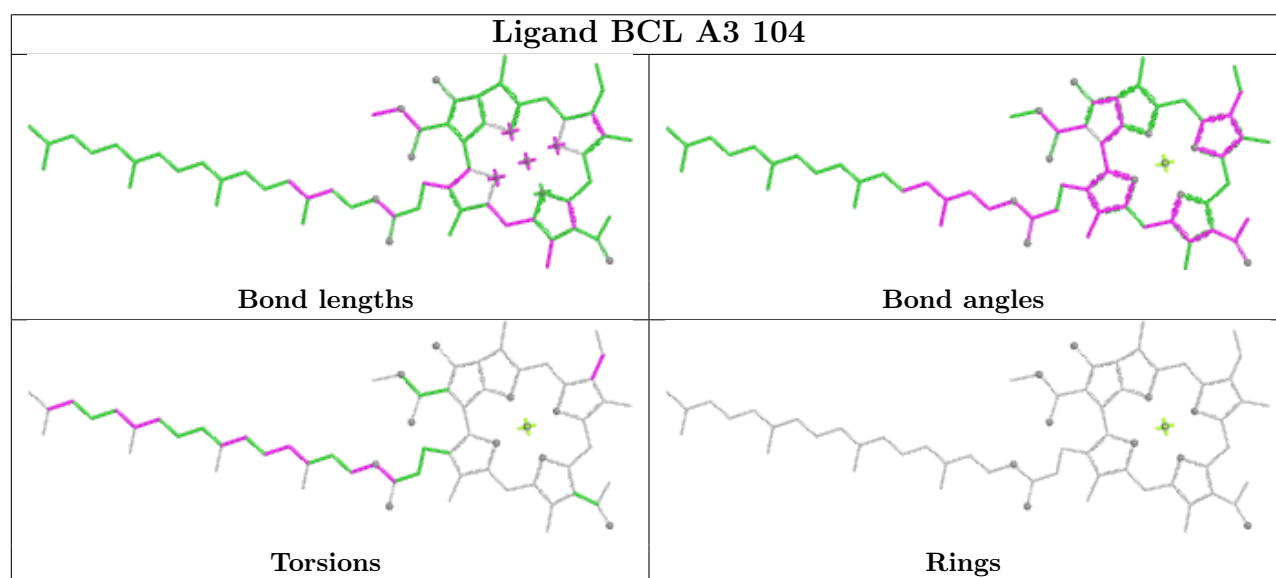
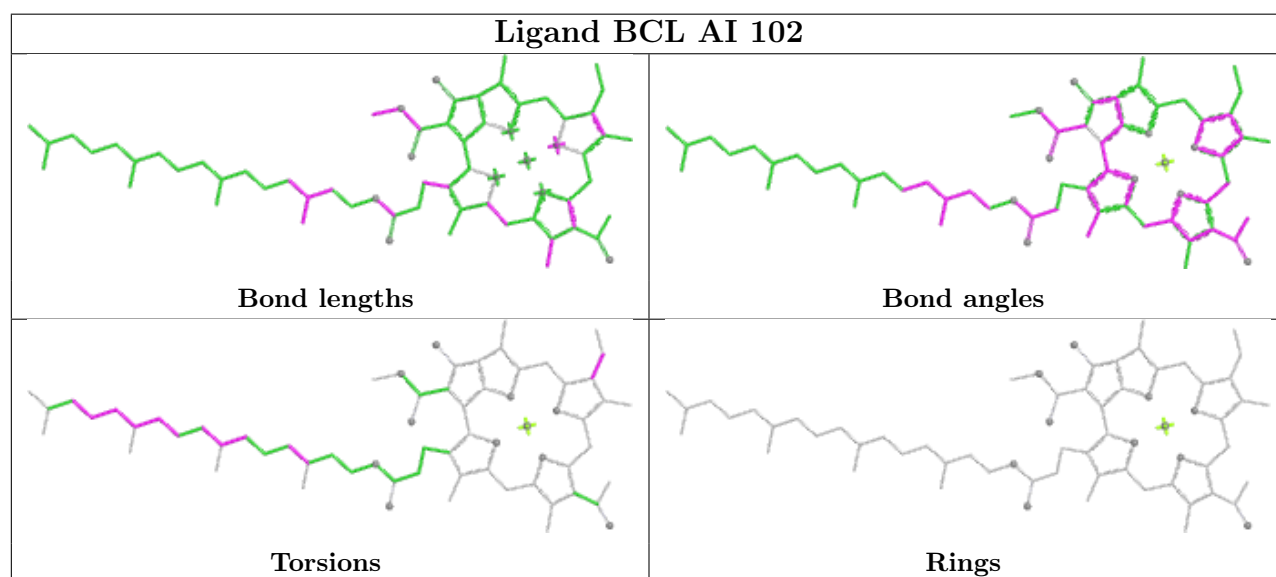
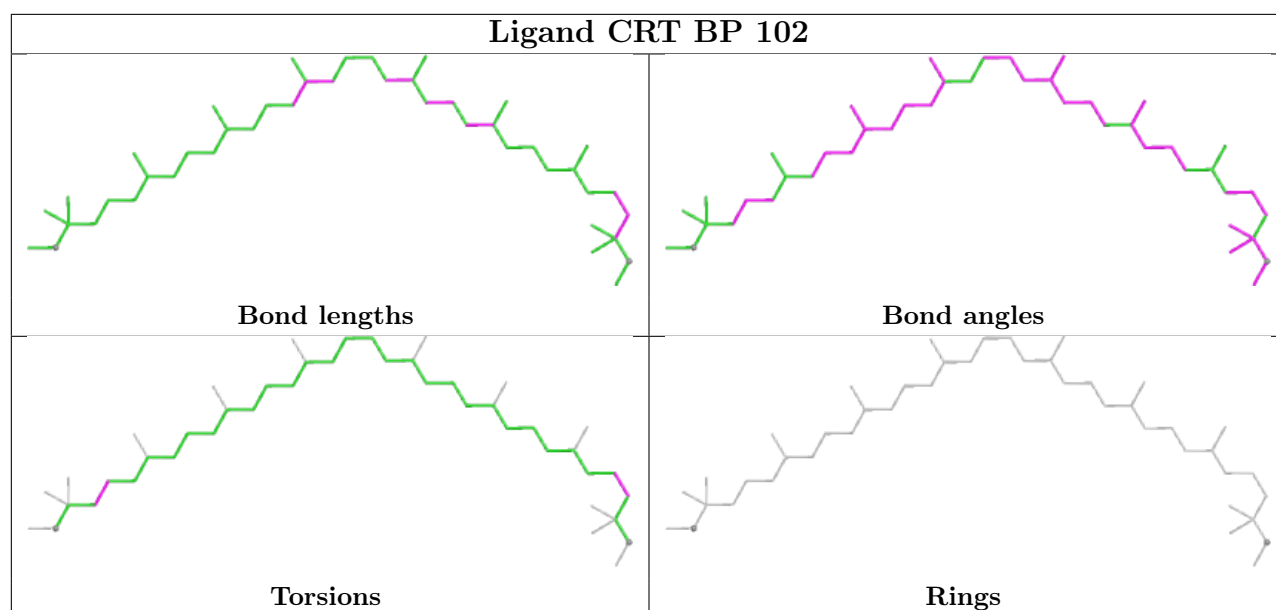


Ligand BCL AE 101

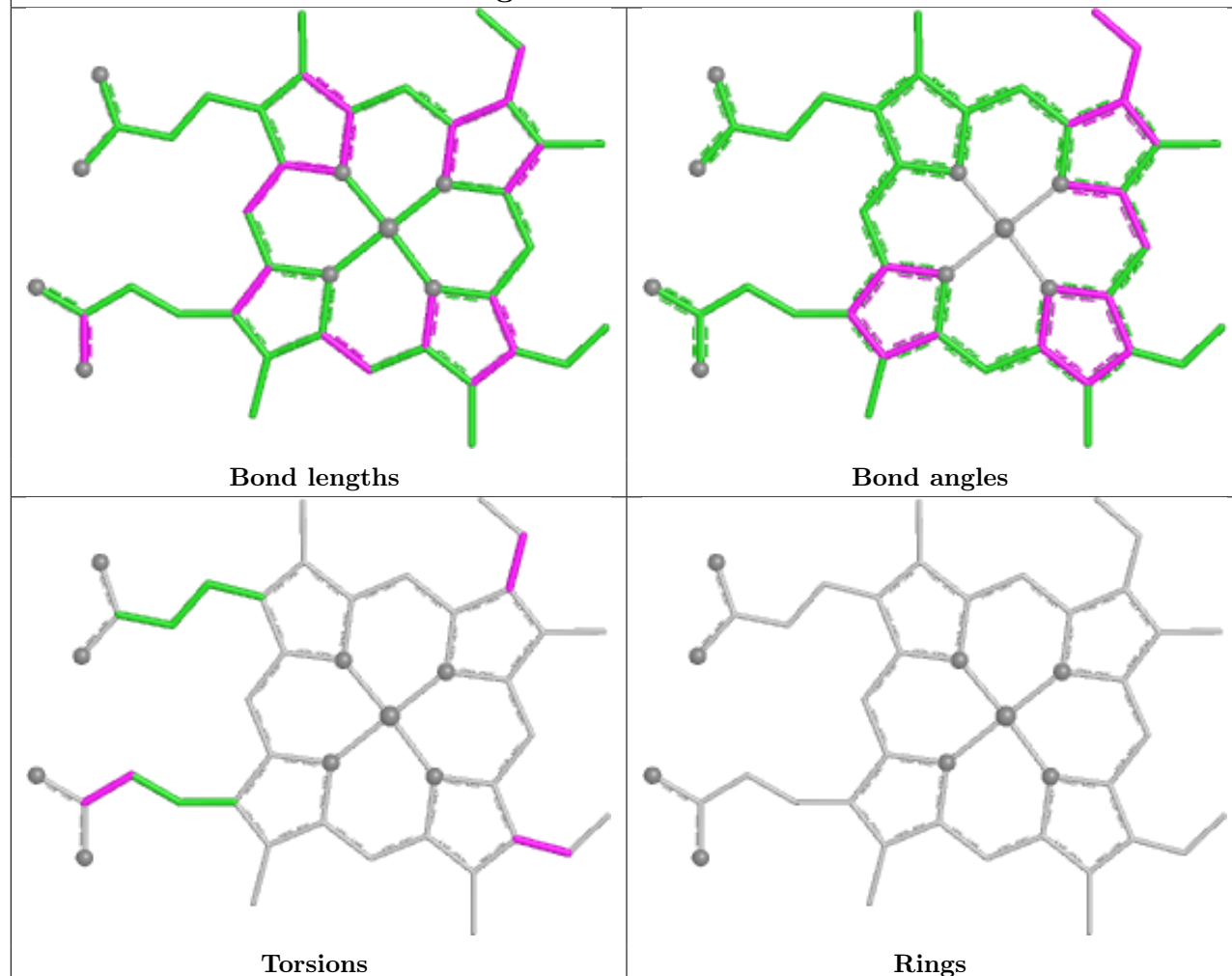


Ligand HEM BC 504

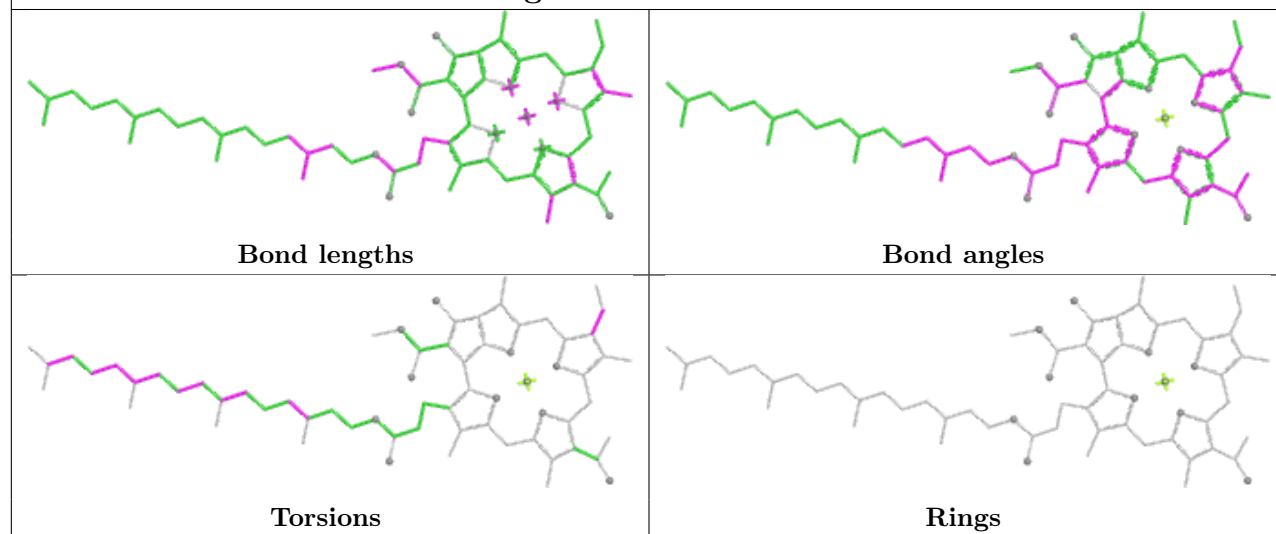


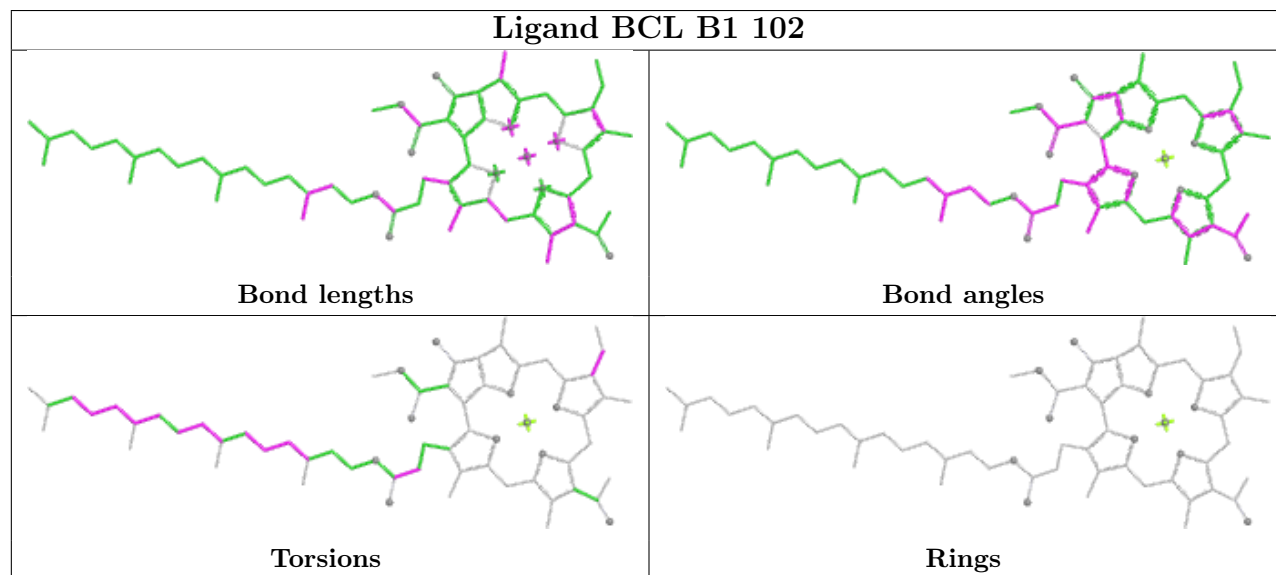
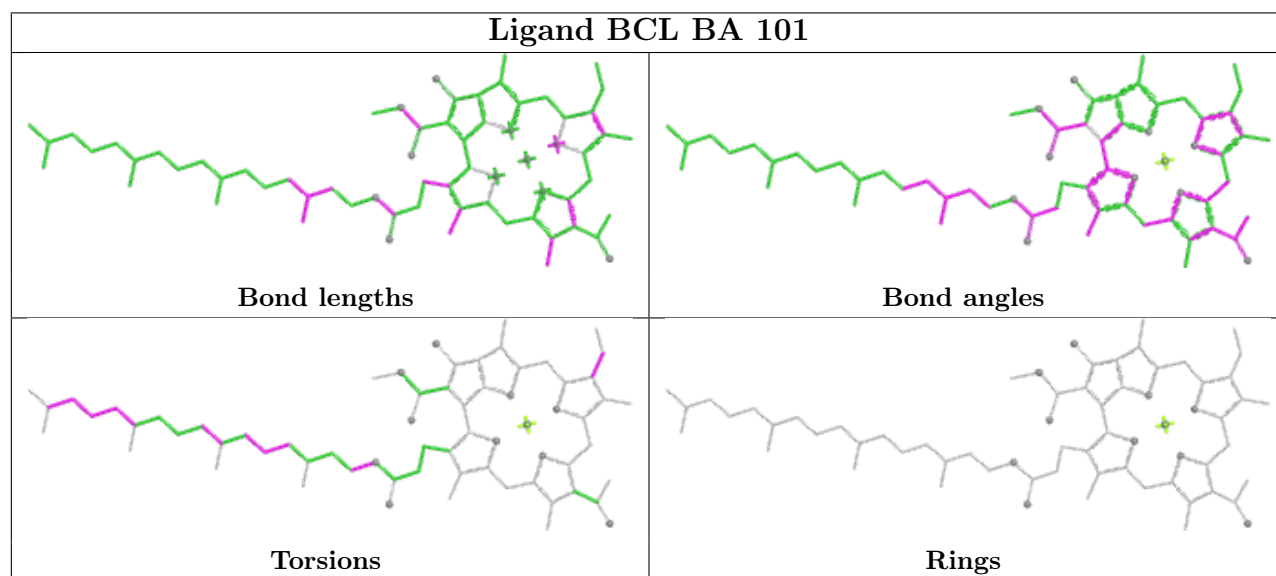
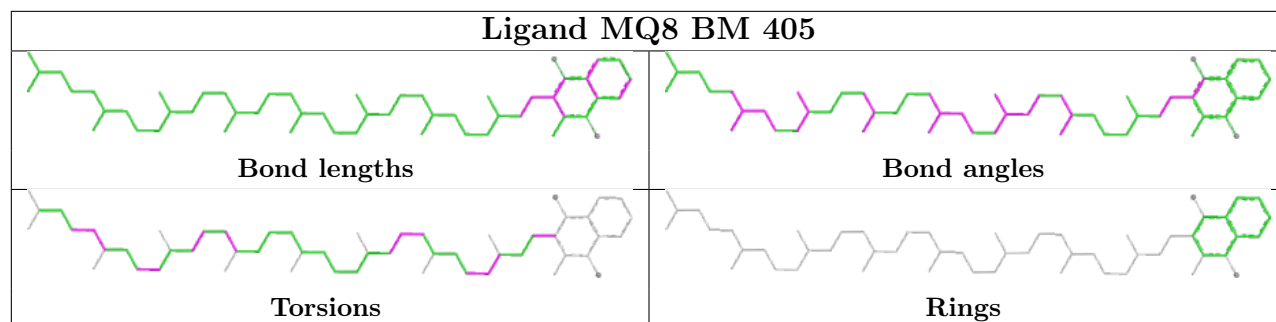


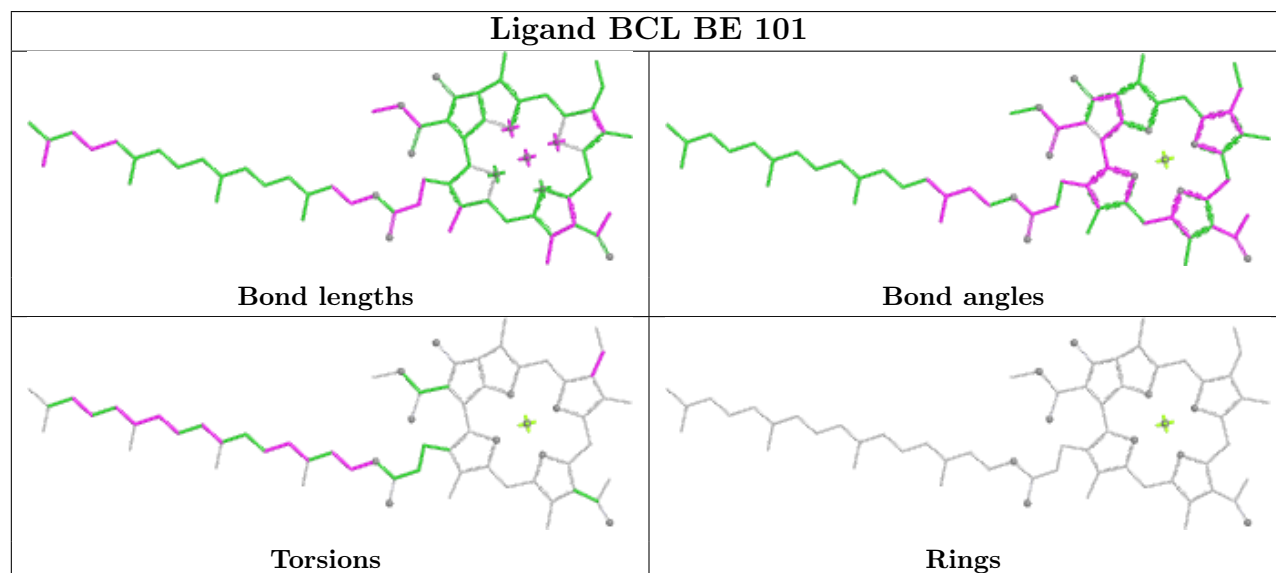
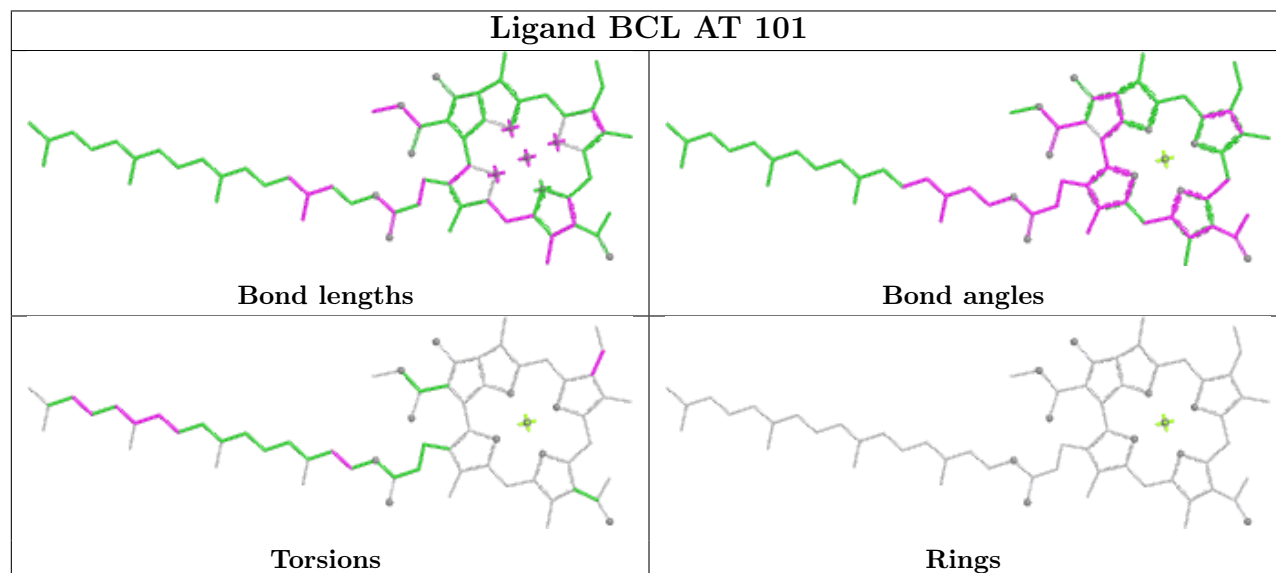
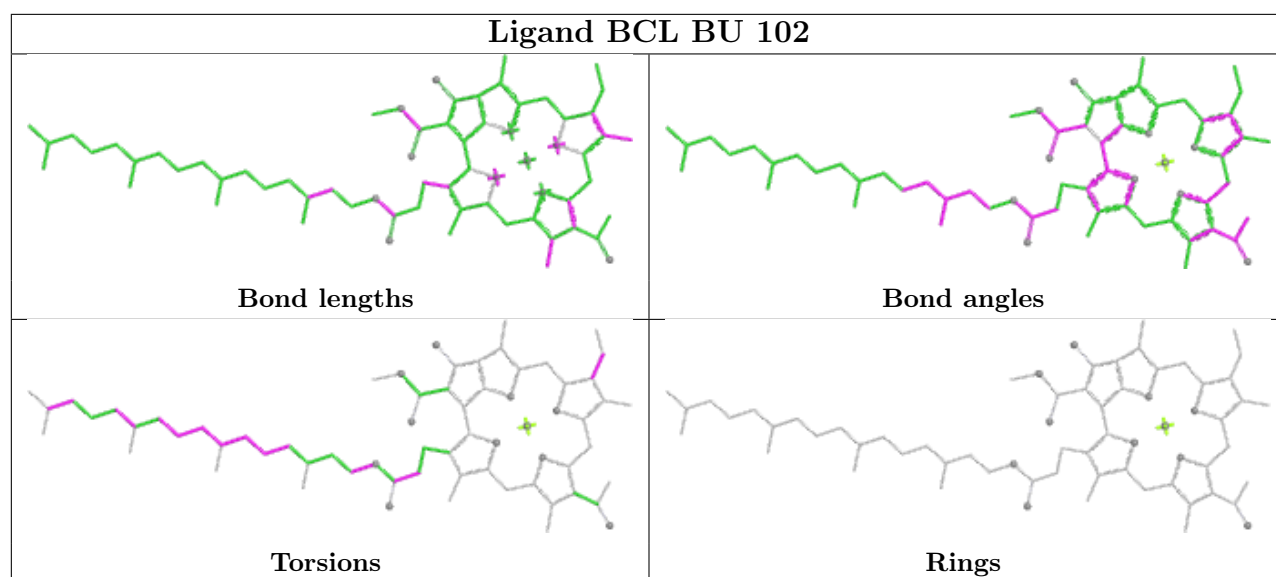
Ligand HEM BC 501

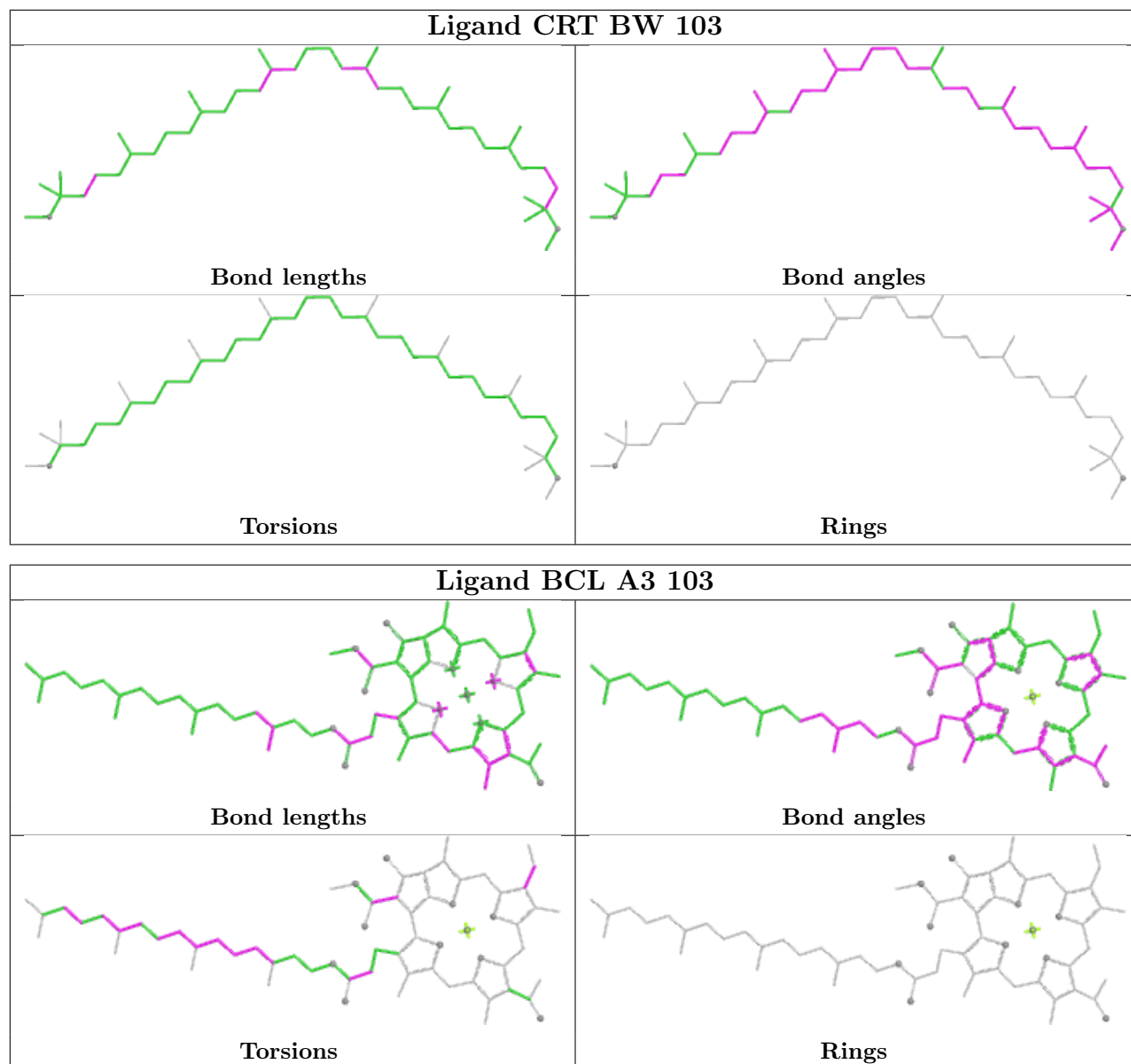


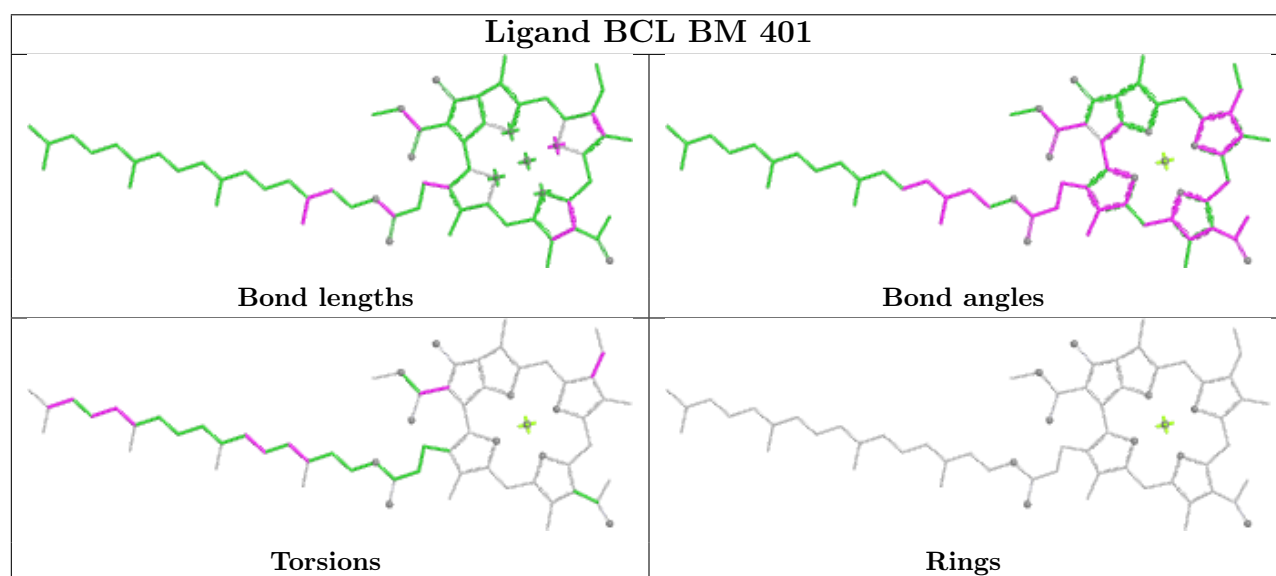
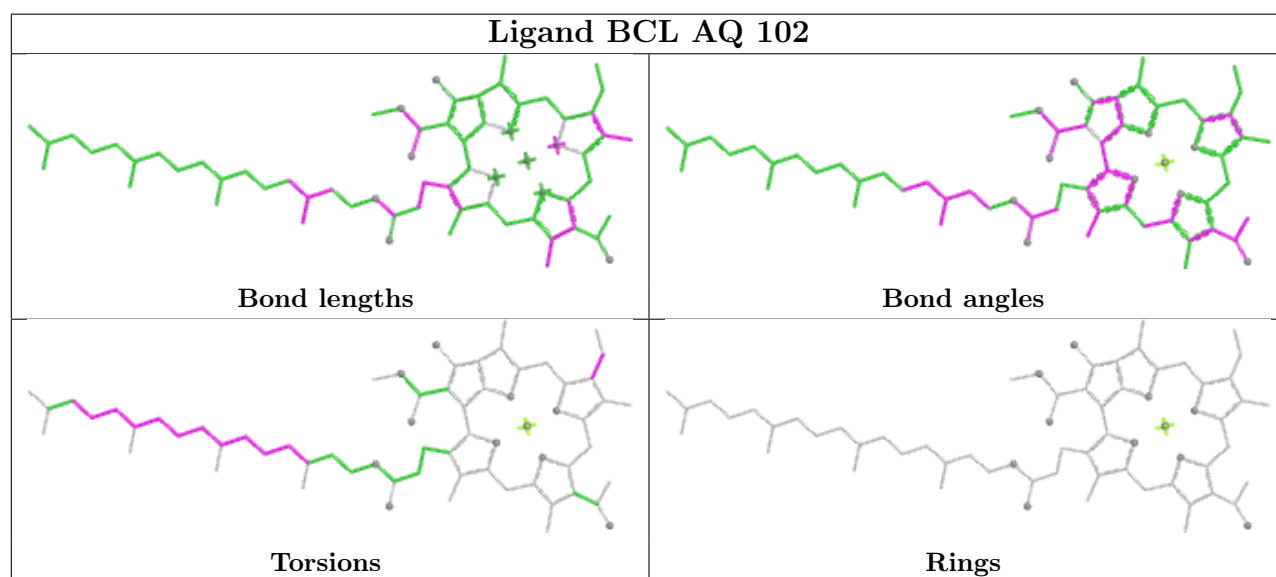
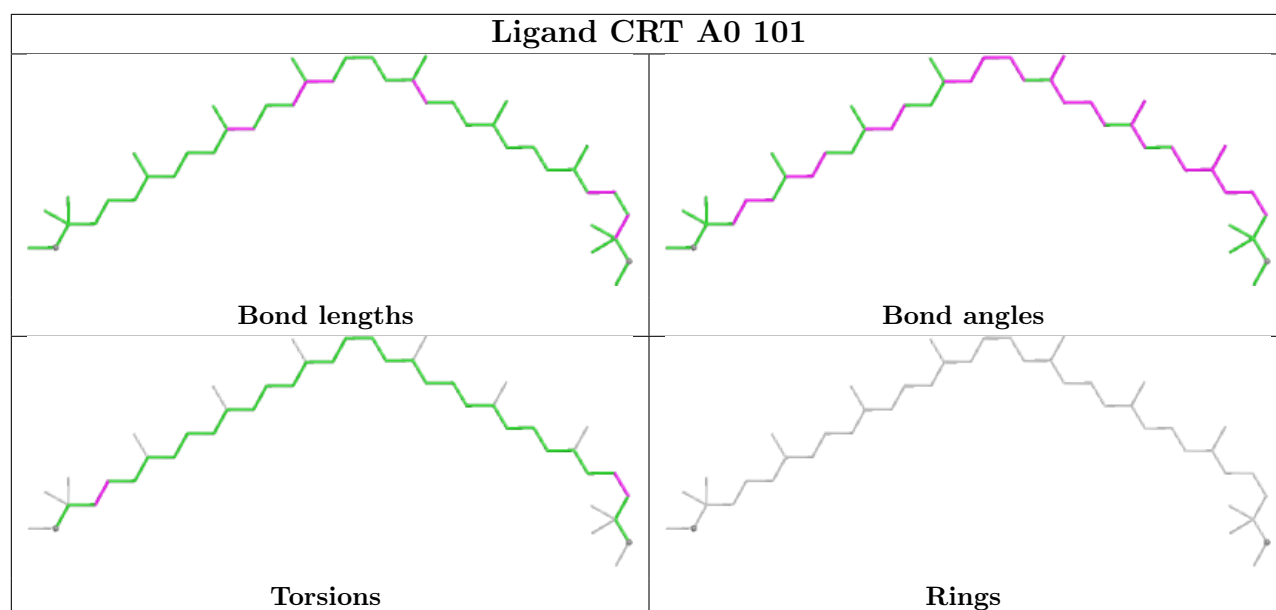
Ligand BCL B0 102

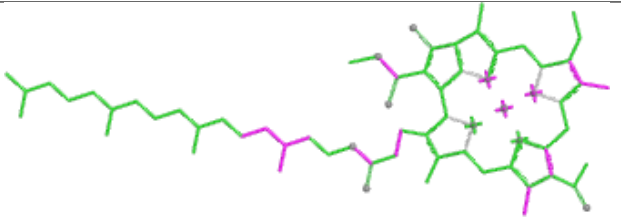
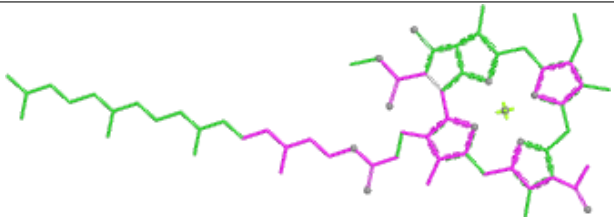
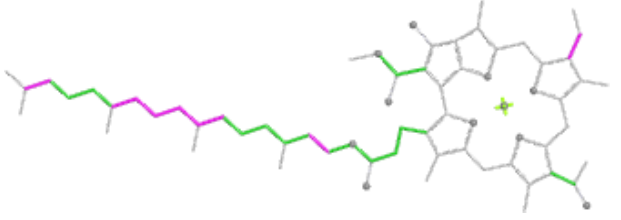
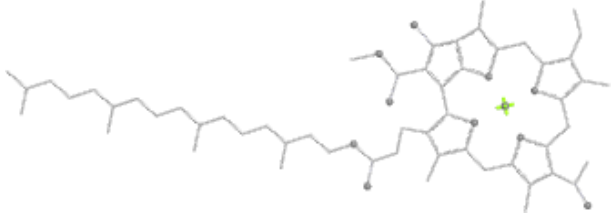


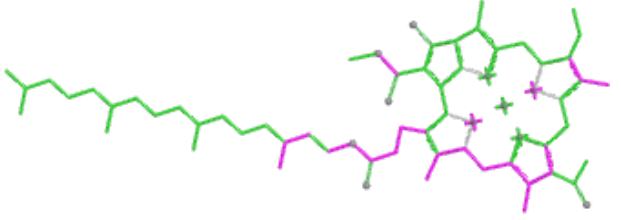
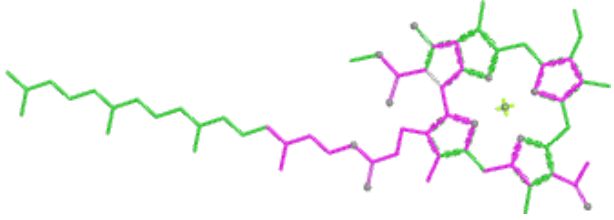
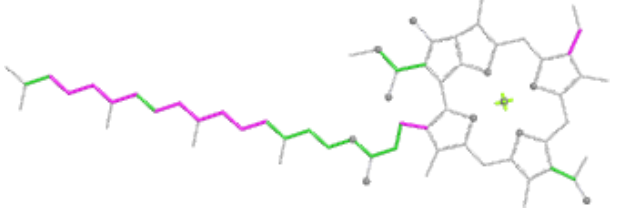
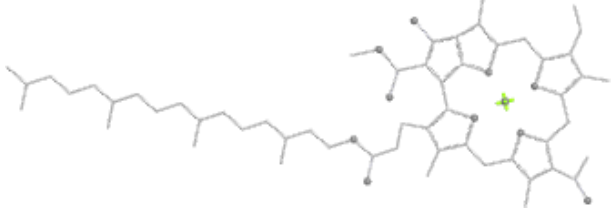


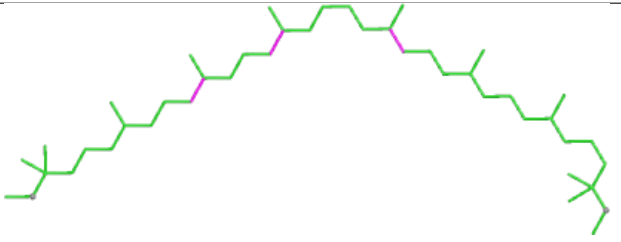
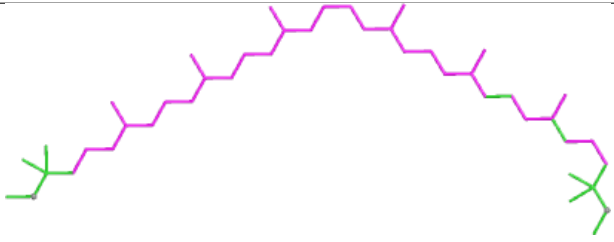
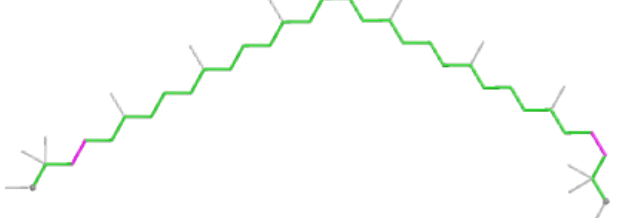


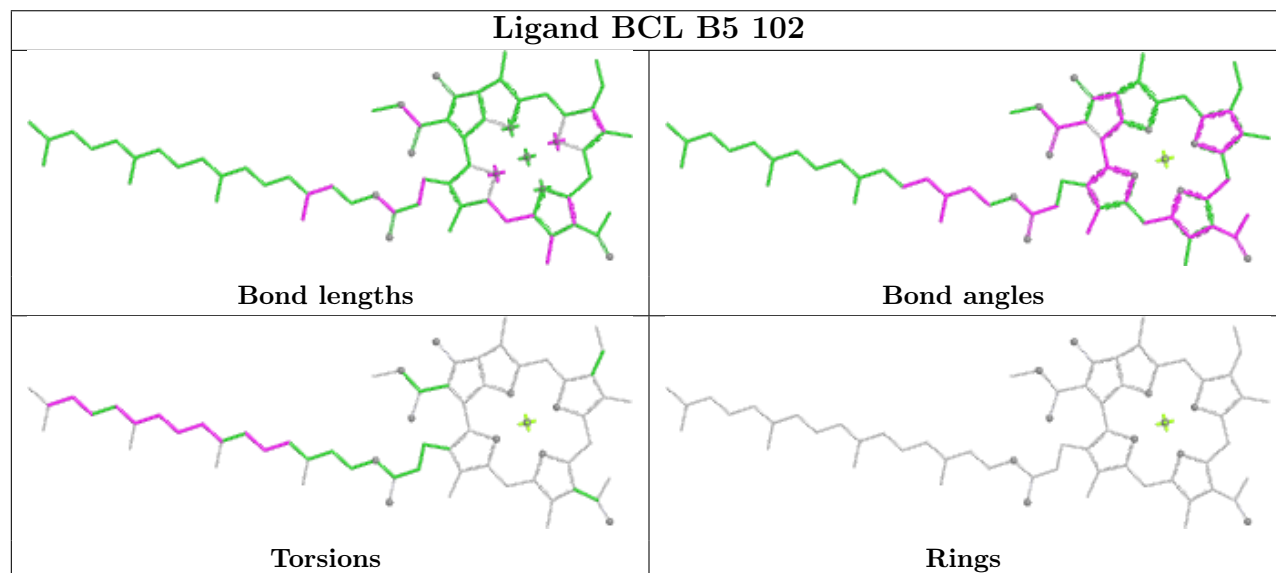
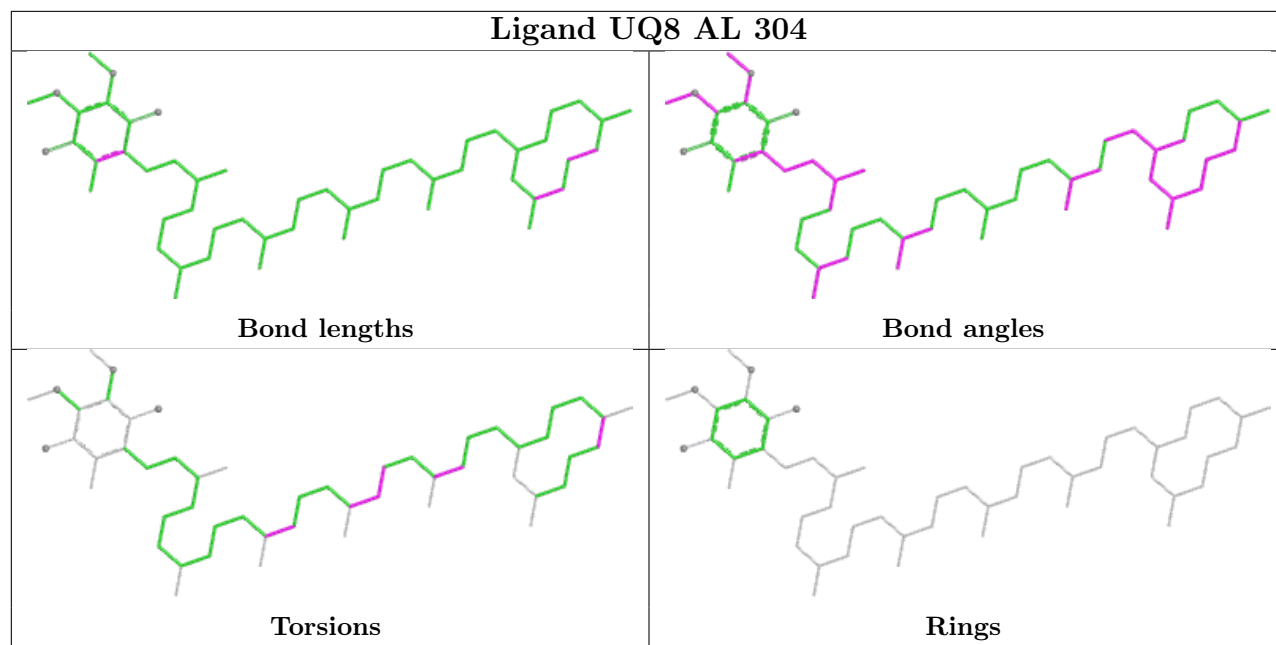


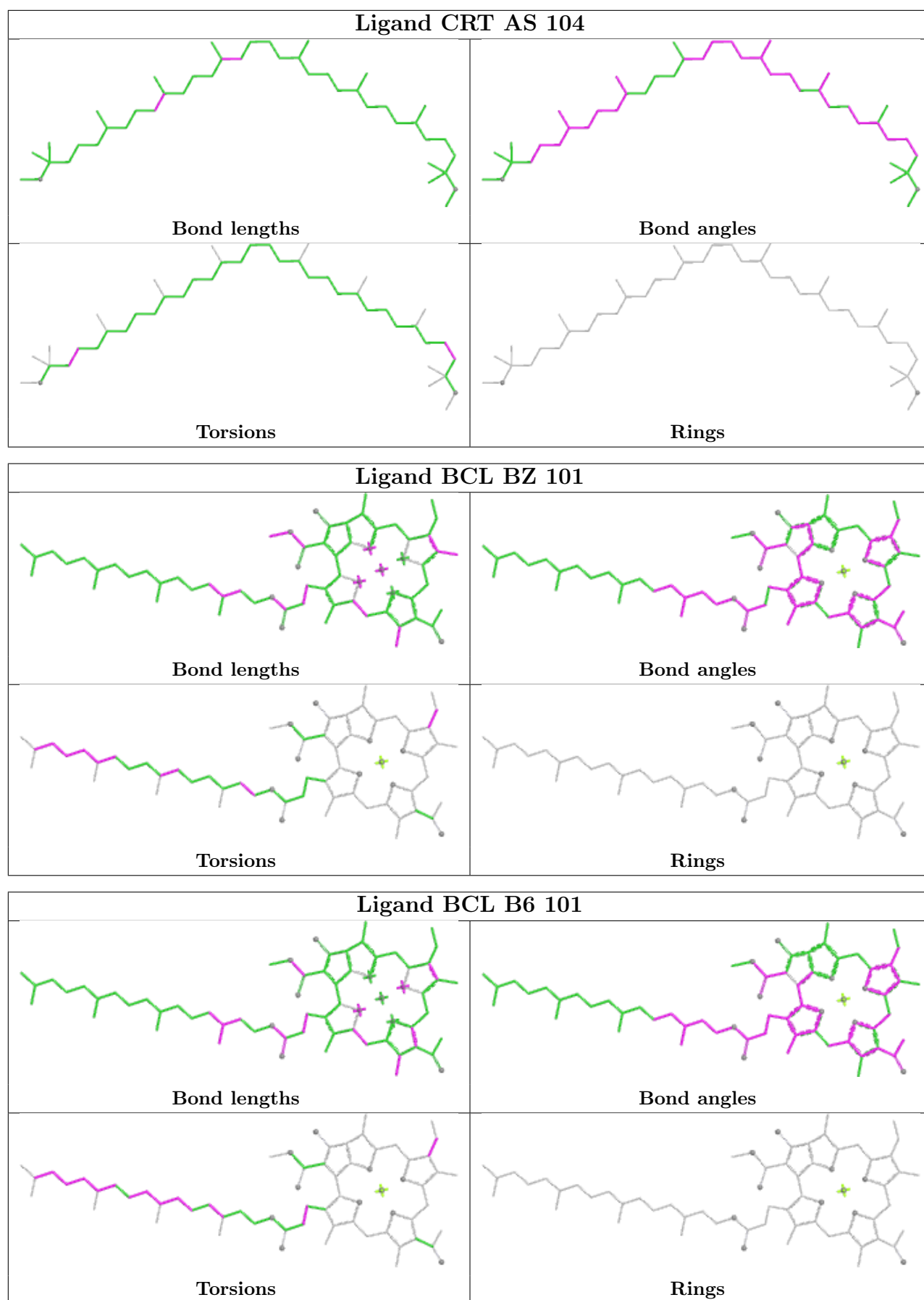


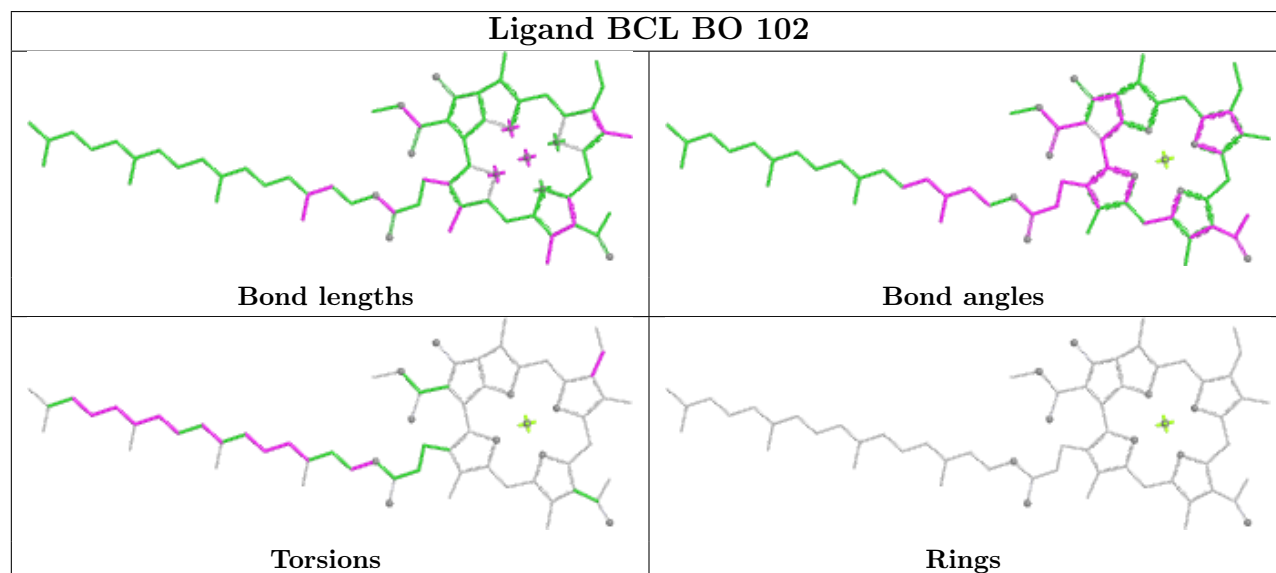
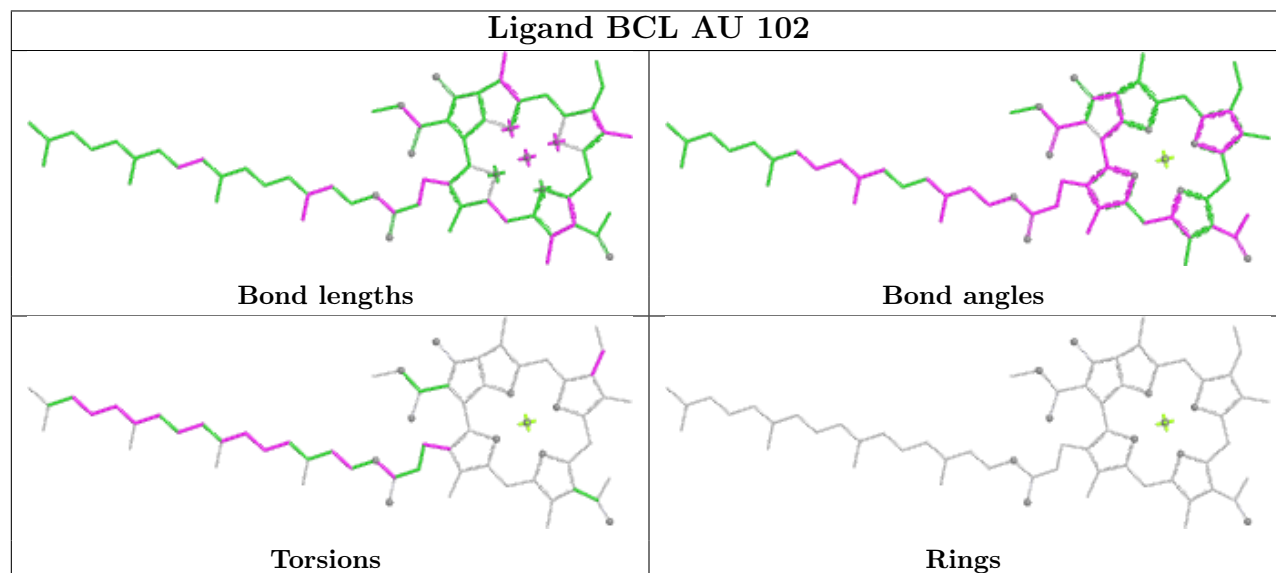
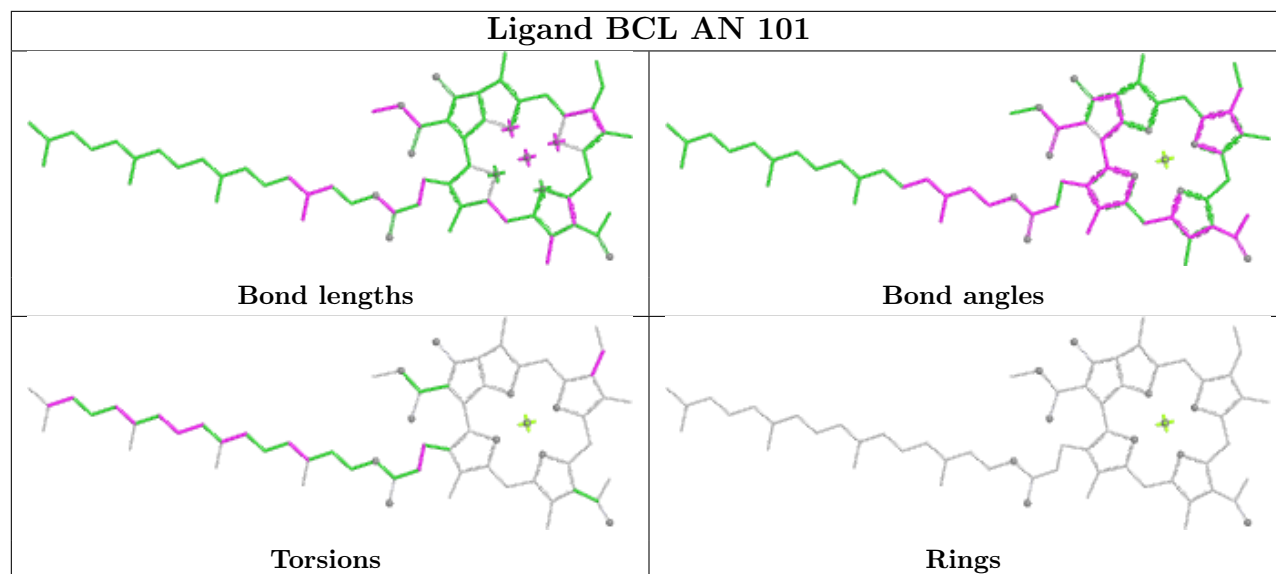
Ligand BCL BN 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

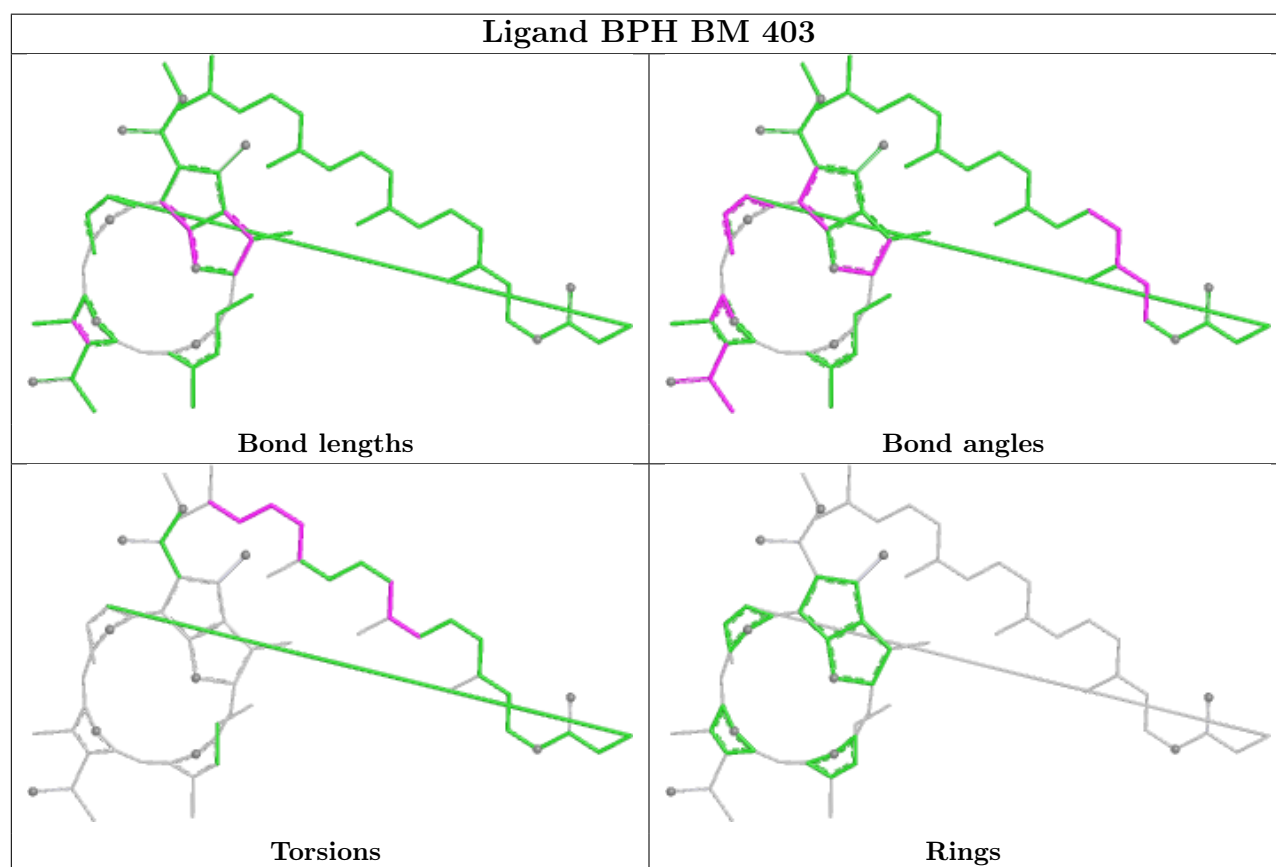
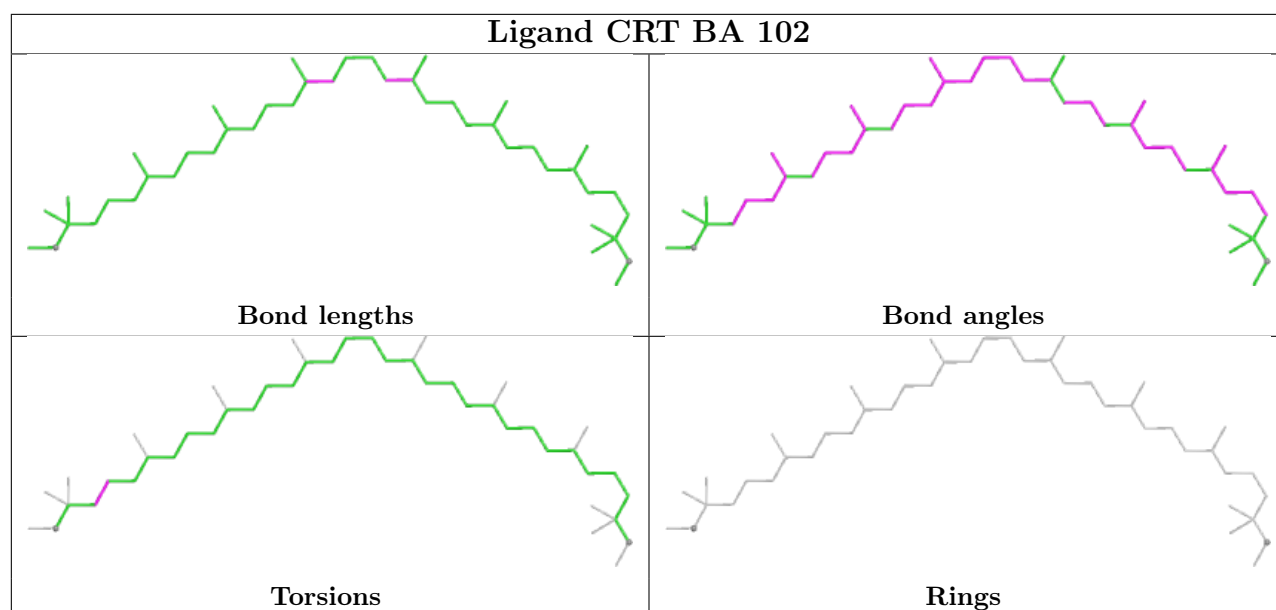
Ligand BCL A1 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

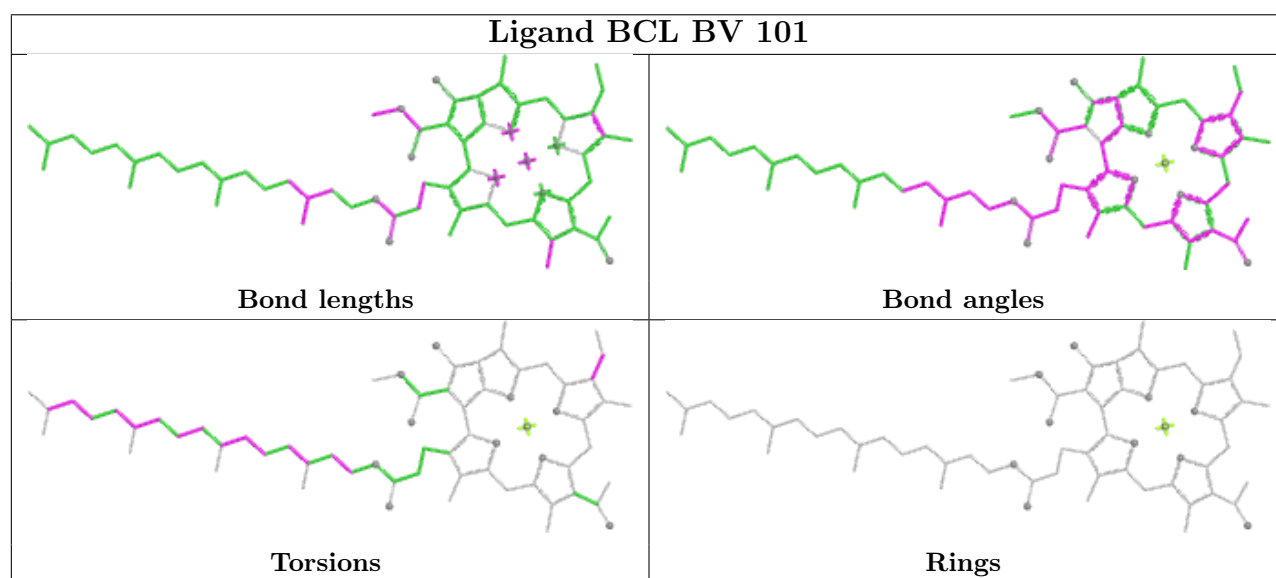
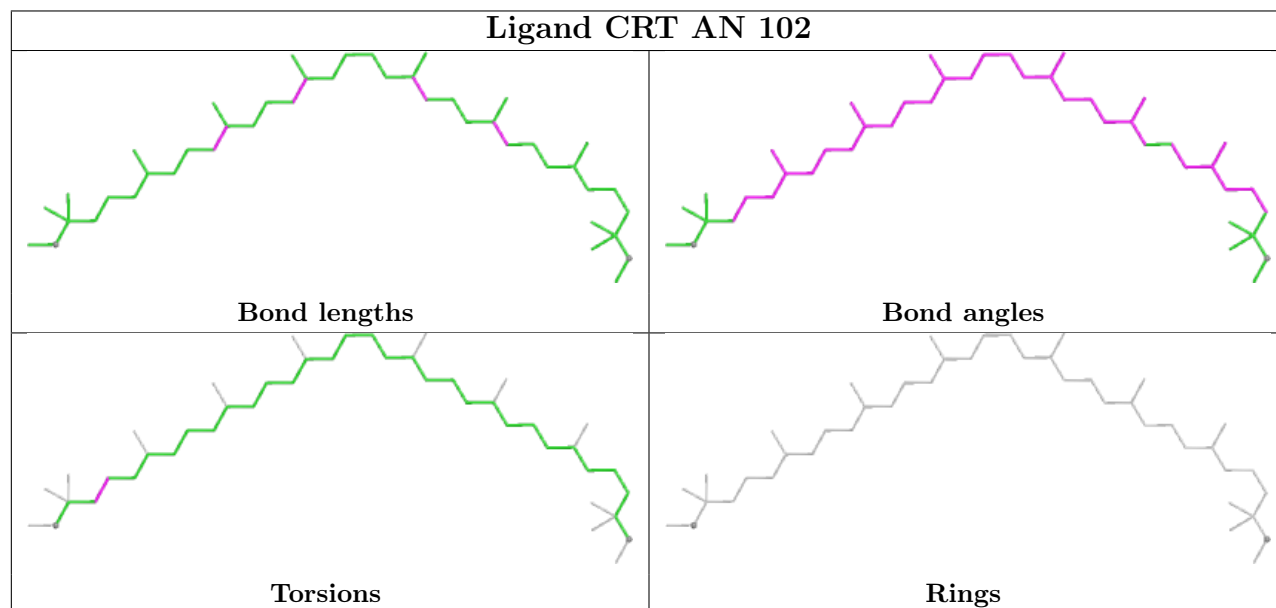
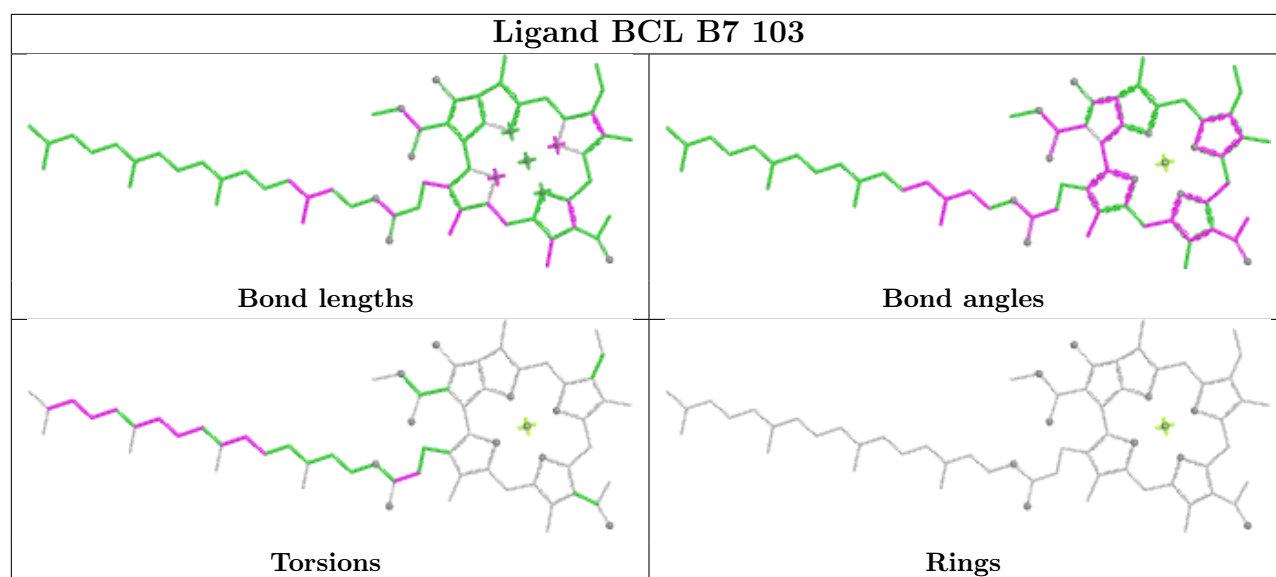
Ligand CRT B1 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

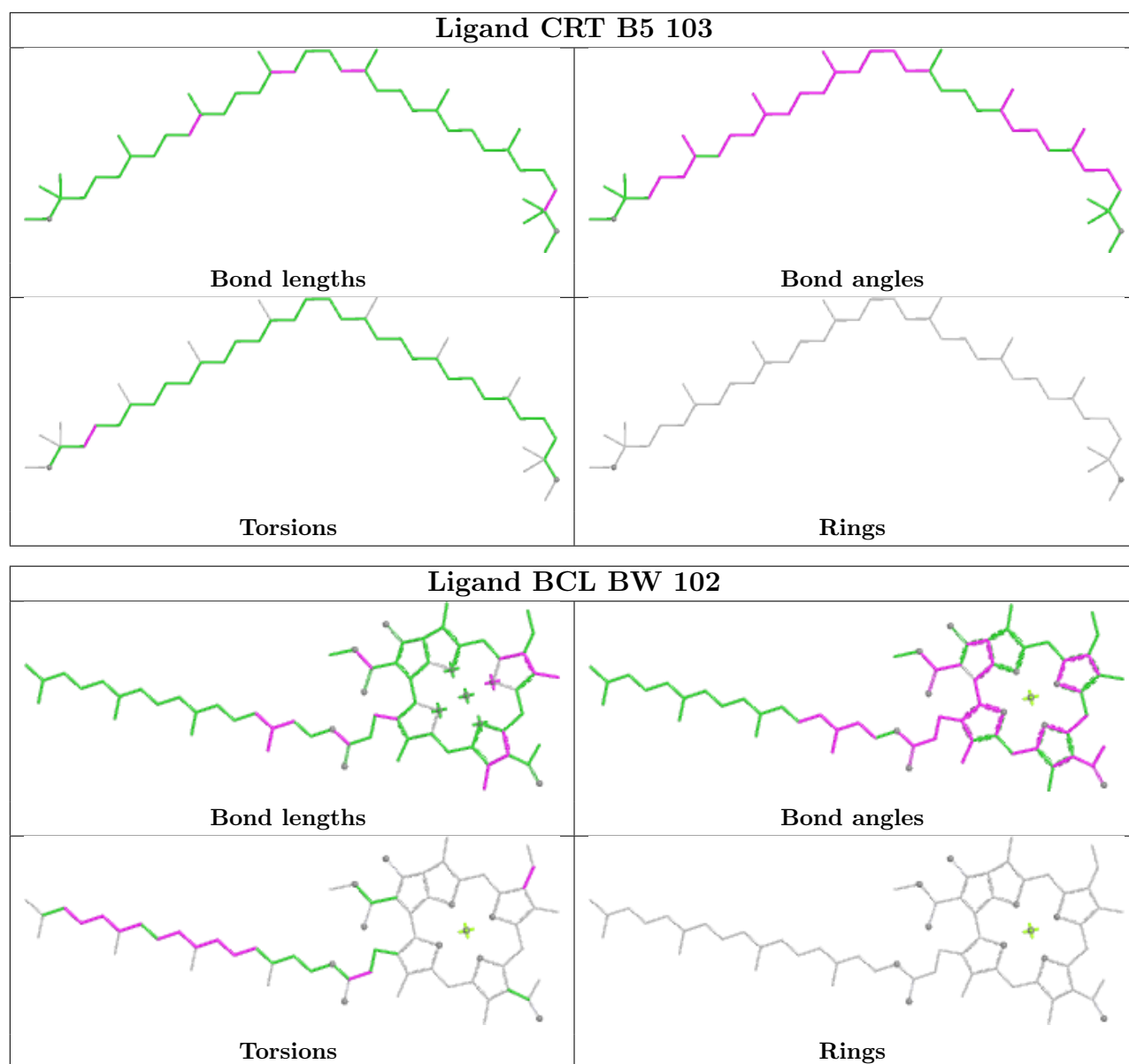


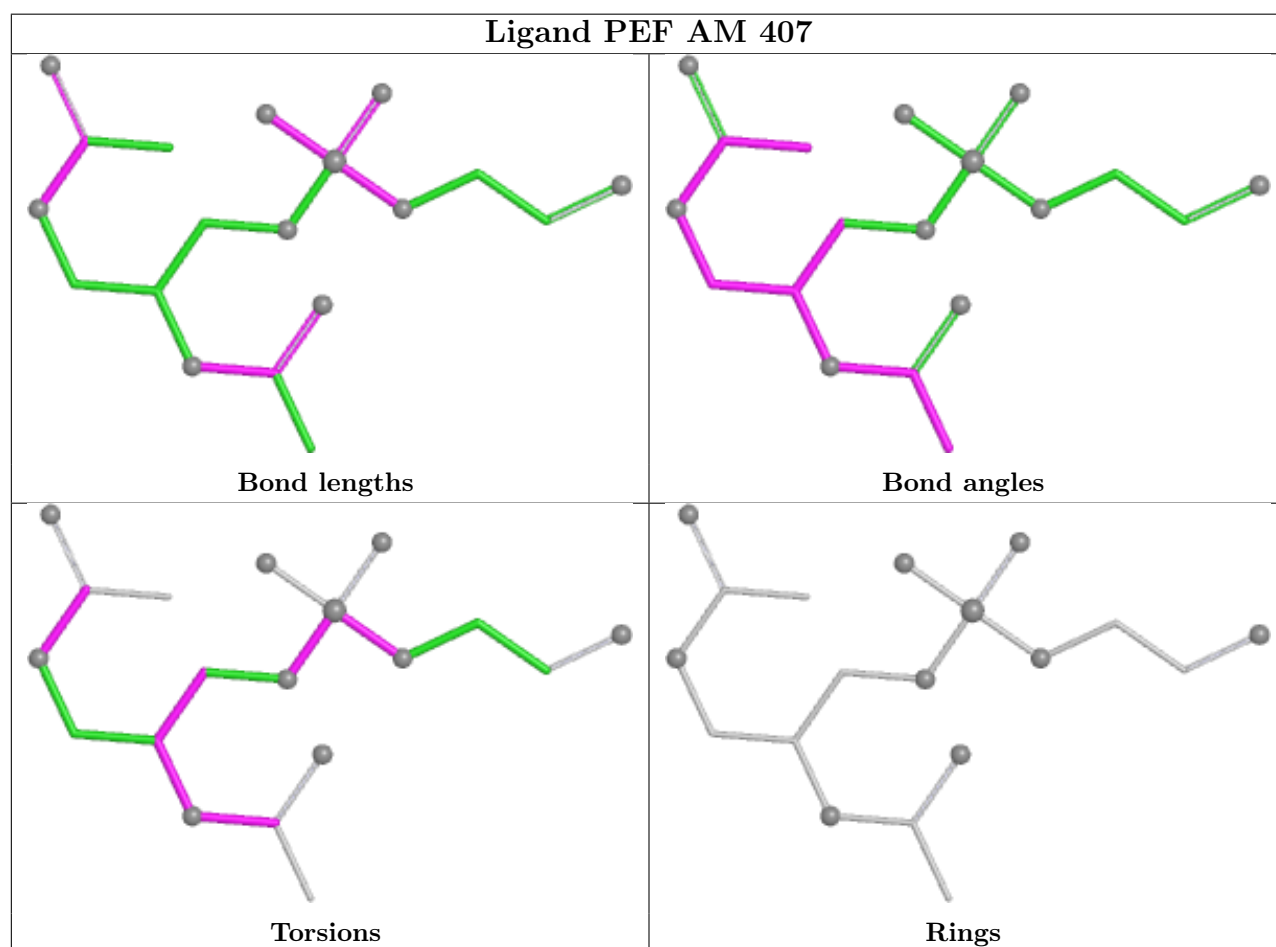
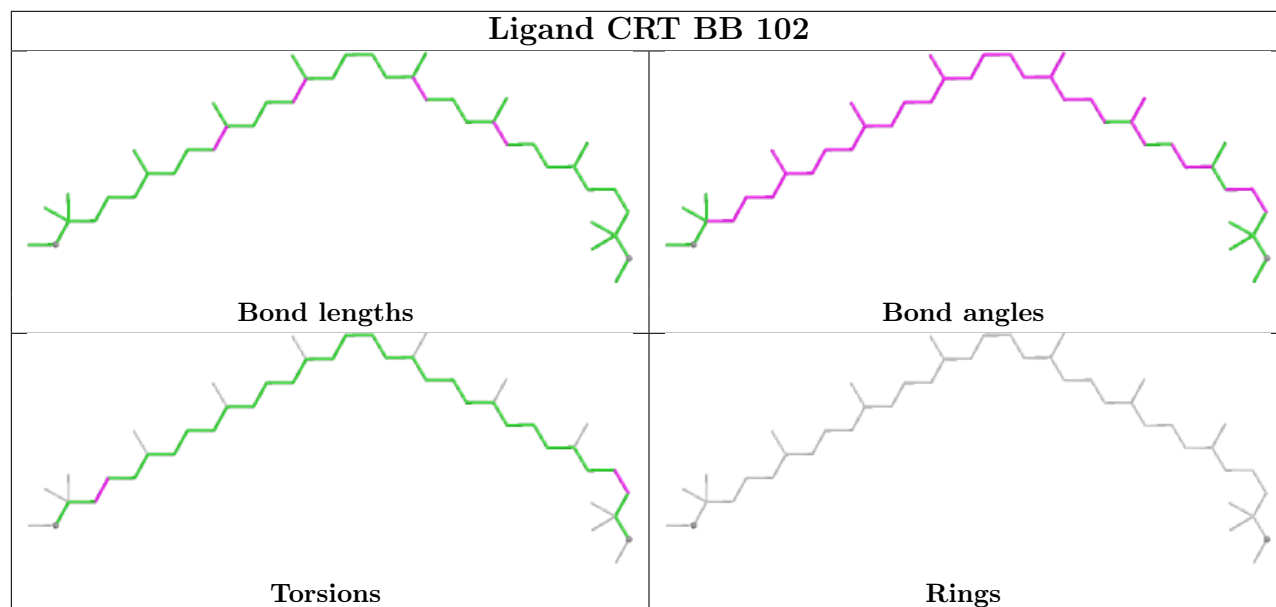


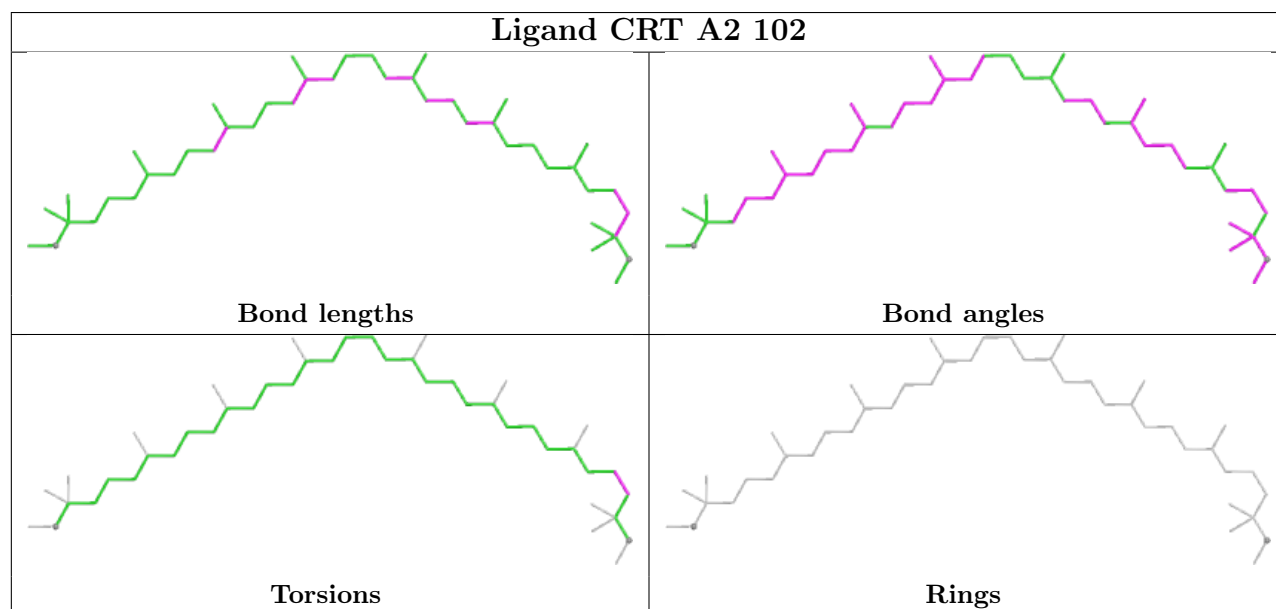
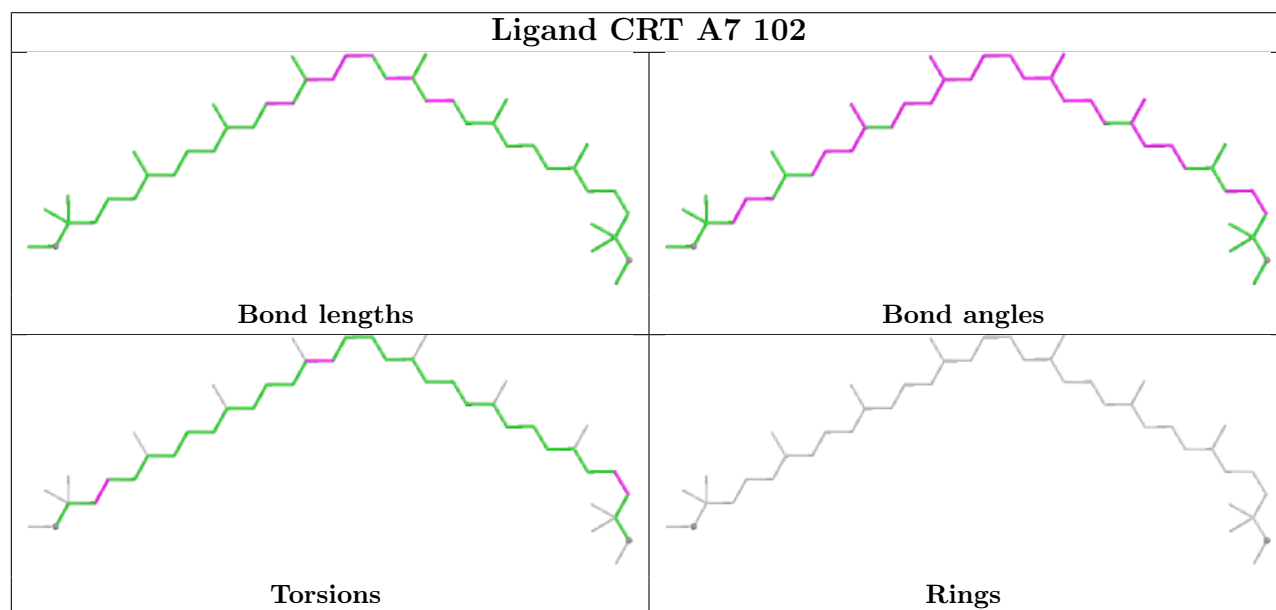
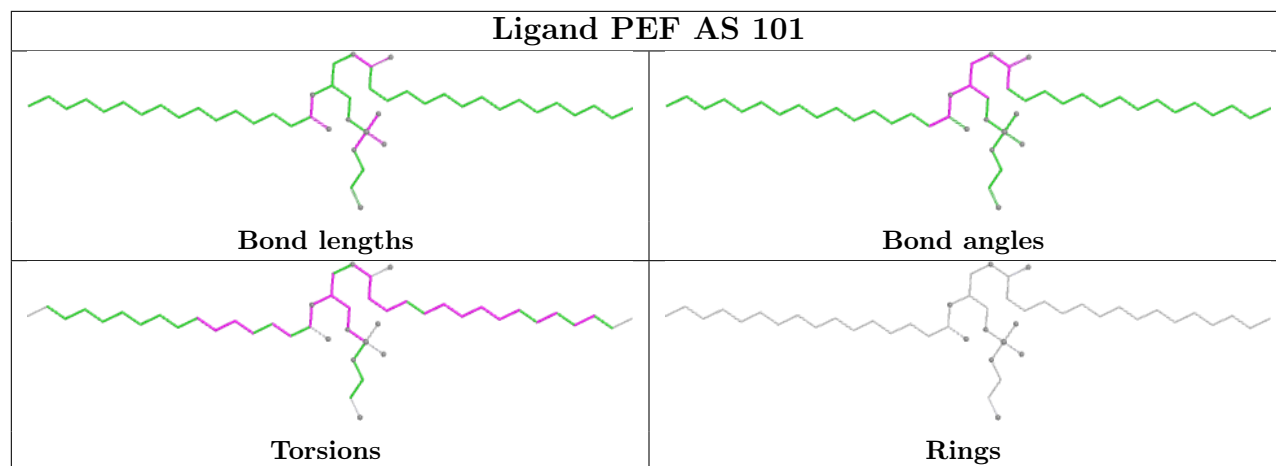


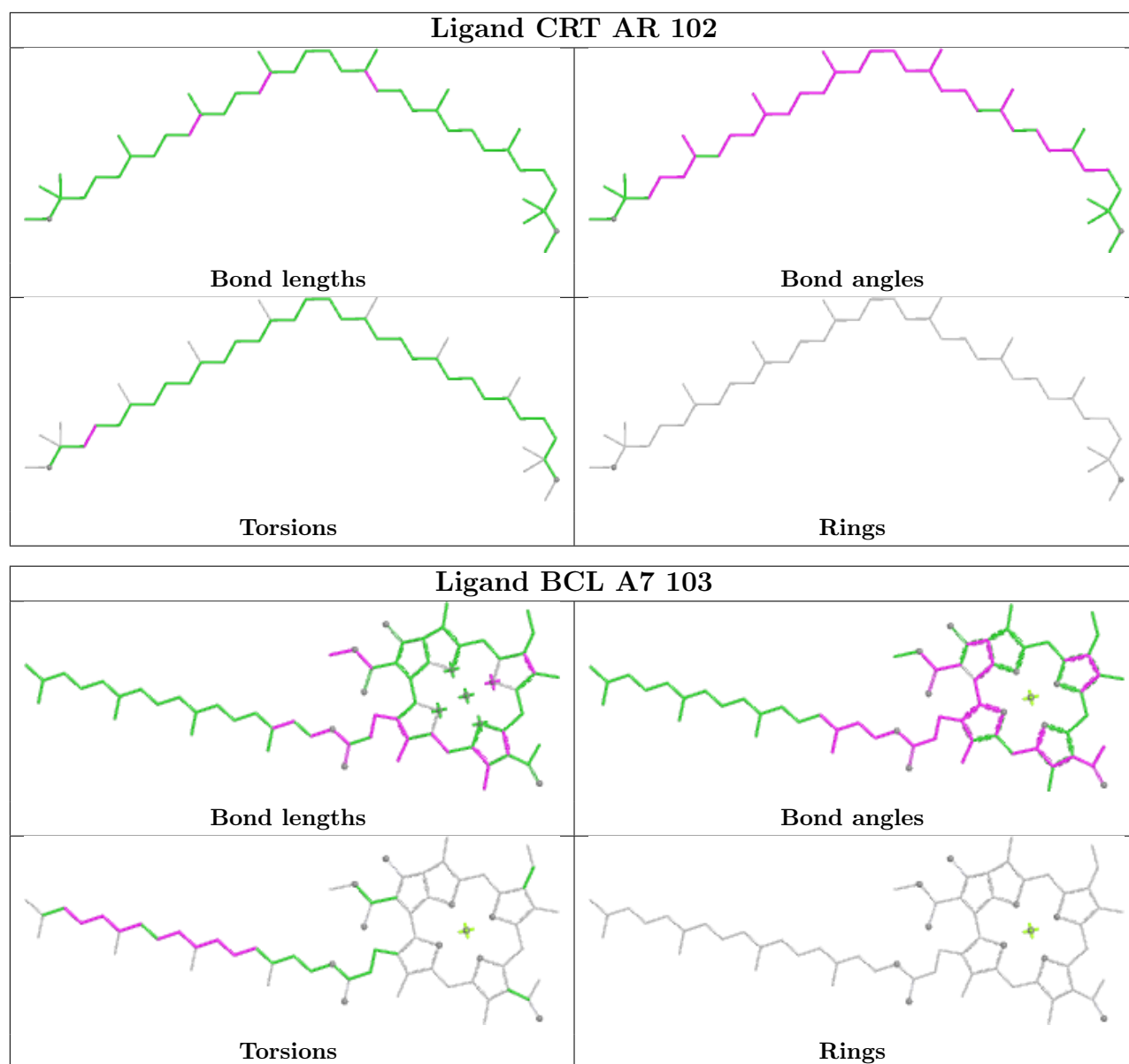


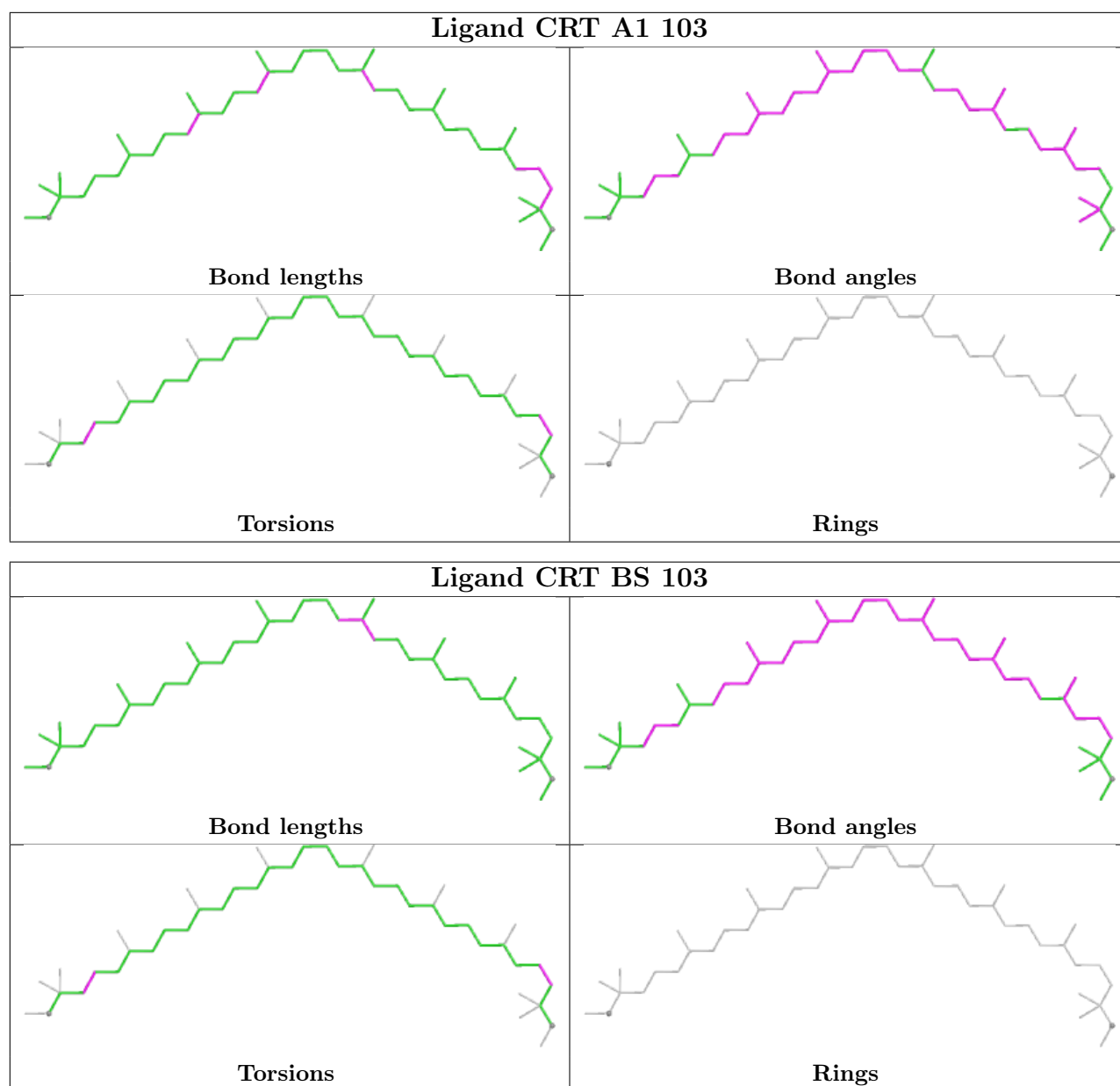




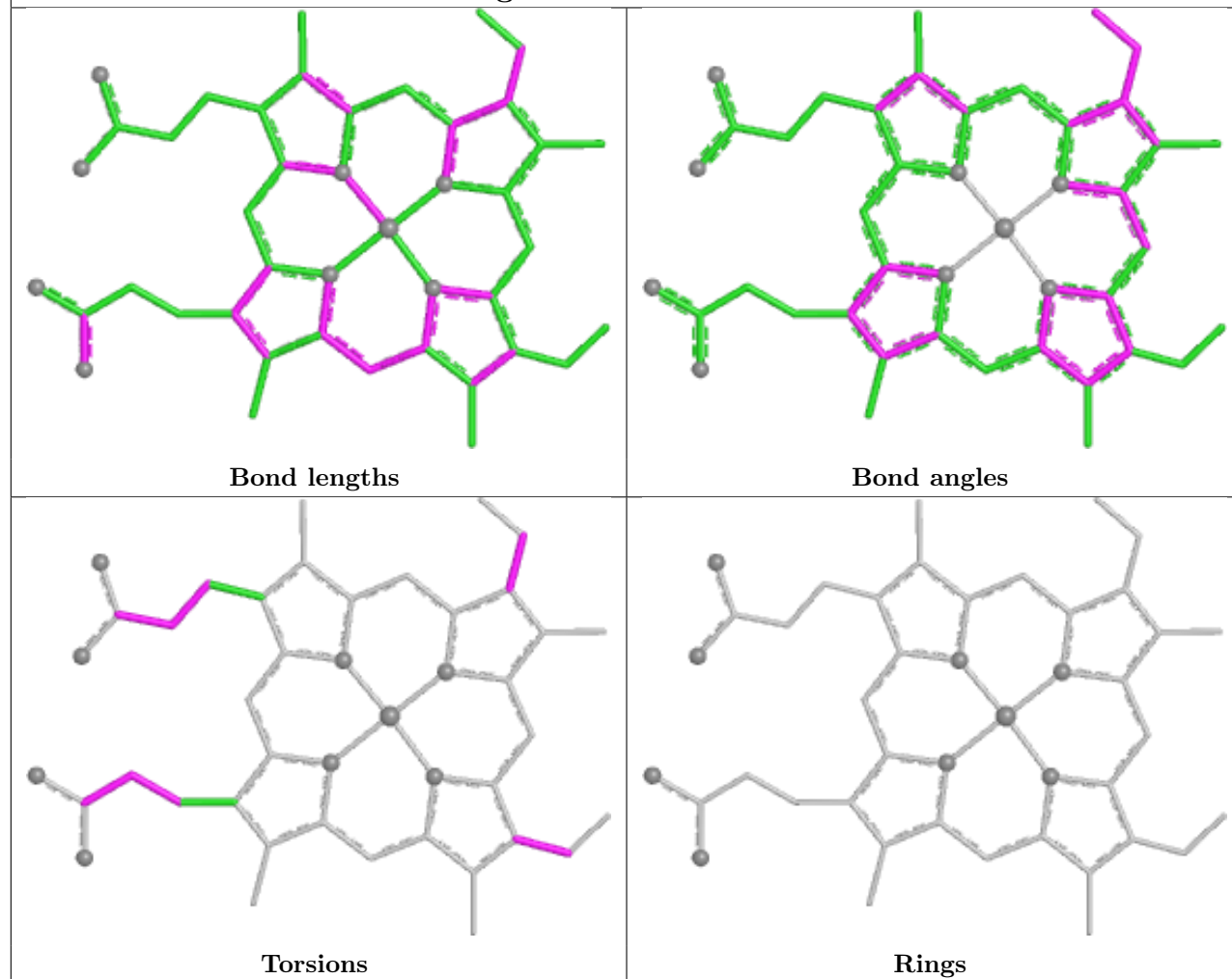




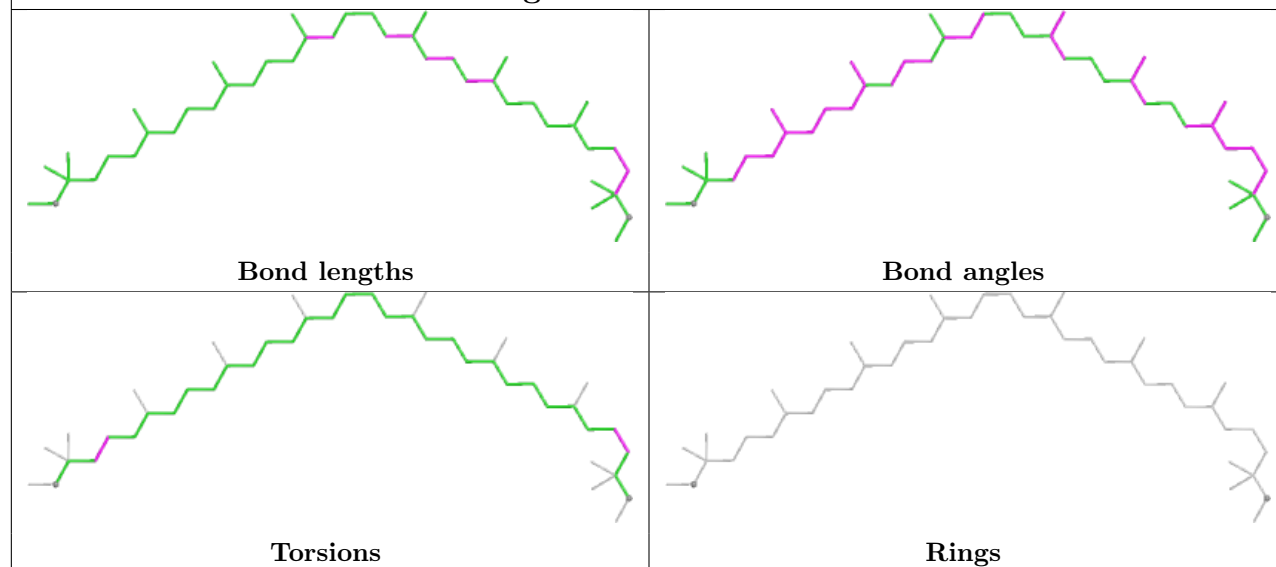


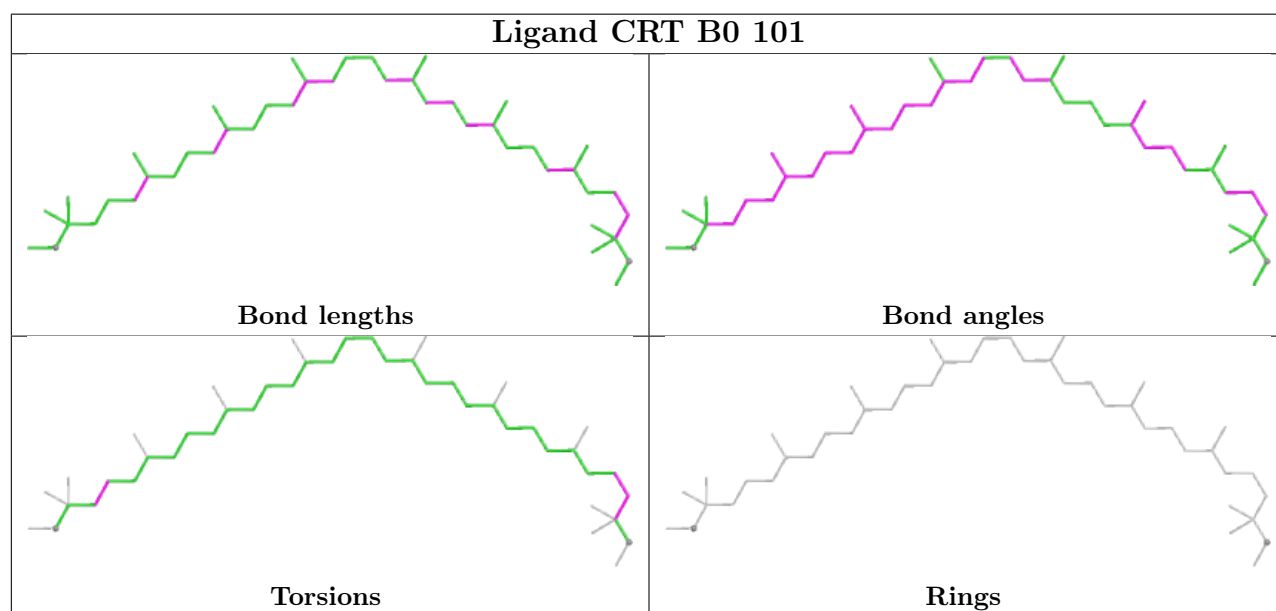
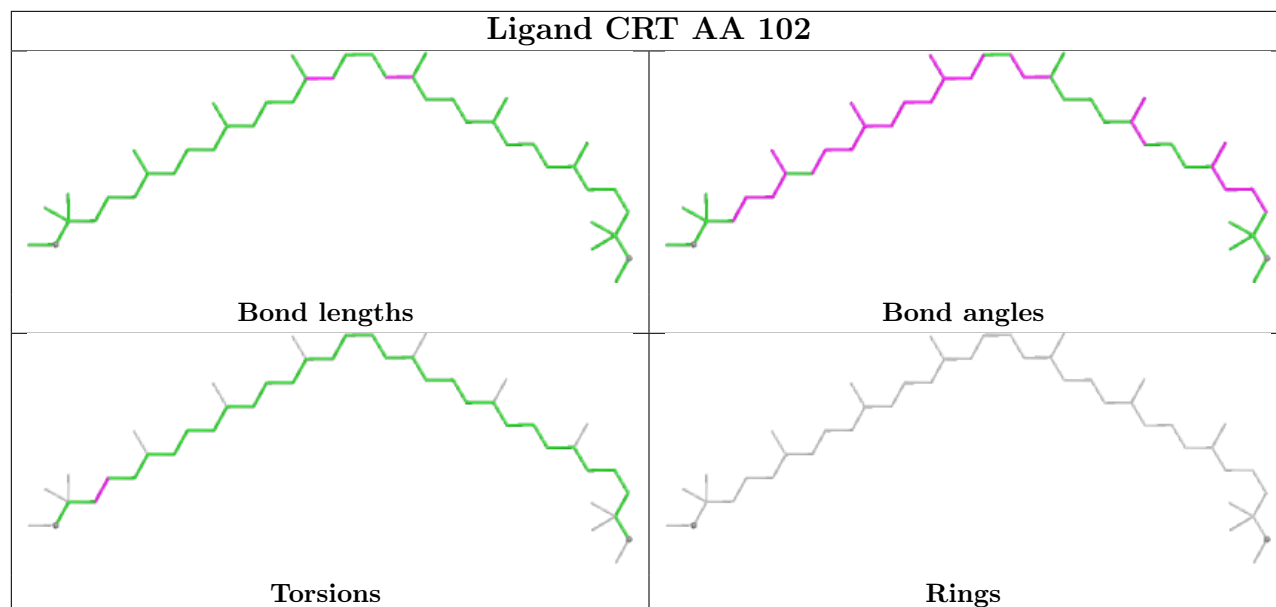


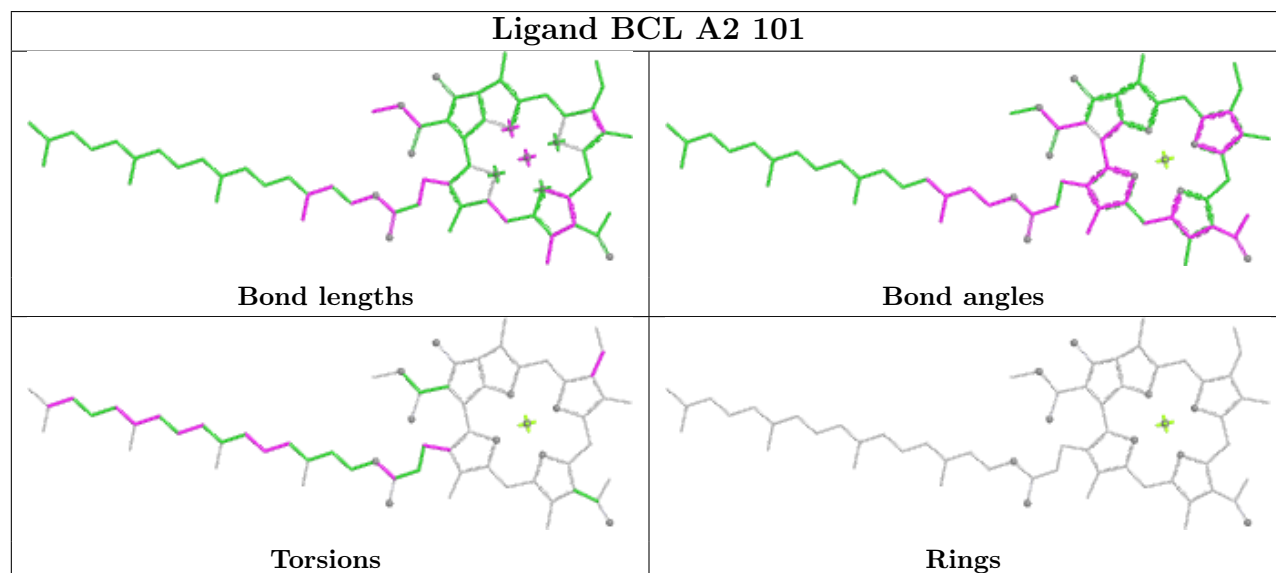
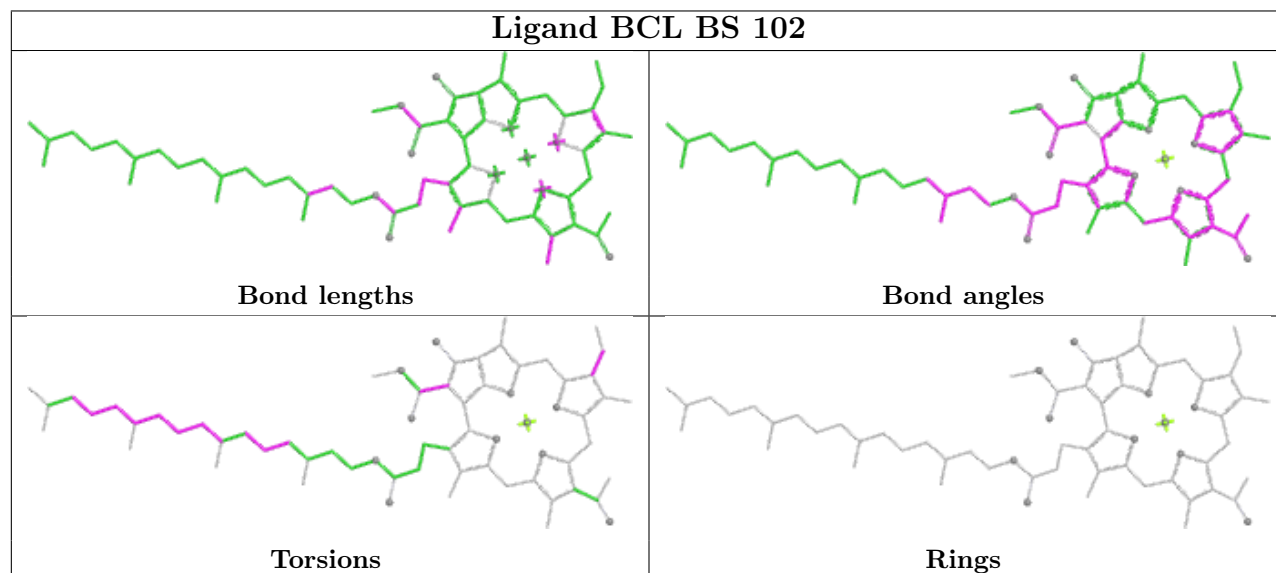
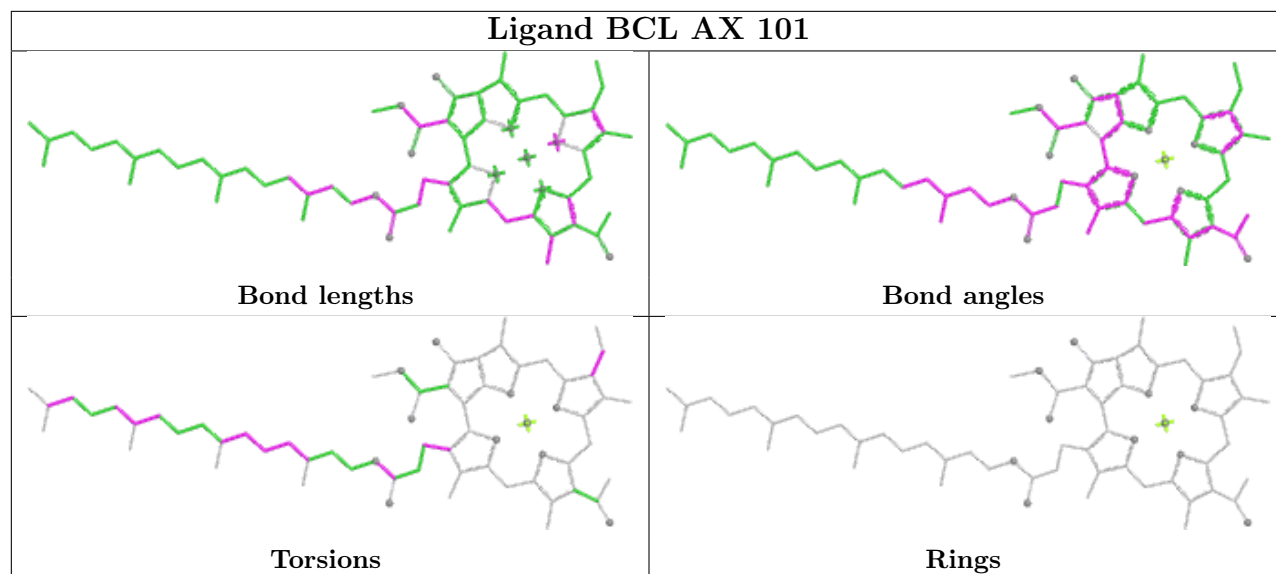
Ligand HEM BC 503

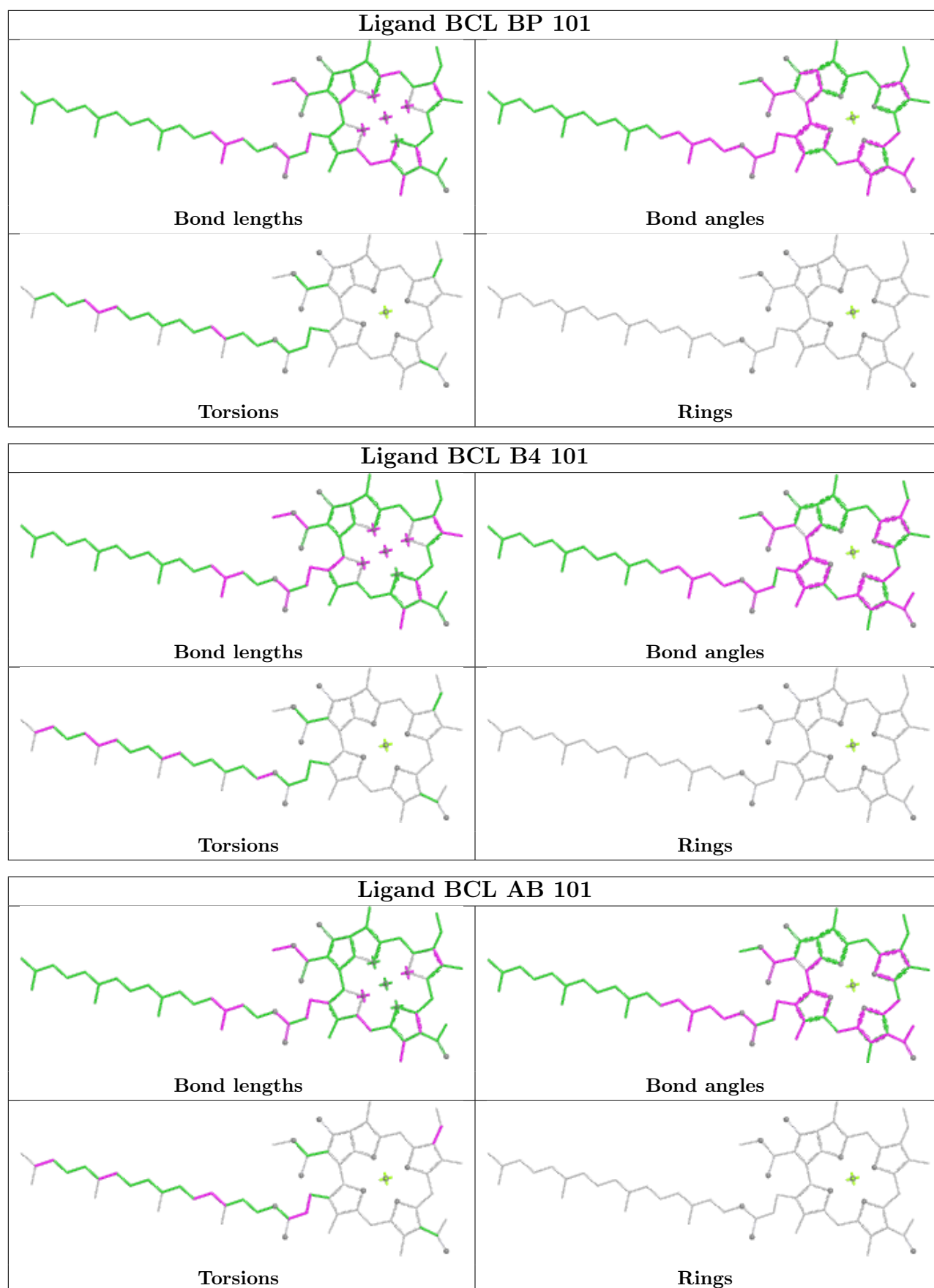


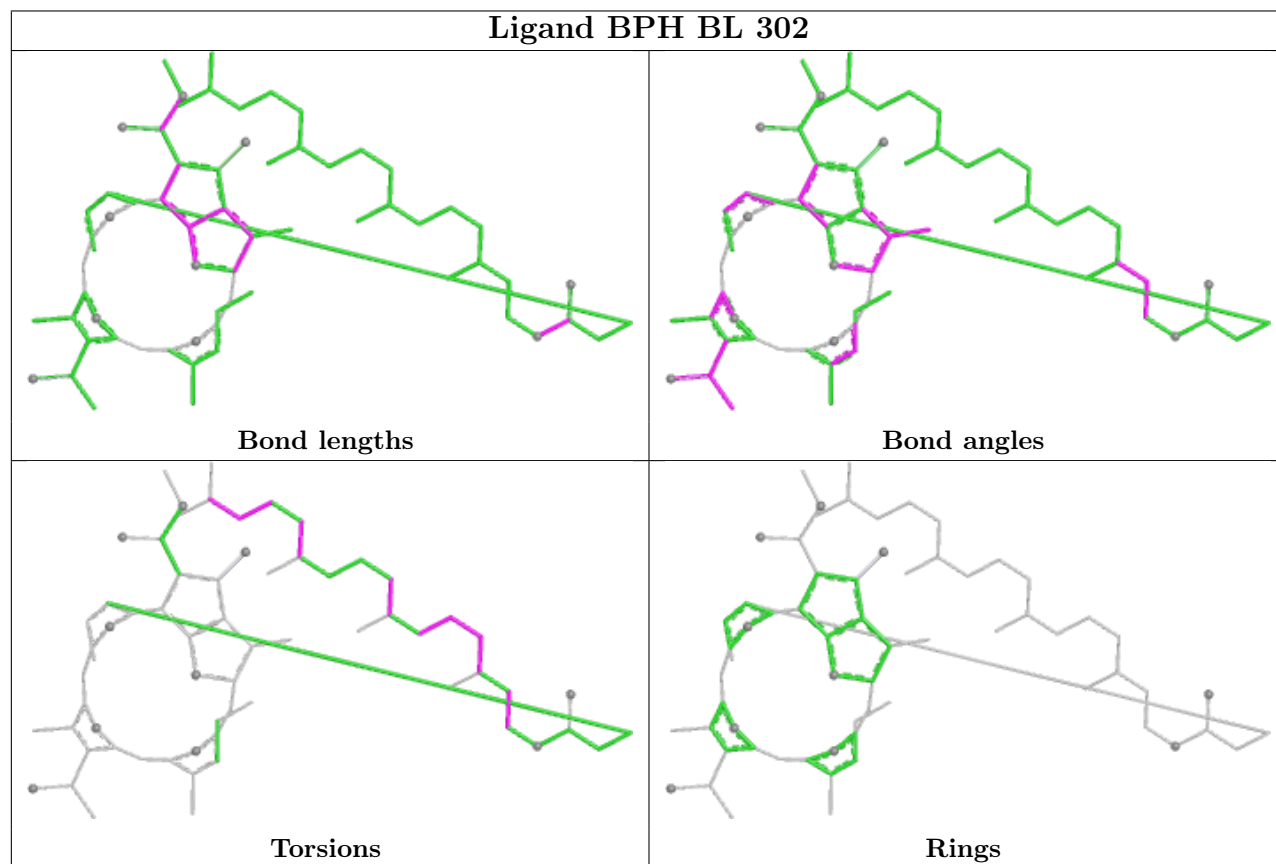
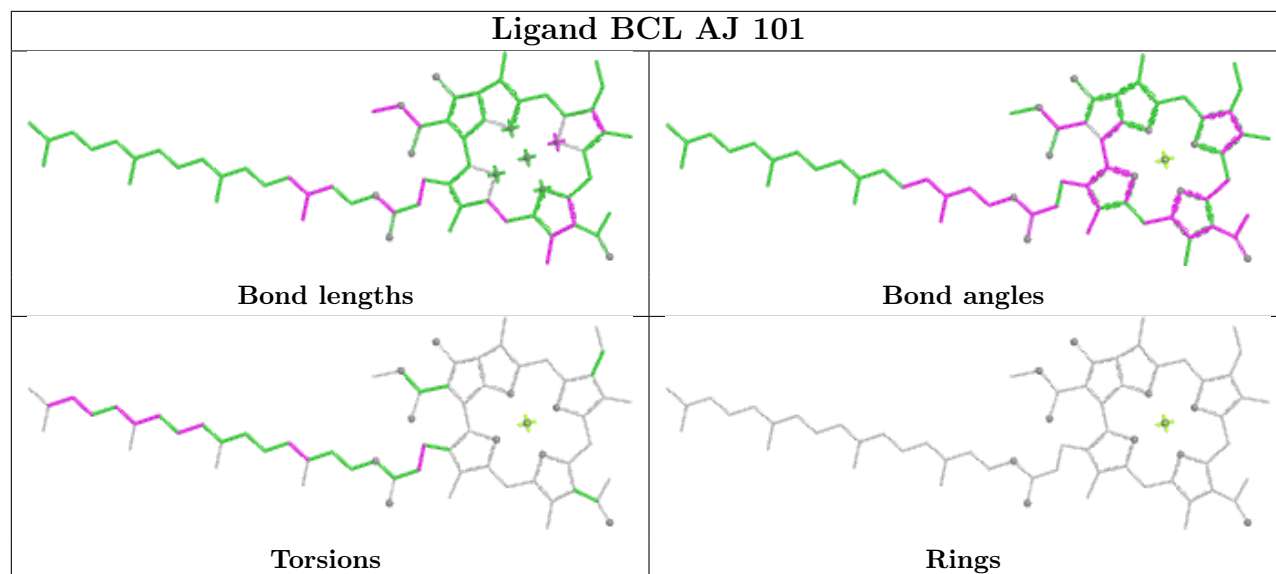
Ligand CRT B7 102

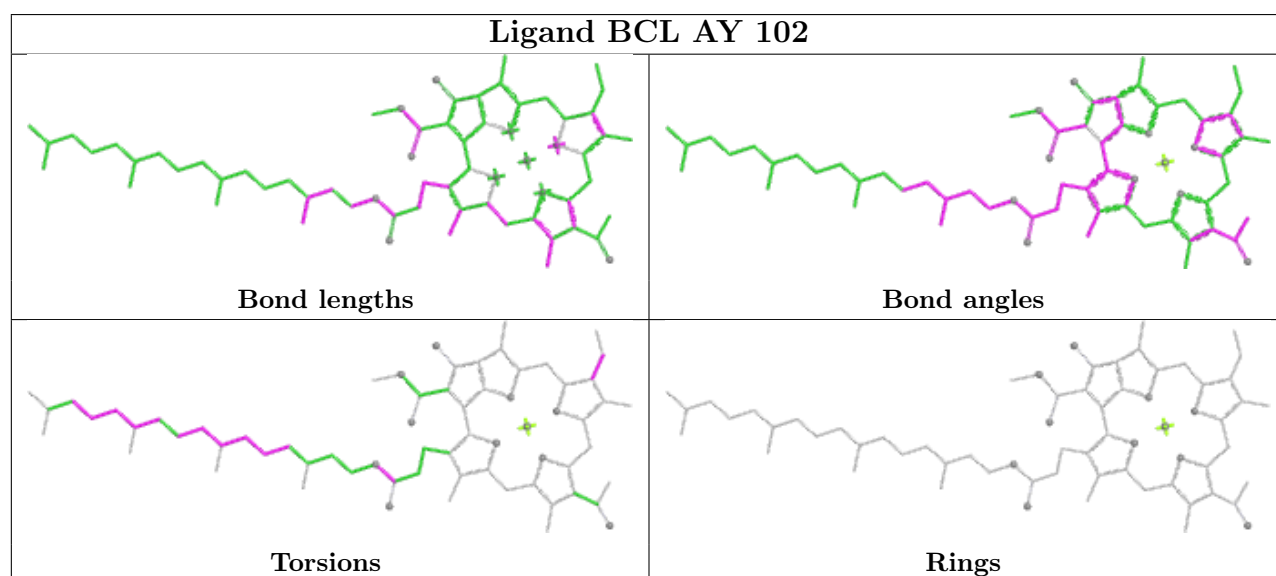
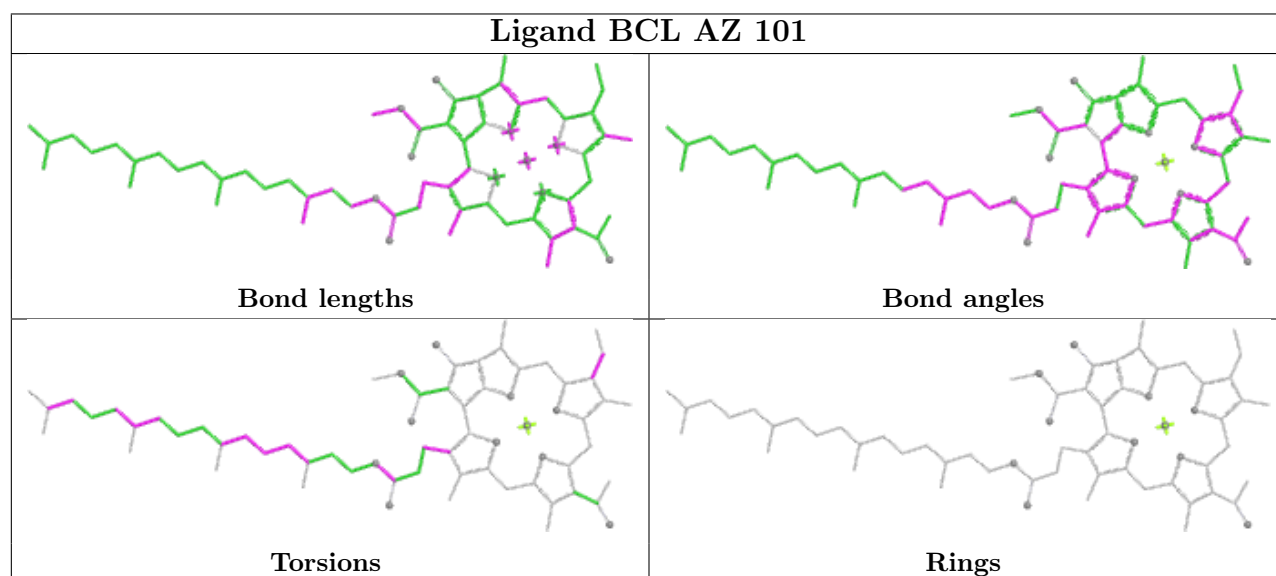
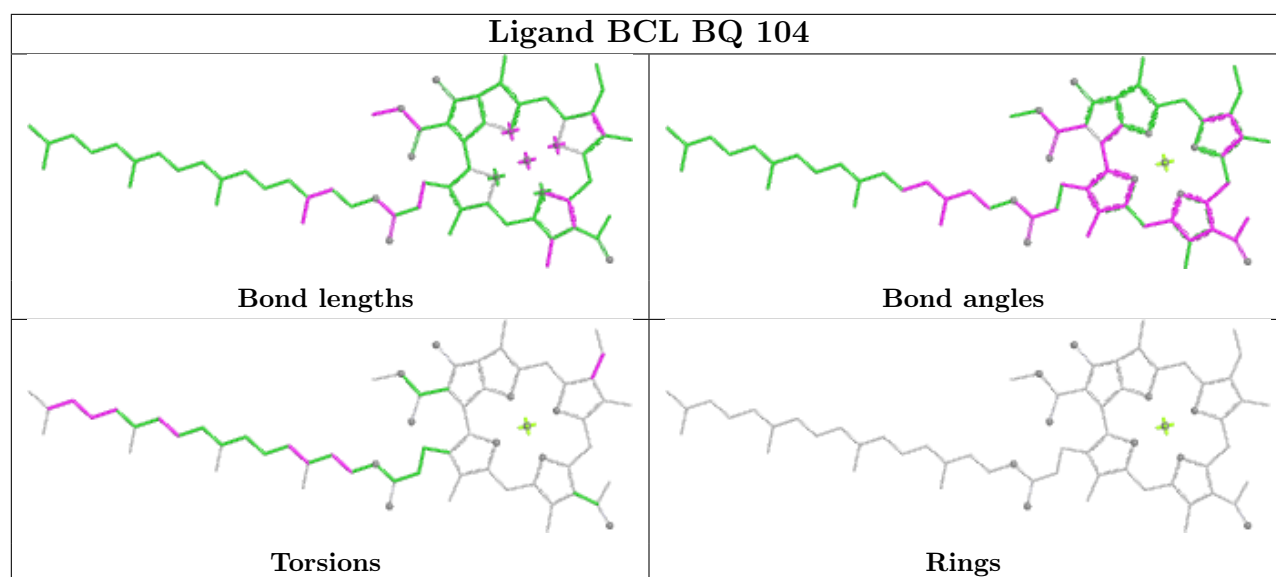


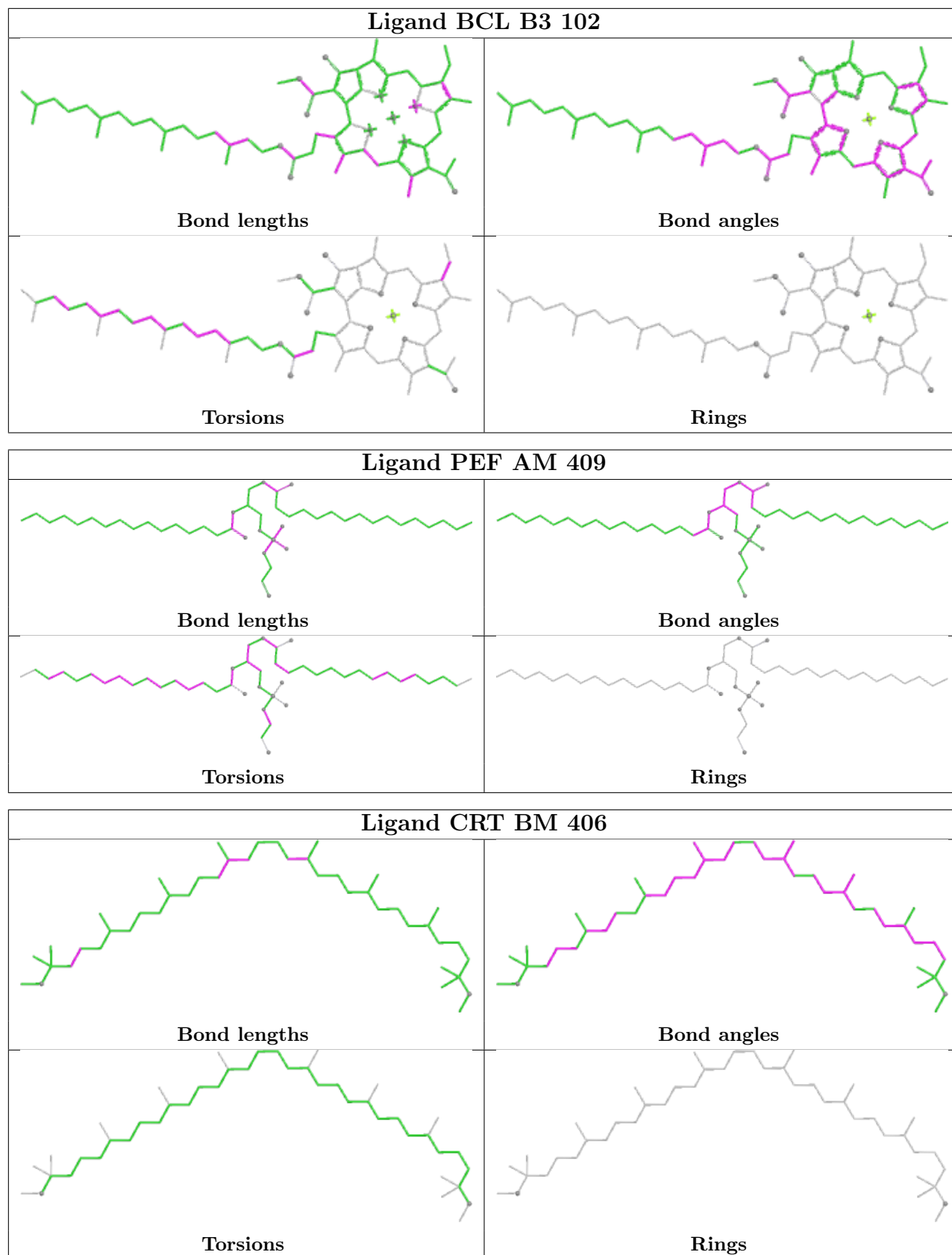












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AC	317/404 (78%)	-0.60	4 (1%) 75 53	5, 84, 141, 197	1 (0%)
1	BC	317/404 (78%)	-0.48	3 (0%) 81 61	8, 91, 139, 165	1 (0%)
2	AL	280/281 (99%)	-0.66	1 (0%) 88 76	21, 58, 119, 145	0
2	BL	280/281 (99%)	-0.60	1 (0%) 88 76	33, 77, 136, 156	0
3	AM	319/325 (98%)	-0.61	2 (0%) 85 69	19, 65, 107, 121	0
3	BM	319/325 (98%)	-0.67	0 100 100	37, 80, 125, 184	0
4	AH	258/259 (99%)	-0.55	4 (1%) 70 47	46, 95, 149, 183	0
4	BH	258/259 (99%)	-0.57	1 (0%) 88 76	57, 104, 164, 183	0
5	A1	58/61 (95%)	-0.37	3 (5%) 33 17	73, 163, 300, 305	0
5	A3	57/61 (93%)	-0.55	0 100 100	117, 162, 318, 320	0
5	A5	56/61 (91%)	-0.40	3 (5%) 31 16	70, 165, 320, 321	0
5	A7	51/61 (83%)	-0.35	0 100 100	111, 148, 234, 251	0
5	A9	60/61 (98%)	-0.39	0 100 100	96, 151, 319, 319	0
5	AA	48/61 (78%)	-0.52	0 100 100	92, 144, 241, 257	0
5	AD	57/61 (93%)	-0.12	4 (7%) 22 12	97, 145, 222, 239	0
5	AF	59/61 (96%)	-0.31	1 (1%) 69 45	99, 130, 226, 235	0
5	AI	59/61 (96%)	-0.13	3 (5%) 33 17	81, 143, 236, 267	0
5	AK	58/61 (95%)	-0.57	0 100 100	81, 140, 226, 261	0
5	AO	59/61 (96%)	-0.19	2 (3%) 48 27	88, 158, 258, 262	0
5	AQ	57/61 (93%)	-0.56	2 (3%) 47 27	56, 135, 277, 280	0
5	AS	59/61 (96%)	-0.24	3 (5%) 33 17	86, 158, 300, 309	0
5	AU	60/61 (98%)	-0.04	4 (6%) 24 12	144, 167, 252, 254	0
5	AW	60/61 (98%)	-0.34	4 (6%) 24 12	68, 135, 239, 250	0
5	AY	60/61 (98%)	-0.24	2 (3%) 49 28	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%)	-0.45	0 100 100	88, 126, 237, 238	0
5	B3	60/61 (98%)	-0.22	2 (3%) 49 28	103, 151, 262, 263	0
5	B5	51/61 (83%)	-0.57	0 100 100	131, 174, 234, 237	0
5	B7	54/61 (88%)	-0.34	1 (1%) 66 43	120, 191, 255, 261	0
5	B9	51/61 (83%)	-0.58	0 100 100	101, 150, 240, 241	0
5	BA	55/61 (90%)	-0.30	3 (5%) 30 15	112, 161, 261, 269	0
5	BD	45/61 (73%)	-0.08	3 (6%) 24 12	135, 140, 226, 247	0
5	BF	56/61 (91%)	-0.26	4 (7%) 22 11	135, 168, 237, 251	0
5	BI	50/61 (81%)	-0.57	1 (2%) 65 41	107, 134, 223, 229	0
5	BK	60/61 (98%)	-0.35	2 (3%) 49 28	152, 166, 314, 318	0
5	BO	59/61 (96%)	-0.66	1 (1%) 69 45	76, 129, 292, 295	0
5	BQ	59/61 (96%)	-0.29	2 (3%) 48 27	150, 168, 266, 274	0
5	BS	59/61 (96%)	-0.46	2 (3%) 48 27	91, 159, 250, 253	0
5	BU	58/61 (95%)	-0.21	1 (1%) 69 45	109, 150, 280, 282	0
5	BW	58/61 (95%)	-0.42	1 (1%) 69 45	49, 114, 230, 232	0
5	BY	54/61 (88%)	-0.44	0 100 100	46, 95, 222, 230	0
6	A0	40/47 (85%)	-0.35	0 100 100	166, 177, 205, 220	0
6	A2	40/47 (85%)	-0.59	0 100 100	122, 146, 202, 211	0
6	A4	40/47 (85%)	-0.60	2 (5%) 34 18	147, 151, 221, 222	0
6	A6	40/47 (85%)	-0.63	1 (2%) 58 35	140, 155, 199, 213	0
6	A8	40/47 (85%)	-0.35	3 (7%) 20 10	129, 187, 225, 229	0
6	AB	40/47 (85%)	-0.39	1 (2%) 58 35	122, 162, 189, 190	0
6	AE	40/47 (85%)	-0.30	2 (5%) 34 18	120, 145, 169, 184	0
6	AG	40/47 (85%)	-0.63	0 100 100	74, 116, 140, 145	0
6	AJ	40/47 (85%)	-0.59	1 (2%) 58 35	118, 129, 154, 159	0
6	AN	40/47 (85%)	-0.69	1 (2%) 58 35	101, 121, 155, 161	0
6	AP	40/47 (85%)	-0.63	1 (2%) 58 35	106, 142, 245, 248	0
6	AR	40/47 (85%)	-0.30	2 (5%) 34 18	122, 157, 194, 199	0
6	AT	40/47 (85%)	-0.52	0 100 100	119, 148, 198, 205	0
6	AV	40/47 (85%)	-0.30	1 (2%) 58 35	130, 167, 222, 225	0
6	AX	40/47 (85%)	-0.23	0 100 100	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%)	-0.52	0 100 100	111, 137, 238, 240	0
6	B0	40/47 (85%)	-0.35	2 (5%) 34 18	197, 208, 220, 221	0
6	B2	40/47 (85%)	-0.90	0 100 100	116, 127, 158, 162	0
6	B4	40/47 (85%)	-0.48	2 (5%) 34 18	134, 156, 191, 199	0
6	B6	40/47 (85%)	-0.73	0 100 100	115, 152, 213, 215	0
6	B8	40/47 (85%)	-0.59	0 100 100	123, 199, 232, 234	0
6	BB	40/47 (85%)	-0.78	0 100 100	155, 164, 228, 231	0
6	BE	40/47 (85%)	-0.73	0 100 100	148, 170, 194, 212	0
6	BG	40/47 (85%)	-0.13	4 (10%) 12 7	185, 204, 218, 220	0
6	BJ	40/47 (85%)	-0.56	0 100 100	199, 204, 208, 209	0
6	BN	40/47 (85%)	-0.66	0 100 100	152, 160, 194, 200	0
6	BP	40/47 (85%)	-0.90	1 (2%) 58 35	124, 149, 226, 230	0
6	BR	40/47 (85%)	-0.25	4 (10%) 12 7	138, 171, 206, 213	0
6	BT	40/47 (85%)	-0.64	0 100 100	132, 157, 227, 233	0
6	BV	40/47 (85%)	-0.75	1 (2%) 58 35	91, 143, 170, 174	0
6	BX	40/47 (85%)	-0.77	0 100 100	100, 127, 169, 172	0
6	BZ	40/47 (85%)	-0.72	0 100 100	121, 135, 178, 186	0
All	All	5429/5994 (90%)	-0.50	99 (1%) 67 44	5, 123, 236, 321	2 (0%)

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	BD	41	SER	8.9
5	AI	13	LEU	7.4
5	BS	5	ASN	5.8
5	AW	46	TRP	5.3
5	AS	48	ASP	5.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CA	AO	101	1/1	0.94	0.07	267,267,267,267	0
16	PO4	A3	101	5/5	0.94	0.08	153,154,154,154	0
8	CA	B9	101	1/1	0.95	0.05	150,150,150,150	0
14	CRT	AN	102	44/44	0.95	0.15	133,135,140,140	0
14	CRT	A0	101	44/44	0.95	0.17	179,184,194,195	0
14	CRT	BV	102	44/44	0.95	0.19	208,214,218,220	0
15	PEF	BQ	101	47/47	0.95	0.17	121,145,161,161	0
8	CA	AS	102	1/1	0.95	0.06	190,190,190,190	0
14	CRT	AB	102	44/44	0.96	0.14	170,172,177,178	0
8	CA	A5	101	1/1	0.96	0.04	255,255,255,255	0
9	BCL	AM	402	66/66	0.96	0.11	40,48,81,101	0
14	CRT	BG	102	44/44	0.96	0.10	122,130,143,145	0
14	CRT	BP	102	44/44	0.96	0.13	149,151,153,154	0
9	BCL	A3	103	66/66	0.96	0.14	127,137,178,178	0
14	CRT	B1	103	44/44	0.96	0.15	205,224,238,240	0
9	BCL	BQ	104	66/66	0.96	0.14	181,191,253,254	0
11	UQ8	AL	304	53/53	0.96	0.14	74,107,143,151	0
9	BCL	AR	101	66/66	0.97	0.10	187,200,230,231	0
9	BCL	A2	101	66/66	0.97	0.14	122,133,201,203	0
8	CA	AK	101	1/1	0.97	0.06	216,216,216,216	0
9	BCL	A3	104	66/66	0.97	0.12	151,177,223,224	0
9	BCL	A6	101	66/66	0.97	0.12	238,254,268,272	0
9	BCL	A8	101	66/66	0.97	0.09	201,214,245,247	0
9	BCL	BL	301	66/66	0.97	0.09	36,53,94,100	0
9	BCL	BM	402	66/66	0.97	0.11	41,58,73,79	0
9	BCL	BA	101	66/66	0.97	0.10	206,224,237,238	0
9	BCL	BD	102	66/66	0.97	0.11	147,182,237,238	0
9	BCL	BF	102	66/66	0.97	0.12	143,168,206,210	0
9	BCL	BI	102	66/66	0.97	0.10	131,159,208,208	0
9	BCL	BJ	101	66/66	0.97	0.10	202,204,207,208	0
9	BCL	BP	101	66/66	0.97	0.09	156,173,208,209	0
8	CA	BD	101	1/1	0.97	0.04	236,236,236,236	0
9	BCL	BU	102	66/66	0.97	0.12	144,161,240,240	0
9	BCL	BW	102	66/66	0.97	0.15	129,145,213,213	0
9	BCL	BX	101	66/66	0.97	0.11	126,139,204,205	0
9	BCL	BZ	101	66/66	0.97	0.10	125,139,192,193	0
9	BCL	B8	101	66/66	0.97	0.09	226,245,252,258	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	BCL	B9	102	66/66	0.97	0.11	205,229,236,237	0
10	BPH	AM	403	65/65	0.97	0.10	43,61,150,153	0
10	BPH	BL	302	65/65	0.97	0.10	36,63,98,116	0
8	CA	BI	101	1/1	0.97	0.05	236,236,236,236	0
11	UQ8	BL	304	53/53	0.97	0.12	66,137,159,166	0
13	MQ8	AM	405	53/53	0.97	0.12	76,93,128,137	0
14	CRT	AA	102	44/44	0.97	0.13	164,164,167,167	0
8	CA	B7	101	1/1	0.97	0.05	259,259,259,259	0
14	CRT	AG	102	44/44	0.97	0.14	126,127,135,138	0
14	CRT	AJ	102	44/44	0.97	0.12	138,140,144,147	0
8	CA	AA	103	1/1	0.97	0.07	275,275,275,275	0
14	CRT	AP	102	44/44	0.97	0.13	137,140,147,148	0
14	CRT	AS	104	44/44	0.97	0.15	165,170,177,180	0
14	CRT	AW	102	44/44	0.97	0.16	127,136,144,147	0
14	CRT	AX	102	44/44	0.97	0.14	218,225,227,229	0
14	CRT	A5	103	44/44	0.97	0.16	167,174,185,187	0
14	CRT	A7	102	44/44	0.97	0.11	126,137,150,152	0
9	BCL	AL	301	66/66	0.97	0.10	38,50,92,96	0
14	CRT	BA	102	44/44	0.97	0.13	143,157,171,174	0
14	CRT	BB	102	44/44	0.97	0.15	169,185,201,205	0
14	CRT	BF	103	44/44	0.97	0.11	134,141,147,149	0
8	CA	AD	101	1/1	0.97	0.06	238,238,238,238	0
14	CRT	BN	102	44/44	0.97	0.11	134,135,140,141	0
14	CRT	BO	103	44/44	0.97	0.15	179,182,185,186	0
9	BCL	AB	101	66/66	0.97	0.11	124,158,224,224	0
14	CRT	BU	103	44/44	0.97	0.15	161,173,176,176	0
9	BCL	AE	101	66/66	0.97	0.12	135,156,211,212	0
9	BCL	AJ	101	66/66	0.97	0.11	134,165,191,193	0
14	CRT	B5	103	44/44	0.97	0.17	178,198,221,226	0
14	CRT	B0	101	44/44	0.97	0.19	202,220,238,242	0
15	PEF	AM	409	47/47	0.97	0.15	129,183,183,183	0
15	PEF	AS	101	47/47	0.97	0.12	178,225,225,225	0
9	BCL	AK	102	66/66	0.97	0.12	142,154,184,184	0
9	BCL	AN	101	66/66	0.97	0.10	106,126,157,171	0
9	BCL	BT	101	66/66	0.98	0.11	176,191,253,254	0
8	CA	AV	101	1/1	0.98	0.05	168,168,168,168	0
9	BCL	BV	101	66/66	0.98	0.14	172,194,218,220	0
9	BCL	AF	102	66/66	0.98	0.14	156,175,222,222	0
9	BCL	AG	101	66/66	0.98	0.11	105,132,177,178	0
9	BCL	BY	102	66/66	0.98	0.09	110,129,169,169	0
9	BCL	AI	102	66/66	0.98	0.11	148,163,190,191	0
9	BCL	B1	102	66/66	0.98	0.09	87,118,185,186	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	BCL	B2	101	66/66	0.98	0.11	136,152,203,204	0
9	BCL	B3	102	66/66	0.98	0.07	104,112,169,170	0
9	BCL	B4	101	66/66	0.98	0.10	149,166,212,214	0
9	BCL	B5	102	66/66	0.98	0.09	154,171,221,221	0
9	BCL	B6	101	66/66	0.98	0.12	238,251,261,264	0
9	BCL	B7	103	66/66	0.98	0.11	232,250,259,260	0
8	CA	A3	102	1/1	0.98	0.08	256,256,256,256	0
7	HEM	AC	502	43/43	0.98	0.09	53,68,81,88	0
9	BCL	B0	102	66/66	0.98	0.10	198,202,205,207	0
10	BPH	AL	302	65/65	0.98	0.09	31,54,75,84	0
8	CA	A9	101	1/1	0.98	0.04	268,268,268,268	0
8	CA	BA	103	1/1	0.98	0.05	283,283,283,283	0
10	BPH	BM	403	65/65	0.98	0.10	72,96,164,176	0
9	BCL	AS	103	66/66	0.98	0.12	206,220,229,233	0
9	BCL	AT	101	66/66	0.98	0.10	187,198,247,248	0
9	BCL	AV	102	66/66	0.98	0.11	183,194,249,250	0
13	MQ8	BM	405	53/53	0.98	0.11	68,99,166,168	0
14	CRT	AM	406	44/44	0.98	0.09	58,70,105,107	0
9	BCL	AX	101	66/66	0.98	0.12	157,171,252,255	0
9	BCL	AZ	101	66/66	0.98	0.12	120,142,217,218	0
7	HEM	AC	503	43/43	0.98	0.10	71,84,106,112	0
8	CA	AI	101	1/1	0.98	0.04	224,224,224,224	0
8	CA	BO	101	1/1	0.98	0.04	238,238,238,238	0
9	BCL	A5	102	66/66	0.98	0.11	152,159,199,200	0
14	CRT	AR	102	44/44	0.98	0.12	189,193,200,201	0
8	CA	BU	101	1/1	0.98	0.04	237,237,237,237	0
14	CRT	AT	102	44/44	0.98	0.14	200,205,209,210	0
9	BCL	A7	103	66/66	0.98	0.12	239,243,267,268	0
8	CA	BW	101	1/1	0.98	0.04	204,204,204,204	0
14	CRT	A1	103	44/44	0.98	0.10	110,123,135,138	0
14	CRT	A2	102	44/44	0.98	0.13	107,117,146,149	0
9	BCL	A9	102	66/66	0.98	0.14	213,227,251,252	0
9	BCL	A0	102	66/66	0.98	0.11	199,210,239,240	0
7	HEM	AC	504	43/43	0.98	0.09	39,76,101,104	0
9	BCL	BL	303	66/66	0.98	0.08	39,55,82,90	0
9	BCL	BM	401	66/66	0.98	0.08	33,56,137,146	0
7	HEM	BC	502	43/43	0.98	0.09	50,80,94,103	0
8	CA	AQ	101	1/1	0.98	0.05	207,207,207,207	0
9	BCL	AL	303	66/66	0.98	0.08	32,54,95,104	0
9	BCL	AM	401	66/66	0.98	0.09	19,34,93,96	0
9	BCL	BG	101	66/66	0.98	0.09	201,207,214,217	0
14	CRT	BS	103	44/44	0.98	0.12	193,197,199,200	0

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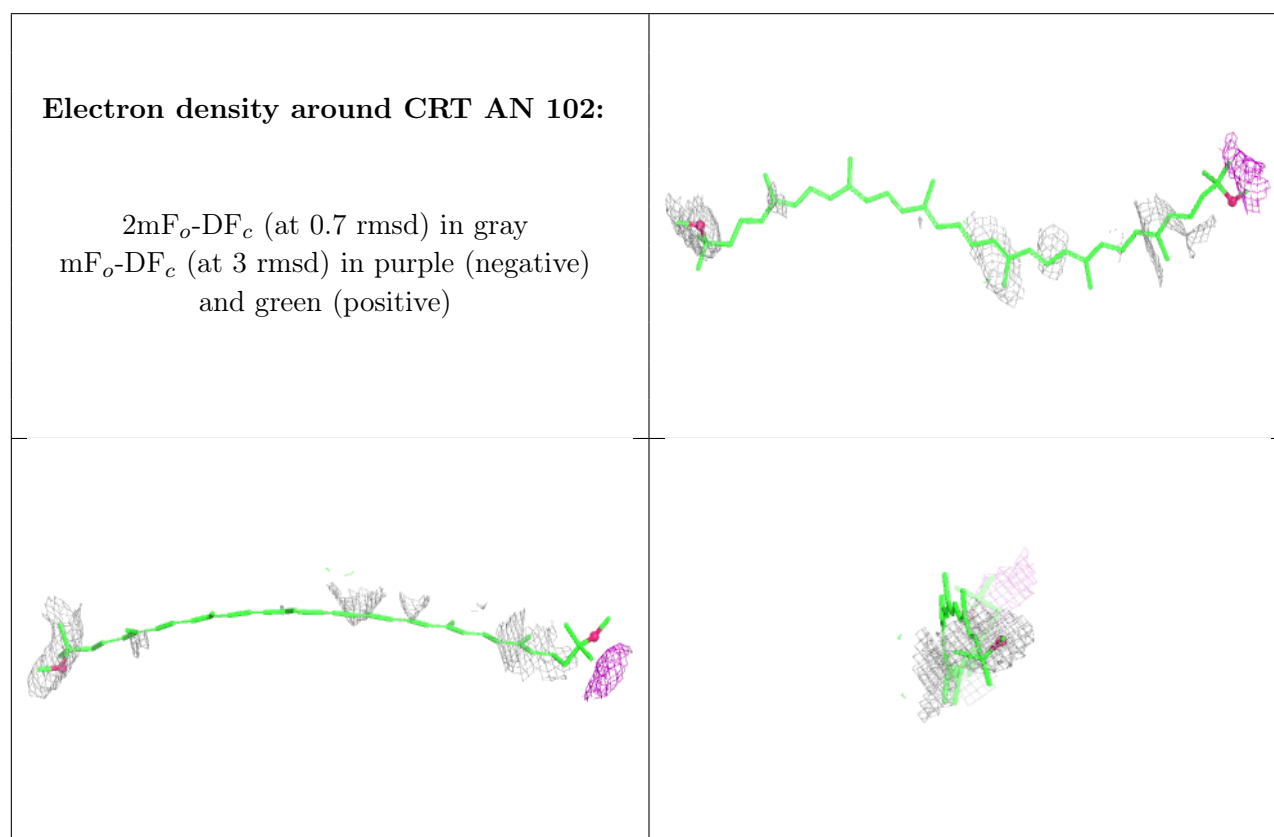
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	HEM	BC	504	43/43	0.98	0.08	55,78,92,106	0
9	BCL	AA	101	66/66	0.98	0.16	235,252,257,260	0
14	CRT	BW	103	44/44	0.98	0.11	129,145,156,161	0
9	BCL	BK	102	66/66	0.98	0.10	194,257,267,269	0
14	CRT	B2	102	44/44	0.98	0.14	132,151,166,171	0
9	BCL	BN	101	66/66	0.98	0.10	153,170,192,193	0
14	CRT	B7	102	44/44	0.98	0.12	173,194,212,217	0
9	BCL	BO	102	66/66	0.98	0.09	153,180,189,193	0
15	PEF	AM	407	19/47	0.98	0.10	114,165,177,177	0
8	CA	AU	101	1/1	0.98	0.05	223,223,223,223	0
15	PEF	AH	301	19/47	0.98	0.08	128,144,161,167	0
9	BCL	BQ	103	66/66	0.98	0.13	168,191,225,226	0
15	PEF	BM	407	19/47	0.98	0.11	102,136,173,178	0
9	BCL	AD	102	66/66	0.98	0.14	179,196,260,263	0
9	BCL	BS	102	66/66	0.98	0.11	152,193,231,231	0
16	PO4	BH	301	5/5	0.98	0.07	108,109,109,110	0
8	CA	B5	101	1/1	0.99	0.03	226,226,226,226	0
9	BCL	BE	101	66/66	0.99	0.08	146,170,225,227	0
8	CA	A7	101	1/1	0.99	0.03	213,213,213,213	0
14	CRT	BM	406	44/44	0.99	0.08	69,74,96,109	0
8	CA	AF	101	1/1	0.99	0.05	254,254,254,254	0
9	BCL	AU	102	66/66	0.99	0.11	161,175,231,234	0
8	CA	BC	505	1/1	0.99	0.06	69,69,69,69	0
9	BCL	AW	101	66/66	0.99	0.10	143,191,243,243	0
7	HEM	BC	501	43/43	0.99	0.07	52,60,117,131	0
9	BCL	AY	102	66/66	0.99	0.10	133,140,195,196	0
8	CA	AC	505	1/1	0.99	0.09	30,30,30,30	0
12	FE	AM	404	1/1	0.99	0.04	47,47,47,47	0
9	BCL	A1	102	66/66	0.99	0.10	96,135,194,194	0
8	CA	BF	101	1/1	0.99	0.03	276,276,276,276	0
8	CA	AY	101	1/1	0.99	0.06	197,197,197,197	0
8	CA	BK	101	1/1	0.99	0.05	275,275,275,275	0
8	CA	A1	101	1/1	0.99	0.05	212,212,212,212	0
8	CA	BQ	102	1/1	0.99	0.04	249,249,249,249	0
8	CA	BS	101	1/1	0.99	0.04	222,222,222,222	0
7	HEM	AC	501	43/43	0.99	0.08	86,86,86,96	0
7	HEM	BC	503	43/43	0.99	0.10	84,110,135,146	0
15	PEF	AM	408	14/47	0.99	0.07	12,90,119,125	0
8	CA	BY	101	1/1	0.99	0.03	148,148,148,148	0
8	CA	B1	101	1/1	0.99	0.06	184,184,184,184	0
8	CA	B3	101	1/1	0.99	0.07	222,222,222,222	0
9	BCL	AO	102	66/66	0.99	0.09	199,207,214,219	0

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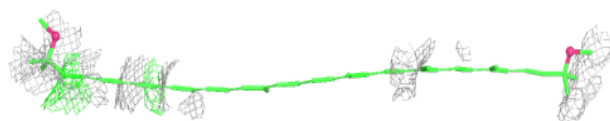
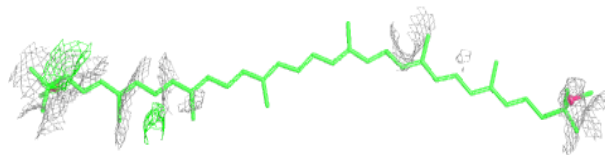
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	BCL	AP	101	66/66	0.99	0.09	107,127,189,190	0
16	PO4	AM	410	5/5	0.99	0.09	83,84,84,84	0
16	PO4	AH	302	5/5	0.99	0.04	102,103,104,104	0
9	BCL	AQ	102	66/66	0.99	0.08	187,198,210,221	0
9	BCL	BB	101	66/66	0.99	0.11	187,209,245,245	0
12	FE	BM	404	1/1	1.00	0.05	44,44,44,44	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.

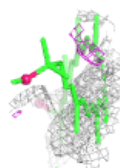
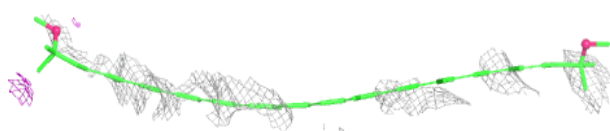
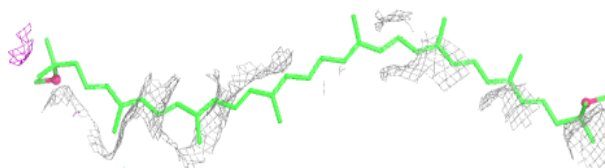


Electron density around CRT A0 101:

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

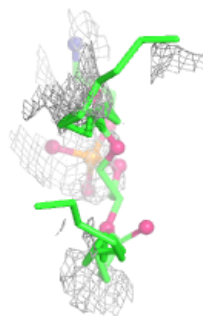
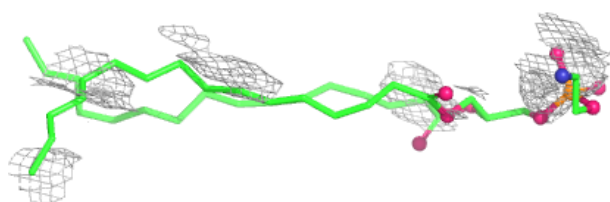
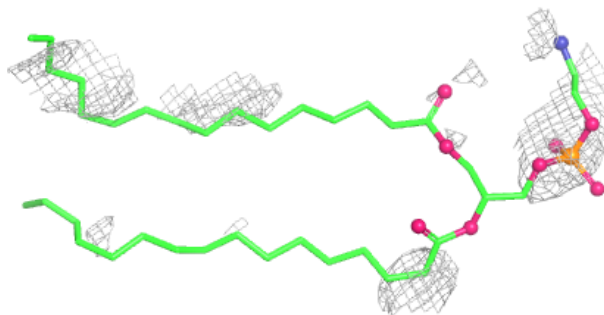
**Electron density around CRT BV 102:**

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

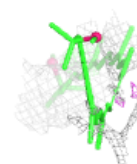
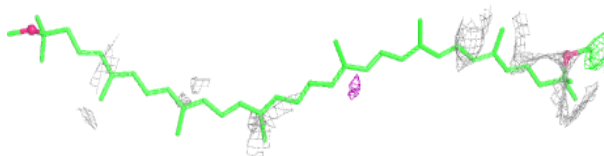


Electron density around PEF BQ 101:

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

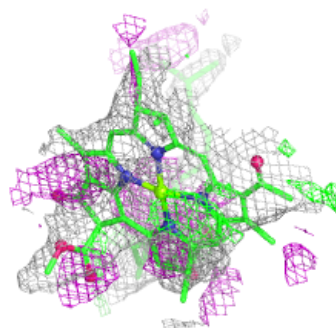
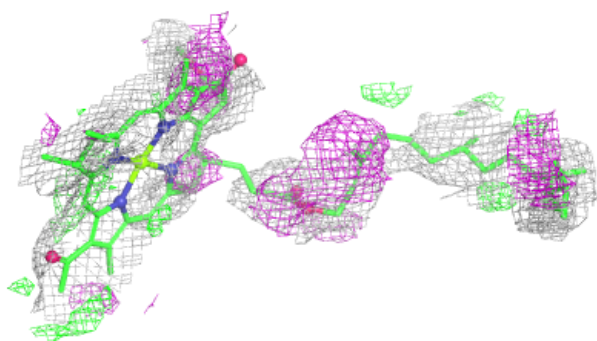
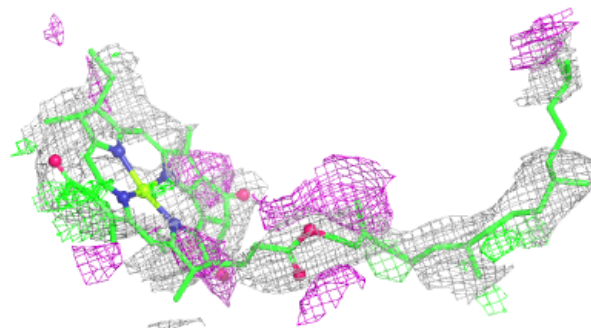
**Electron density around CRT AB 102:**

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

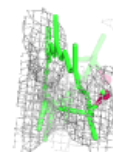
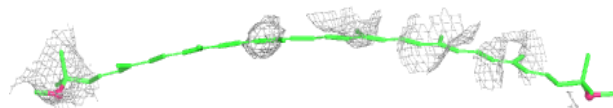
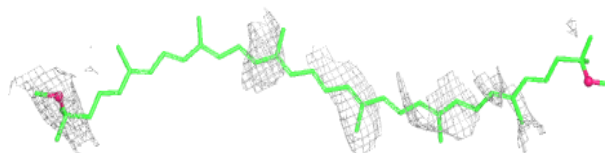


Electron density around BCL AM 402:

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

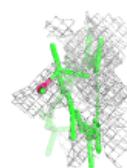
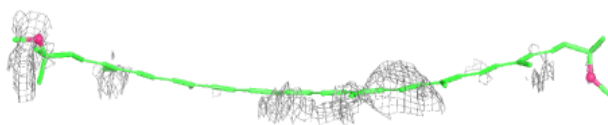
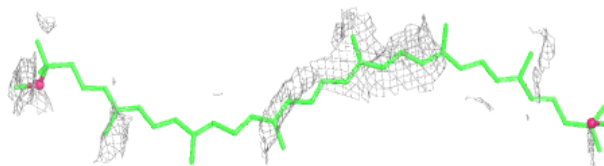
**Electron density around CRT BG 102:**

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

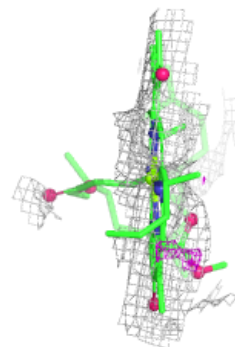
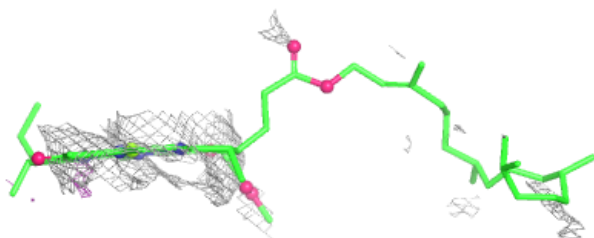
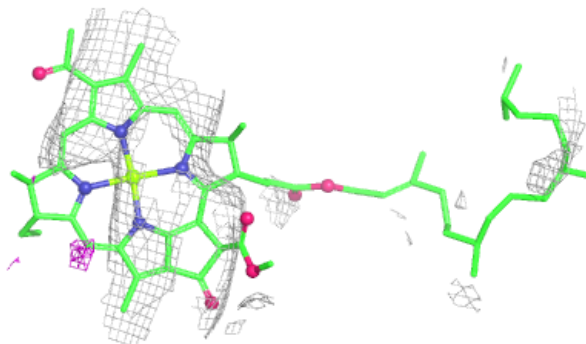


Electron density around CRT BP 102:

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

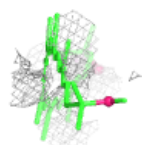
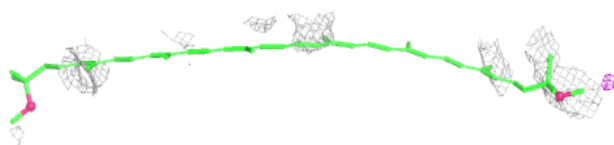
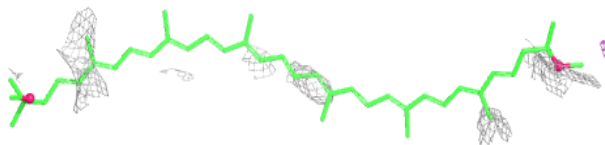
**Electron density around BCL A3 103:**

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



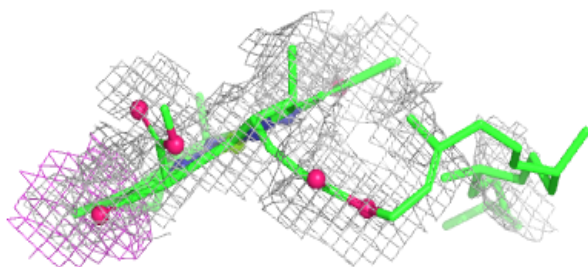
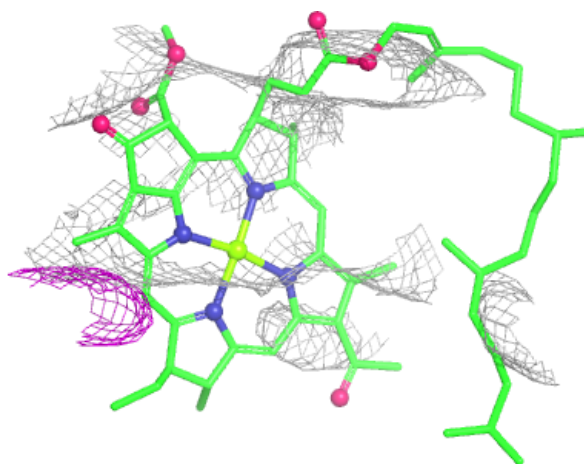
Electron density around CRT B1 103:

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



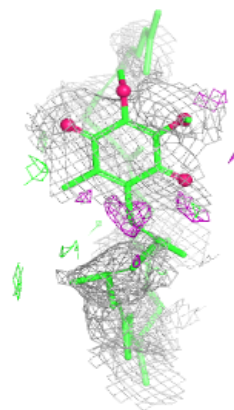
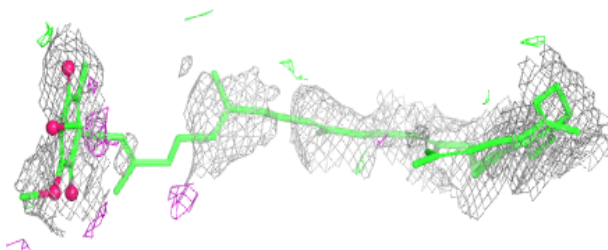
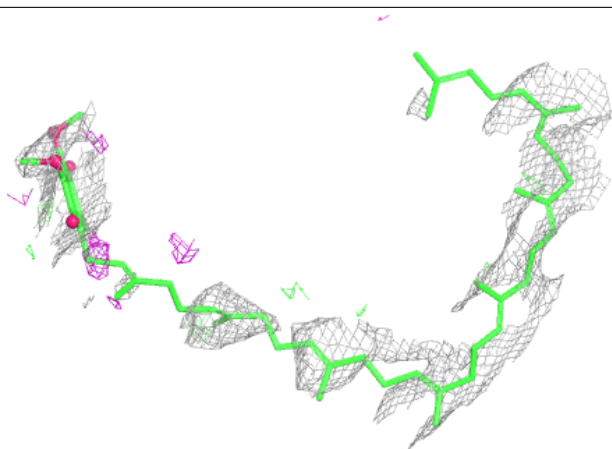
Electron density around BCL BQ 104:

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



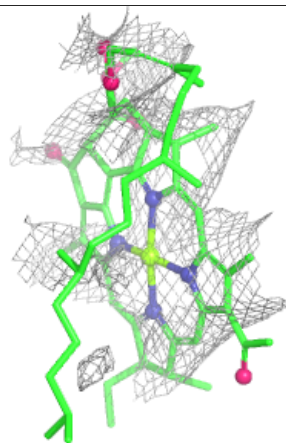
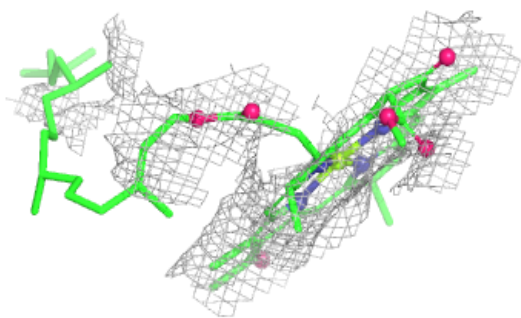
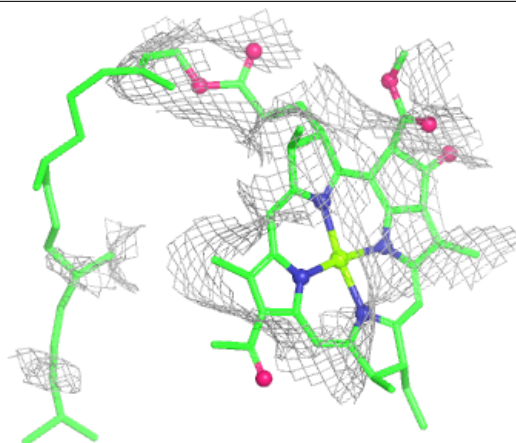
Electron density around UQ8 AL 304:

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



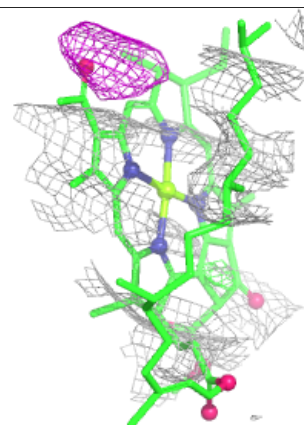
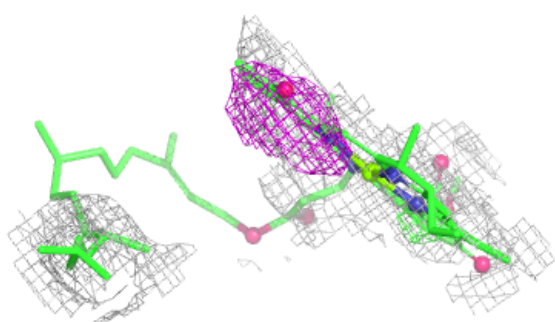
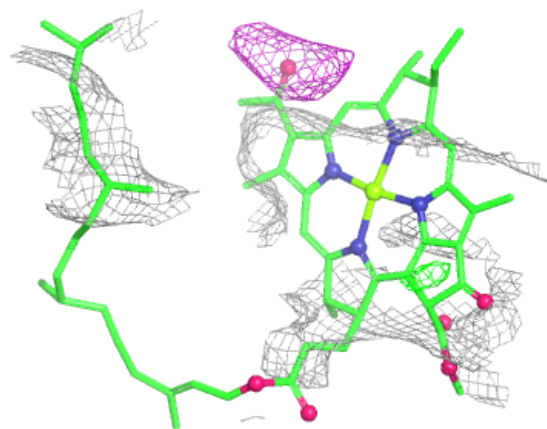
Electron density around BCL AR 101:

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



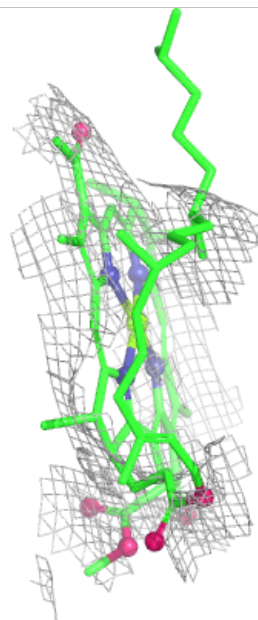
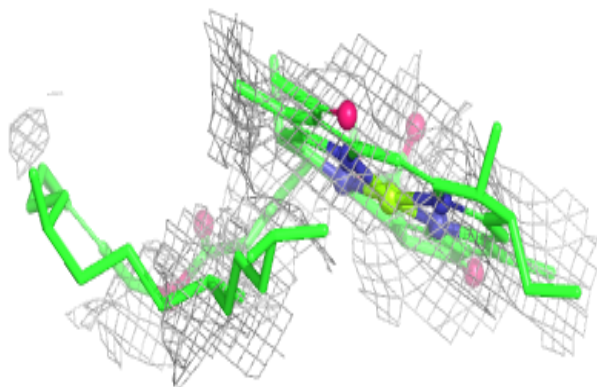
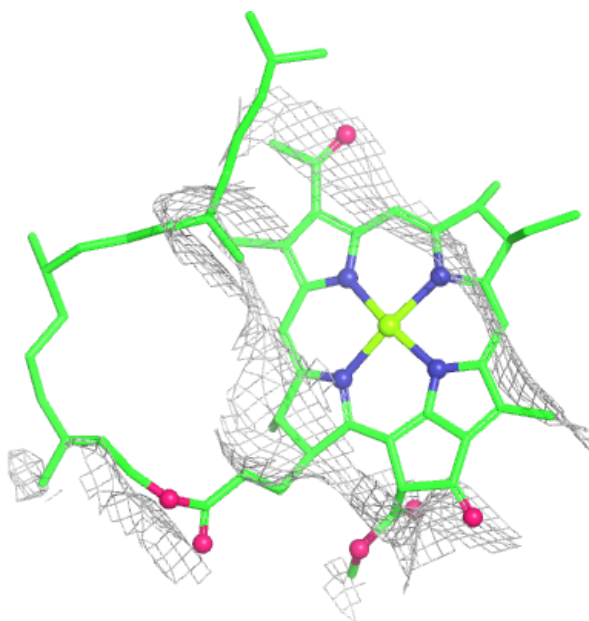
Electron density around BCL A2 101:

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



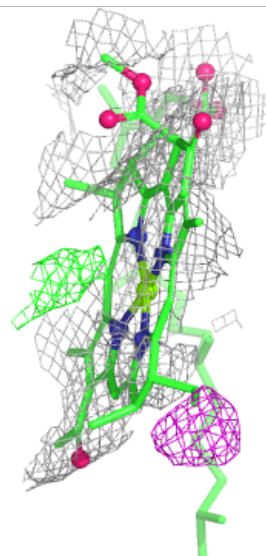
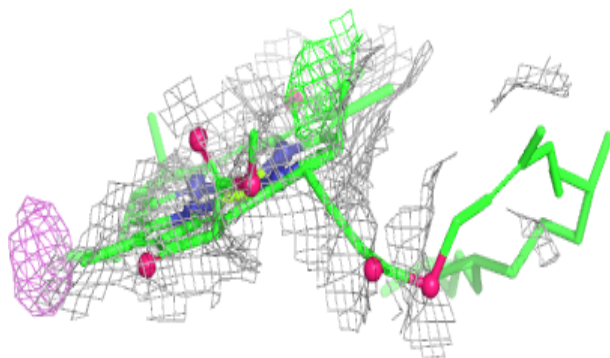
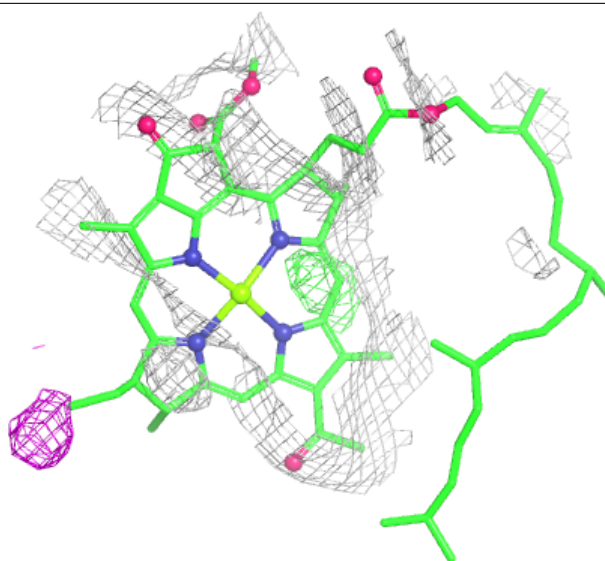
Electron density around BCL A3 104:

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



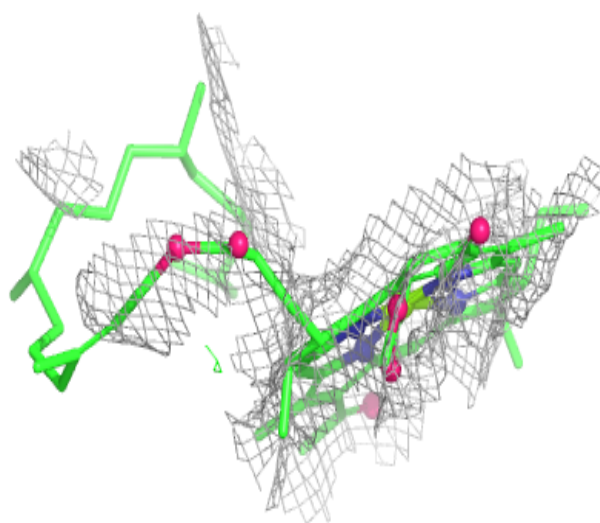
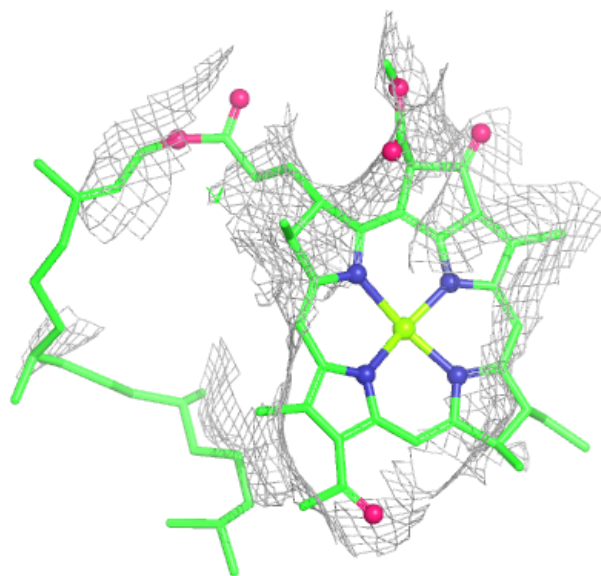
Electron density around BCL A6 101:

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



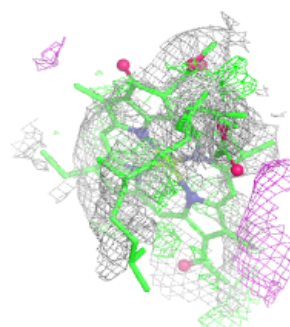
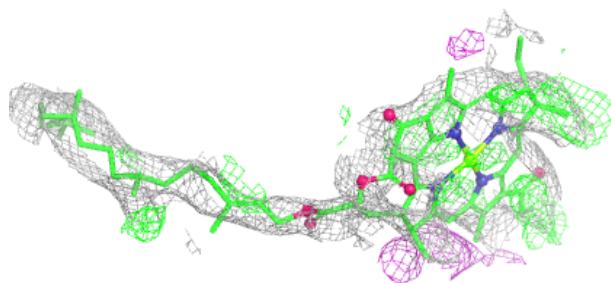
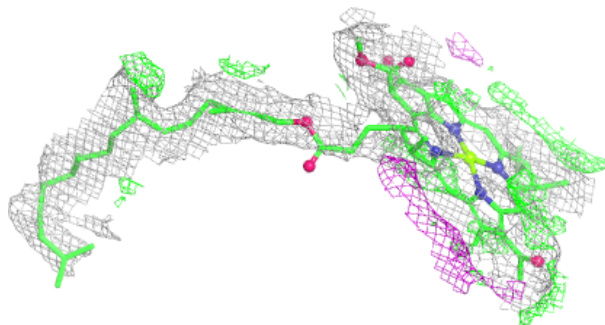
Electron density around BCL A8 101:

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

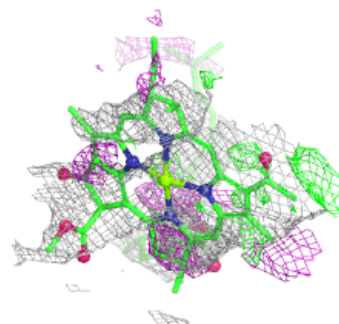
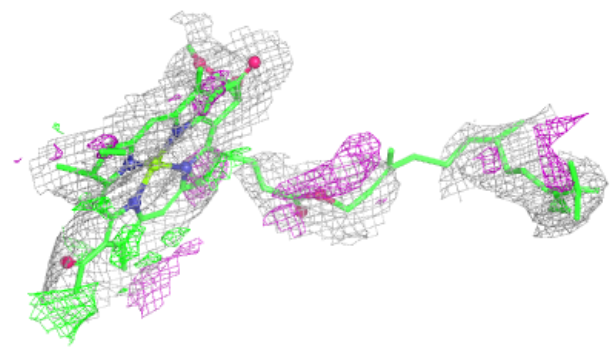
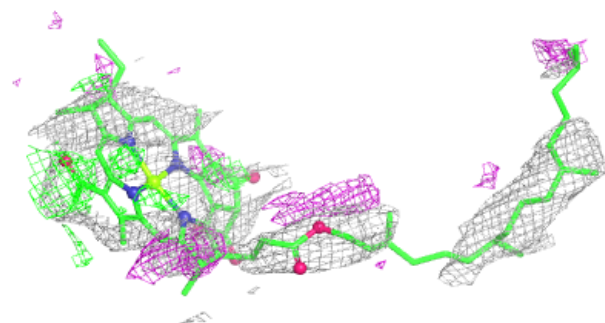


Electron density around BCL BL 301:

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

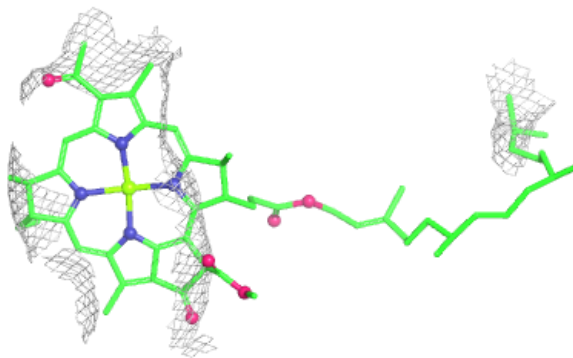
**Electron density around BCL BM 402:**

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

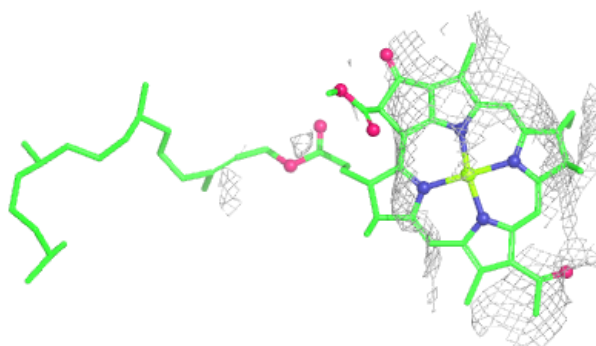


Electron density around BCL BA 101:

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

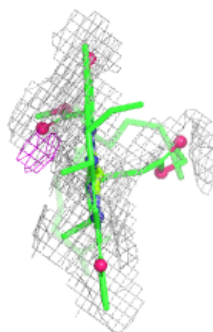
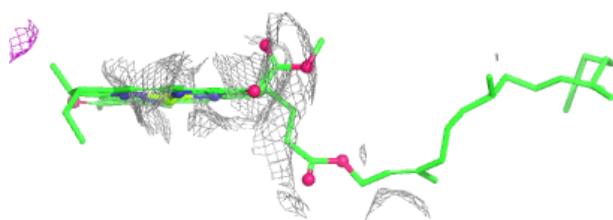
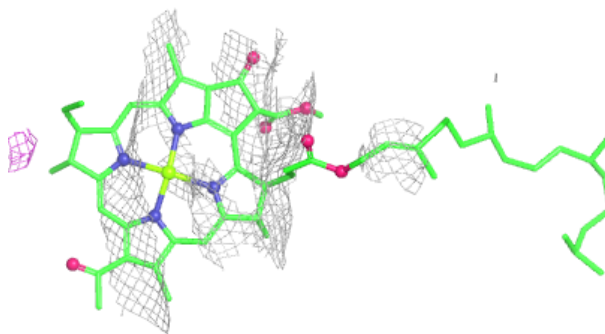
**Electron density around BCL BD 102:**

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

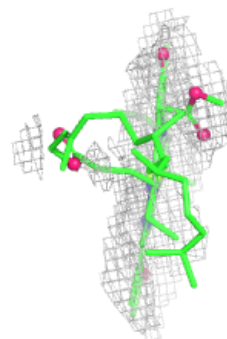
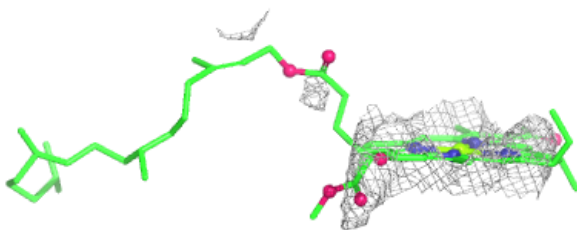
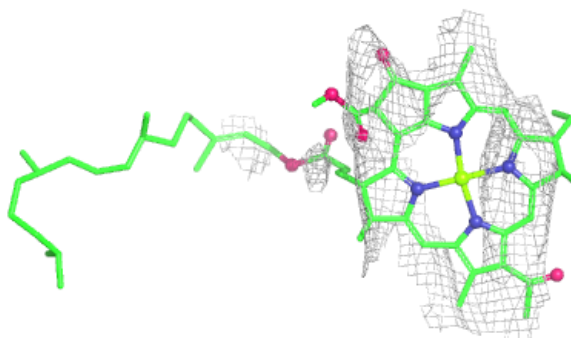


Electron density around BCL BF 102:

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

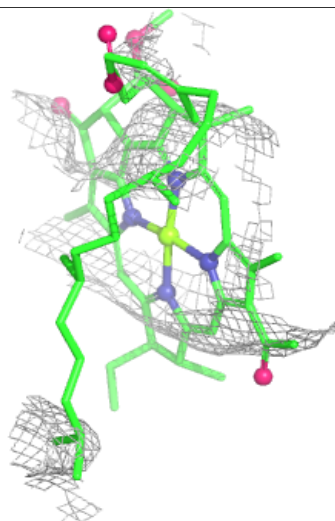
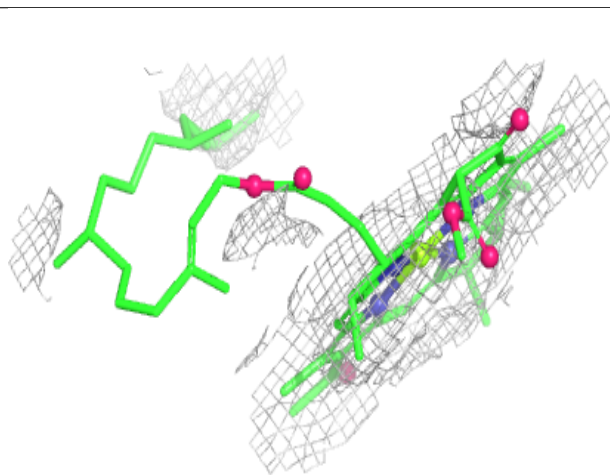
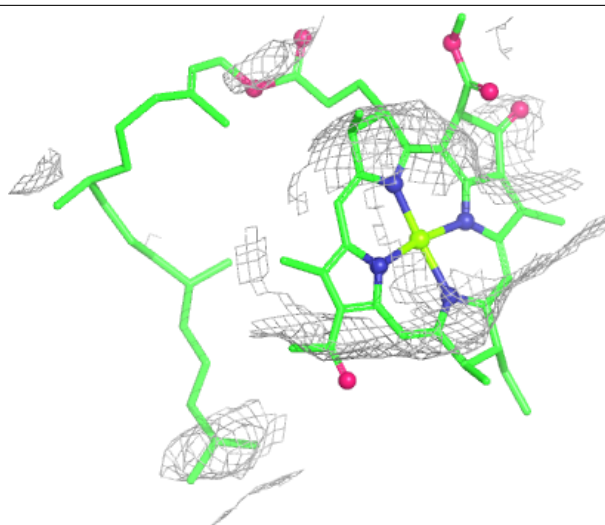
**Electron density around BCL BI 102:**

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



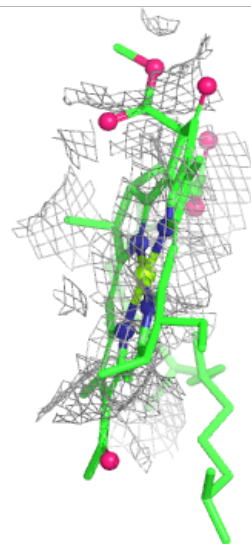
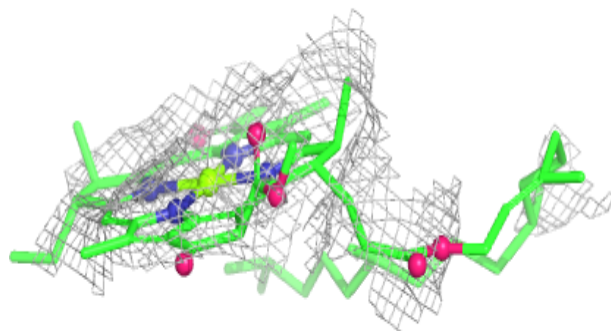
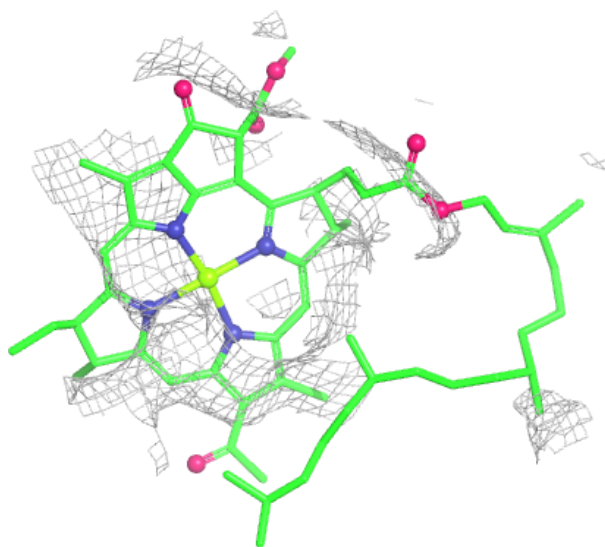
Electron density around BCL BJ 101:

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



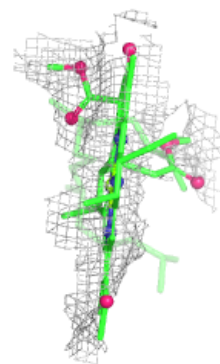
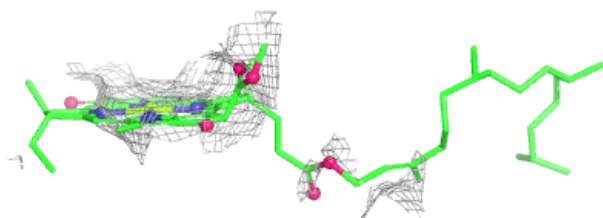
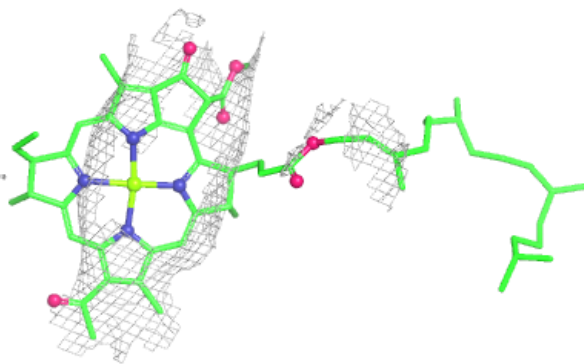
Electron density around BCL BP 101:

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

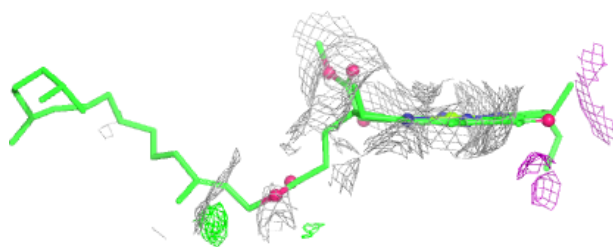
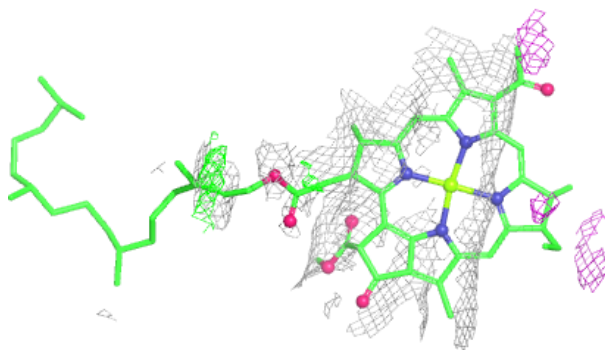


Electron density around BCL BU 102:

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

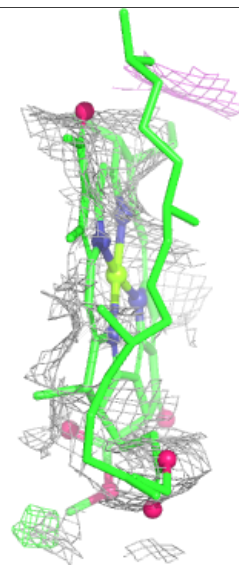
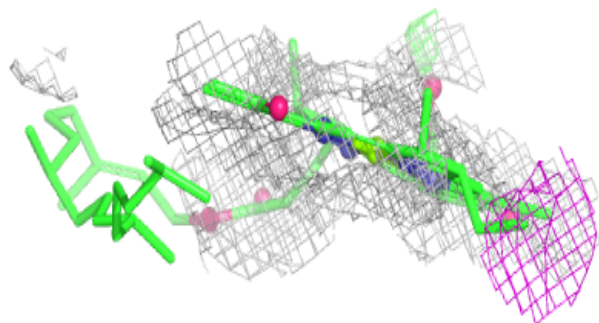
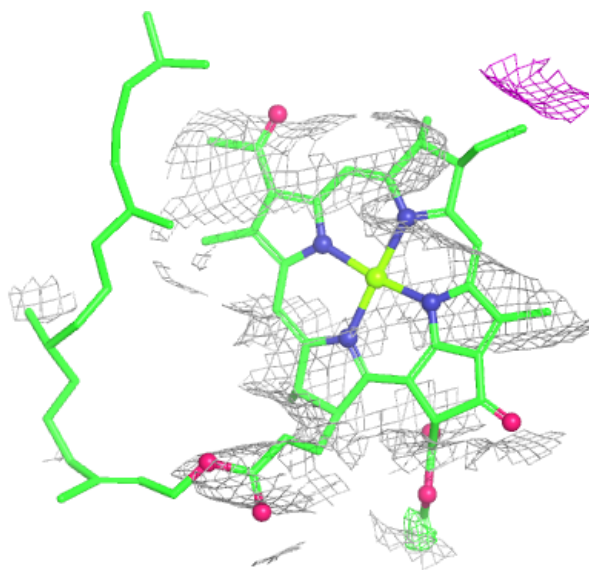
**Electron density around BCL BW 102:**

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



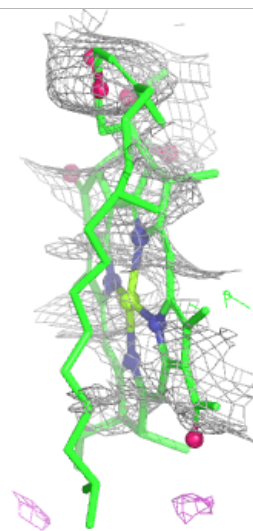
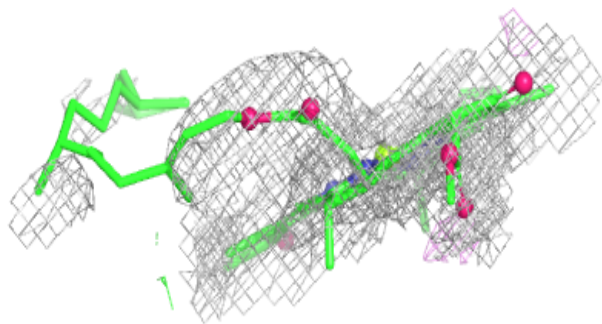
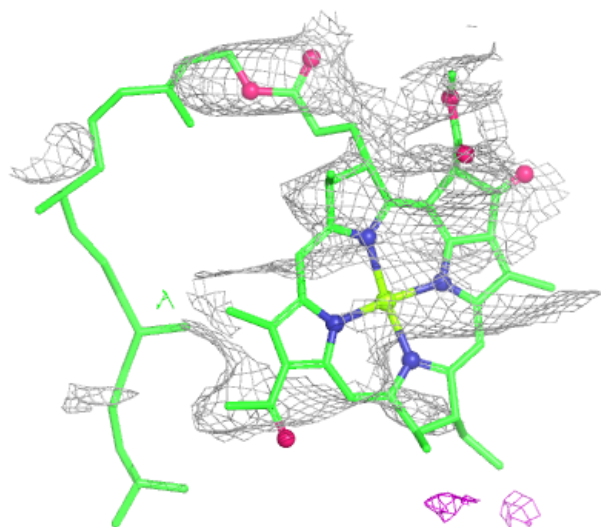
Electron density around BCL BX 101:

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



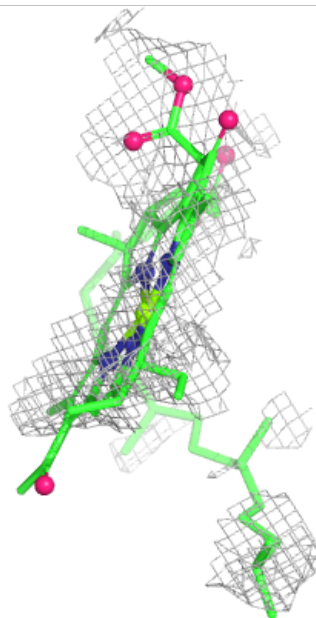
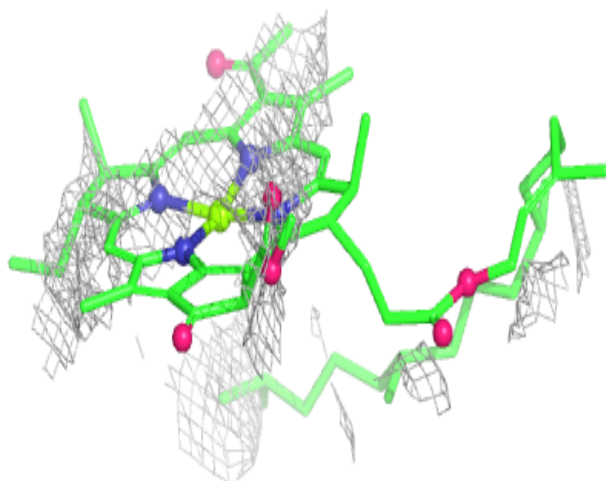
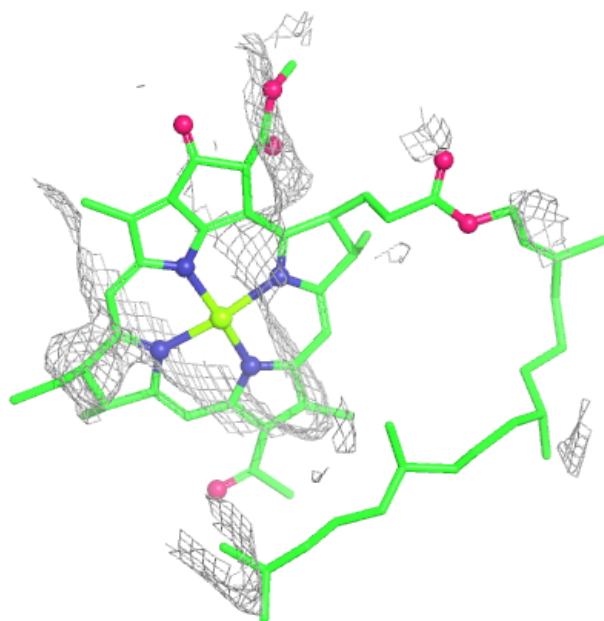
Electron density around BCL BZ 101:

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



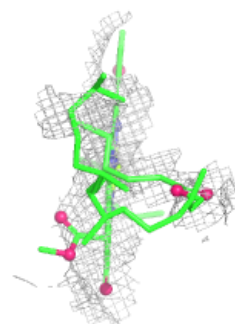
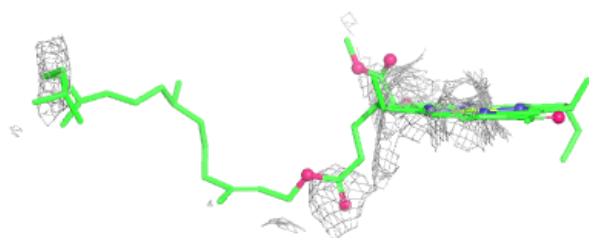
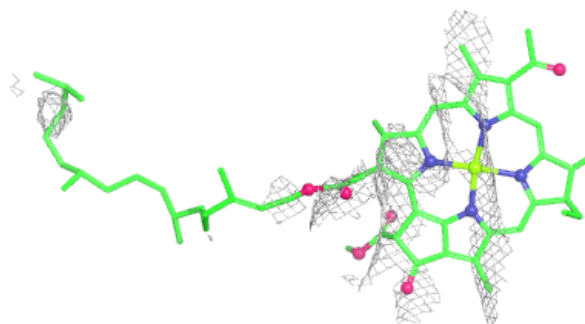
Electron density around BCL B8 101:

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

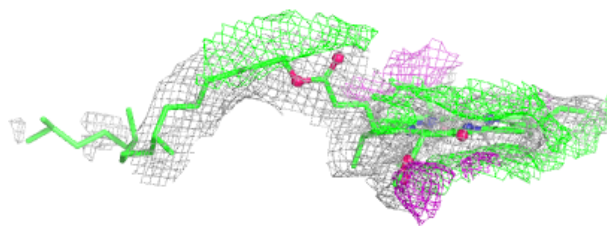
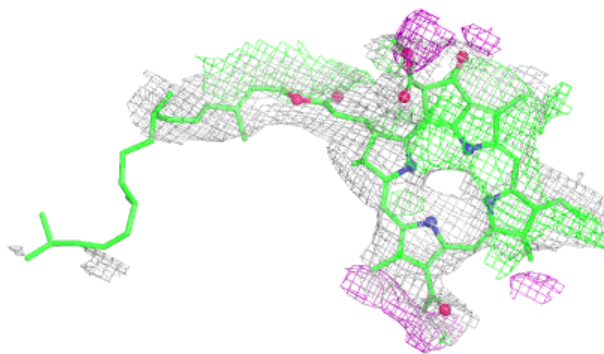


Electron density around BCL B9 102:

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

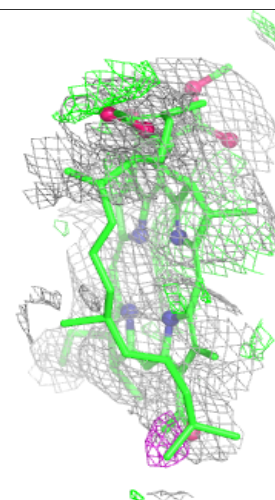
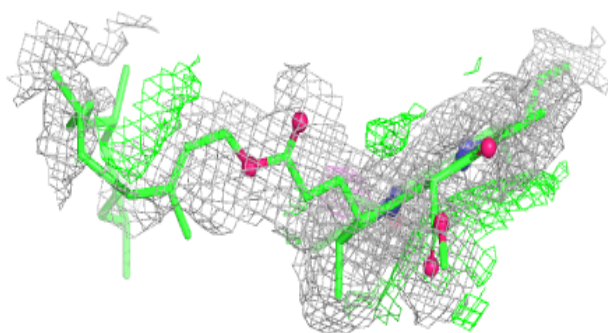
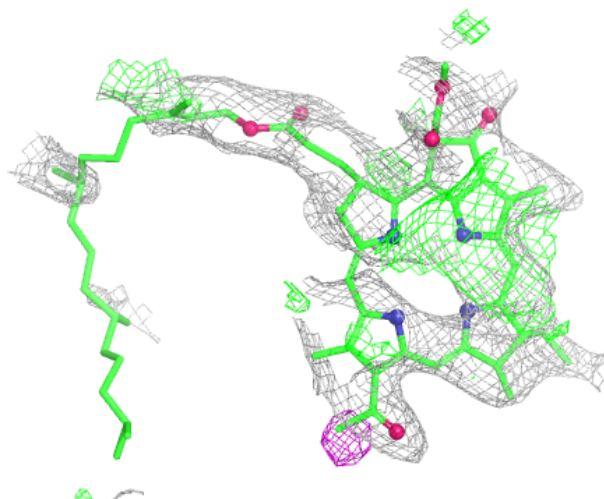
**Electron density around BPH AM 403:**

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



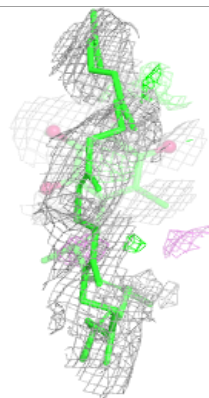
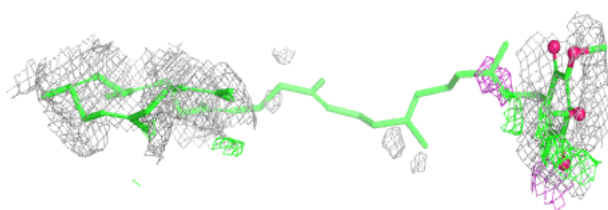
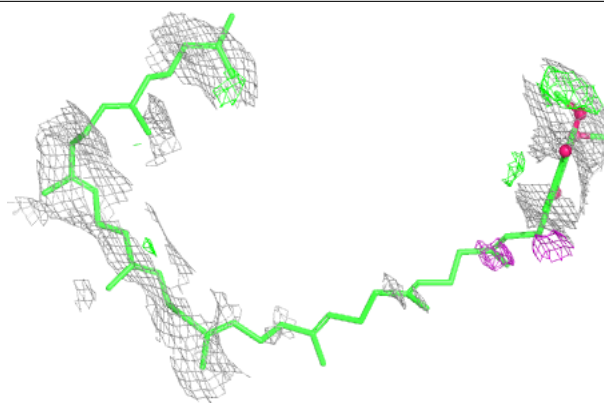
Electron density around BPH BL 302:

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

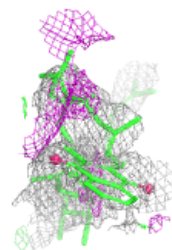
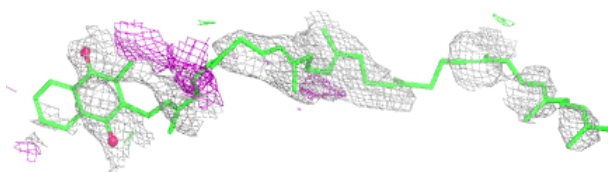
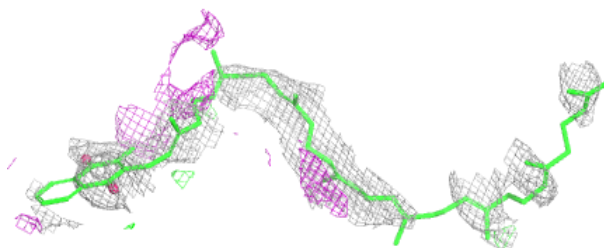


Electron density around UQ8 BL 304:

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

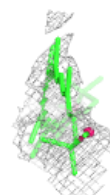
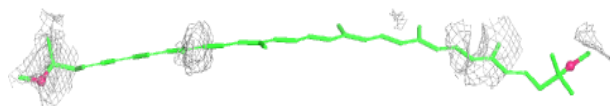
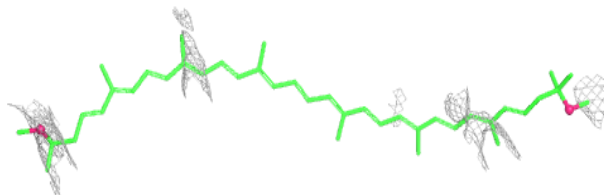
**Electron density around MQ8 AM 405:**

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

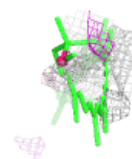
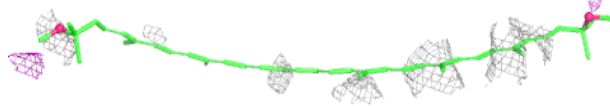
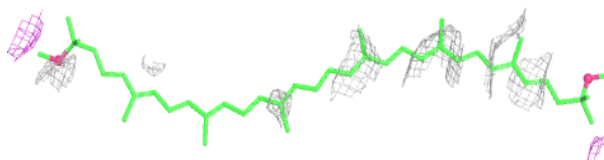


Electron density around CRT AA 102:

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

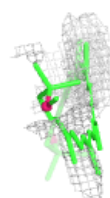
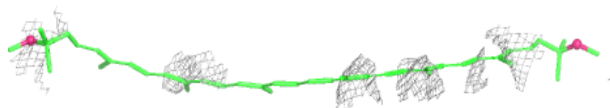
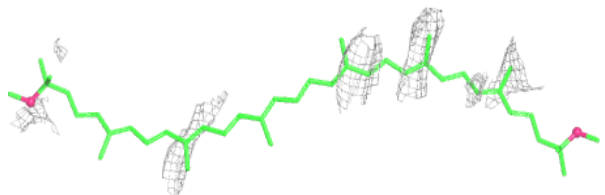
**Electron density around CRT AG 102:**

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

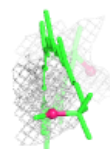
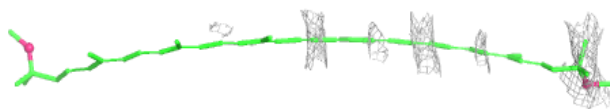
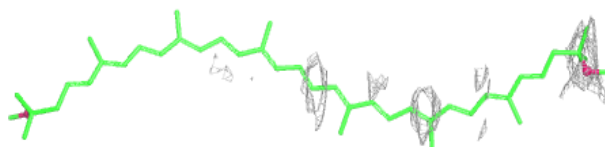


Electron density around CRT AJ 102:

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

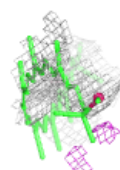
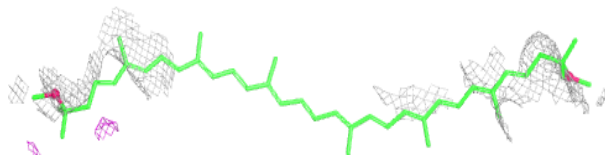
**Electron density around CRT AP 102:**

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

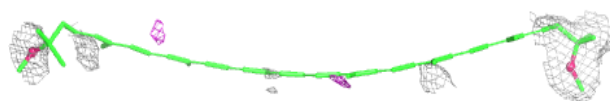
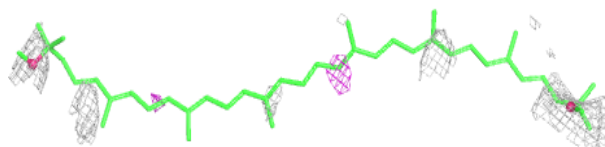


Electron density around CRT AS 104:

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

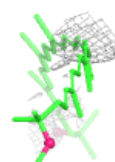
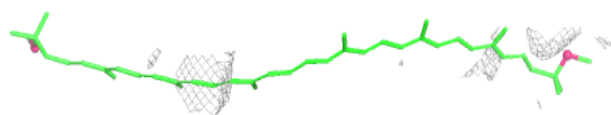
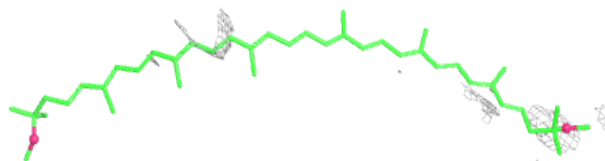
**Electron density around CRT AW 102:**

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

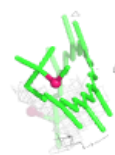
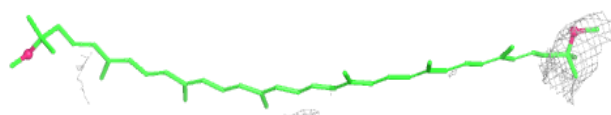
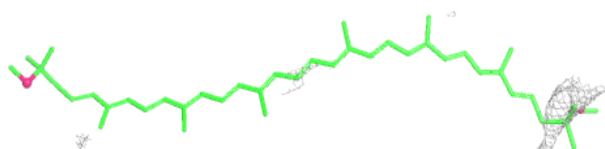


Electron density around CRT AX 102:

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

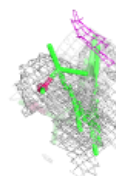
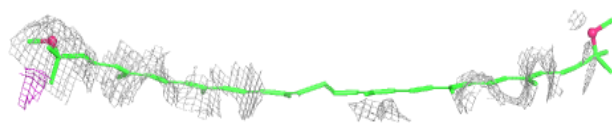
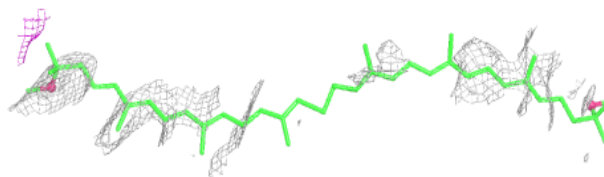
**Electron density around CRT A5 103:**

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

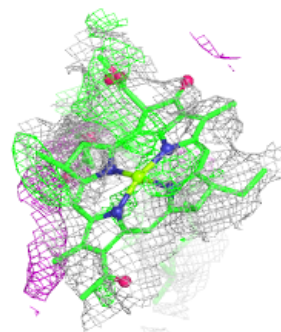
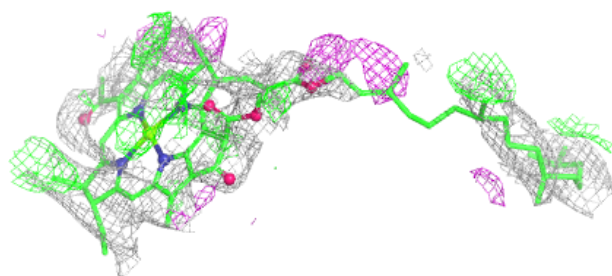
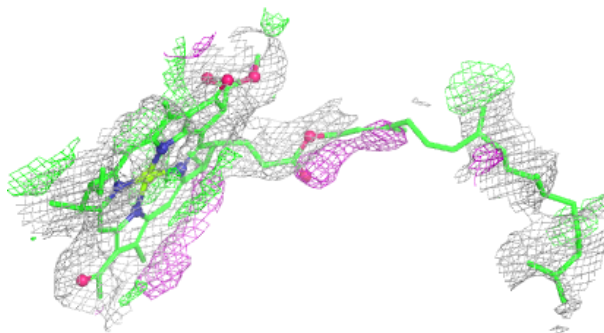


Electron density around CRT A7 102:

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

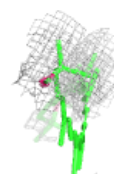
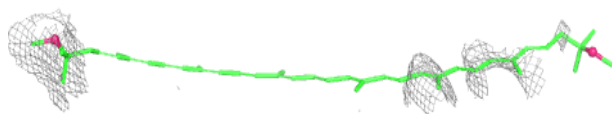
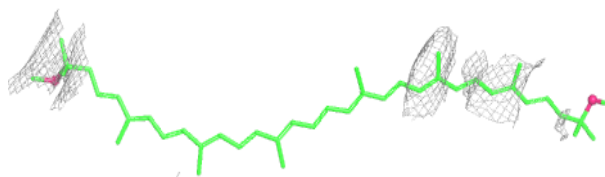
**Electron density around BCL AL 301:**

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

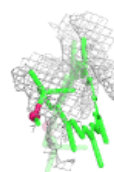
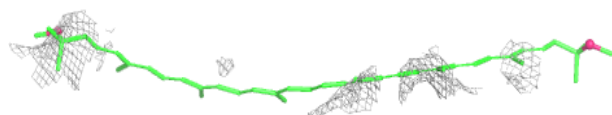
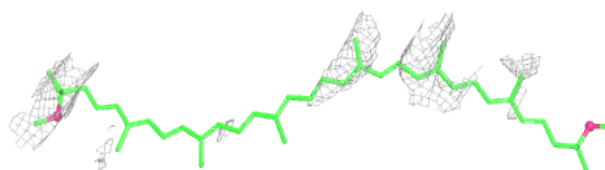


Electron density around CRT BA 102:

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

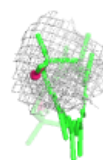
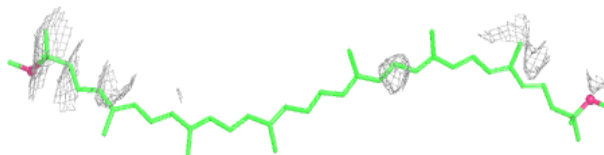
**Electron density around CRT BB 102:**

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

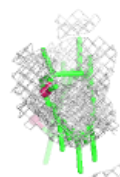
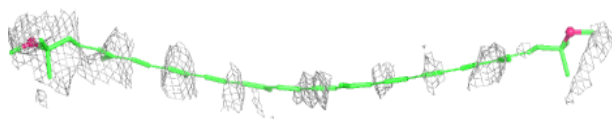
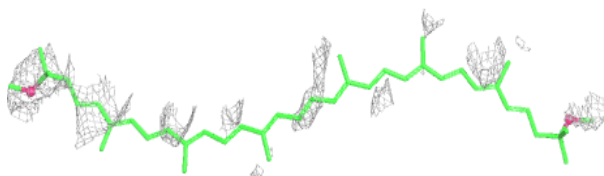


Electron density around CRT BF 103:

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

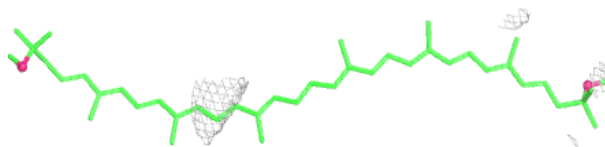
**Electron density around CRT BN 102:**

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



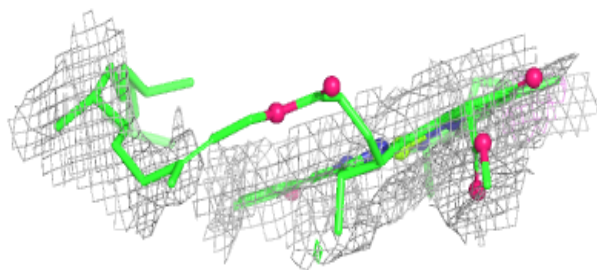
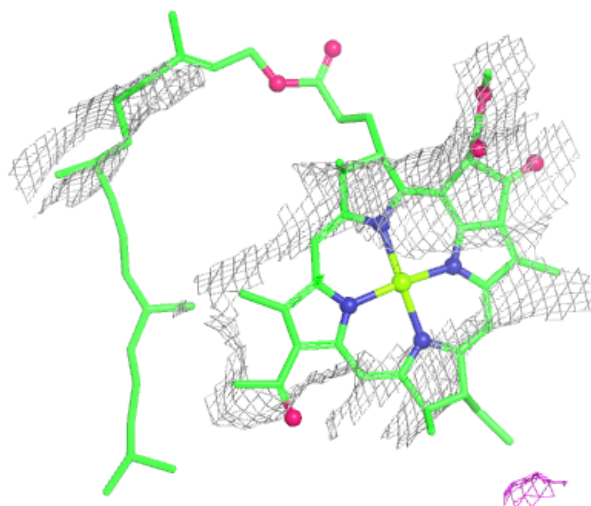
Electron density around CRT BO 103:

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



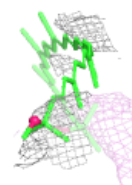
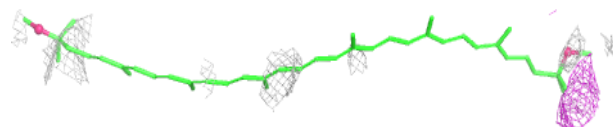
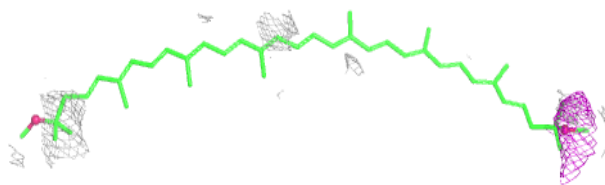
Electron density around BCL AB 101:

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



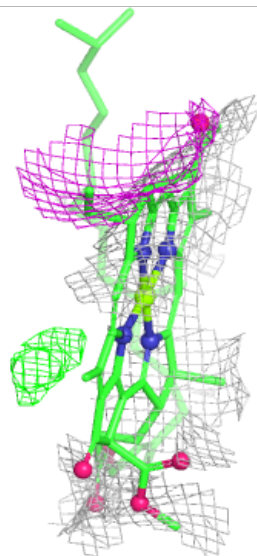
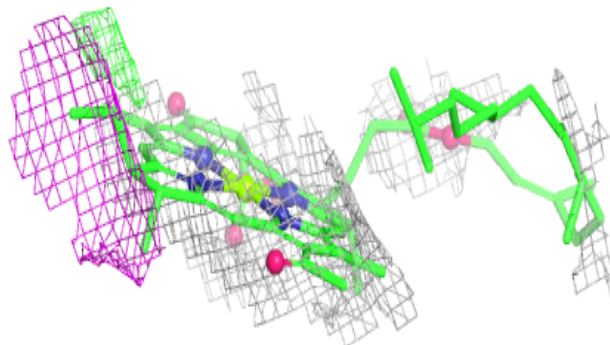
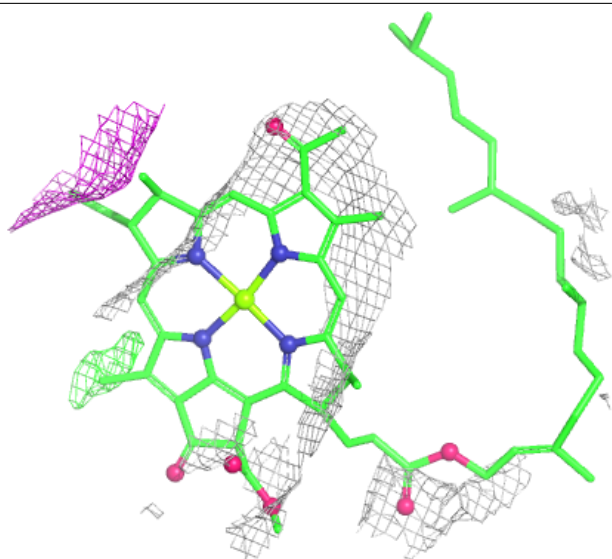
Electron density around CRT BU 103:

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



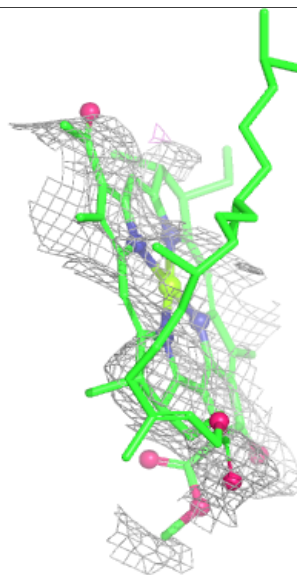
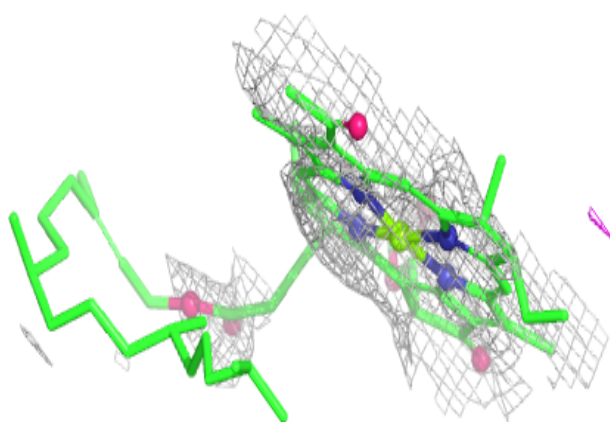
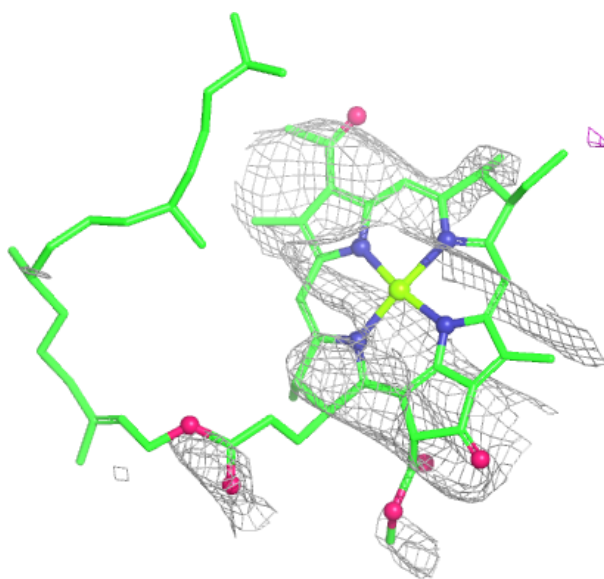
Electron density around BCL AE 101:

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



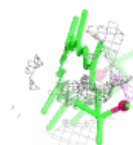
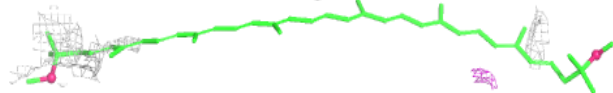
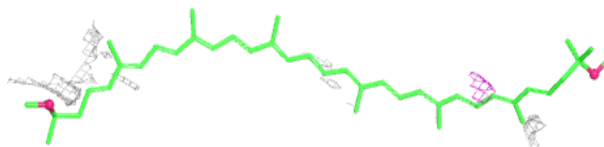
Electron density around BCL AJ 101:

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

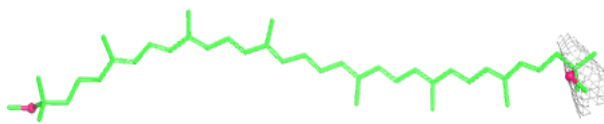


Electron density around CRT B5 103:

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

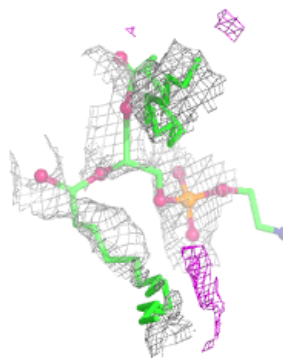
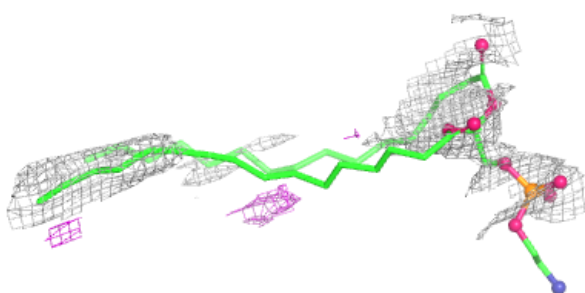
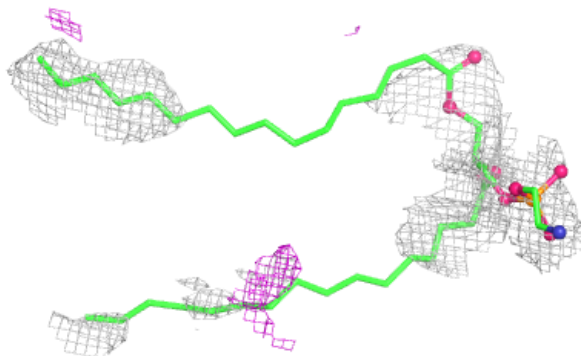
**Electron density around CRT B0 101:**

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

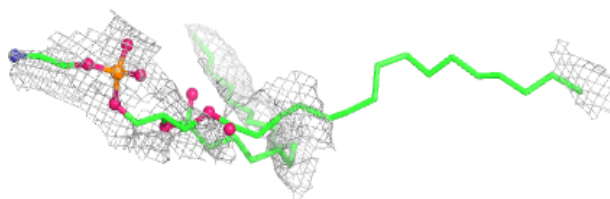
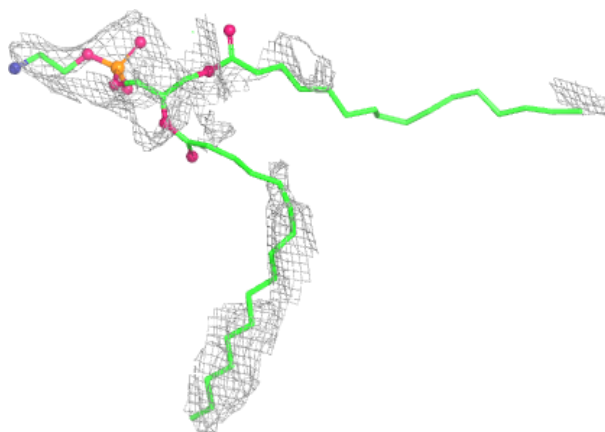


Electron density around PEF AM 409:

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

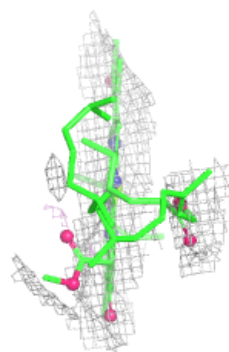
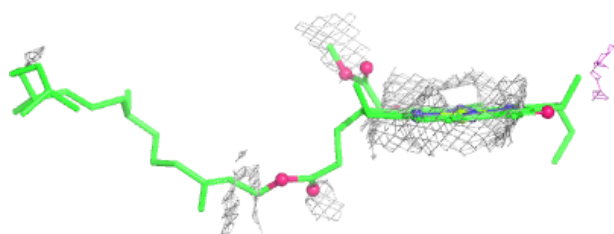
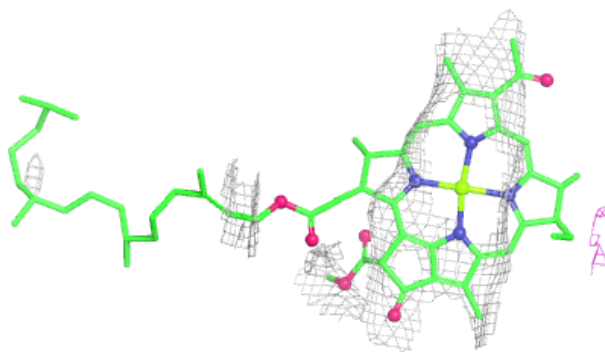
**Electron density around PEF AS 101:**

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



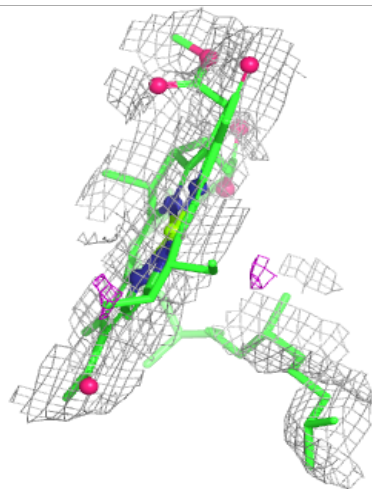
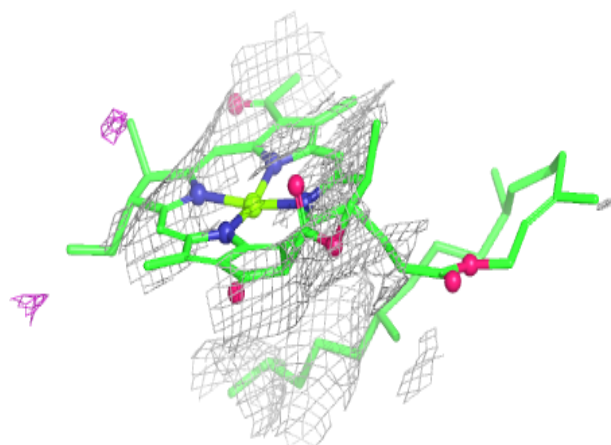
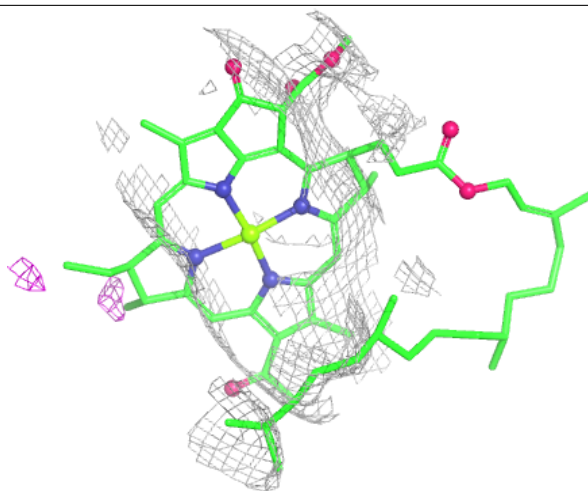
Electron density around BCL AK 102:

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



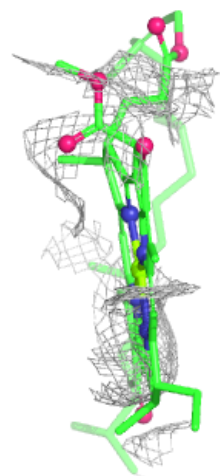
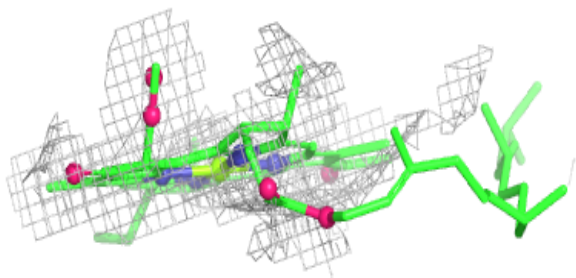
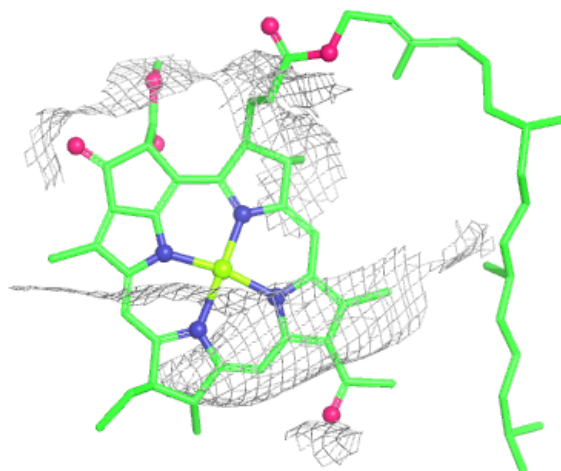
Electron density around BCL AN 101:

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



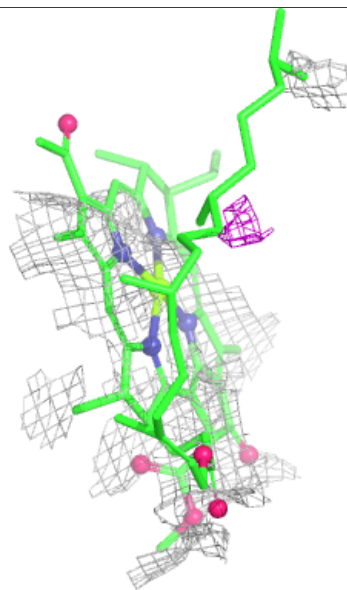
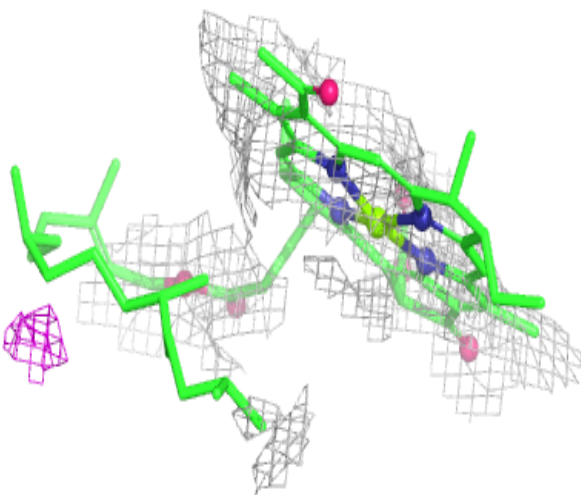
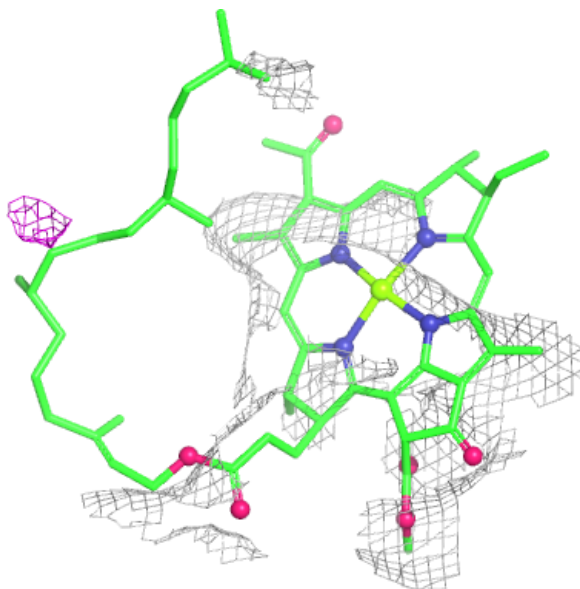
Electron density around BCL BT 101:

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



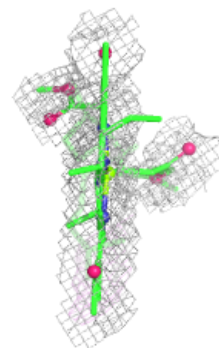
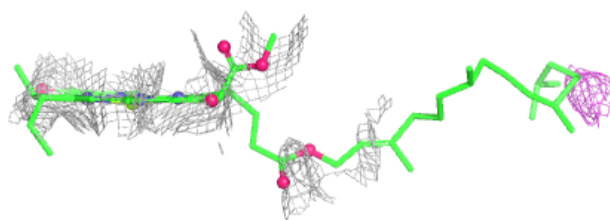
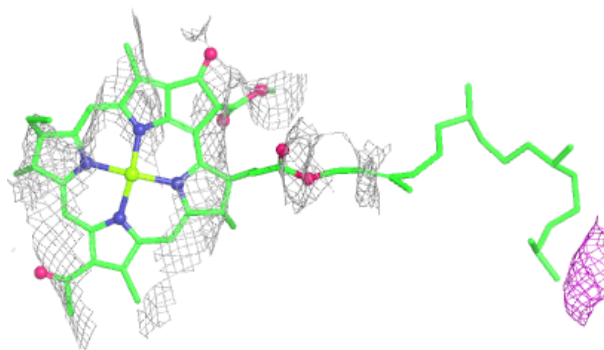
Electron density around BCL BV 101:

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



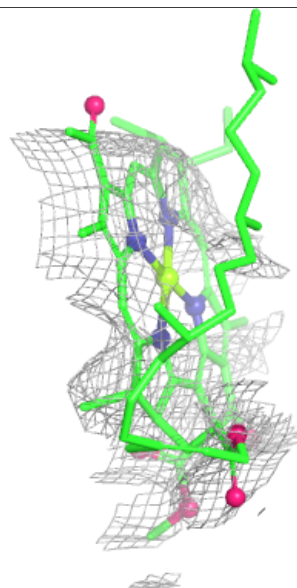
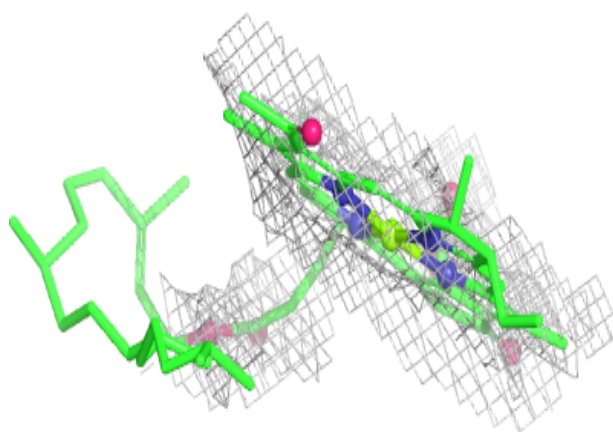
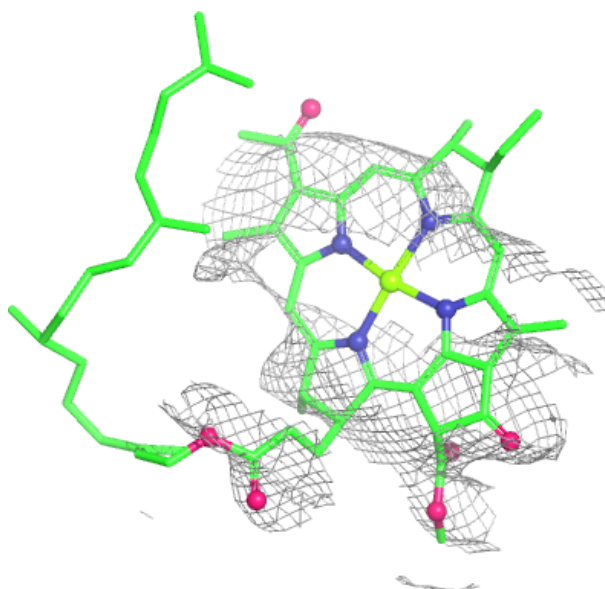
Electron density around BCL AF 102:

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



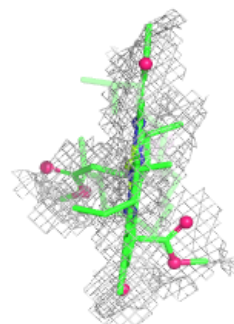
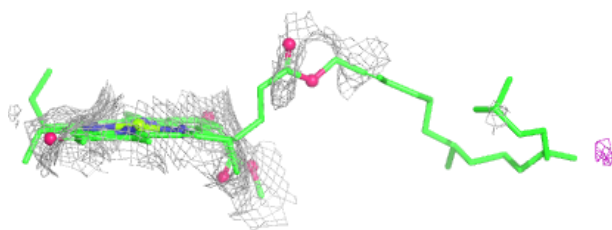
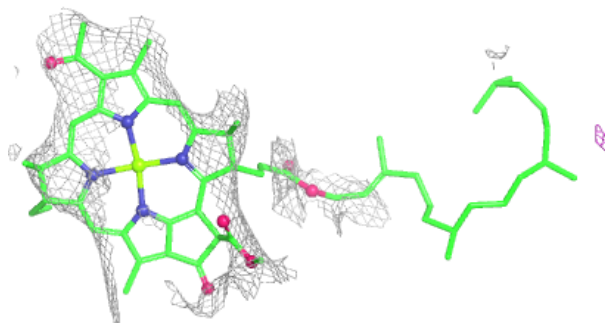
Electron density around BCL AG 101:

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

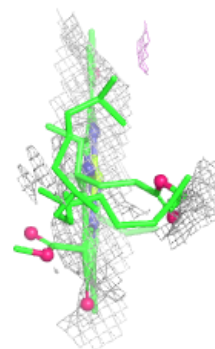
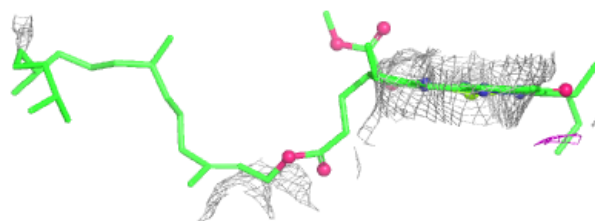
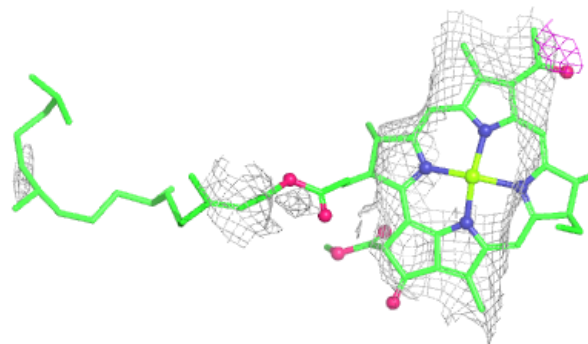


Electron density around BCL BY 102:

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

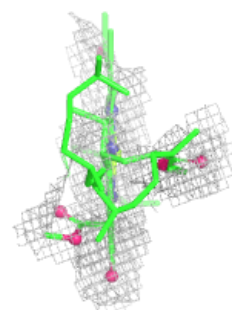
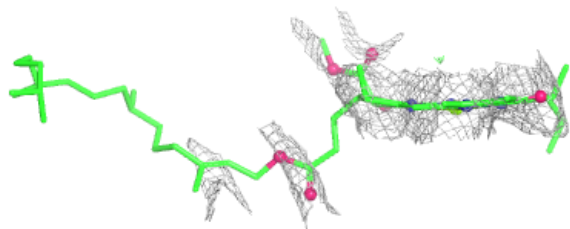
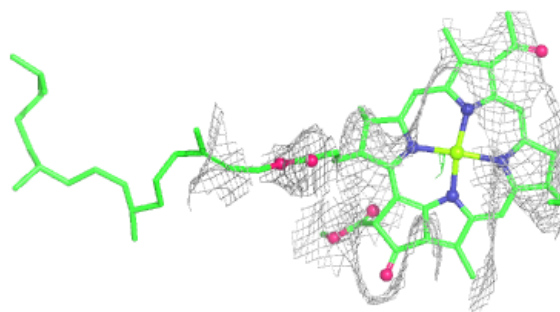
**Electron density around BCL AI 102:**

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



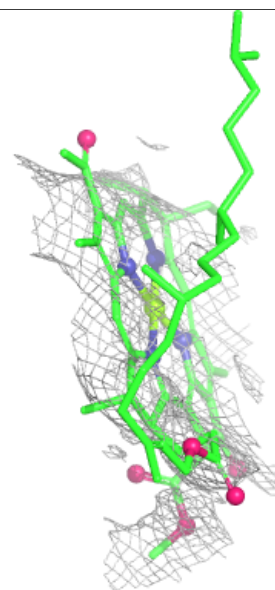
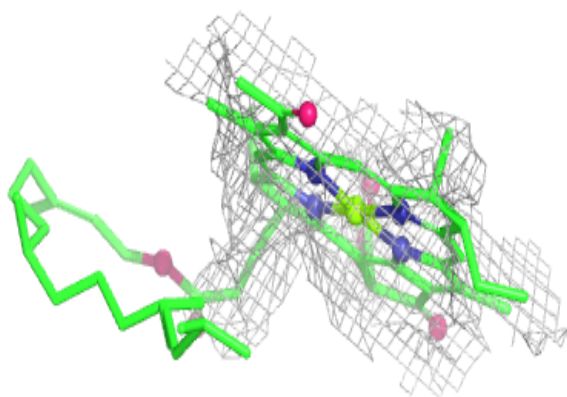
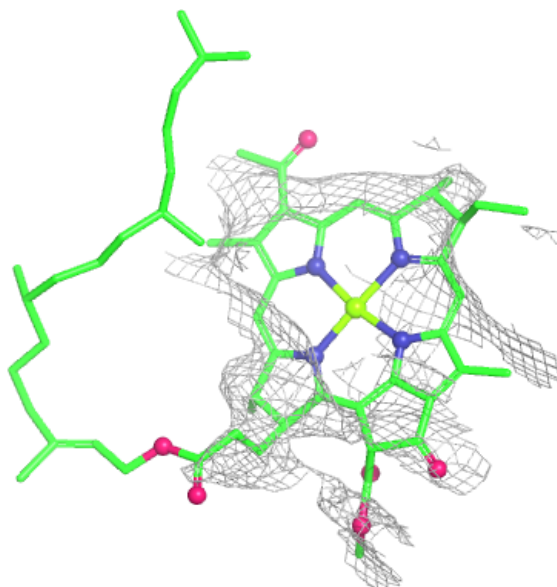
Electron density around BCL B1 102:

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



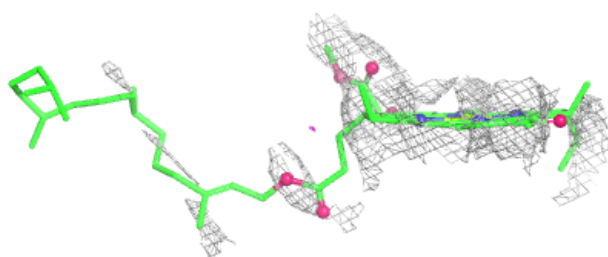
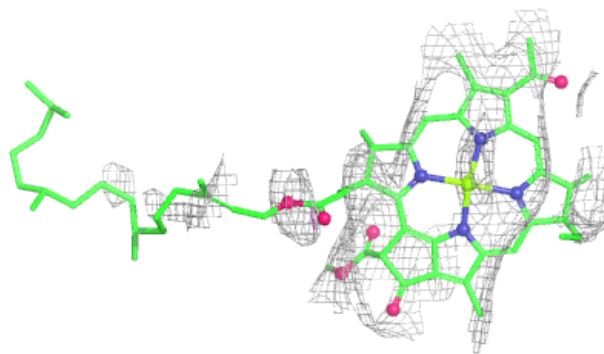
Electron density around BCL B2 101:

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



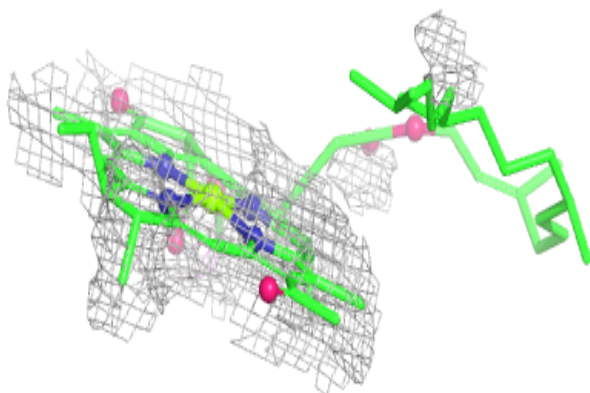
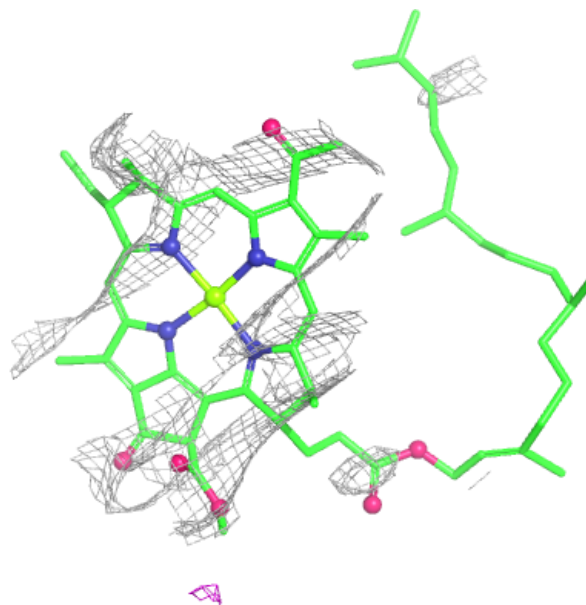
Electron density around BCL B3 102:

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



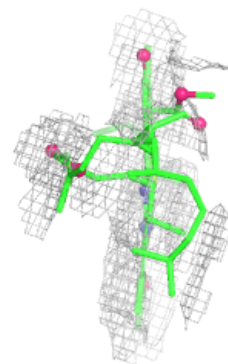
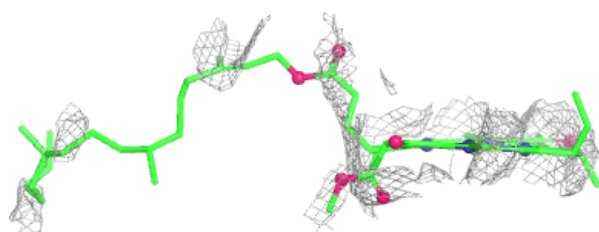
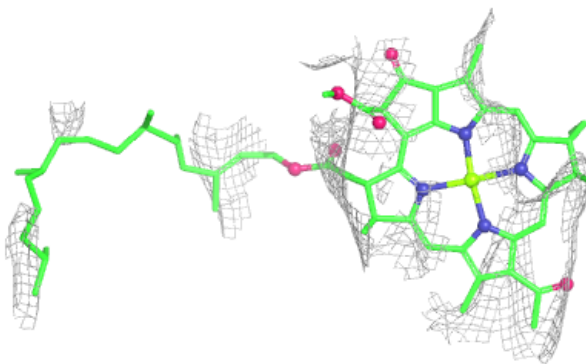
Electron density around BCL B4 101:

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



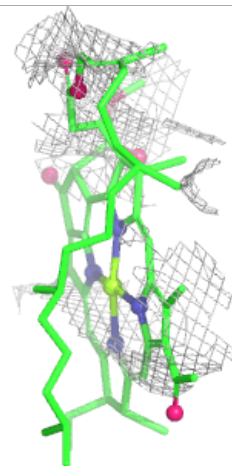
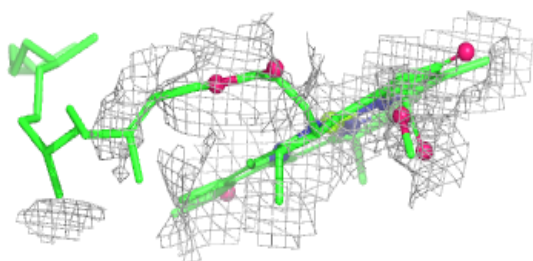
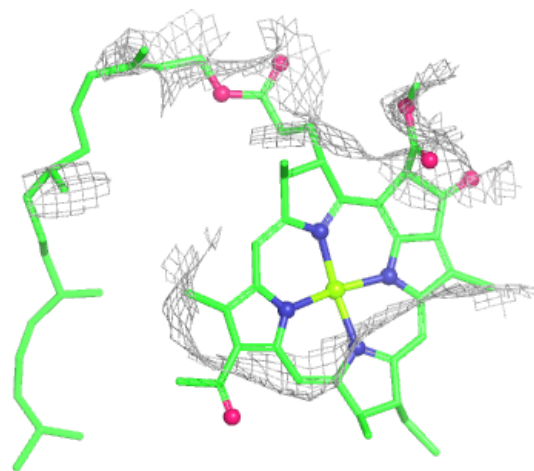
Electron density around BCL B5 102:

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



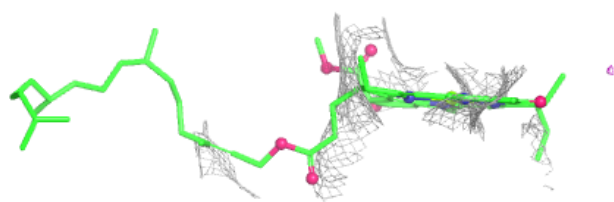
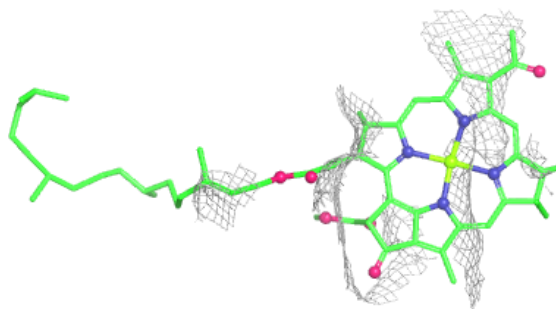
Electron density around BCL B6 101:

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



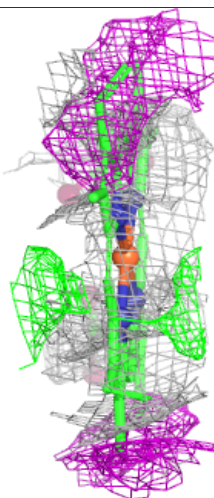
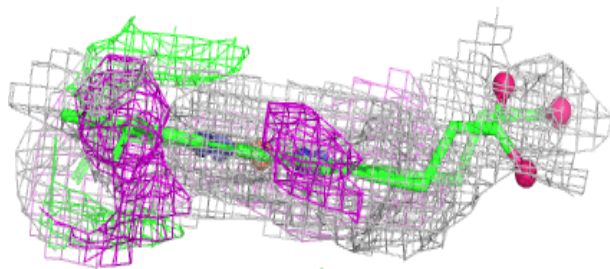
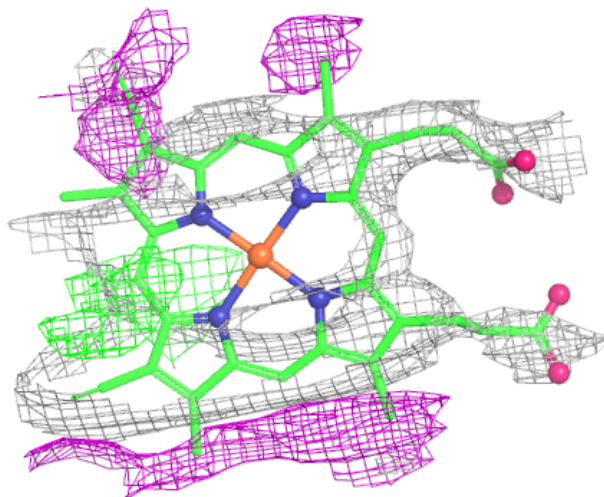
Electron density around BCL B7 103:

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



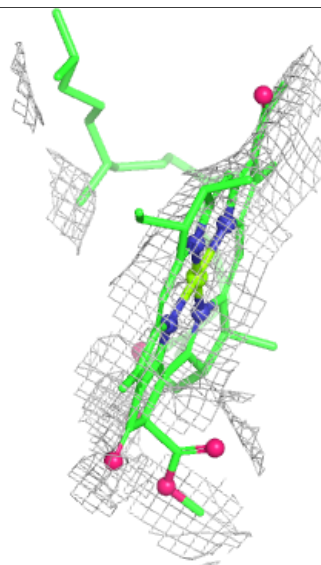
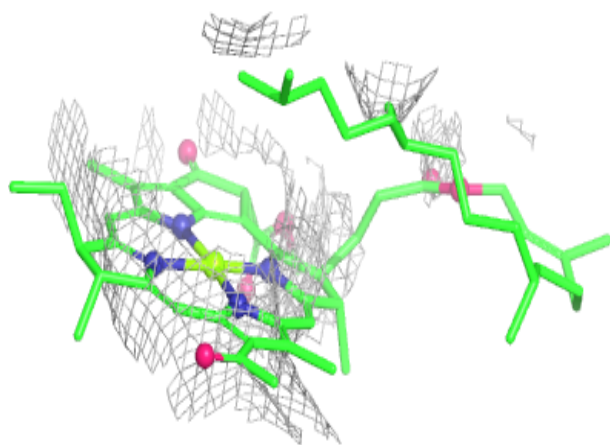
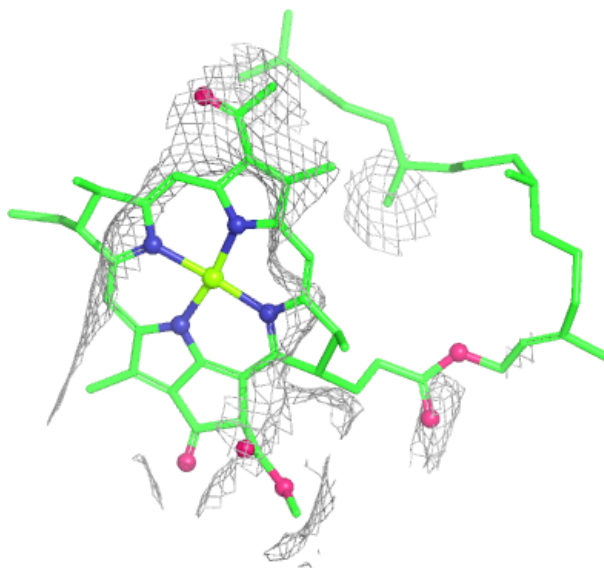
Electron density around HEM AC 502:

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



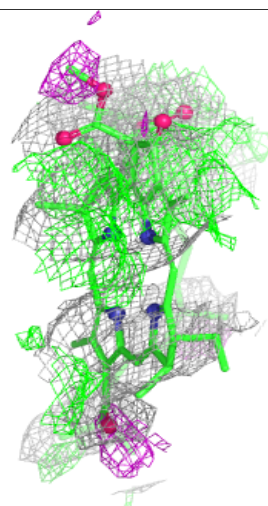
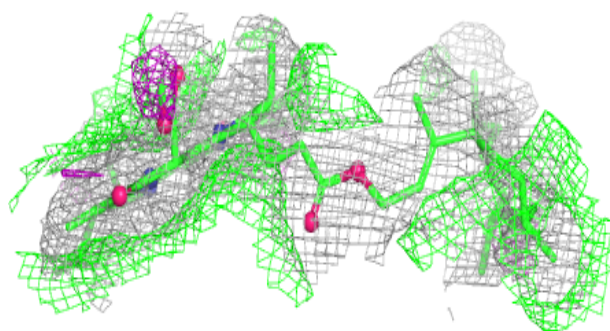
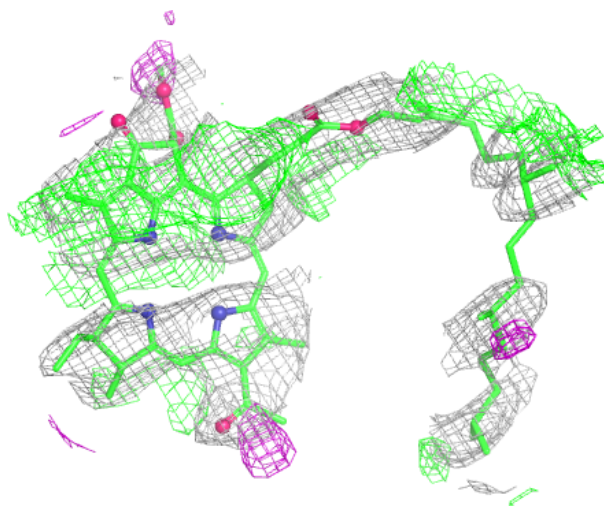
Electron density around BCL B0 102:

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



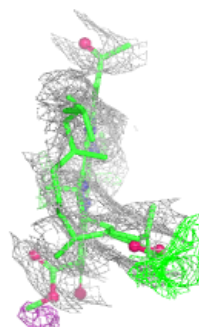
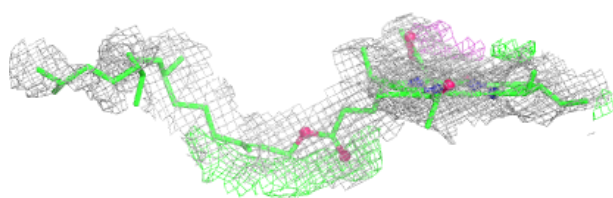
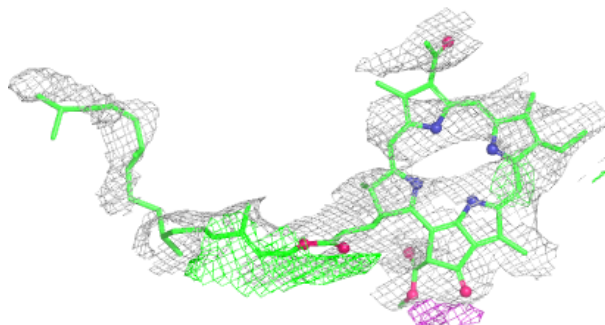
Electron density around BPH AL 302:

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

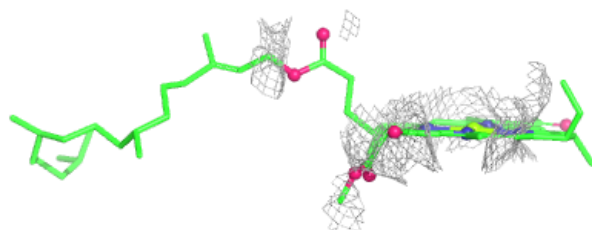
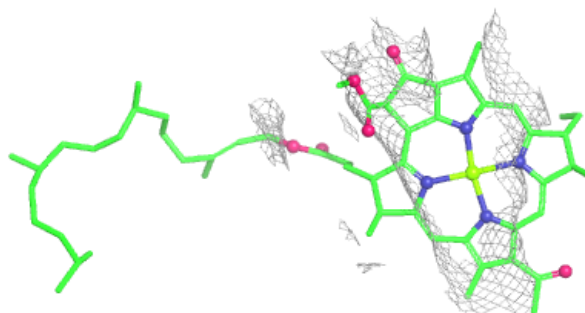


Electron density around BPH BM 403:

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

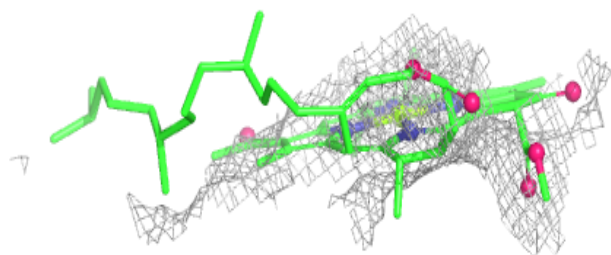
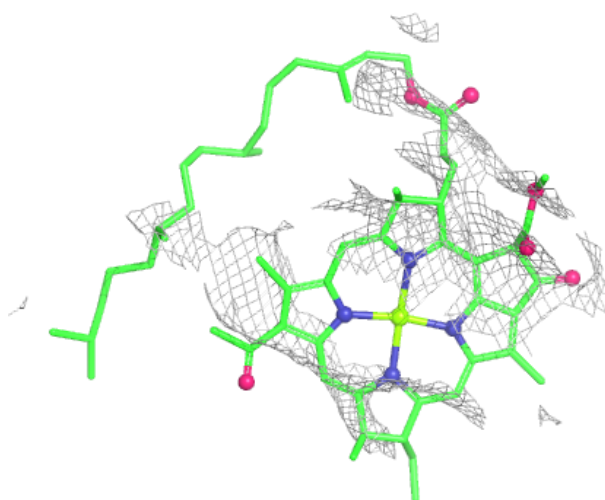
**Electron density around BCL AS 103:**

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



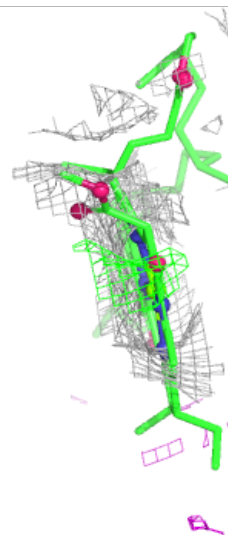
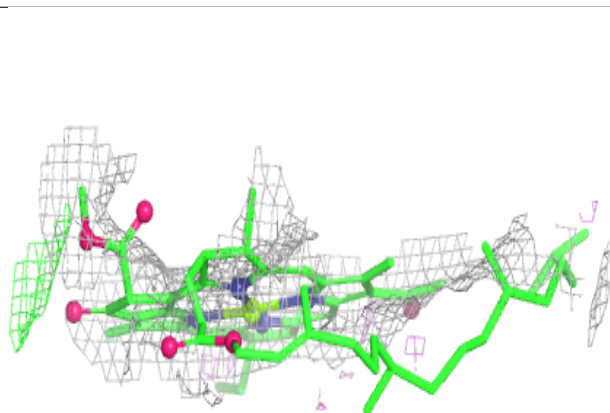
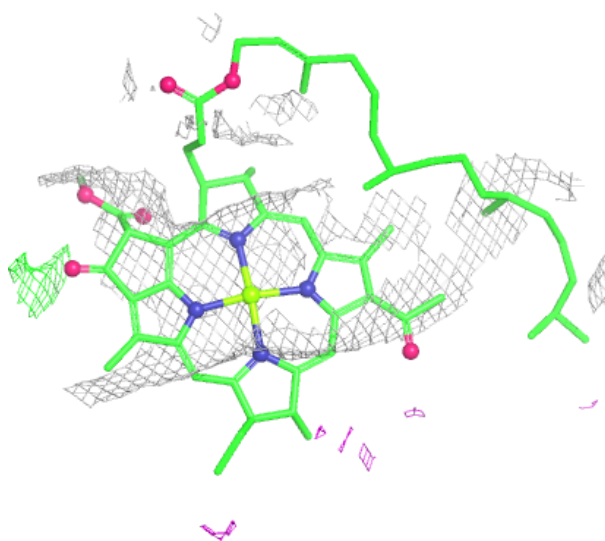
Electron density around BCL AT 101:

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



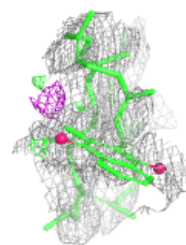
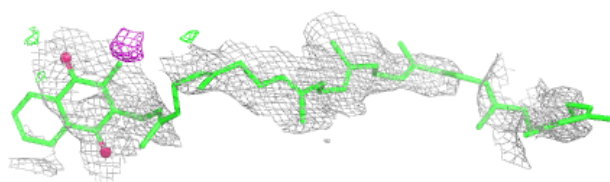
Electron density around BCL AV 102:

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

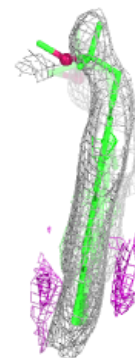
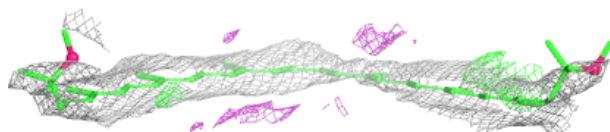
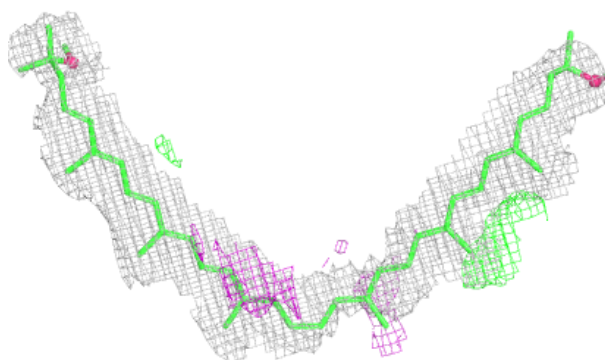


Electron density around MQ8 BM 405:

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

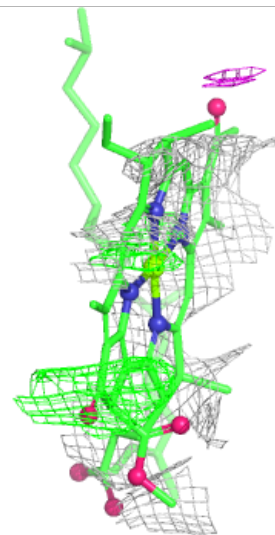
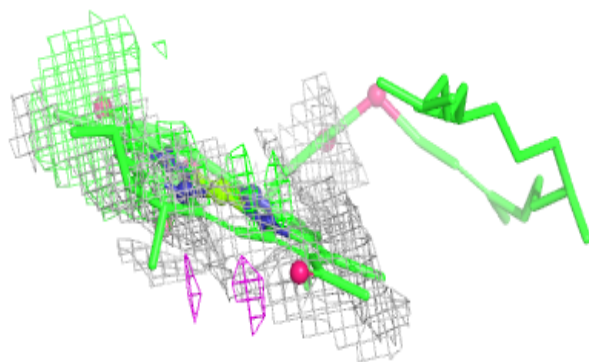
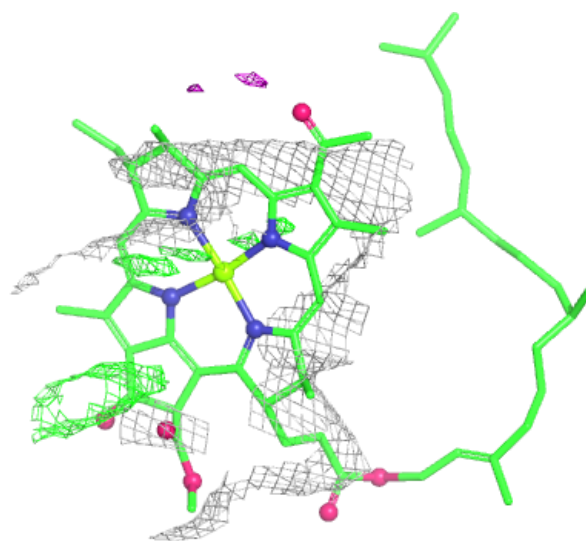
**Electron density around CRT AM 406:**

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



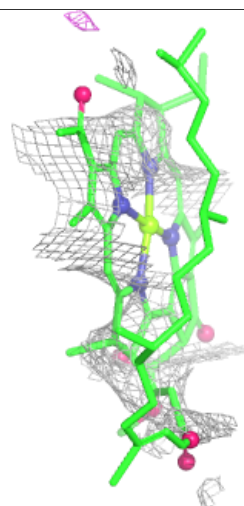
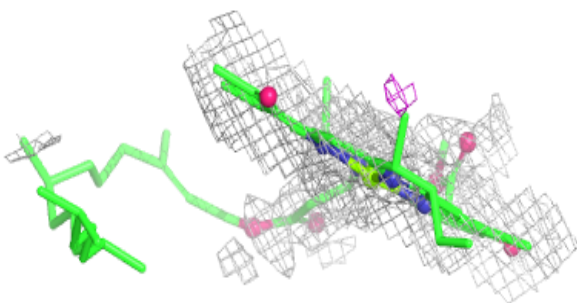
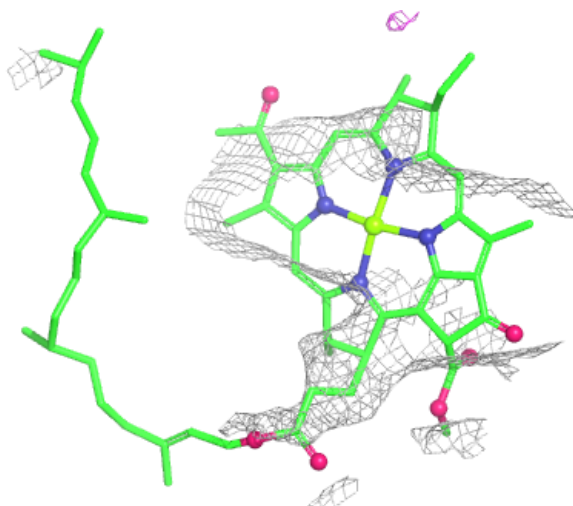
Electron density around BCL AX 101:

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



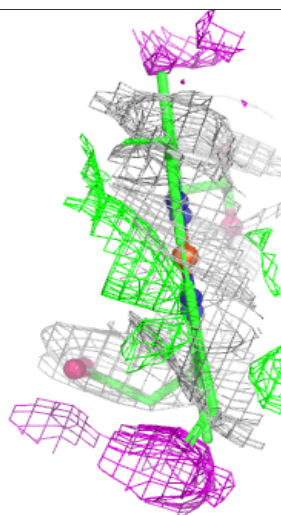
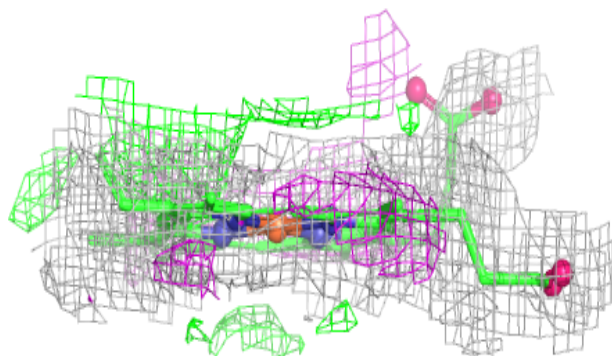
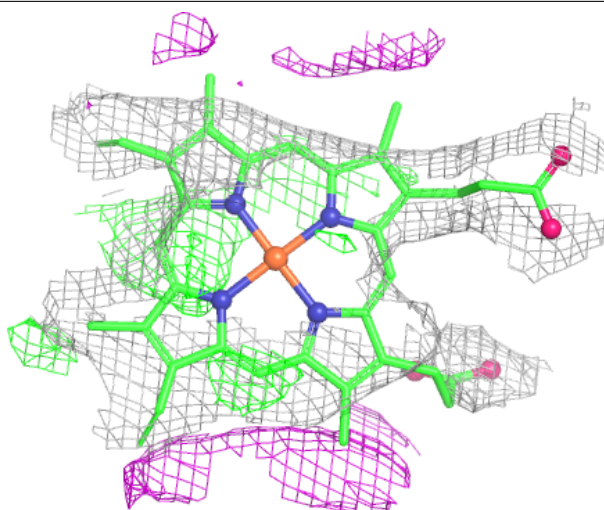
Electron density around BCL AZ 101:

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



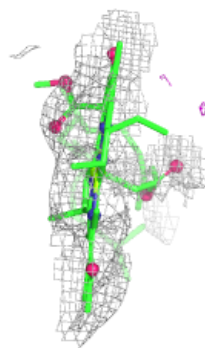
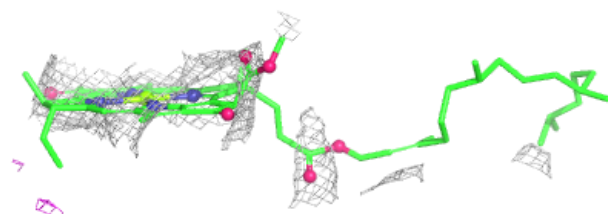
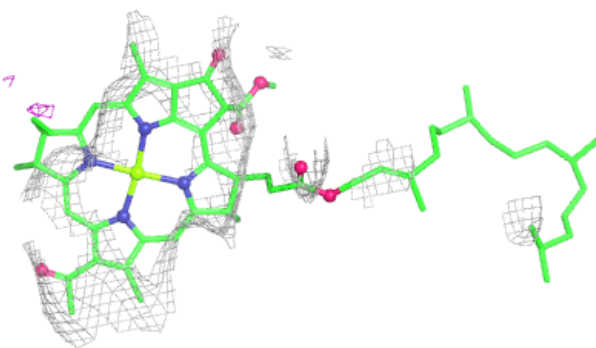
Electron density around HEM AC 503:

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

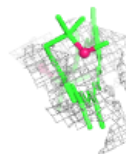
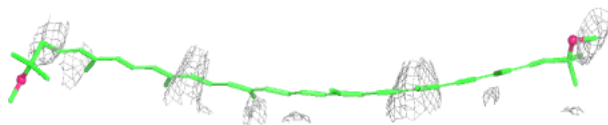
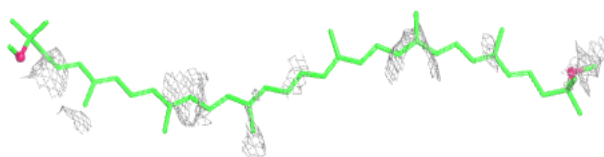


Electron density around BCL A5 102:

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

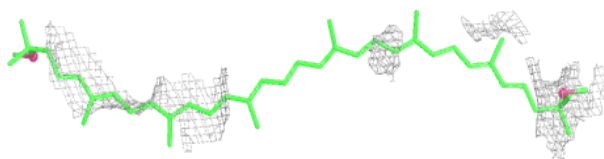
**Electron density around CRT AR 102:**

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

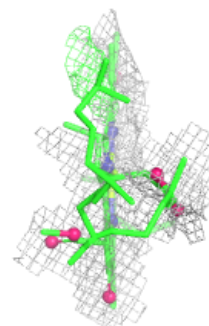
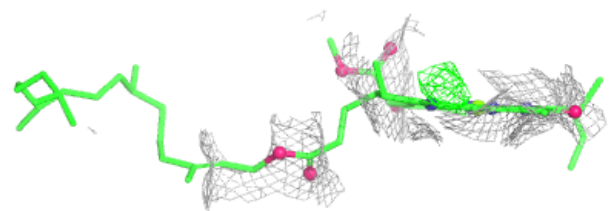
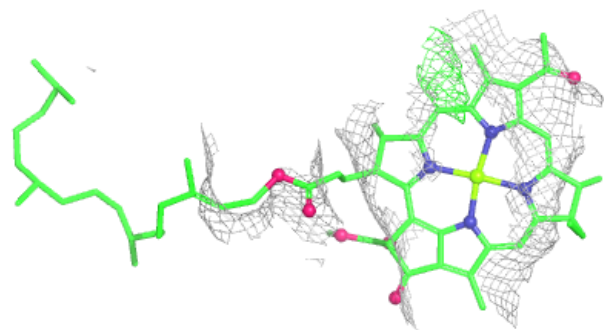


Electron density around CRT AT 102:

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

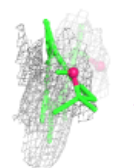
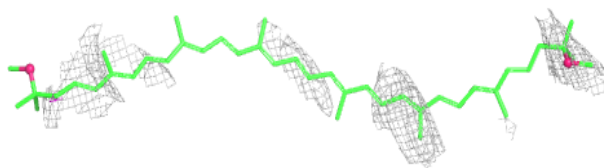
**Electron density around BCL A7 103:**

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

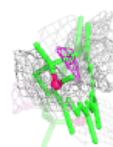
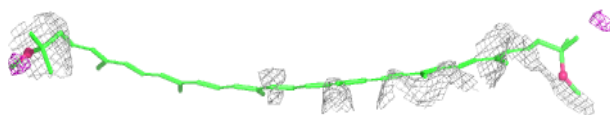
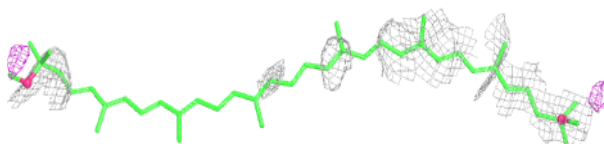


Electron density around CRT A1 103:

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

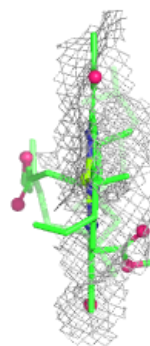
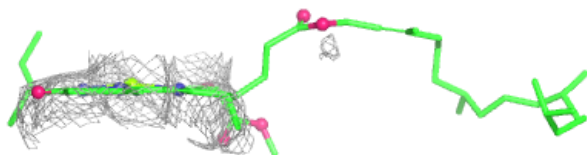
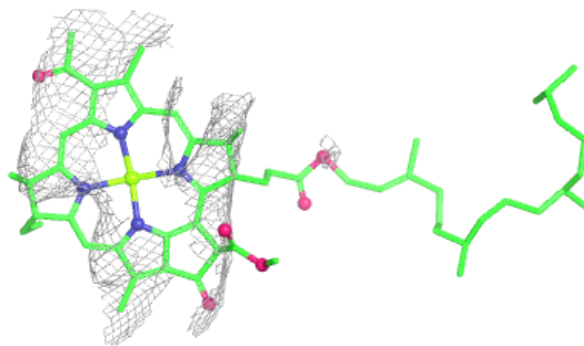
**Electron density around CRT A2 102:**

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



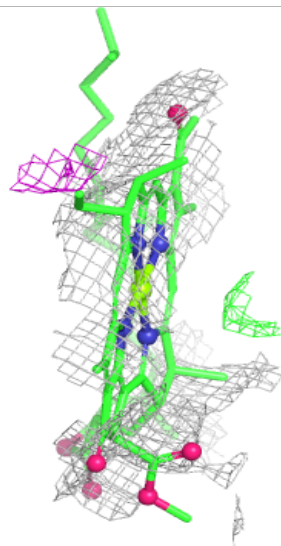
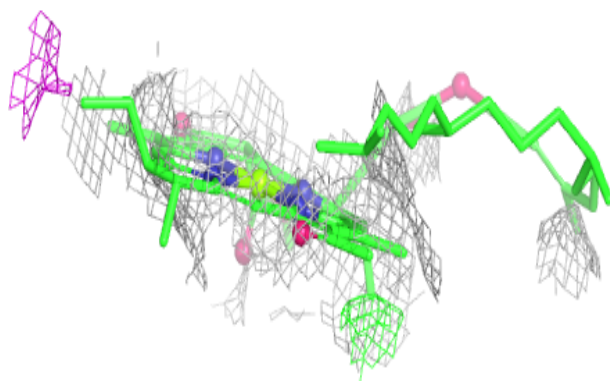
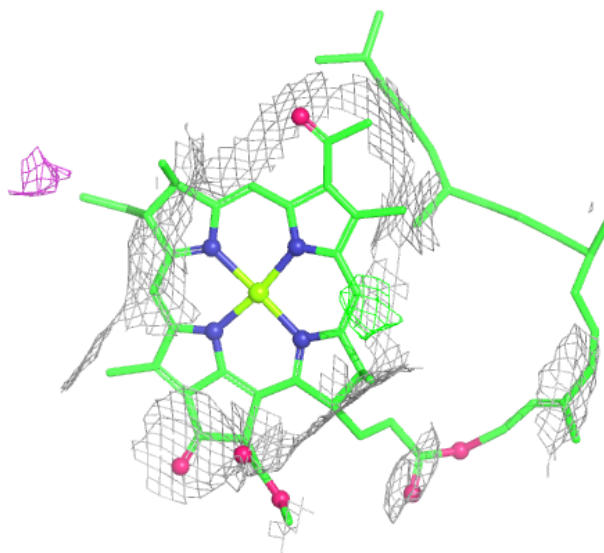
Electron density around BCL A9 102:

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



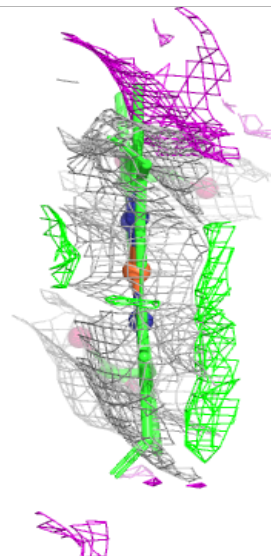
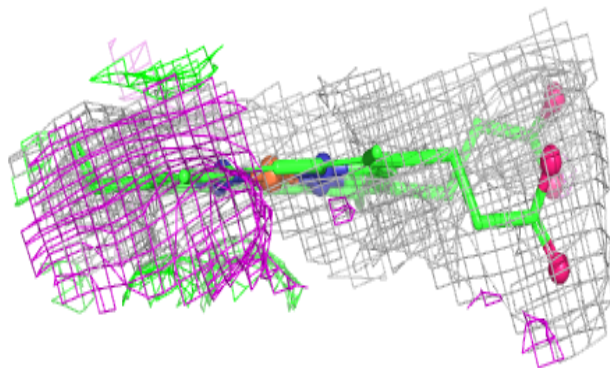
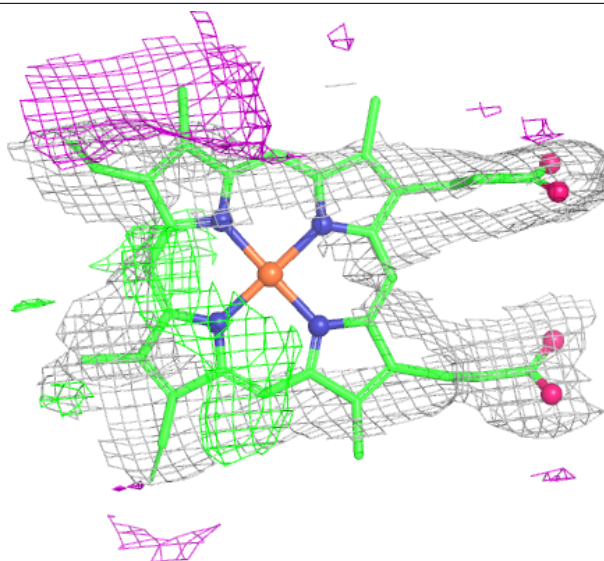
Electron density around BCL A0 102:

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



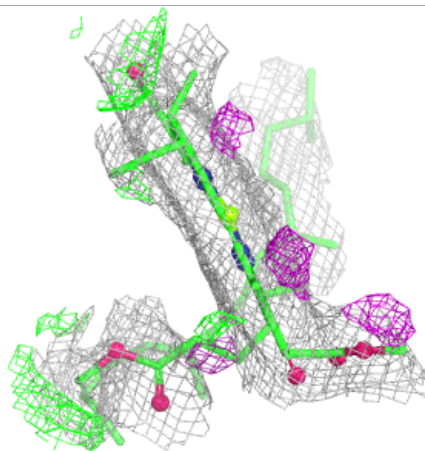
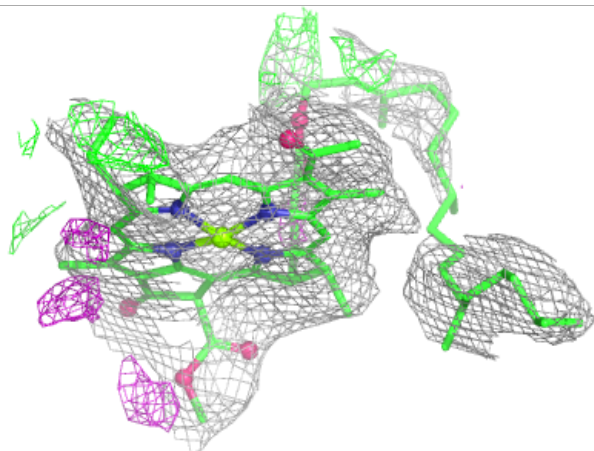
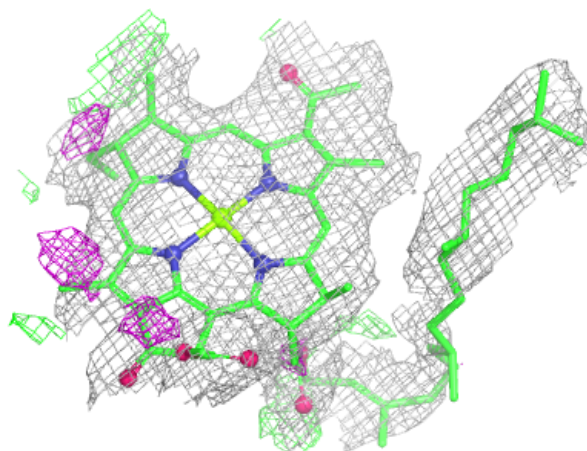
Electron density around HEM AC 504:

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



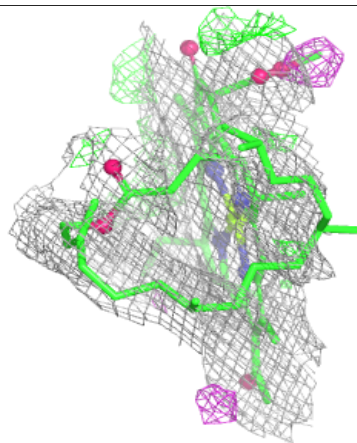
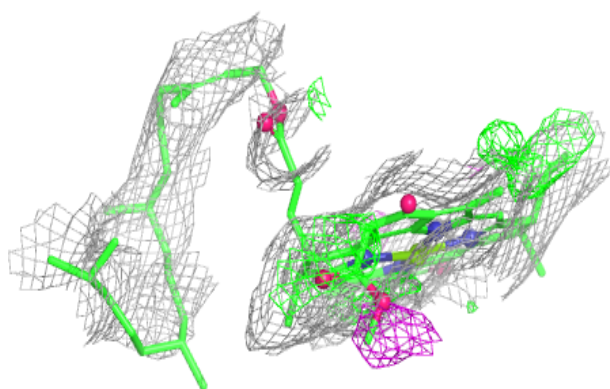
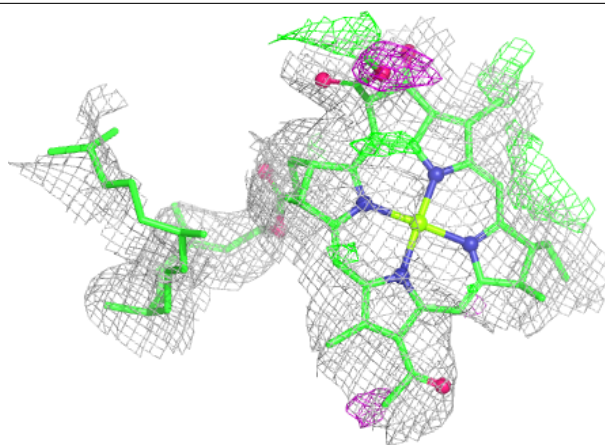
Electron density around BCL BL 303:

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



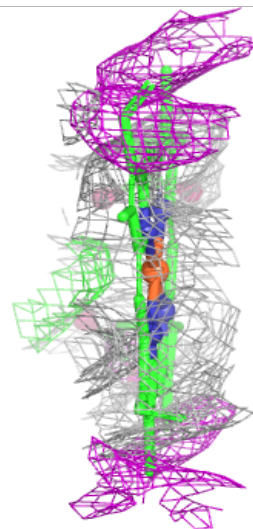
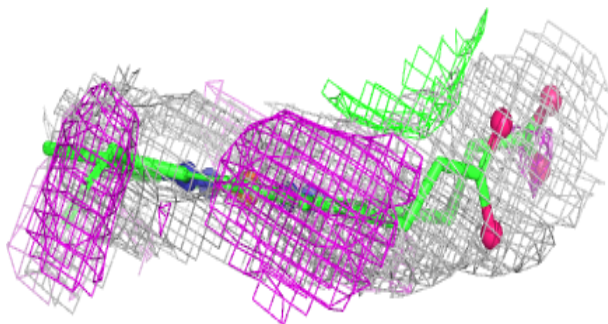
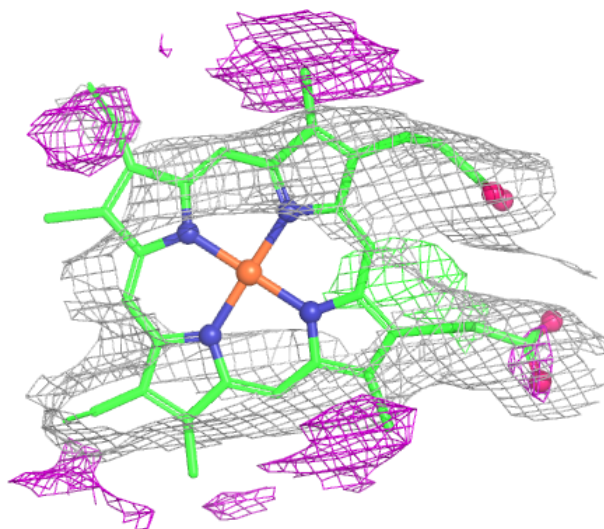
Electron density around BCL BM 401:

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



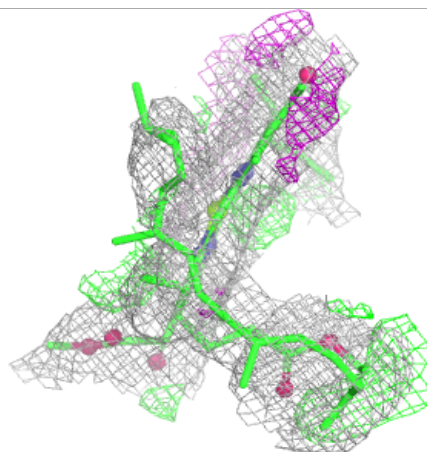
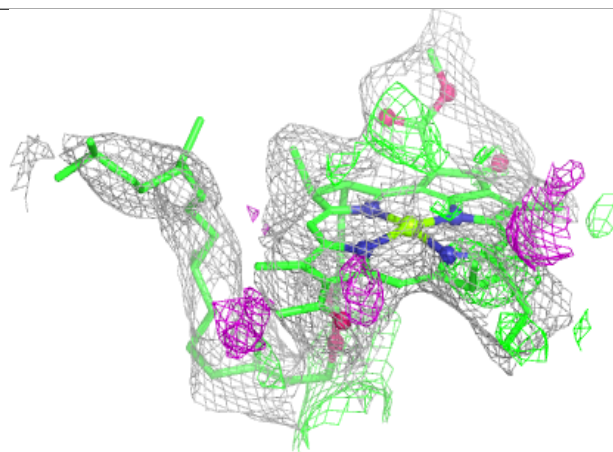
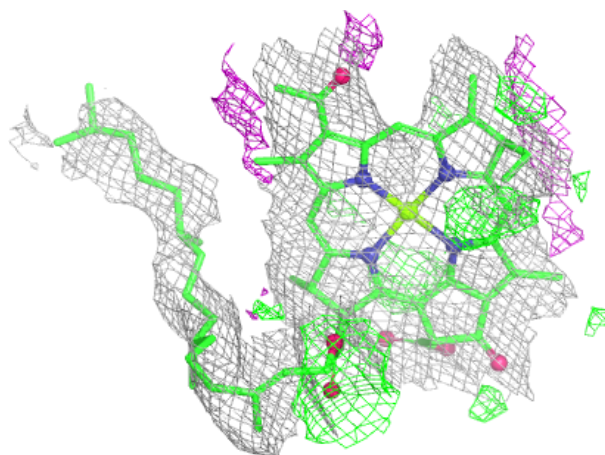
Electron density around HEM BC 502:

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



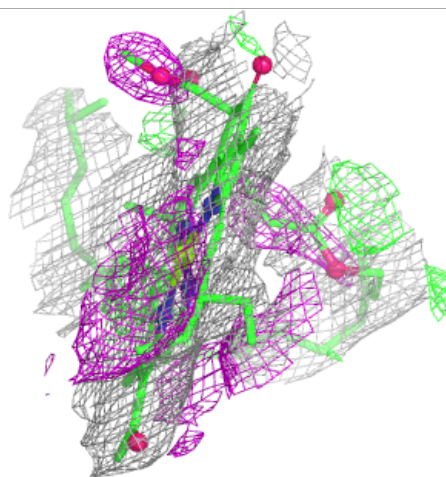
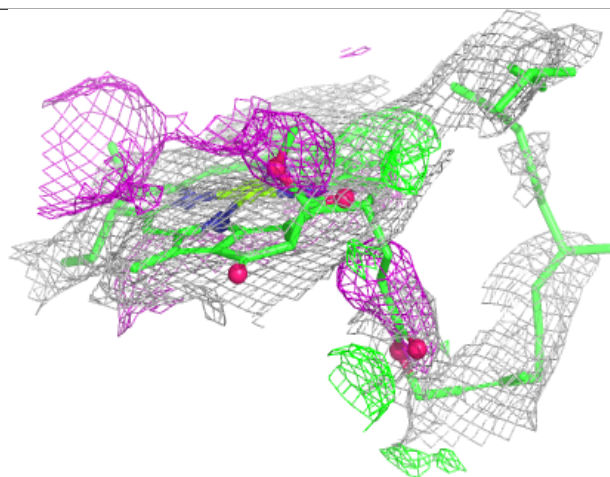
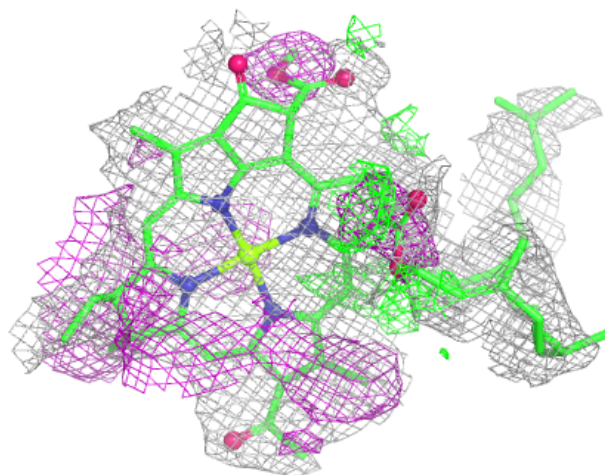
Electron density around BCL AL 303:

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



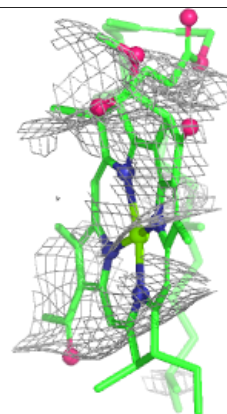
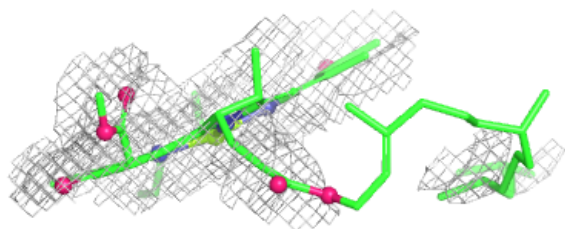
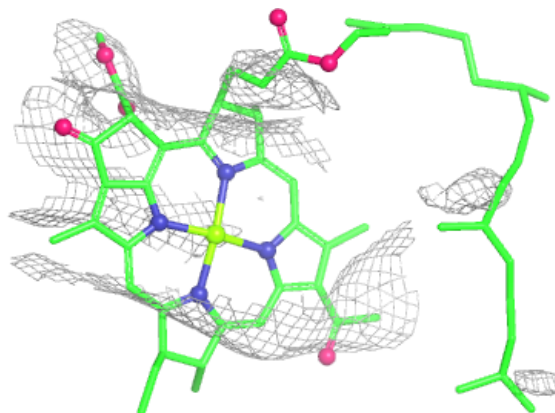
Electron density around BCL AM 401:

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

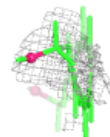
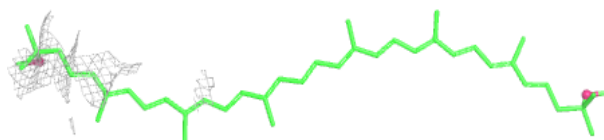


Electron density around BCL BG 101:

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

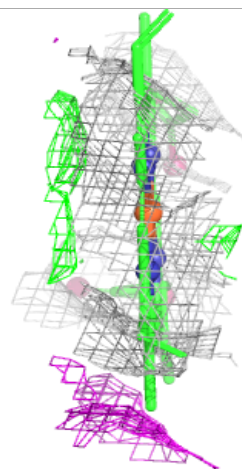
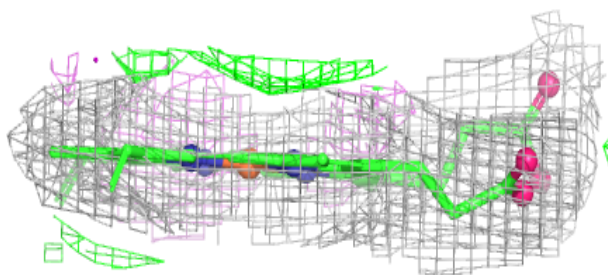
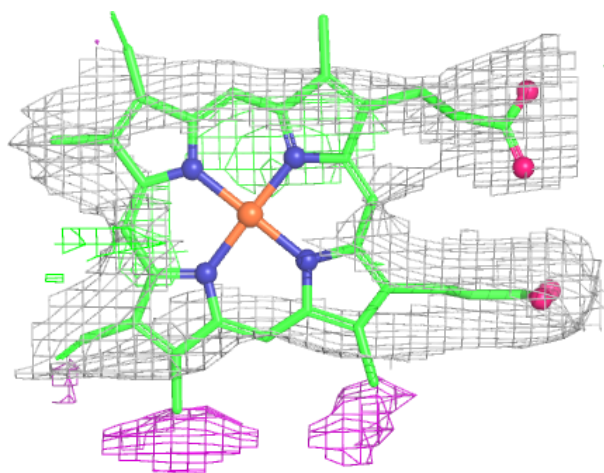
**Electron density around CRT BS 103:**

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



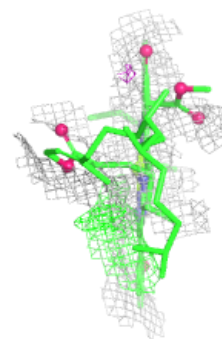
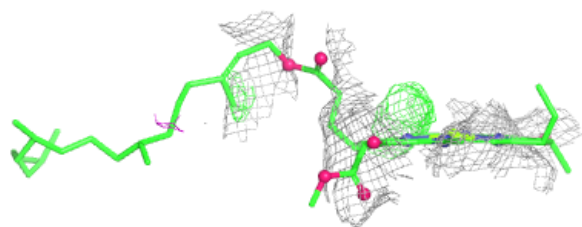
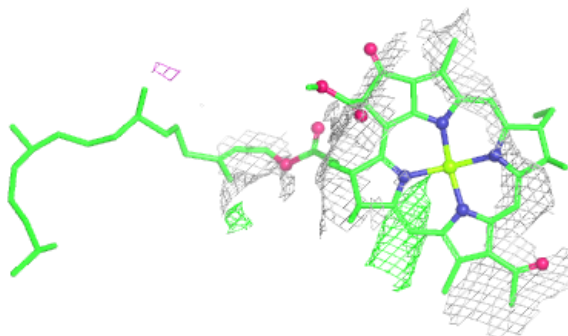
Electron density around HEM BC 504:

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

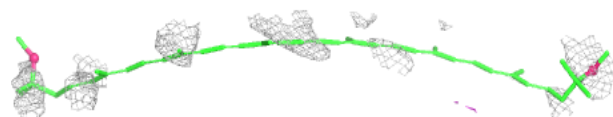
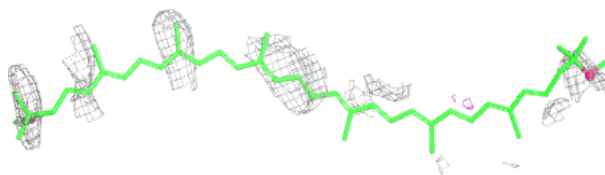


Electron density around BCL AA 101:

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

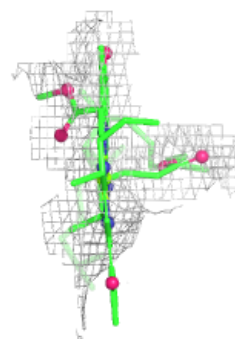
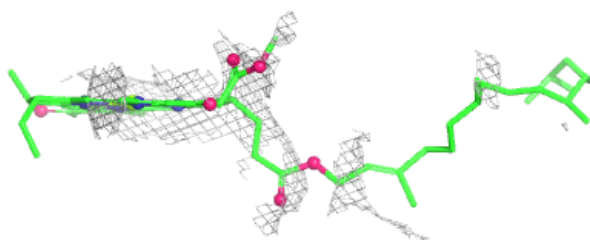
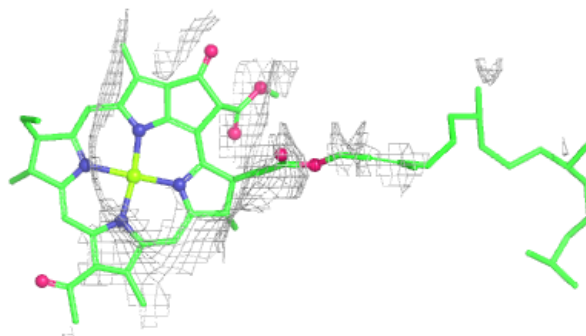
**Electron density around CRT BW 103:**

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

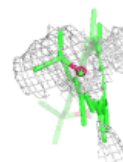
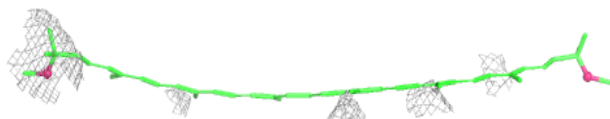
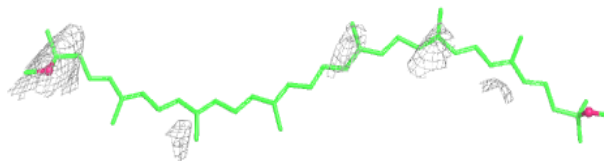


Electron density around BCL BK 102:

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

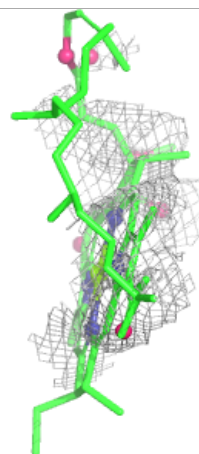
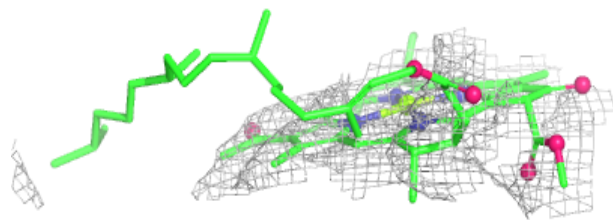
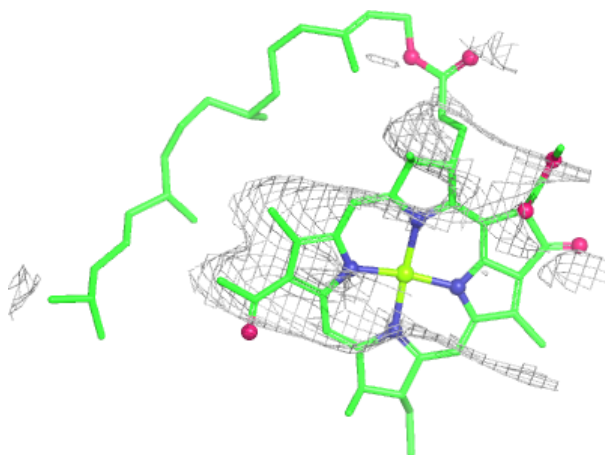
**Electron density around CRT B2 102:**

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



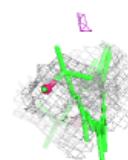
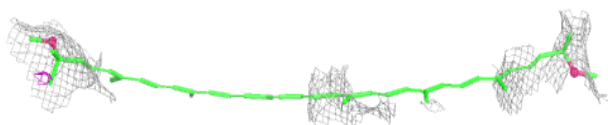
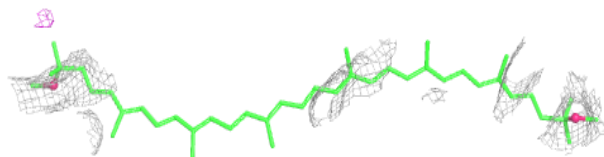
Electron density around BCL BN 101:

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

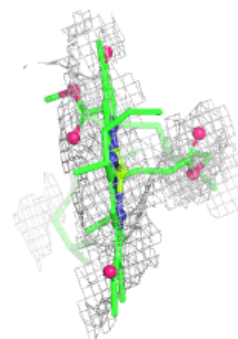
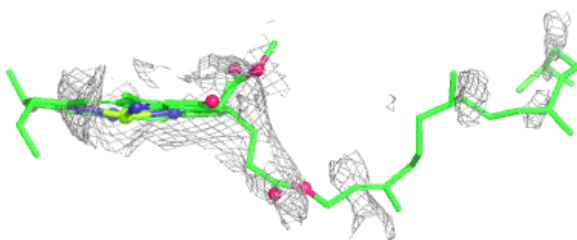
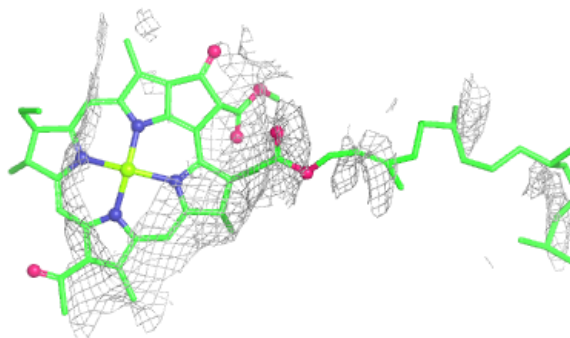


Electron density around CRT B7 102:

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

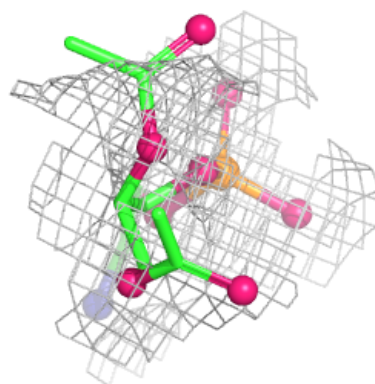
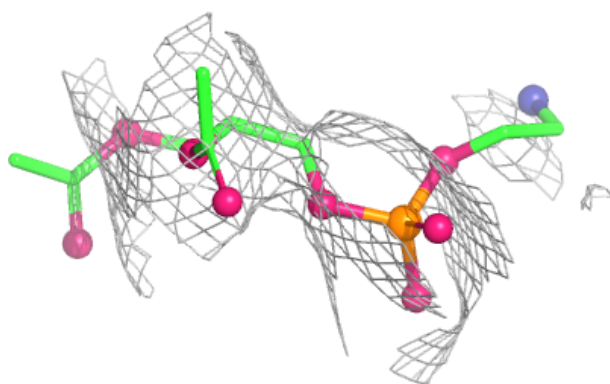
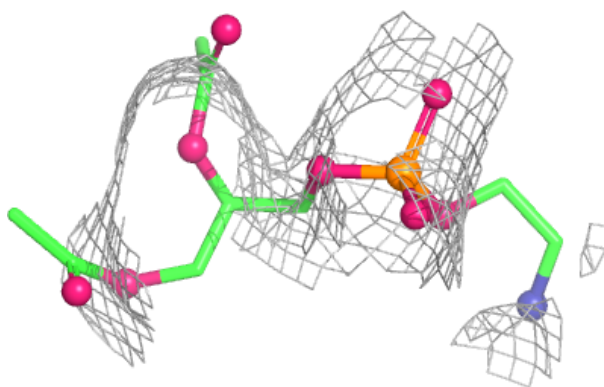
**Electron density around BCL BO 102:**

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



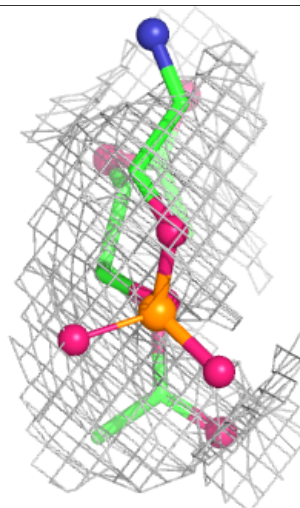
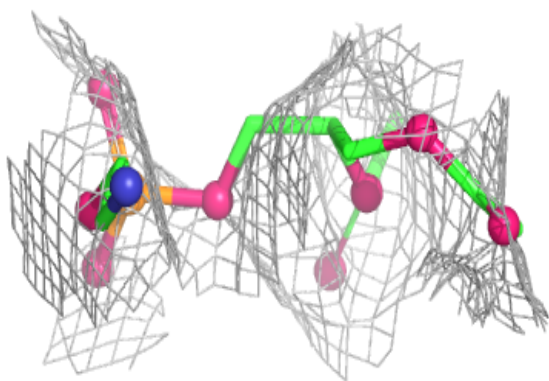
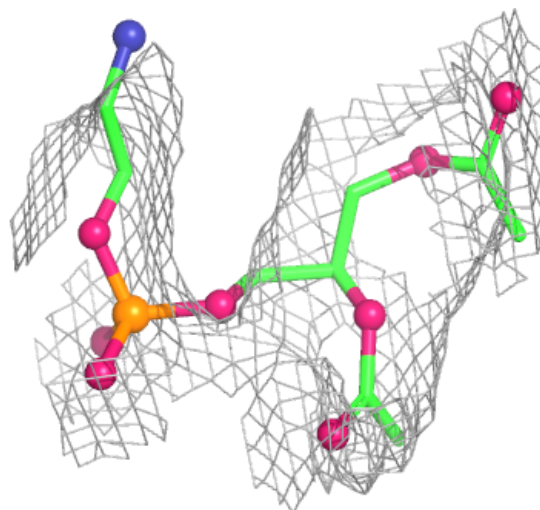
Electron density around PEF AM 407:

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



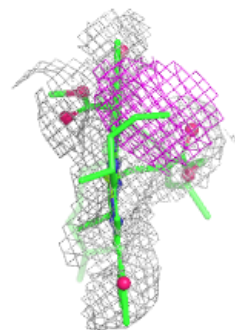
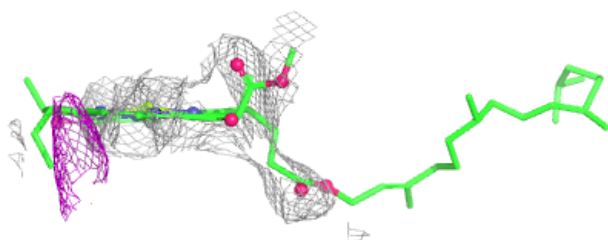
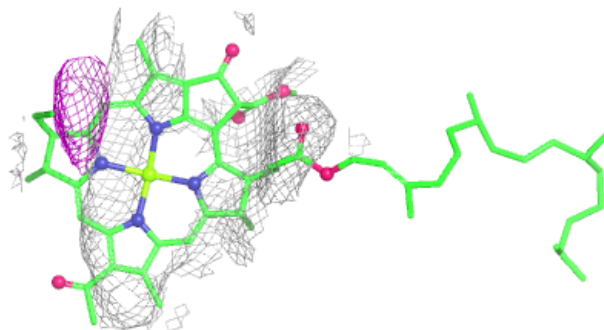
Electron density around PEF AH 301:

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

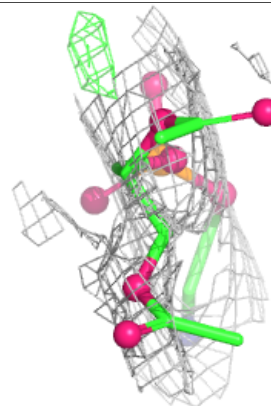
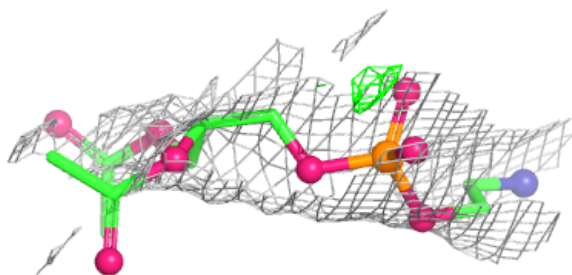
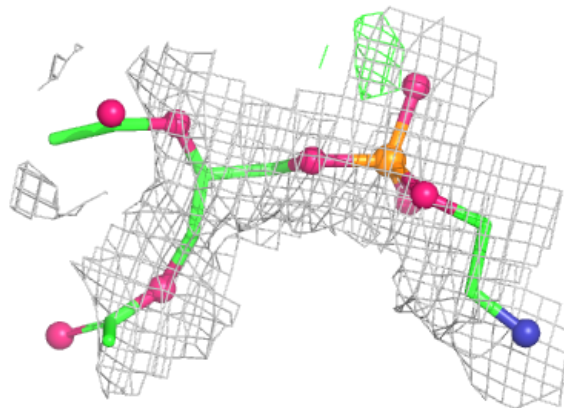


Electron density around BCL BQ 103:

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

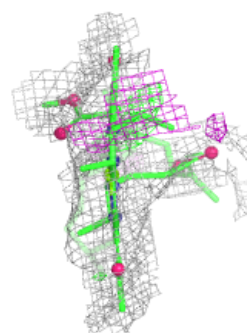
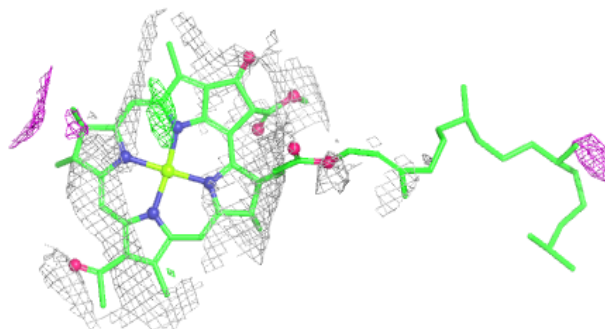
**Electron density around PEF BM 407:**

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

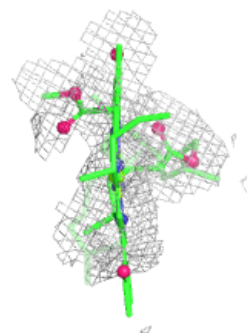
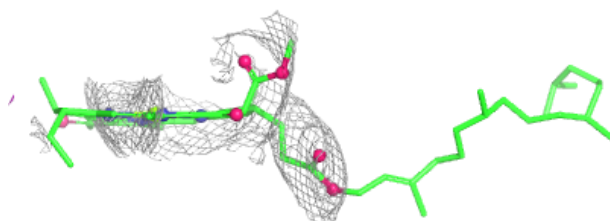
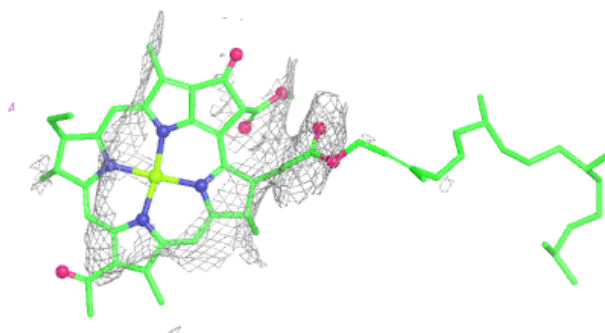


Electron density around BCL AD 102:

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

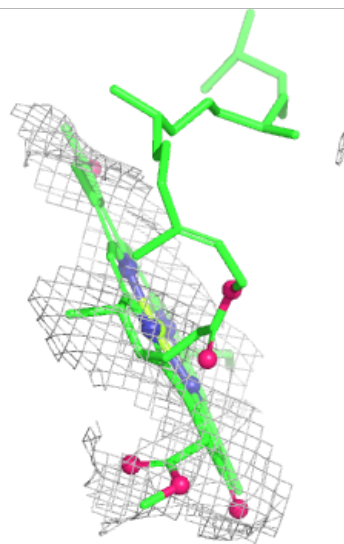
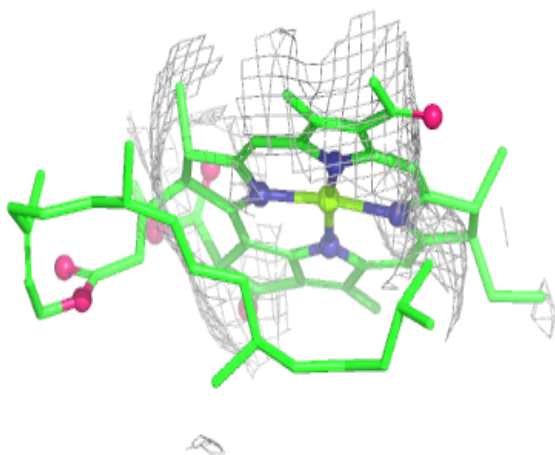
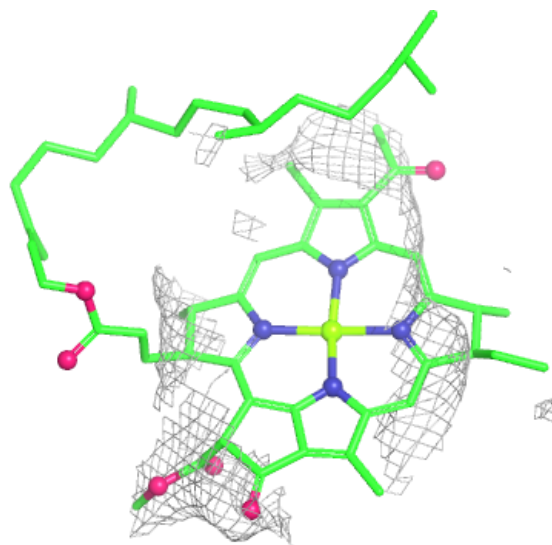
**Electron density around BCL BS 102:**

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



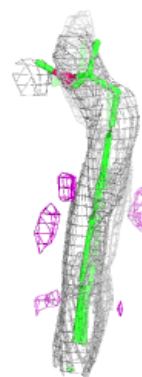
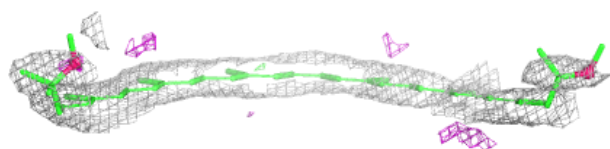
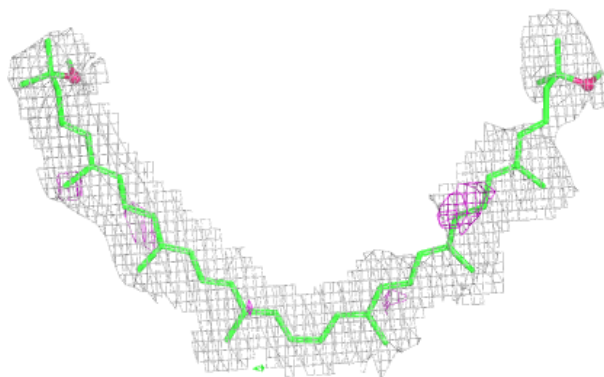
Electron density around BCL BE 101:

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

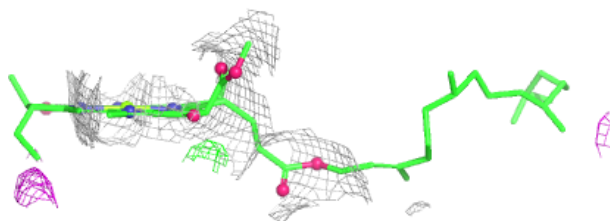
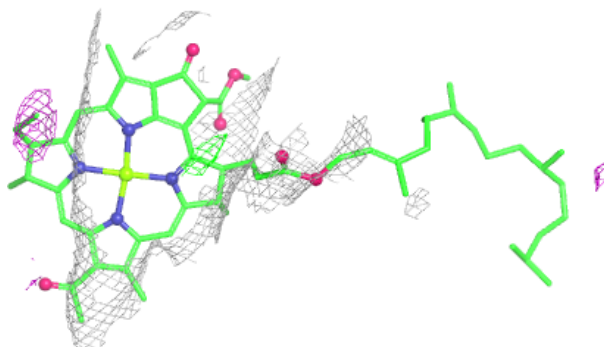


Electron density around CRT BM 406:

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

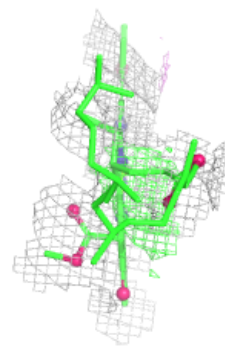
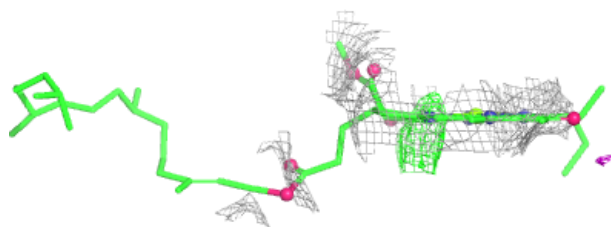
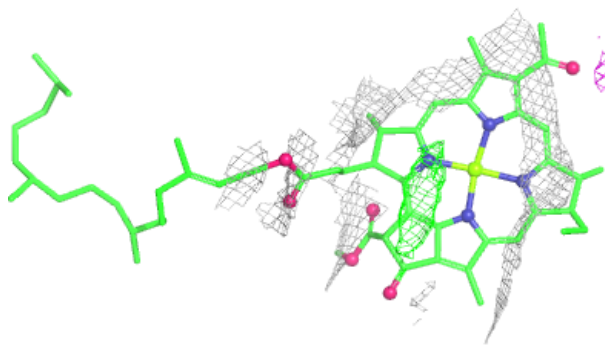
**Electron density around BCL AU 102:**

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



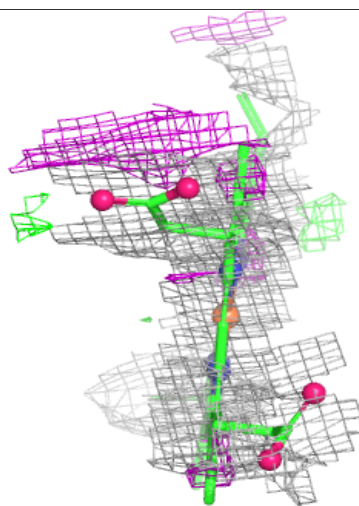
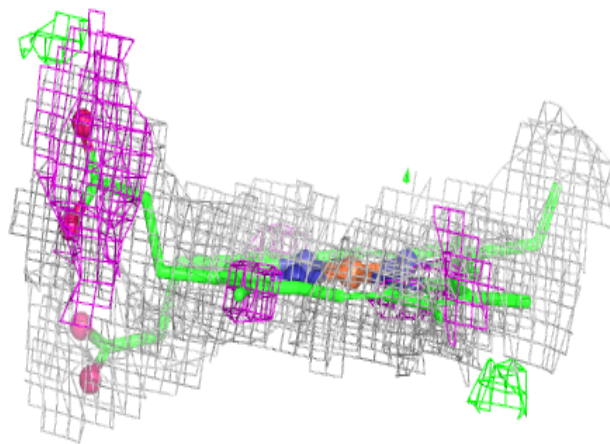
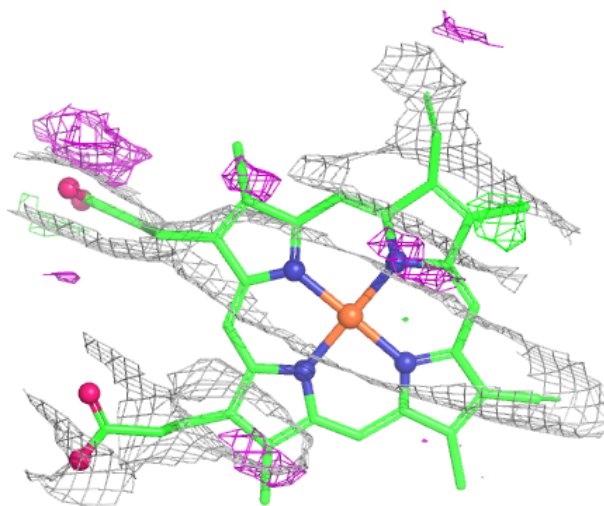
Electron density around BCL AW 101:

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



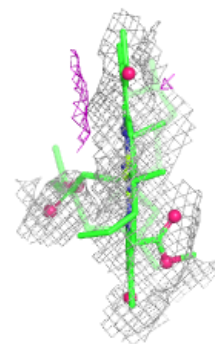
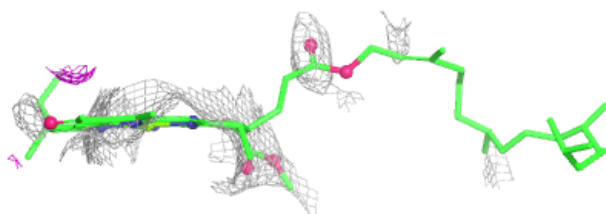
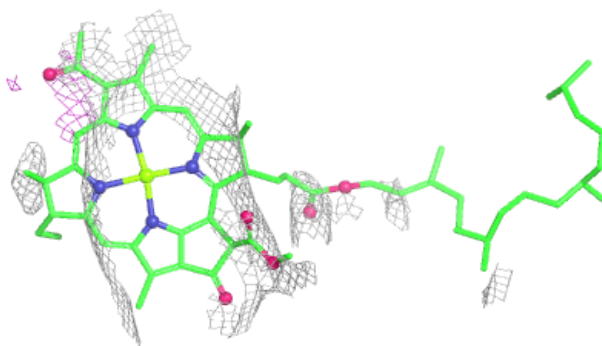
Electron density around HEM BC 501:

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

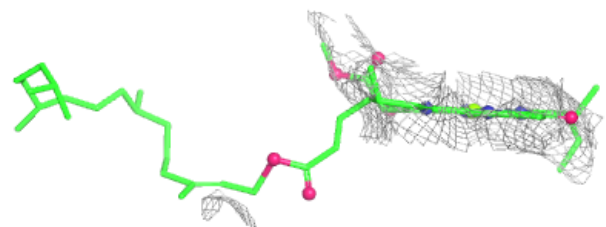
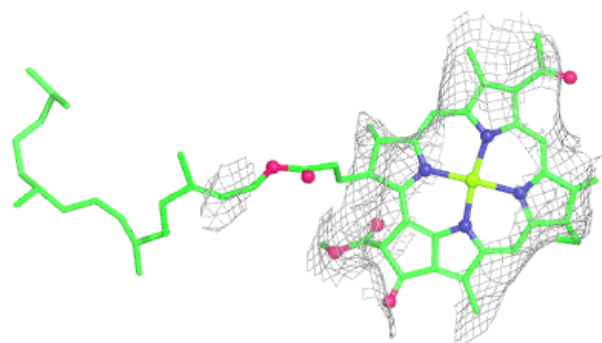


Electron density around BCL AY 102:

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

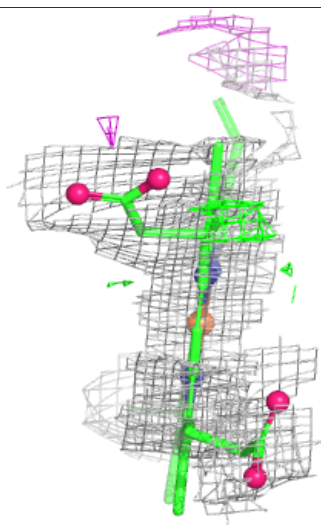
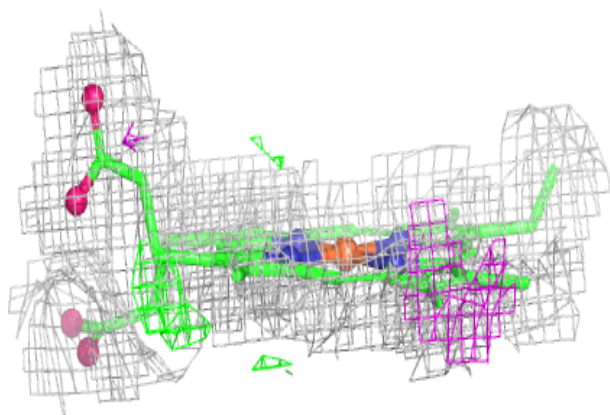
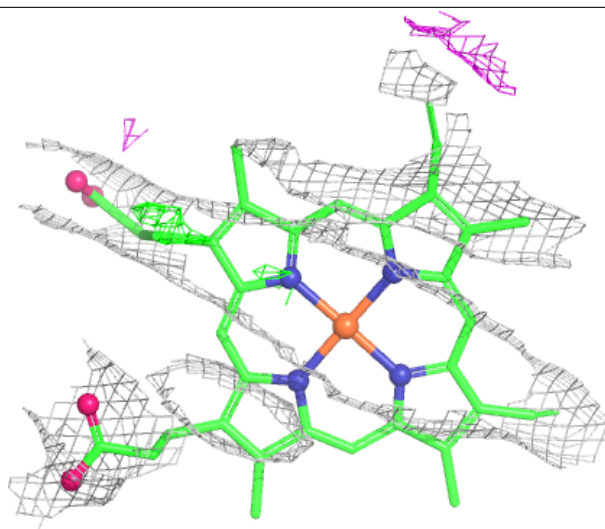
**Electron density around BCL A1 102:**

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



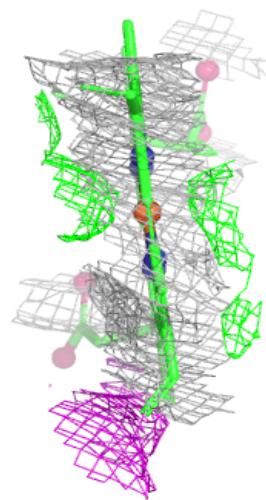
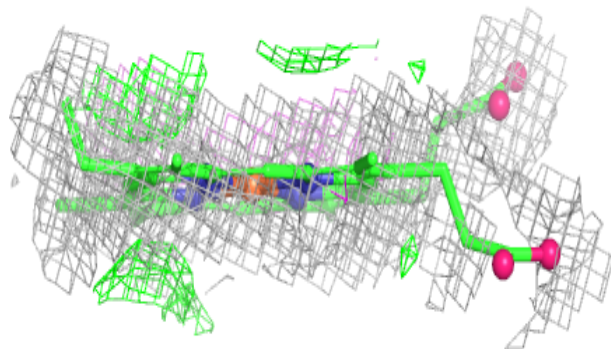
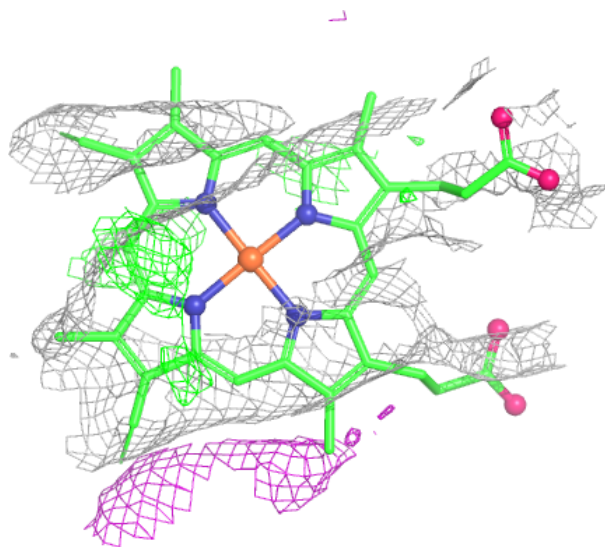
Electron density around HEM AC 501:

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



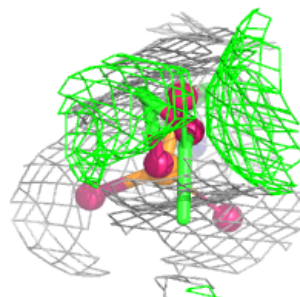
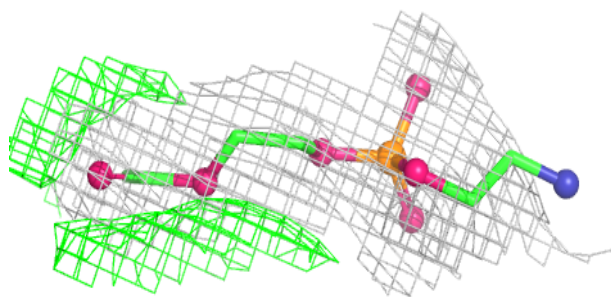
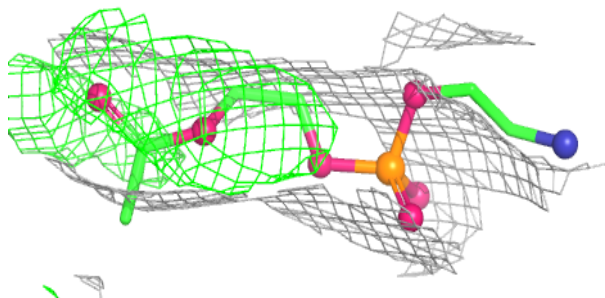
Electron density around HEM BC 503:

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

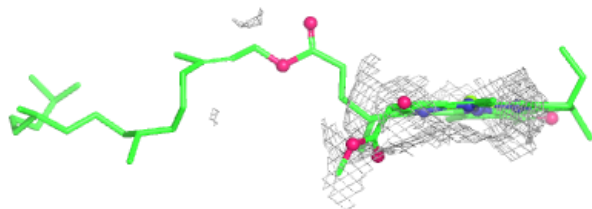
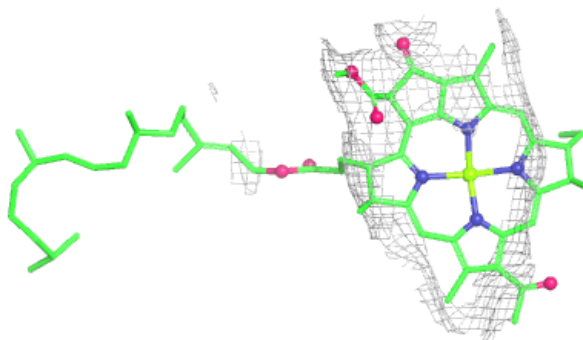


Electron density around PEF AM 408:

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

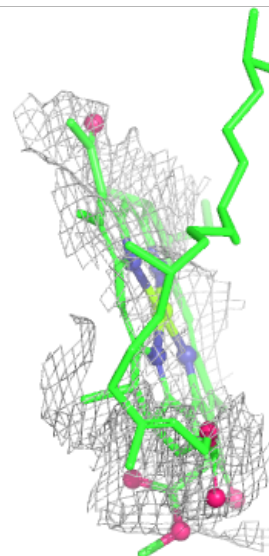
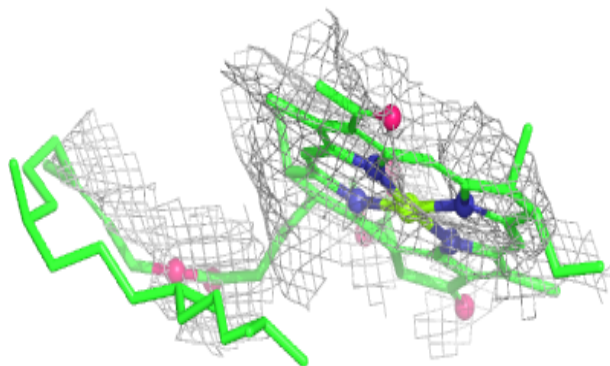
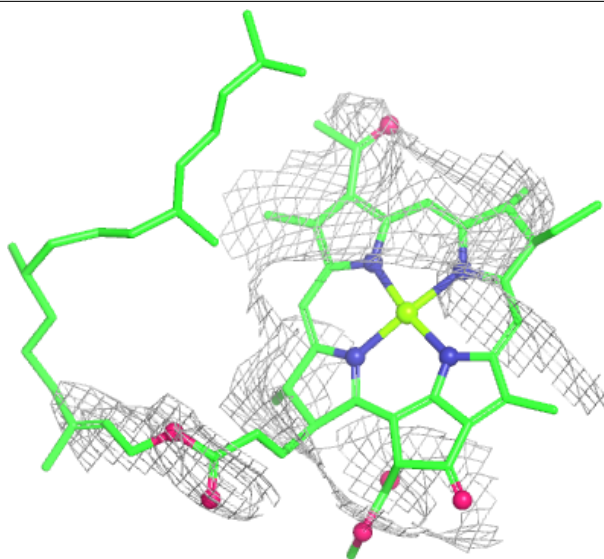
**Electron density around BCL AO 102:**

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



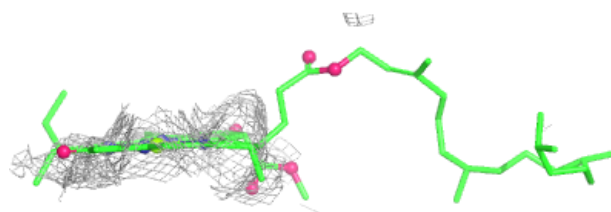
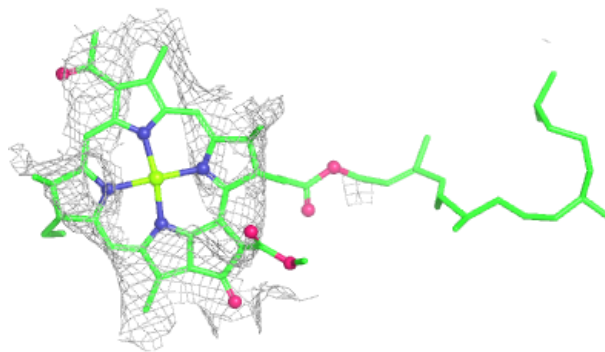
Electron density around BCL AP 101:

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



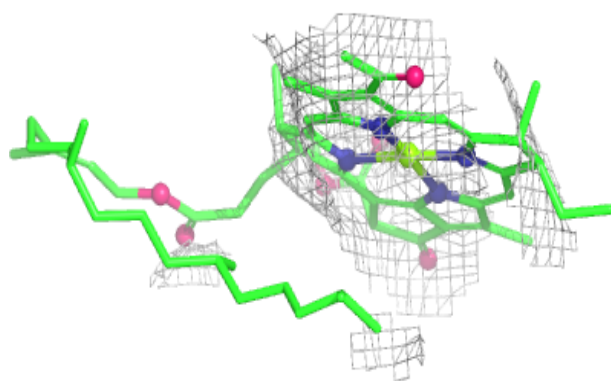
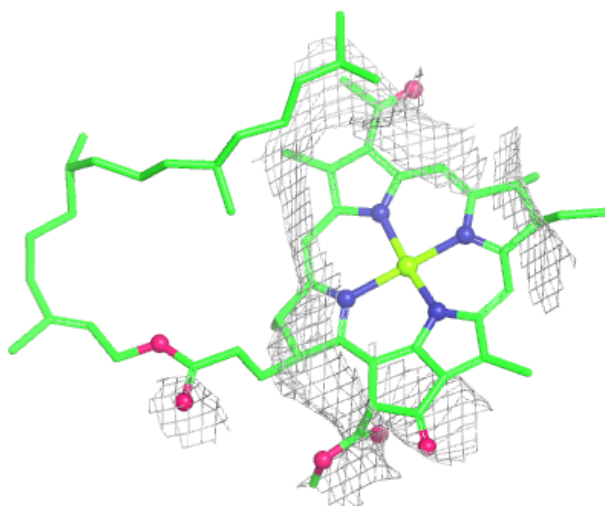
Electron density around BCL AQ 102:

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



Electron density around BCL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.