wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2024 – 04:27 PM EST

PDB ID	:	3WMM
Title	:	Crystal structure of the LH1-RC complex from Thermochromatium tepidum in C2 form
Authors	:	Niwa, S.; Takeda, K.; Wang-Otomo, Z.-Y.; Miki, K.
Deposited on	:	2013-11-22
Resolution	:	3.01 Å(reported)

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

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

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

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

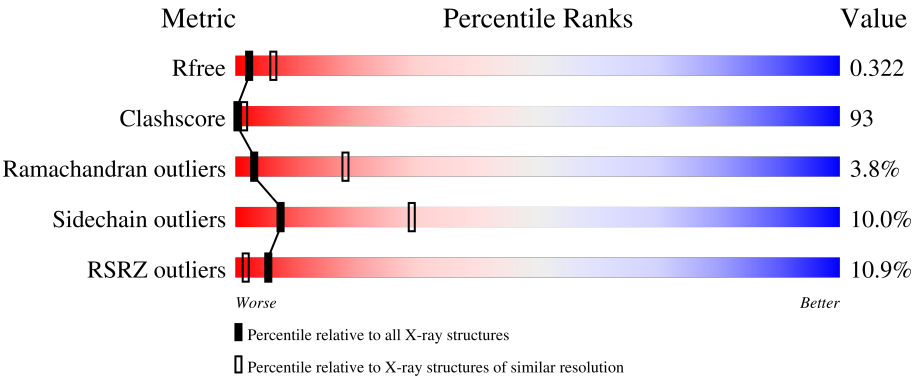
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	404	4% 29% 45% 22%
2	L	281	2% 28% 66% 6%
3	M	325	2% 30% 63% 5%
4	H	259	7% 33% 59% 7%
5	1	61	18% 16% 62% 20%

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Mol	Chain	Length	Quality of chain
5	3	61	10% 11% 72% 15%
5	5	61	20% 20% 61% 18%
5	7	61	20% 18% 62% 18%
5	9	61	23% 23% 62% 13%
5	A	61	25% 15% 74% 10%
5	D	61	15% 8% 82% 8%
5	F	61	20% 18% 66% 13%
5	I	61	26% 21% 64% 13%
5	K	61	33% 26% 57% 15%
5	O	61	21% 18% 67% 13%
5	Q	61	31% 28% 64% 7%
5	S	61	23% 25% 67% 5%
5	U	61	11% 18% 66% 15%
5	W	61	10% 11% 67% 20%
5	Y	61	16% 15% 66% 18%
6	0	47	4% 11% 53% 21% 15%
6	2	47	6% 21% 55% 9% 15%
6	4	47	9% 23% 51% 11% 15%
6	6	47	6% 21% 55% 9% 15%
6	8	47	17% 15% 55% 15% 15%
6	B	47	11% 19% 53% 13% 15%
6	E	47	6% 23% 60% 15%
6	G	47	13% 6% 66% 13% 15%
6	J	47	21% 55% 9% 15%
6	N	47	9% 17% 55% 13% 15%

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Mol	Chain	Length	Quality of chain
6	P	47	13% 11% 62% 13% 15%
6	R	47	13% 19% 55% 11% 15%
6	T	47	11% 17% 51% 17% 15%
6	V	47	6% 19% 53% 13% 15%
6	X	47	11% 66% 6% 15%
6	Z	47	6% 26% 45% 13% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	UQ8	L	304	-	-	-	X
12	PO4	H	304	-	-	X	-
15	CRT	2	102	-	-	X	X
15	CRT	3	103	-	-	-	X
15	CRT	4	102	-	-	X	X
15	CRT	8	101	-	-	X	X
15	CRT	A	101	-	-	X	X
15	CRT	A	103	-	-	X	X
15	CRT	B	102	-	-	X	X
15	CRT	G	102	-	-	X	X
15	CRT	J	101	-	-	X	X
15	CRT	N	102	-	-	X	X
15	CRT	P	102	-	-	X	X
15	CRT	R	102	-	-	X	X
15	CRT	T	102	-	-	X	X
15	CRT	V	102	-	-	X	X
15	CRT	W	103	-	-	X	X
15	CRT	X	102	-	-	X	X
17	PEF	H	301	-	X	-	-
9	BCL	0	101	-	-	X	-
9	BCL	3	102	-	-	X	-
9	BCL	4	101	-	-	X	-
9	BCL	5	102	-	-	X	-
9	BCL	6	101	-	-	X	-
9	BCL	7	102	-	-	X	-
9	BCL	7	103	-	-	X	-
9	BCL	9	102	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BCL	A	102	-	-	X	-
9	BCL	B	101	-	-	X	-
9	BCL	D	102	-	-	X	-
9	BCL	E	101	-	-	X	-
9	BCL	F	102	-	-	X	-
9	BCL	G	101	-	-	X	-
9	BCL	I	102	-	-	X	-
9	BCL	I	103	-	-	X	-
9	BCL	K	102	-	-	X	-
9	BCL	M	401	-	-	X	-
9	BCL	N	101	-	-	X	-
9	BCL	O	102	-	-	X	-
9	BCL	P	101	-	-	X	-
9	BCL	Q	102	-	-	X	-
9	BCL	R	101	-	-	X	-
9	BCL	S	102	-	-	X	-
9	BCL	T	101	-	-	X	-
9	BCL	U	102	-	-	X	-
9	BCL	W	102	-	-	X	-
9	BCL	X	101	-	-	X	-
9	BCL	Y	102	-	-	X	-
9	BCL	Z	101	-	-	X	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 25819 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 C subunit.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	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	H	258	Total	C	N	O	S	0	0	0
			1983	1275	339	364	5			

- Molecule 5 is a protein called LH1 alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	D	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	F	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	I	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	O	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	Q	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	S	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	U	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	W	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	Y	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	1	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	3	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	5	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	7	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	9	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			

- Molecule 6 is a protein called LH1 beta polypeptide.

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

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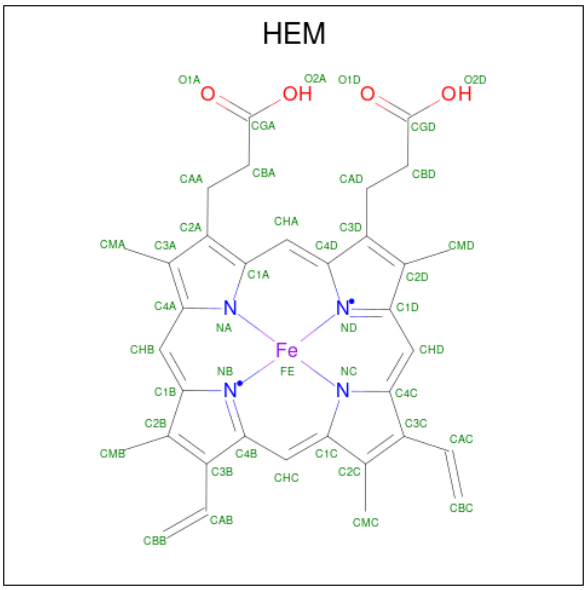
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	T	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	V	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	X	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	Z	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	2	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	4	40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

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



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

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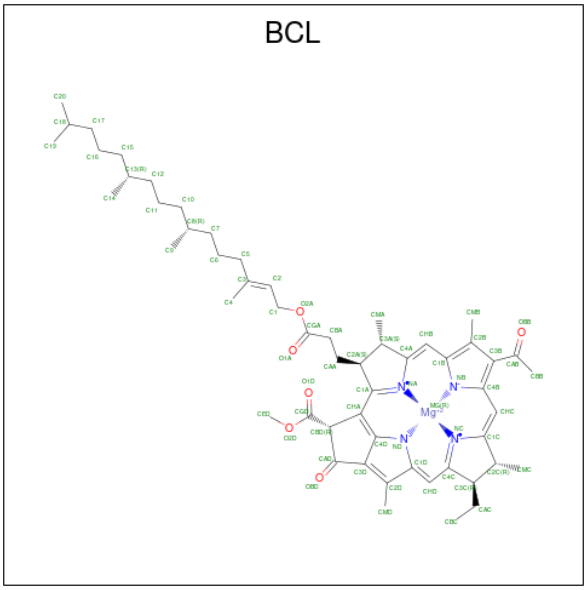
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca	0	0
			1	1		
8	A	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		
8	F	1	Total	Ca	0	0
			1	1		
8	I	1	Total	Ca	0	0
			1	1		
8	K	1	Total	Ca	0	0
			1	1		
8	O	1	Total	Ca	0	0
			1	1		
8	Q	1	Total	Ca	0	0
			1	1		
8	S	1	Total	Ca	0	0
			1	1		
8	U	1	Total	Ca	0	0
			1	1		
8	W	1	Total	Ca	0	0
			1	1		
8	Y	1	Total	Ca	0	0
			1	1		
8	1	1	Total	Ca	0	0
			1	1		
8	3	1	Total	Ca	0	0
			1	1		
8	5	1	Total	Ca	0	0
			1	1		
8	7	1	Total	Ca	0	0
			1	1		
8	9	1	Total	Ca	0	0
			1	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	K	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	N	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	O	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	P	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	Q	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	T	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	U	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	V	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	W	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	X	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	Y	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	Z	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	1	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	2	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	3	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	4	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	5	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	6	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	7	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	7	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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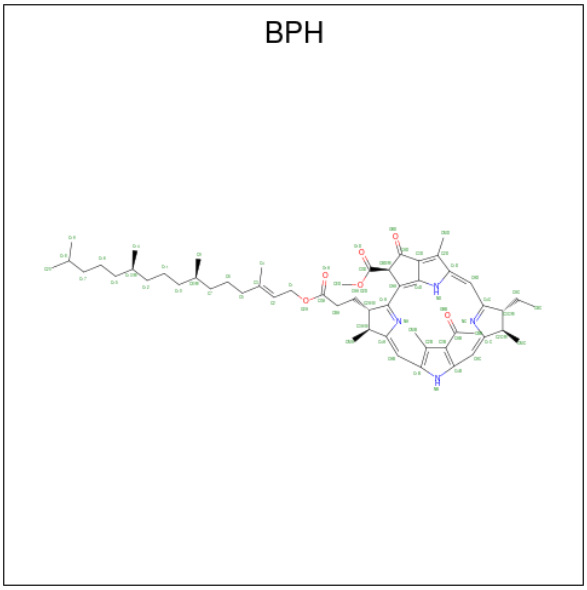
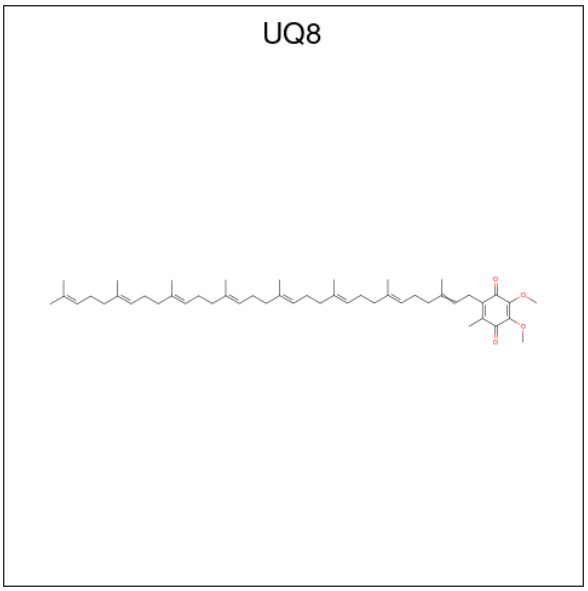
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	0	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



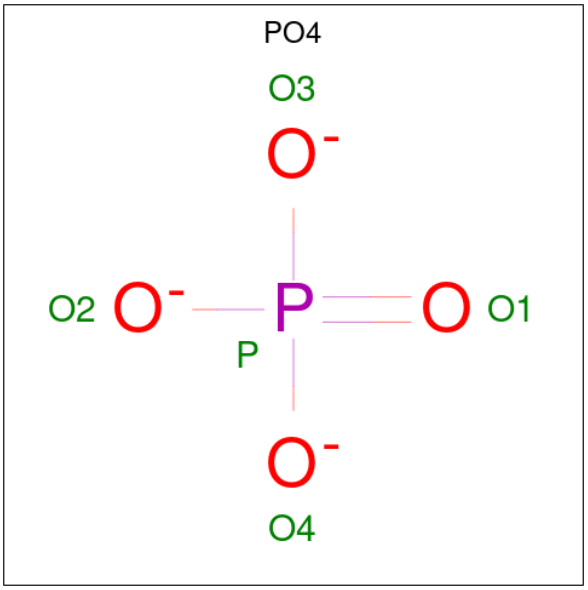
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total O P 5 4 1	0	0
12	M	1	Total O P 5 4 1	0	0
12	H	1	Total O P 5 4 1	0	0

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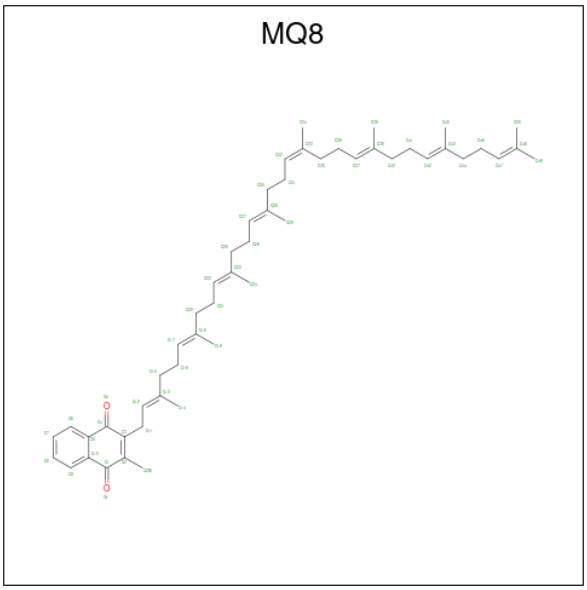
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	H	1	Total O P 5 4 1	0	0

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

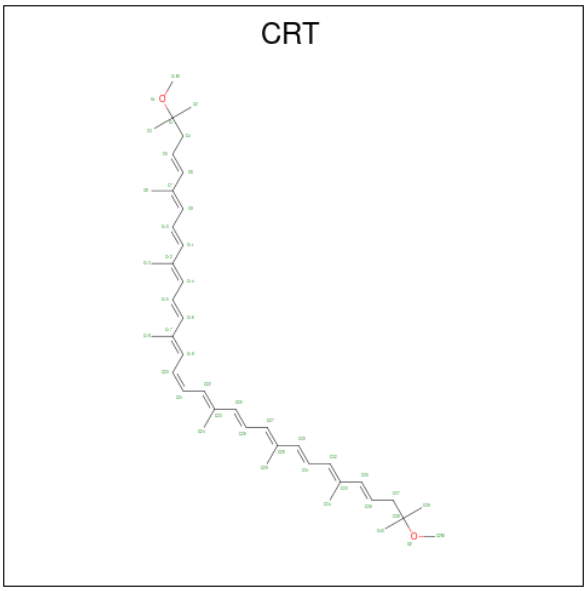
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total Fe 1 1	0	0

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



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	M	1	Total C O 44 42 2	0	0
15	A	1	Total C O 44 42 2	0	0
15	A	1	Total C O 44 42 2	0	0
15	B	1	Total C O 44 42 2	0	0
15	G	1	Total C O 44 42 2	0	0
15	J	1	Total C O 44 42 2	0	0
15	N	1	Total C O 44 42 2	0	0
15	P	1	Total C O 44 42 2	0	0
15	R	1	Total C O 44 42 2	0	0
15	T	1	Total C O 44 42 2	0	0
15	V	1	Total C O 44 42 2	0	0
15	W	1	Total C O 44 42 2	0	0
15	X	1	Total C O 44 42 2	0	0
15	2	1	Total C O 44 42 2	0	0

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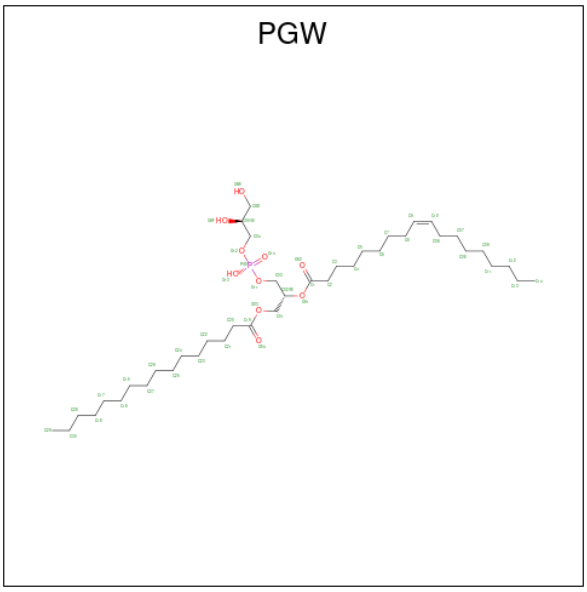
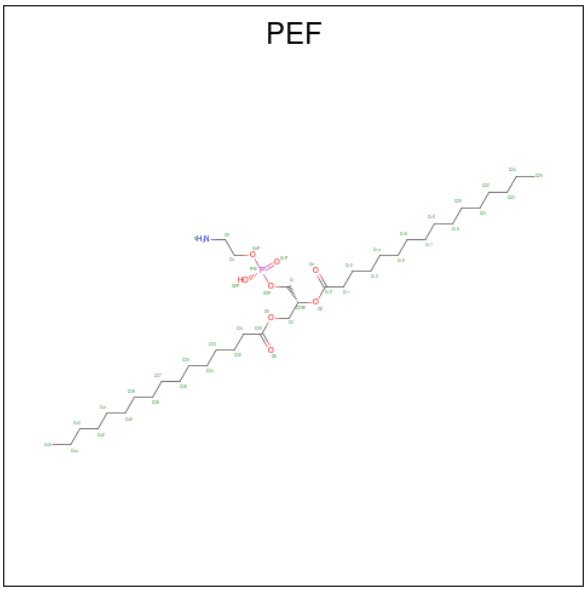
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	3	1	Total C O 44 42 2	0	0
15	4	1	Total C O 44 42 2	0	0
15	8	1	Total C O 44 42 2	0	0

- Molecule 16 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total C O P 21 10 10 1	0	0
16	H	1	Total C O P 21 10 10 1	0	0

- Molecule 17 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

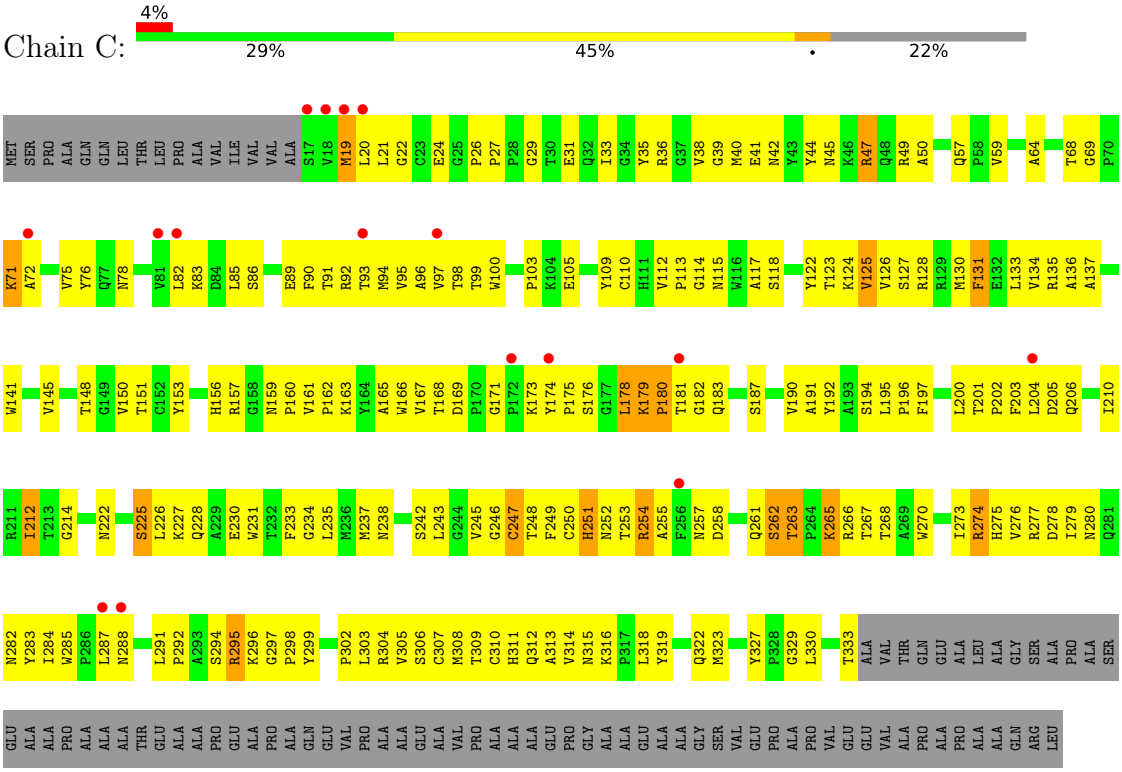
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	4	Total	O	0	0
			4	4		
18	H	1	Total	O	0	0
			1	1		

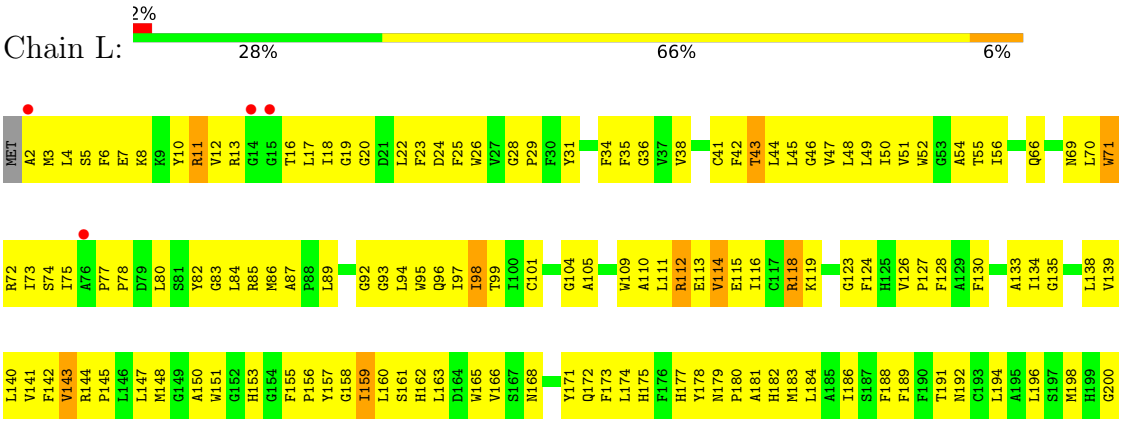
3 Residue-property plots (i)

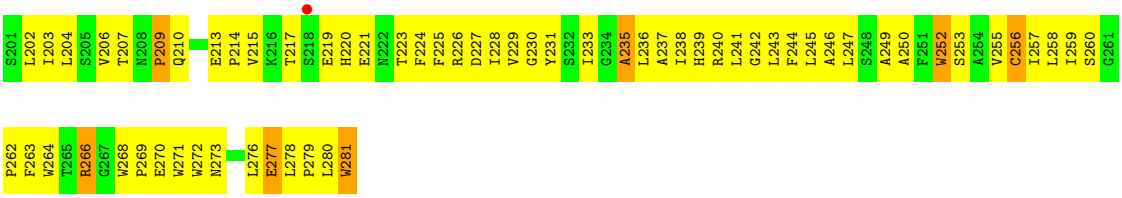
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Photosynthetic reaction center C subunit



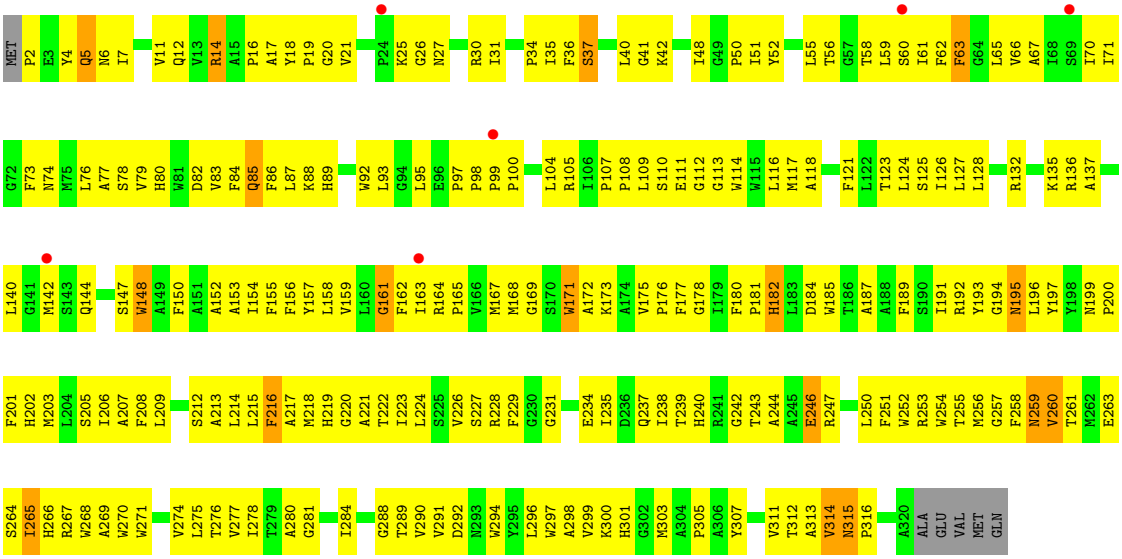
• Molecule 2: Photosynthetic reaction center L subunit





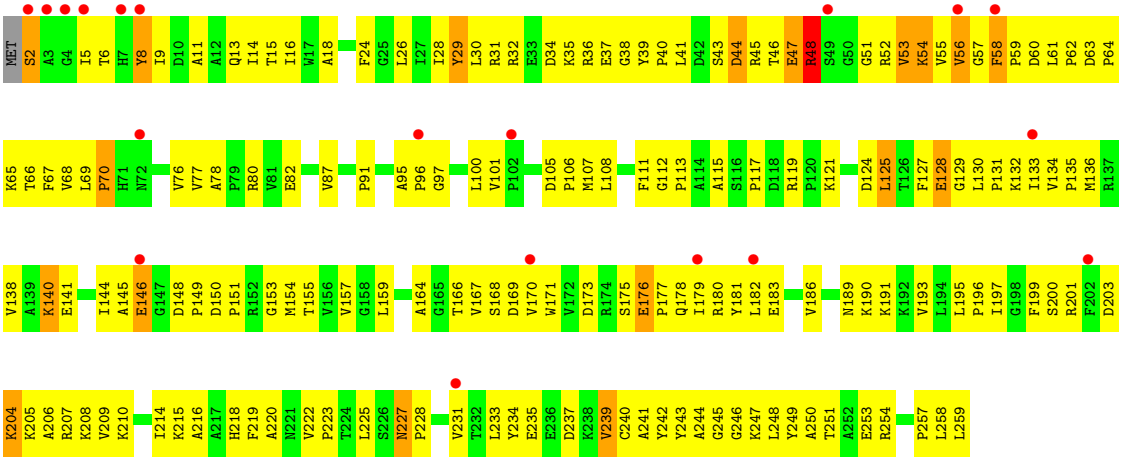
• Molecule 3: Photosynthetic reaction center M subunit

Chain M:



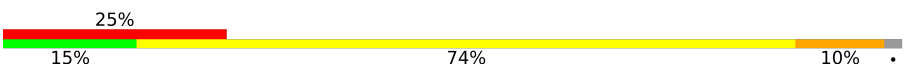
• Molecule 4: Photosynthetic reaction center H subunit

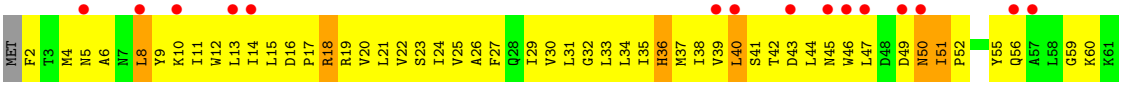
Chain H:



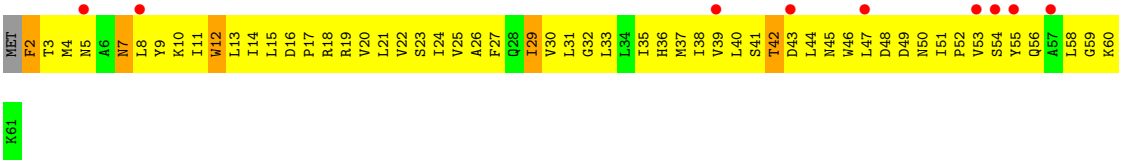
• Molecule 5: LH1 alpha polypeptide

Chain A:

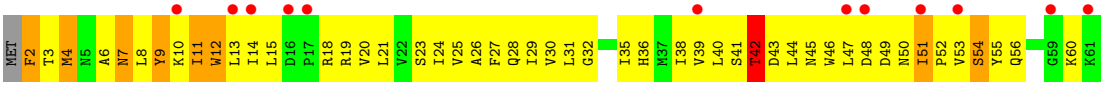




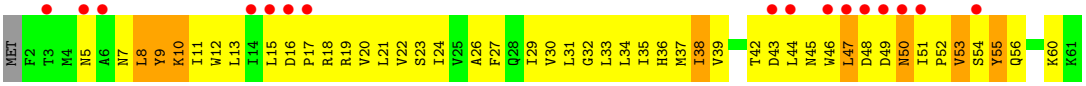
• Molecule 5: LH1 alpha polypeptide



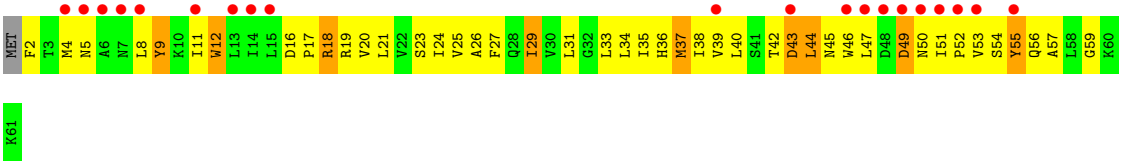
• Molecule 5: LH1 alpha polypeptide



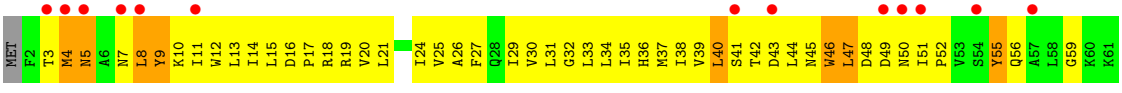
• Molecule 5: LH1 alpha polypeptide



• Molecule 5: LH1 alpha polypeptide



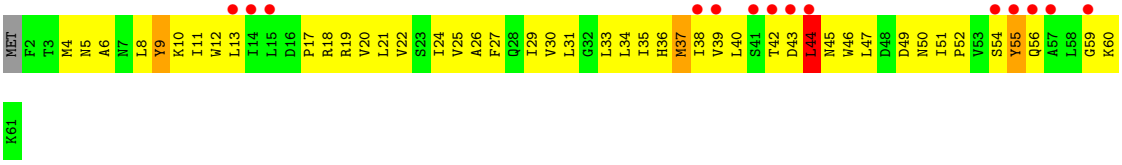
• Molecule 5: LH1 alpha polypeptide



• Molecule 5: LH1 alpha polypeptide

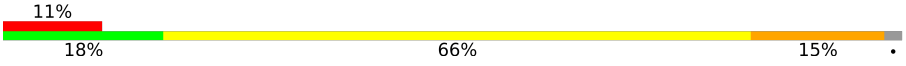
• Molecule 5: LH1 alpha polypeptide

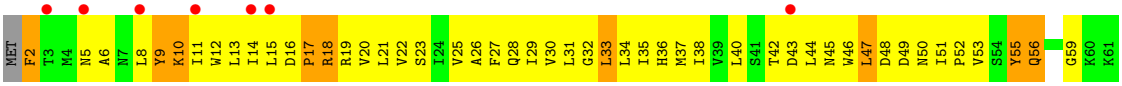
Chain S:



• Molecule 5: LH1 alpha polypeptide

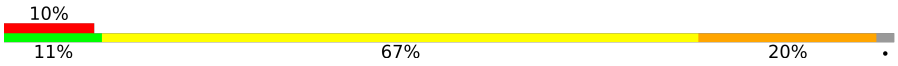
Chain U:

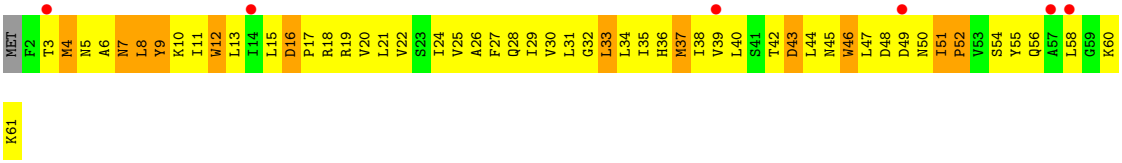




• Molecule 5: LH1 alpha polypeptide

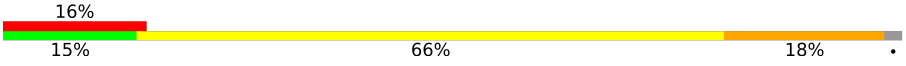
Chain W:

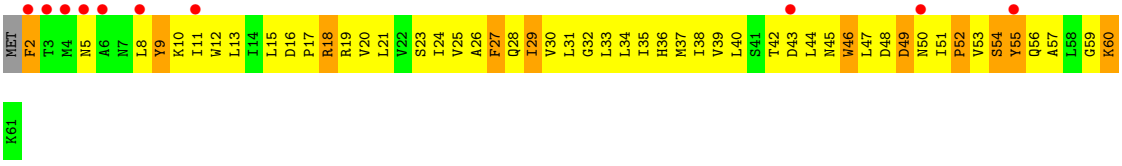




• Molecule 5: LH1 alpha polypeptide

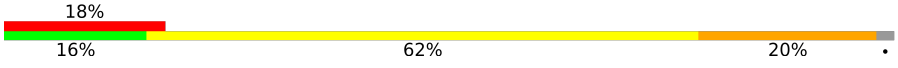
Chain Y:





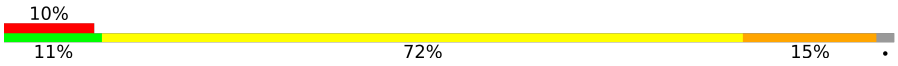
• Molecule 5: LH1 alpha polypeptide

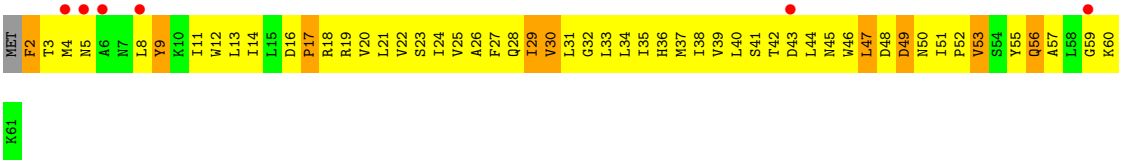
Chain 1:



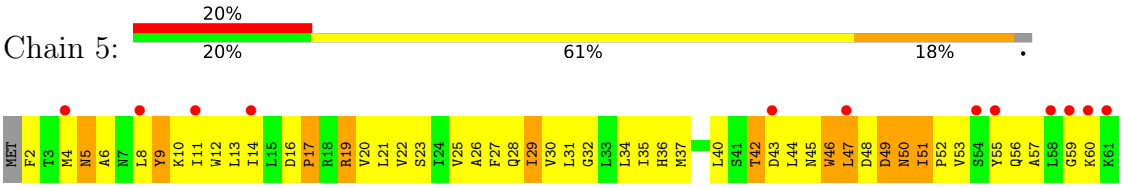
• Molecule 5: LH1 alpha polypeptide

Chain 3:

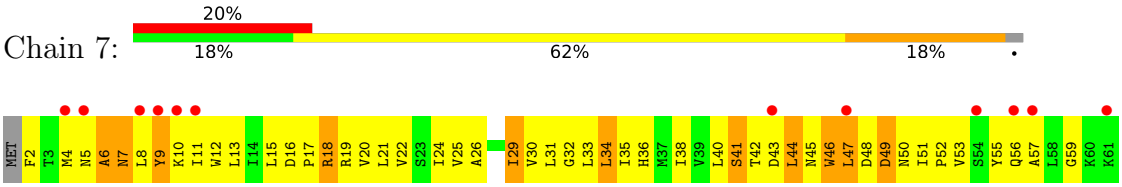




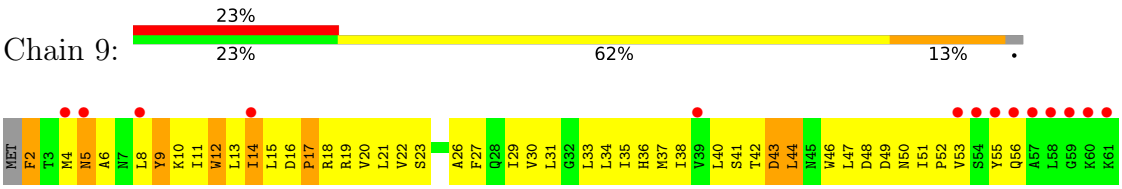
• Molecule 5: LH1 alpha polypeptide



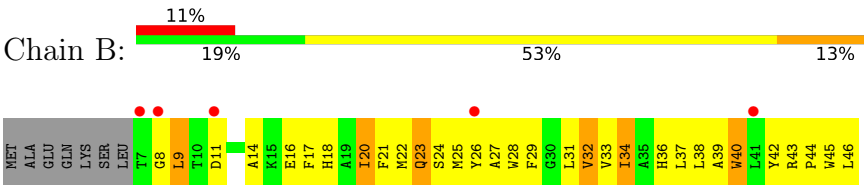
• Molecule 5: LH1 alpha polypeptide



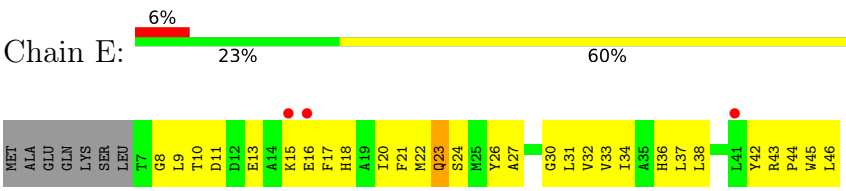
• Molecule 5: LH1 alpha polypeptide



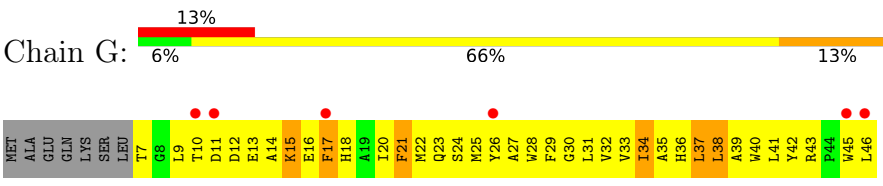
• Molecule 6: LH1 beta polypeptide



• Molecule 6: LH1 beta polypeptide

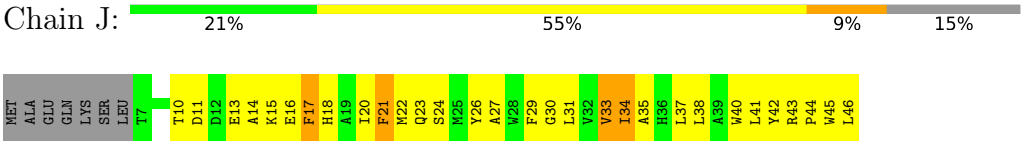


• Molecule 6: LH1 beta polypeptide



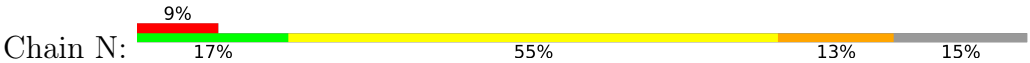
• Molecule 6: LH1 beta polypeptide

Chain J:



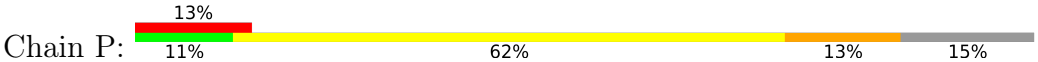
• Molecule 6: LH1 beta polypeptide

Chain N:



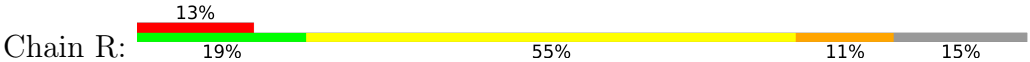
• Molecule 6: LH1 beta polypeptide

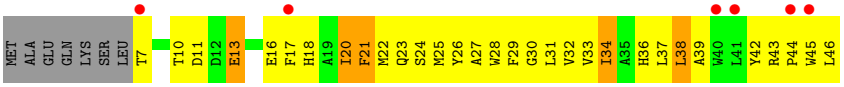
Chain P:



• Molecule 6: LH1 beta polypeptide

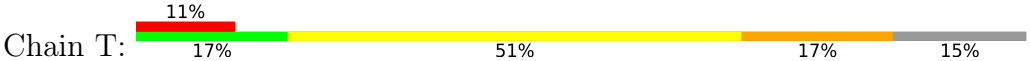
Chain R:

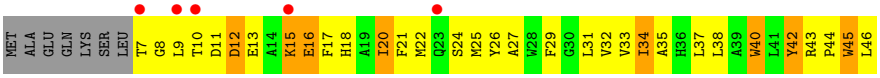




• Molecule 6: LH1 beta polypeptide

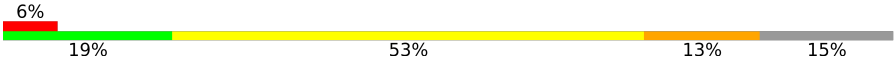
Chain T:

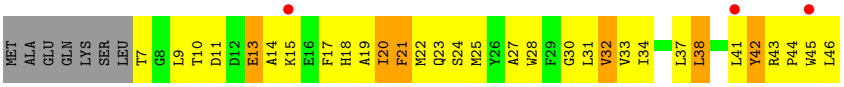




• Molecule 6: LH1 beta polypeptide

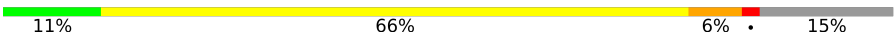
Chain V:





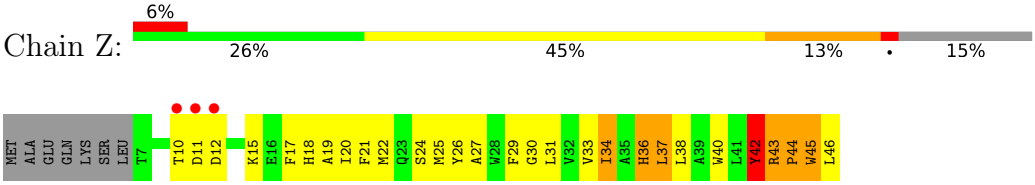
• Molecule 6: LH1 beta polypeptide

Chain X:



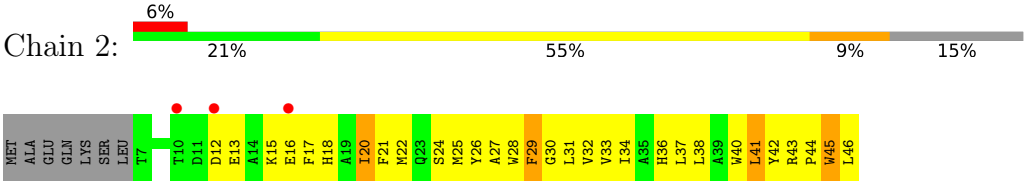
• Molecule 6: LH1 beta polypeptide

Chain Z:



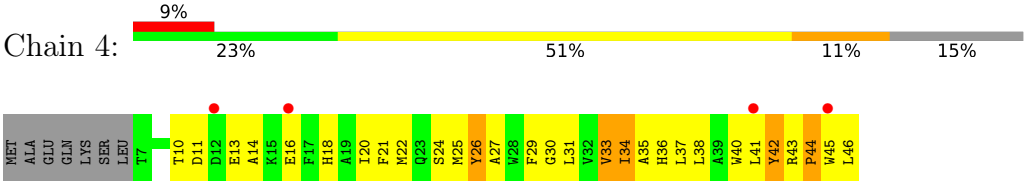
• Molecule 6: LH1 beta polypeptide

Chain 2:



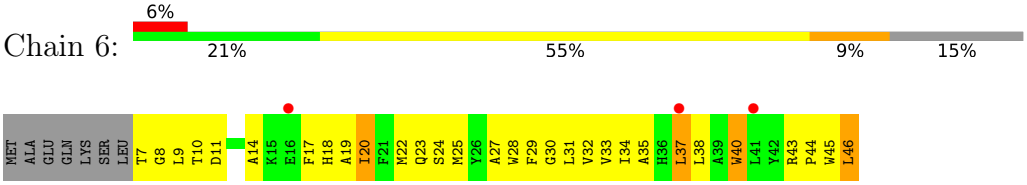
• Molecule 6: LH1 beta polypeptide

Chain 4:



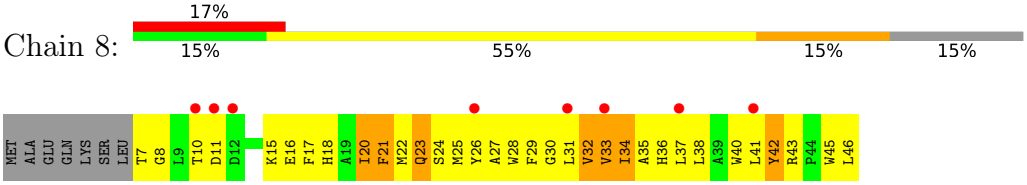
• Molecule 6: LH1 beta polypeptide

Chain 6:



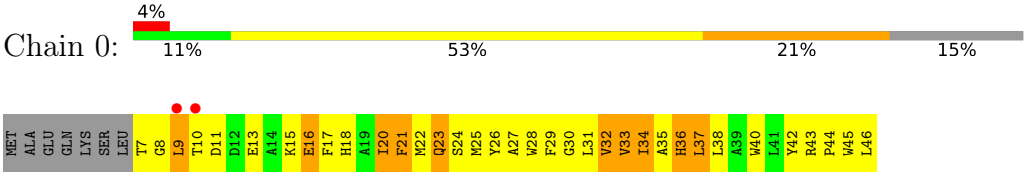
• Molecule 6: LH1 beta polypeptide

Chain 8:



• Molecule 6: LH1 beta polypeptide

Chain 0:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.34Å 148.24Å 161.79Å 90.00° 117.59° 90.00°	Depositor
Resolution (Å)	47.99 – 3.01 47.99 – 3.01	Depositor EDS
% Data completeness (in resolution range)	83.0 (47.99-3.01) 83.0 (47.99-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.314 , 0.337 0.315 , 0.322	Depositor DCC
R_{free} test set	3884 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	25819	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.38	0/2528	0.63	0/3451
2	L	0.37	0/2318	0.57	1/3167 (0.0%)
3	M	0.30	0/2651	0.51	1/3628 (0.0%)
4	H	0.37	0/2038	0.57	1/2776 (0.0%)
5	1	0.42	0/483	0.63	0/660
5	3	0.37	0/483	0.68	0/660
5	5	0.34	0/483	0.71	0/660
5	7	0.39	0/483	0.75	0/660
5	9	0.38	0/483	0.67	0/660
5	A	0.43	0/483	0.74	0/660
5	D	0.33	0/483	0.61	0/660
5	F	0.42	0/483	0.66	0/660
5	I	0.33	0/483	0.63	0/660
5	K	0.38	0/483	0.63	0/660
5	O	0.36	0/483	0.68	0/660
5	Q	0.31	0/483	0.58	0/660
5	S	0.31	0/483	0.61	0/660
5	U	0.36	0/483	0.69	1/660 (0.2%)
5	W	0.41	1/483 (0.2%)	0.59	0/660
5	Y	0.37	0/483	0.68	0/660
6	0	0.42	0/350	0.57	0/476
6	2	0.33	0/350	0.58	0/476
6	4	0.44	0/350	0.67	0/476
6	6	0.33	0/350	0.59	1/476 (0.2%)
6	8	0.47	0/350	0.63	0/476
6	B	0.39	0/350	0.49	0/476
6	E	0.40	0/350	0.51	0/476
6	G	0.43	0/350	0.61	0/476
6	J	0.45	0/350	0.56	0/476
6	N	0.40	0/350	0.58	0/476
6	P	0.42	0/350	0.60	0/476
6	R	0.39	0/350	0.55	0/476

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	T	0.35	0/350	0.52	0/476
6	V	0.40	0/350	0.64	0/476
6	X	0.40	0/350	0.56	0/476
6	Z	0.34	0/350	0.59	0/476
All	All	0.37	1/22863 (0.0%)	0.61	5/31198 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	X	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	61	LYS	C-OXT	5.31	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	58	PHE	C-N-CD	6.24	141.50	128.40
3	M	5	GLN	N-CA-C	-5.97	94.89	111.00
5	U	10	LYS	CB-CA-C	-5.35	99.70	110.40
2	L	98	ILE	CB-CA-C	-5.10	101.39	111.60
6	6	46	LEU	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	X	37	LEU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2458	0	2377	294	0
2	L	2231	0	2192	349	0
3	M	2551	0	2526	413	0
4	H	1983	0	1981	326	0
5	1	473	0	476	149	0
5	3	473	0	476	148	0
5	5	473	0	476	150	0
5	7	473	0	476	149	0
5	9	473	0	476	137	0
5	A	473	0	476	204	0
5	D	473	0	476	152	0
5	F	473	0	476	160	0
5	I	473	0	476	150	0
5	K	473	0	476	133	0
5	O	473	0	476	133	0
5	Q	473	0	476	119	0
5	S	473	0	476	119	0
5	U	473	0	476	142	0
5	W	473	0	476	184	0
5	Y	473	0	476	165	0
6	0	337	0	323	78	0
6	2	337	0	323	88	0
6	4	337	0	323	114	0
6	6	337	0	323	55	0
6	8	337	0	323	103	0
6	B	337	0	323	77	0
6	E	337	0	323	77	0
6	G	337	0	323	92	0
6	J	337	0	323	89	0
6	N	337	0	323	75	0
6	P	337	0	323	125	0
6	R	337	0	323	80	0
6	T	337	0	323	71	0
6	V	337	0	323	106	0
6	X	337	0	323	93	0
6	Z	337	0	323	74	0
7	C	172	0	120	17	0
8	1	1	0	0	0	0
8	3	1	0	0	0	0
8	5	1	0	0	0	0
8	7	1	0	0	0	0
8	9	1	0	0	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
8	O	1	0	0	0	0
8	Q	1	0	0	0	0
8	S	1	0	0	0	0
8	U	1	0	0	0	0
8	W	1	0	0	0	0
8	Y	1	0	0	0	0
9	0	66	0	74	24	0
9	1	66	0	74	18	0
9	2	66	0	74	19	0
9	3	66	0	74	28	0
9	4	66	0	74	36	0
9	5	66	0	74	23	0
9	6	66	0	74	22	0
9	7	132	0	148	51	0
9	9	66	0	74	29	0
9	A	66	0	74	35	0
9	B	66	0	74	38	0
9	D	66	0	74	22	0
9	E	66	0	74	33	0
9	F	66	0	74	45	0
9	G	66	0	74	37	0
9	I	132	0	148	53	0
9	K	66	0	74	27	0
9	L	132	0	148	20	0
9	M	132	0	148	43	0
9	N	66	0	74	23	0
9	O	66	0	74	55	0
9	P	66	0	74	30	0
9	Q	66	0	74	28	0
9	R	66	0	74	31	0
9	S	66	0	74	26	0
9	T	66	0	74	24	0
9	U	66	0	74	23	0
9	V	66	0	74	14	0
9	W	66	0	74	37	0
9	X	66	0	74	39	0
9	Y	66	0	74	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Z	66	0	74	29	0
10	L	65	0	76	8	0
10	M	65	0	76	19	0
11	L	53	0	74	13	0
12	H	10	0	0	4	0
12	L	5	0	0	0	0
12	M	5	0	0	1	0
13	M	1	0	0	0	0
14	M	53	0	72	13	0
15	2	44	0	60	40	0
15	3	44	0	60	20	0
15	4	44	0	60	68	0
15	8	44	0	60	80	0
15	A	88	0	120	70	0
15	B	44	0	60	35	0
15	G	44	0	60	27	0
15	J	44	0	60	35	0
15	M	44	0	60	12	0
15	N	44	0	60	54	0
15	P	44	0	60	61	0
15	R	44	0	60	34	0
15	T	44	0	58	23	0
15	V	44	0	60	65	0
15	W	44	0	60	29	0
15	X	44	0	60	27	0
16	H	21	0	12	7	0
16	M	21	0	12	16	0
17	H	19	0	11	18	0
18	H	1	0	0	0	0
18	L	4	0	0	3	0
All	All	25819	0	25995	4814	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 93.

The worst 5 of 4814 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:27:PHE:CE2	5:Y:29:ILE:HD11	1.30	1.64
5:U:27:PHE:CE2	5:W:29:ILE:HD11	1.30	1.63
6:V:21:PHE:CD2	15:V:102:CRT:H14	1.37	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:10:LYS:HD2	15:8:101:CRT:C2	1.27	1.58
6:P:17:PHE:CD1	15:P:102:CRT:H6	1.39	1.57

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	315/404 (78%)	230 (73%)	79 (25%)	6 (2%)	8 36
2	L	278/281 (99%)	219 (79%)	51 (18%)	8 (3%)	4 24
3	M	317/325 (98%)	254 (80%)	60 (19%)	3 (1%)	17 55
4	H	256/259 (99%)	204 (80%)	43 (17%)	9 (4%)	3 20
5	1	58/61 (95%)	34 (59%)	15 (26%)	9 (16%)	0 1
5	3	58/61 (95%)	38 (66%)	15 (26%)	5 (9%)	1 3
5	5	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0 1
5	7	58/61 (95%)	37 (64%)	15 (26%)	6 (10%)	0 2
5	9	58/61 (95%)	39 (67%)	13 (22%)	6 (10%)	0 2
5	A	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	9 39
5	D	58/61 (95%)	40 (69%)	18 (31%)	0	100 100
5	F	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	2 12
5	I	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	2 12
5	K	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2 12
5	O	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	9 39
5	Q	58/61 (95%)	42 (72%)	14 (24%)	2 (3%)	3 20
5	S	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	2 12
5	U	58/61 (95%)	34 (59%)	23 (40%)	1 (2%)	9 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	W	58/61 (95%)	41 (71%)	12 (21%)	5 (9%)	1 3
5	Y	58/61 (95%)	39 (67%)	12 (21%)	7 (12%)	0 1
6	0	38/47 (81%)	29 (76%)	9 (24%)	0	100 100
6	2	38/47 (81%)	28 (74%)	8 (21%)	2 (5%)	2 11
6	4	38/47 (81%)	31 (82%)	6 (16%)	1 (3%)	5 27
6	6	38/47 (81%)	35 (92%)	3 (8%)	0	100 100
6	8	38/47 (81%)	27 (71%)	10 (26%)	1 (3%)	5 27
6	B	38/47 (81%)	33 (87%)	5 (13%)	0	100 100
6	E	38/47 (81%)	33 (87%)	5 (13%)	0	100 100
6	G	38/47 (81%)	32 (84%)	6 (16%)	0	100 100
6	J	38/47 (81%)	29 (76%)	9 (24%)	0	100 100
6	N	38/47 (81%)	33 (87%)	4 (10%)	1 (3%)	5 27
6	P	38/47 (81%)	25 (66%)	12 (32%)	1 (3%)	5 27
6	R	38/47 (81%)	31 (82%)	7 (18%)	0	100 100
6	T	38/47 (81%)	30 (79%)	5 (13%)	3 (8%)	1 4
6	V	38/47 (81%)	35 (92%)	2 (5%)	1 (3%)	5 27
6	X	38/47 (81%)	32 (84%)	6 (16%)	0	100 100
6	Z	38/47 (81%)	28 (74%)	6 (16%)	4 (10%)	0 2
All	All	2702/2997 (90%)	2030 (75%)	570 (21%)	102 (4%)	3 18

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	235	ALA
4	H	53	VAL
5	I	50	ASN
5	I	53	VAL
5	Q	46	TRP

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	265/317 (84%)	245 (92%)	20 (8%)	13 43
2	L	228/229 (100%)	220 (96%)	8 (4%)	36 71
3	M	256/261 (98%)	239 (93%)	17 (7%)	16 49
4	H	210/211 (100%)	198 (94%)	12 (6%)	20 56
5	1	50/56 (89%)	47 (94%)	3 (6%)	19 53
5	3	50/56 (89%)	44 (88%)	6 (12%)	5 22
5	5	50/56 (89%)	45 (90%)	5 (10%)	7 29
5	7	50/56 (89%)	44 (88%)	6 (12%)	5 22
5	9	50/56 (89%)	44 (88%)	6 (12%)	5 22
5	A	50/56 (89%)	45 (90%)	5 (10%)	7 29
5	D	50/56 (89%)	45 (90%)	5 (10%)	7 29
5	F	50/56 (89%)	43 (86%)	7 (14%)	3 16
5	I	50/56 (89%)	44 (88%)	6 (12%)	5 22
5	K	50/56 (89%)	43 (86%)	7 (14%)	3 16
5	O	50/56 (89%)	42 (84%)	8 (16%)	2 12
5	Q	50/56 (89%)	47 (94%)	3 (6%)	19 53
5	S	50/56 (89%)	46 (92%)	4 (8%)	12 40
5	U	50/56 (89%)	43 (86%)	7 (14%)	3 16
5	W	50/56 (89%)	43 (86%)	7 (14%)	3 16
5	Y	50/56 (89%)	45 (90%)	5 (10%)	7 29
6	0	33/39 (85%)	23 (70%)	10 (30%)	0 1
6	2	33/39 (85%)	29 (88%)	4 (12%)	5 21
6	4	33/39 (85%)	29 (88%)	4 (12%)	5 21
6	6	33/39 (85%)	30 (91%)	3 (9%)	9 34
6	8	33/39 (85%)	26 (79%)	7 (21%)	1 5
6	B	33/39 (85%)	27 (82%)	6 (18%)	1 9
6	E	33/39 (85%)	32 (97%)	1 (3%)	41 75
6	G	33/39 (85%)	26 (79%)	7 (21%)	1 5
6	J	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	N	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	P	33/39 (85%)	28 (85%)	5 (15%)	3 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	R	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	T	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	V	33/39 (85%)	27 (82%)	6 (18%)	1 9
6	X	33/39 (85%)	28 (85%)	5 (15%)	3 14
6	Z	33/39 (85%)	29 (88%)	4 (12%)	5 21
All	All	2287/2538 (90%)	2058 (90%)	229 (10%)	7 29

5 of 229 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	O	40	LEU
6	0	20	ILE
5	U	18	ARG
6	0	9	LEU
6	6	40	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
6	8	23	GLN
5	9	7	ASN
3	M	315	ASN
3	M	301	HIS
5	9	45	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 86 ligands modelled in this entry, 18 are monoatomic - leaving 68 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CRT	A	103	-	41,43,43	1.76	10 (24%)	50,54,54	1.63	12 (24%)
9	BCL	A	102	-	64,74,74	1.38	9 (14%)	78,115,115	2.29	20 (25%)
9	BCL	9	102	-	64,74,74	1.47	9 (14%)	78,115,115	2.29	21 (26%)
11	UQ8	L	304	-	53,53,53	1.50	4 (7%)	64,67,67	1.89	19 (29%)
9	BCL	N	101	-	64,74,74	1.48	10 (15%)	78,115,115	2.35	24 (30%)
10	BPH	L	302	-	51,70,70	0.89	3 (5%)	52,101,101	1.15	4 (7%)
15	CRT	V	102	-	41,43,43	1.79	10 (24%)	50,54,54	2.57	20 (40%)
15	CRT	2	102	-	41,43,43	1.52	10 (24%)	50,54,54	1.94	20 (40%)
10	BPH	M	403	-	51,70,70	0.99	2 (3%)	52,101,101	1.18	3 (5%)
15	CRT	4	102	-	41,43,43	1.50	9 (21%)	50,54,54	1.84	18 (36%)
9	BCL	7	103	-	64,74,74	1.48	11 (17%)	78,115,115	2.43	24 (30%)
9	BCL	D	102	-	64,74,74	1.49	11 (17%)	78,115,115	2.33	23 (29%)
9	BCL	1	102	-	64,74,74	1.49	10 (15%)	78,115,115	2.26	20 (25%)
9	BCL	4	101	-	64,74,74	1.50	12 (18%)	78,115,115	2.37	23 (29%)
9	BCL	I	103	-	64,74,74	1.59	13 (20%)	78,115,115	2.31	25 (32%)
9	BCL	3	102	-	64,74,74	1.43	11 (17%)	78,115,115	2.34	24 (30%)
12	PO4	H	304	-	4,4,4	1.62	0	6,6,6	0.41	0
15	CRT	J	101	-	41,43,43	2.16	11 (26%)	50,54,54	2.51	20 (40%)
9	BCL	R	101	-	64,74,74	1.54	10 (15%)	78,115,115	2.37	24 (30%)
15	CRT	A	101	-	41,43,43	2.00	14 (34%)	50,54,54	3.07	21 (42%)
9	BCL	L	301	-	64,74,74	1.45	9 (14%)	78,115,115	2.39	24 (30%)
15	CRT	W	103	-	41,43,43	1.97	10 (24%)	50,54,54	2.14	17 (34%)
17	PEF	H	301	-	18,18,46	3.12	7 (38%)	21,23,51	1.96	5 (23%)
9	BCL	F	102	-	64,74,74	1.50	11 (17%)	78,115,115	2.29	21 (26%)
7	HEM	C	503	1	41,50,50	2.12	13 (31%)	45,82,82	1.54	8 (17%)
9	BCL	Z	101	-	64,74,74	1.46	12 (18%)	78,115,115	2.33	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BCL	5	102	-	64,74,74	1.51	10 (15%)	78,115,115	2.29	21 (26%)
15	CRT	M	406	-	41,43,43	1.60	7 (17%)	50,54,54	1.48	11 (22%)
12	PO4	L	305	-	4,4,4	1.67	0	6,6,6	0.43	0
15	CRT	P	102	-	41,43,43	2.56	16 (39%)	50,54,54	2.55	17 (34%)
15	CRT	8	101	-	41,43,43	1.57	7 (17%)	50,54,54	1.76	13 (26%)
9	BCL	I	102	-	64,74,74	1.50	12 (18%)	78,115,115	2.33	23 (29%)
12	PO4	M	408	-	4,4,4	1.77	1 (25%)	6,6,6	0.44	0
7	HEM	C	504	1	41,50,50	2.17	11 (26%)	45,82,82	1.59	6 (13%)
9	BCL	7	102	-	64,74,74	1.41	9 (14%)	78,115,115	2.30	21 (26%)
9	BCL	G	101	-	64,74,74	1.37	8 (12%)	78,115,115	2.37	25 (32%)
9	BCL	M	402	-	64,74,74	1.55	9 (14%)	78,115,115	2.30	22 (28%)
9	BCL	P	101	-	64,74,74	1.45	12 (18%)	78,115,115	2.32	25 (32%)
9	BCL	E	101	-	64,74,74	1.59	13 (20%)	78,115,115	2.34	26 (33%)
15	CRT	R	102	-	41,43,43	1.67	11 (26%)	50,54,54	2.64	18 (36%)
15	CRT	3	103	-	41,43,43	1.97	12 (29%)	50,54,54	1.83	13 (26%)
9	BCL	V	101	-	64,74,74	1.48	11 (17%)	78,115,115	2.31	24 (30%)
9	BCL	W	102	-	64,74,74	1.39	8 (12%)	78,115,115	2.31	21 (26%)
9	BCL	L	303	-	64,74,74	1.38	9 (14%)	78,115,115	2.33	24 (30%)
15	CRT	N	102	-	41,43,43	1.68	10 (24%)	50,54,54	2.25	14 (28%)
7	HEM	C	501	1	41,50,50	1.90	13 (31%)	45,82,82	1.68	9 (20%)
9	BCL	T	101	-	64,74,74	1.52	11 (17%)	78,115,115	2.34	24 (30%)
9	BCL	U	102	-	64,74,74	1.50	12 (18%)	78,115,115	2.30	20 (25%)
16	PGW	M	407	-	20,20,50	0.96	1 (5%)	23,26,56	1.64	4 (17%)
9	BCL	K	102	-	64,74,74	1.46	11 (17%)	78,115,115	2.31	23 (29%)
9	BCL	B	101	-	64,74,74	1.43	10 (15%)	78,115,115	2.30	23 (29%)
9	BCL	2	101	-	64,74,74	1.52	13 (20%)	78,115,115	2.28	24 (30%)
15	CRT	T	102	-	41,43,43	1.90	9 (21%)	50,54,54	3.30	21 (42%)
9	BCL	6	101	-	64,74,74	1.46	10 (15%)	78,115,115	2.34	25 (32%)
9	BCL	O	102	-	64,74,74	1.42	10 (15%)	78,115,115	2.25	22 (28%)
16	PGW	H	302	-	20,20,50	0.95	1 (5%)	23,26,56	1.63	4 (17%)
9	BCL	S	102	-	64,74,74	1.50	14 (21%)	78,115,115	2.24	21 (26%)
15	CRT	X	102	-	41,43,43	2.93	13 (31%)	50,54,54	2.48	16 (32%)
9	BCL	0	101	-	64,74,74	1.40	12 (18%)	78,115,115	2.37	26 (33%)
9	BCL	M	401	-	64,74,74	1.57	11 (17%)	78,115,115	2.26	23 (29%)
12	PO4	H	303	-	4,4,4	1.68	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CRT	G	102	-	41,43,43	1.44	8 (19%)	50,54,54	1.68	15 (30%)
9	BCL	Y	102	-	64,74,74	1.46	13 (20%)	78,115,115	2.25	21 (26%)
14	MQ8	M	405	-	54,54,54	0.91	2 (3%)	66,69,69	1.67	16 (24%)
7	HEM	C	502	1	41,50,50	2.10	12 (29%)	45,82,82	1.64	9 (20%)
9	BCL	X	101	-	64,74,74	1.54	13 (20%)	78,115,115	2.38	25 (32%)
15	CRT	B	102	-	41,43,43	1.50	6 (14%)	50,54,54	2.42	20 (40%)
9	BCL	Q	102	-	64,74,74	1.49	13 (20%)	78,115,115	2.30	20 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	A	103	-	-	1/51/51/51	-
9	BCL	A	102	-	-	16/37/137/137	-
9	BCL	9	102	-	-	16/37/137/137	-
11	UQ8	L	304	-	-	6/51/75/75	0/1/1/1
9	BCL	N	101	-	-	11/37/137/137	-
10	BPH	L	302	-	-	15/37/105/105	0/5/6/6
15	CRT	V	102	-	-	7/51/51/51	-
15	CRT	2	102	-	-	2/51/51/51	-
10	BPH	M	403	-	-	12/37/105/105	0/5/6/6
15	CRT	4	102	-	-	2/51/51/51	-
9	BCL	7	103	-	-	10/37/137/137	-
9	BCL	D	102	-	-	19/37/137/137	-
9	BCL	1	102	-	-	15/37/137/137	-
9	BCL	4	101	-	-	11/37/137/137	-
9	BCL	I	103	-	-	12/37/137/137	-
9	BCL	3	102	-	-	18/37/137/137	-
15	CRT	J	101	-	-	2/51/51/51	-
17	PEF	H	301	-	-	16/20/20/50	-
9	BCL	R	101	-	-	14/37/137/137	-
15	CRT	A	101	-	-	2/51/51/51	-
9	BCL	L	301	-	-	13/37/137/137	-
15	CRT	W	103	-	-	1/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	F	102	-	-	21/37/137/137	-
7	HEM	C	503	1	-	6/12/54/54	-
9	BCL	Z	101	-	-	12/37/137/137	-
9	BCL	5	102	-	-	21/37/137/137	-
15	CRT	M	406	-	-	0/51/51/51	-
15	CRT	P	102	-	-	2/51/51/51	-
15	CRT	8	101	-	-	2/51/51/51	-
9	BCL	I	102	-	-	19/37/137/137	-
7	HEM	C	504	1	-	6/12/54/54	-
9	BCL	7	102	-	-	15/37/137/137	-
9	BCL	G	101	-	-	8/37/137/137	-
9	BCL	M	402	-	-	15/37/137/137	-
9	BCL	P	101	-	-	12/37/137/137	-
9	BCL	E	101	-	-	8/37/137/137	-
15	CRT	R	102	-	-	2/51/51/51	-
15	CRT	3	103	-	-	2/51/51/51	-
9	BCL	V	101	-	-	17/37/137/137	-
9	BCL	W	102	-	-	22/37/137/137	-
9	BCL	L	303	-	-	9/37/137/137	-
15	CRT	N	102	-	-	2/51/51/51	-
7	HEM	C	501	1	-	7/12/54/54	-
9	BCL	T	101	-	-	12/37/137/137	-
9	BCL	U	102	-	-	15/37/137/137	-
16	PGW	M	407	-	-	11/23/23/55	-
9	BCL	K	102	-	-	17/37/137/137	-
9	BCL	B	101	-	-	15/37/137/137	-
9	BCL	2	101	-	-	14/37/137/137	-
15	CRT	T	102	-	-	5/51/51/51	-
9	BCL	6	101	-	-	19/37/137/137	-
9	BCL	O	102	-	-	21/37/137/137	-
16	PGW	H	302	-	-	10/23/23/55	-
9	BCL	S	102	-	-	20/37/137/137	-
15	CRT	X	102	-	-	2/51/51/51	-
9	BCL	0	101	-	-	16/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	M	401	-	-	19/37/137/137	-
15	CRT	G	102	-	-	1/51/51/51	-
9	BCL	Y	102	-	-	14/37/137/137	-
14	MQ8	M	405	-	-	10/47/67/67	0/2/2/2
7	HEM	C	502	1	-	7/12/54/54	-
9	BCL	X	101	-	-	13/37/137/137	-
15	CRT	B	102	-	-	4/51/51/51	-
9	BCL	Q	102	-	-	21/37/137/137	-

The worst 5 of 635 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	503	HEM	C3C-CAC	-7.90	1.31	1.47
11	L	304	UQ8	C43-C44	7.79	1.54	1.32
15	X	102	CRT	C14-C12	7.74	1.46	1.35
15	X	102	CRT	C4-C5	7.26	1.61	1.50
17	H	301	PEF	O4-C10	7.19	1.47	1.20

The worst 5 of 1198 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	102	CRT	C1-C4-C5	15.40	153.86	113.06
15	A	101	CRT	C36-C35-C33	-10.28	110.36	125.89
15	T	102	CRT	C3-C1-C4	-10.11	95.33	110.86
9	7	103	BCL	C1-C2-C3	9.65	142.73	126.04
9	4	101	BCL	C1-C2-C3	9.19	141.93	126.04

There are no chirality outliers.

5 of 695 torsion outliers are listed below:

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

There are no ring outliers.

67 monomers are involved in 1470 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	103	CRT	23	0
9	A	102	BCL	35	0
9	9	102	BCL	29	0
11	L	304	UQ8	13	0
9	N	101	BCL	23	0
10	L	302	BPH	8	0
15	V	102	CRT	65	0
15	2	102	CRT	40	0
10	M	403	BPH	19	0
15	4	102	CRT	68	0
9	7	103	BCL	32	0
9	D	102	BCL	22	0
9	1	102	BCL	18	0
9	4	101	BCL	36	0
9	I	103	BCL	36	0
9	3	102	BCL	28	0
12	H	304	PO4	3	0
15	J	101	CRT	35	0
9	R	101	BCL	31	0
15	A	101	CRT	47	0
9	L	301	BCL	11	0
15	W	103	CRT	29	0
17	H	301	PEF	18	0
9	F	102	BCL	45	0
7	C	503	HEM	9	0
9	Z	101	BCL	29	0
9	5	102	BCL	23	0
15	M	406	CRT	12	0
15	P	102	CRT	61	0
15	8	101	CRT	80	0
9	I	102	BCL	34	0
12	M	408	PO4	1	0
7	C	504	HEM	2	0
9	7	102	BCL	21	0
9	G	101	BCL	37	0
9	M	402	BCL	13	0
9	P	101	BCL	30	0
9	E	101	BCL	33	0
15	R	102	CRT	34	0
15	3	103	CRT	20	0
9	V	101	BCL	14	0
9	W	102	BCL	37	0
9	L	303	BCL	11	0

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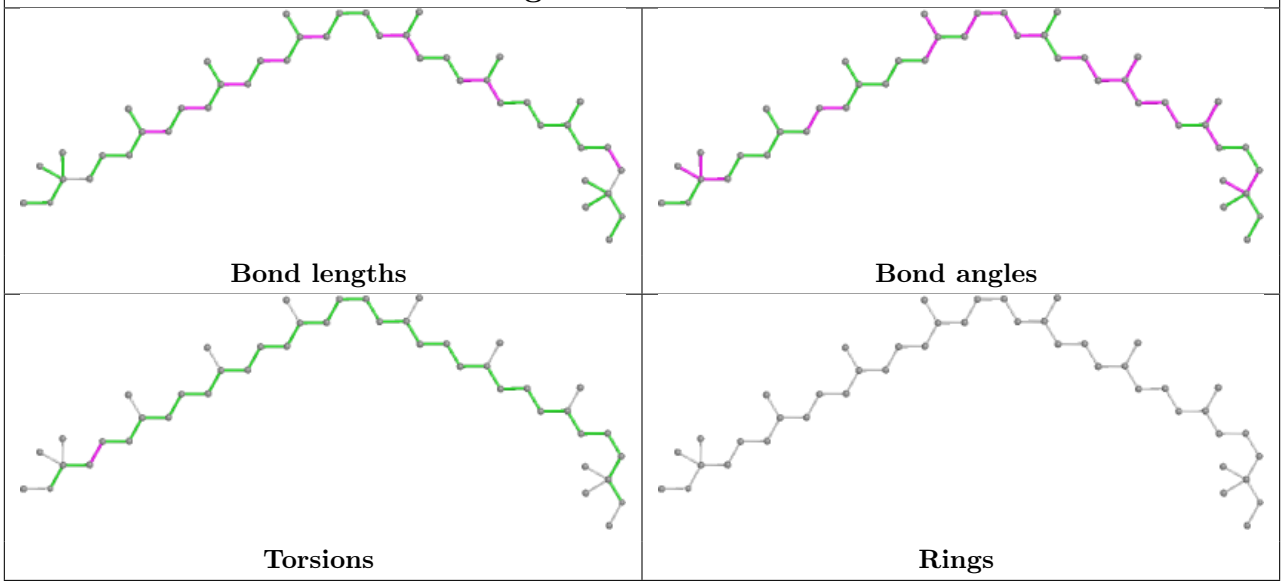
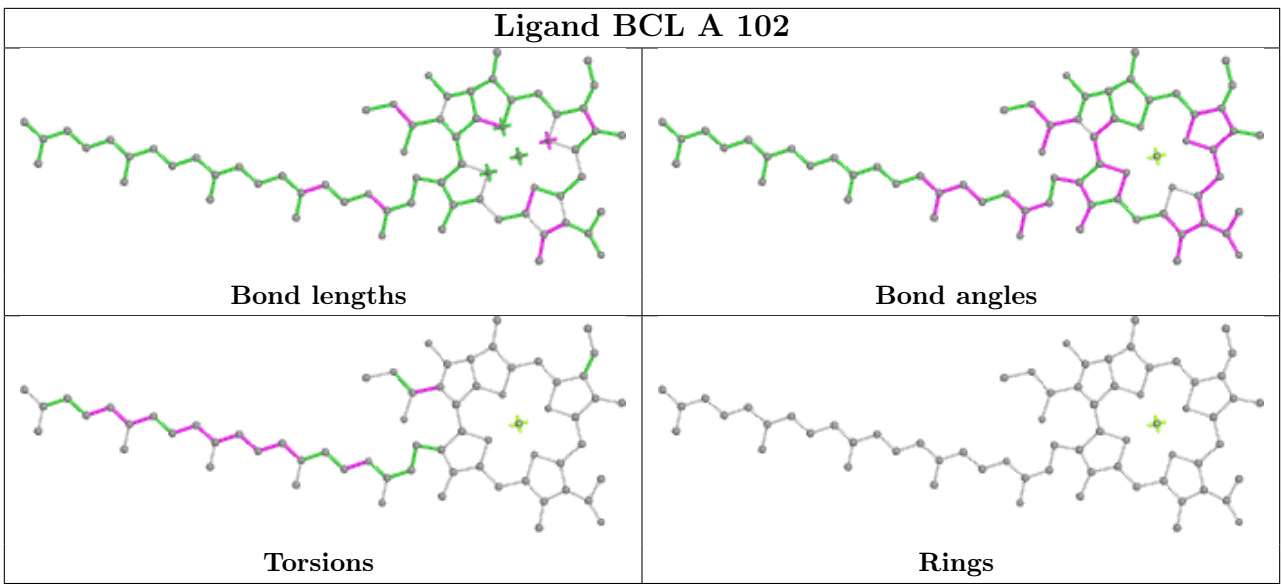
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	102	CRT	54	0
7	C	501	HEM	2	0
9	T	101	BCL	24	0
9	U	102	BCL	23	0
16	M	407	PGW	16	0
9	K	102	BCL	27	0
9	B	101	BCL	38	0
9	2	101	BCL	19	0
15	T	102	CRT	23	0
9	6	101	BCL	22	0
9	O	102	BCL	55	0
16	H	302	PGW	7	0
9	S	102	BCL	26	0
15	X	102	CRT	27	0
9	0	101	BCL	24	0
9	M	401	BCL	31	0
12	H	303	PO4	1	0
15	G	102	CRT	27	0
9	Y	102	BCL	29	0
14	M	405	MQ8	13	0
7	C	502	HEM	4	0
9	X	101	BCL	39	0
15	B	102	CRT	35	0
9	Q	102	BCL	28	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

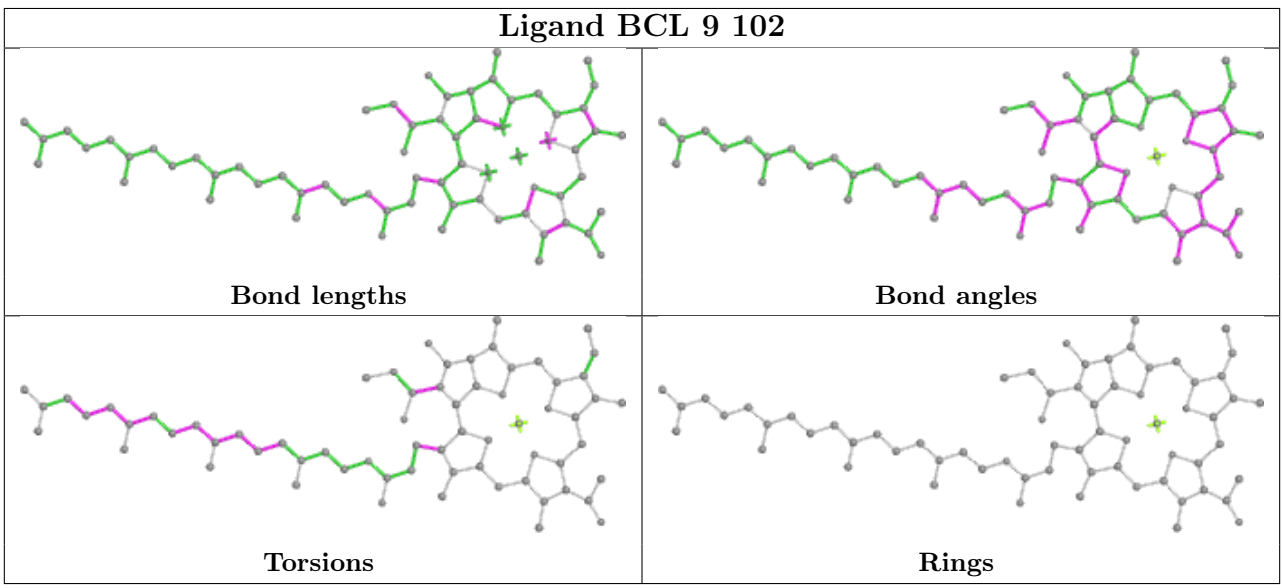
Ligand CRT A 103



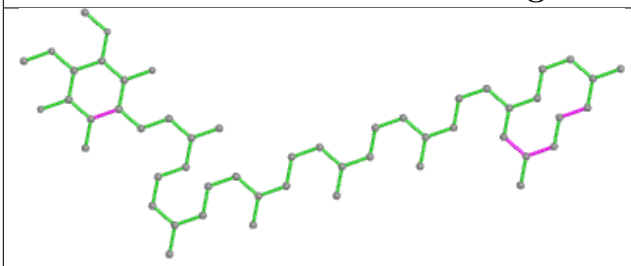
Ligand BCL A 102



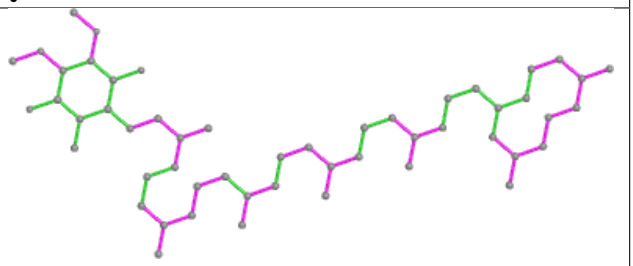
Ligand BCL 9 102



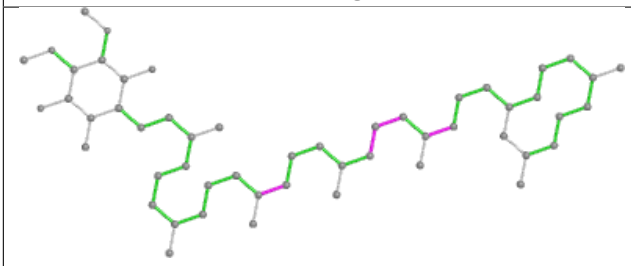
Ligand UQ8 L 304



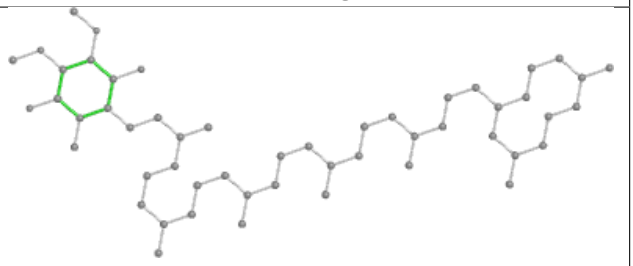
Bond lengths



Bond angles

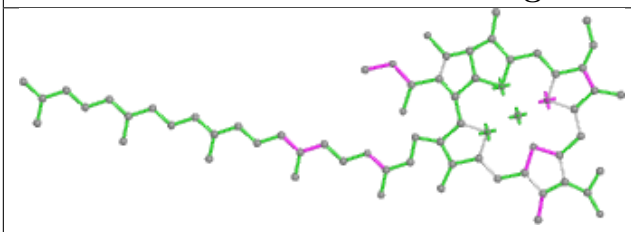


Torsions

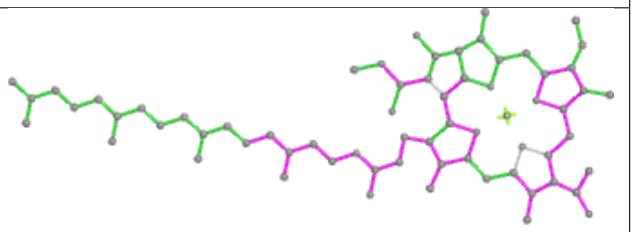


Rings

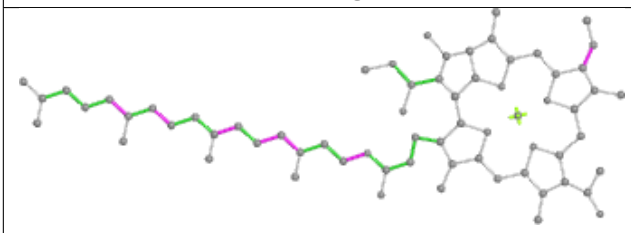
Ligand BCL N 101



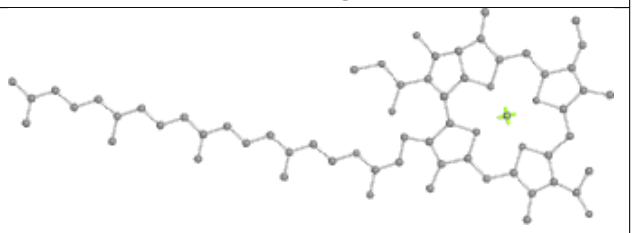
Bond lengths



Bond angles

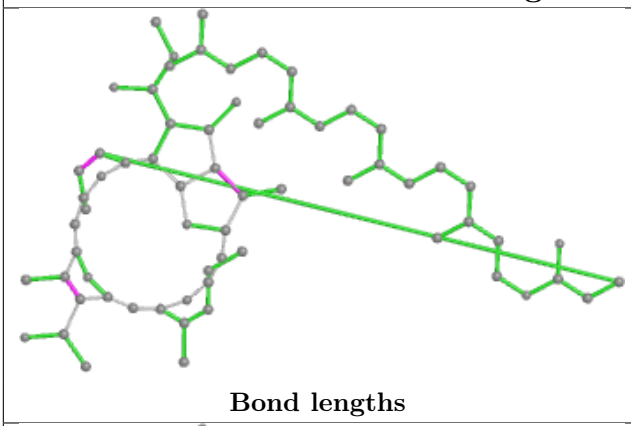


Torsions

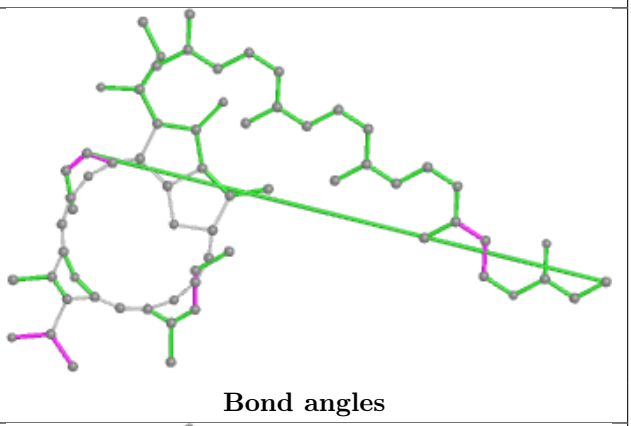


Rings

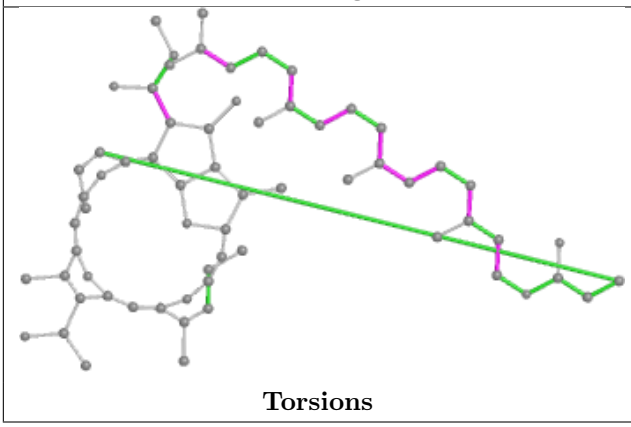
Ligand BPH L 302



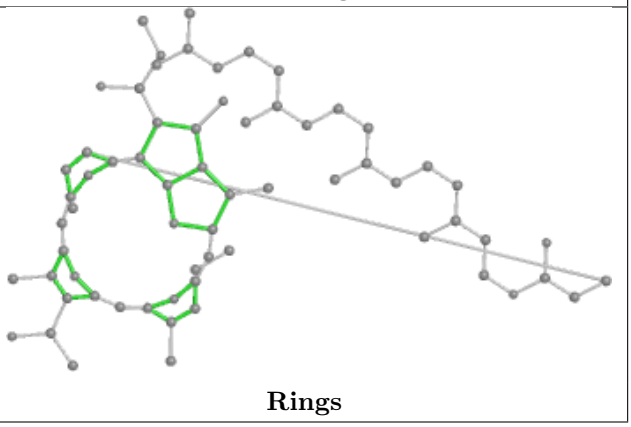
Bond lengths



Bond angles

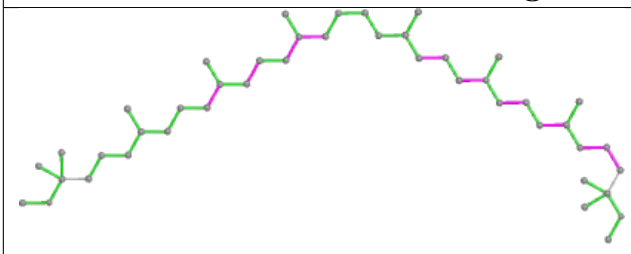


Torsions

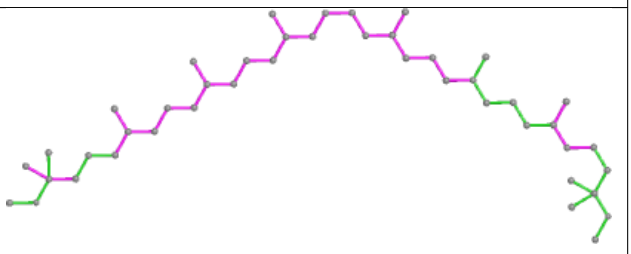


Rings

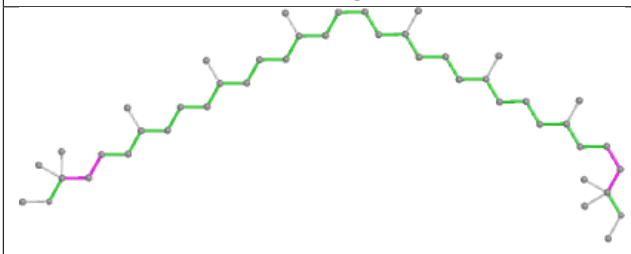
Ligand CRT V 102



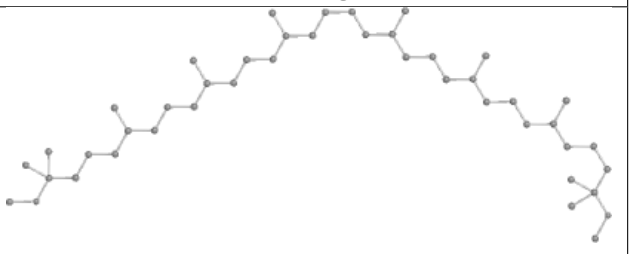
Bond lengths



Bond angles

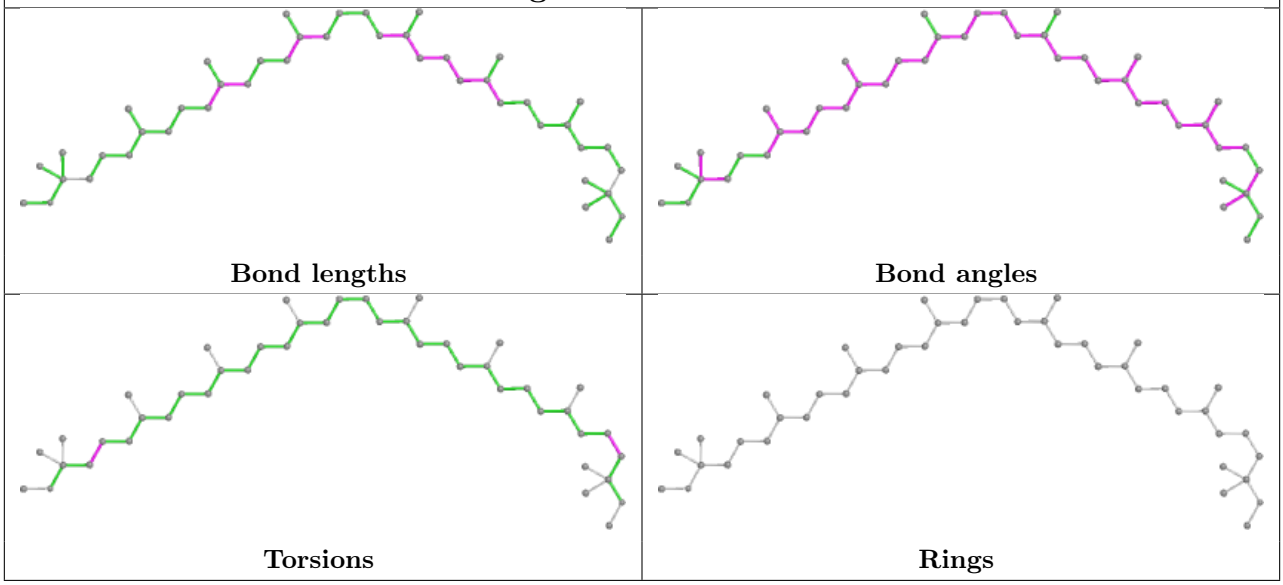


Torsions

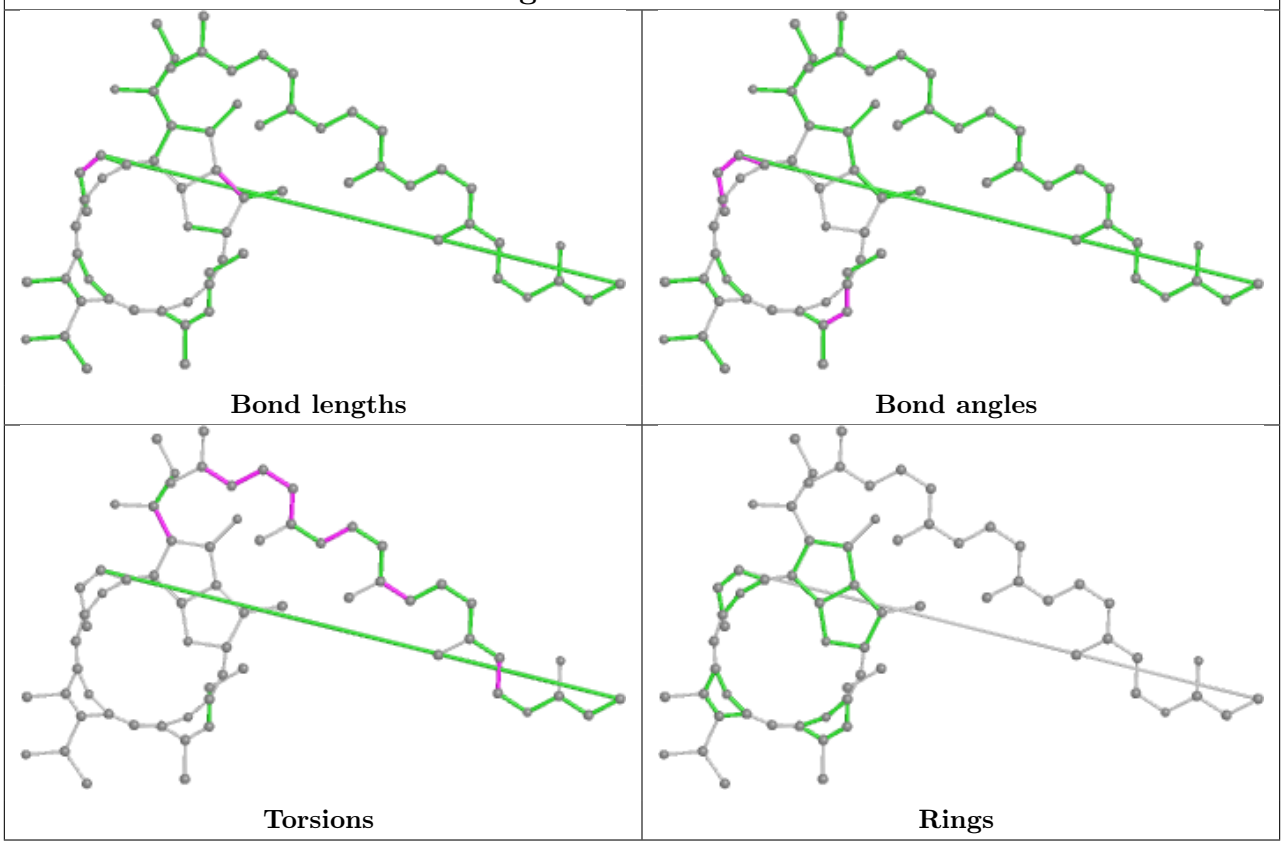


Rings

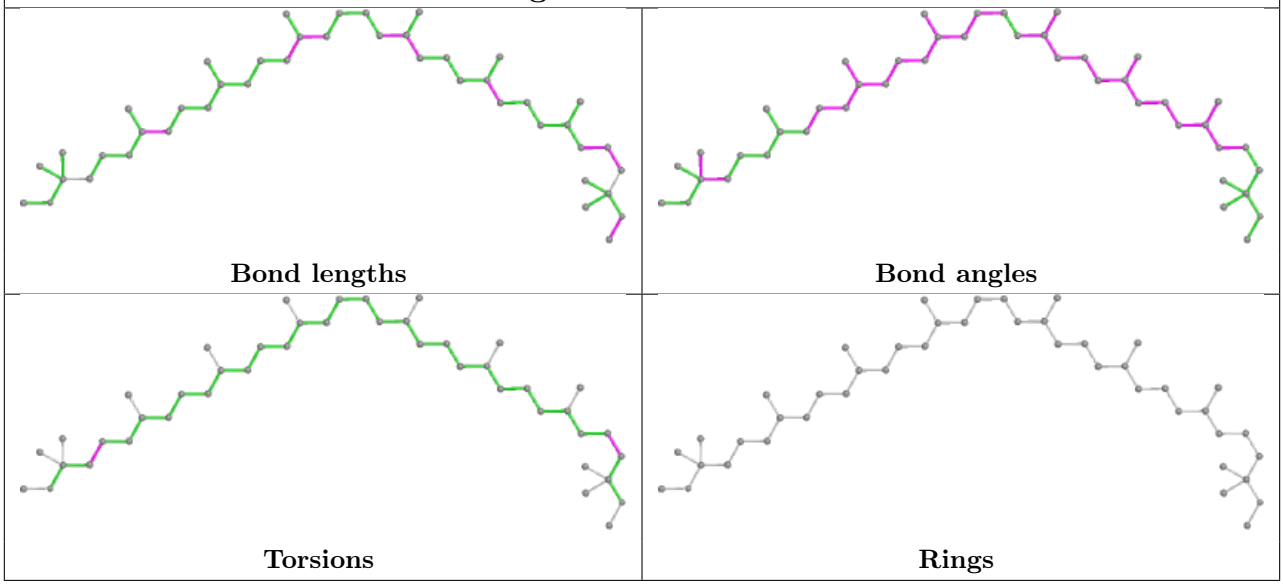
Ligand CRT 2 102



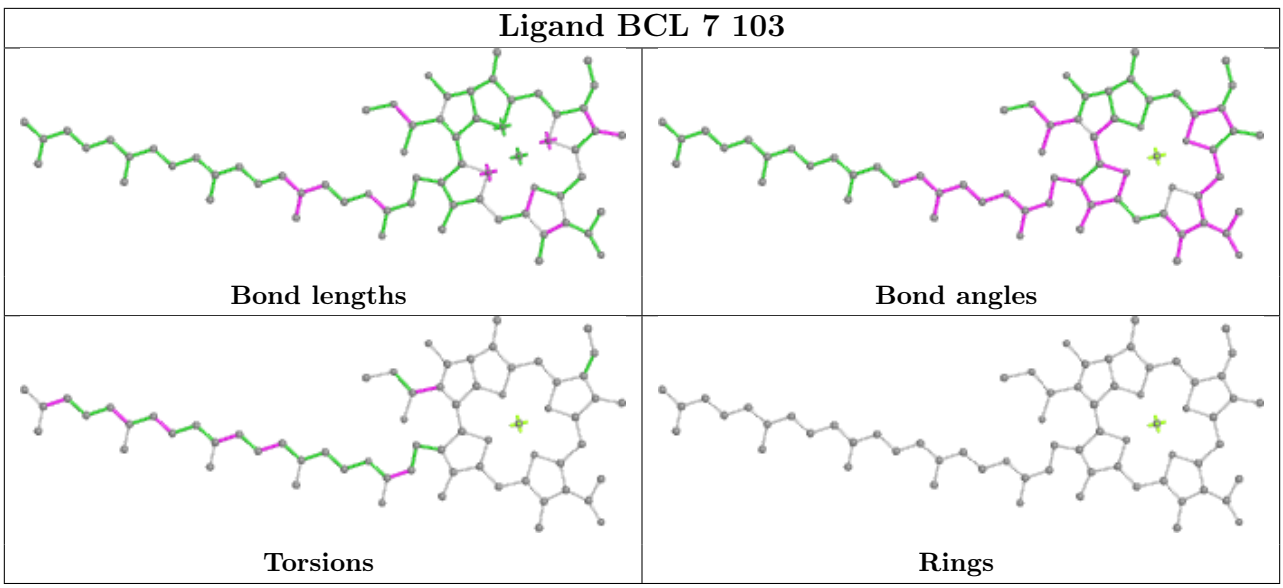
Ligand BPH M 403



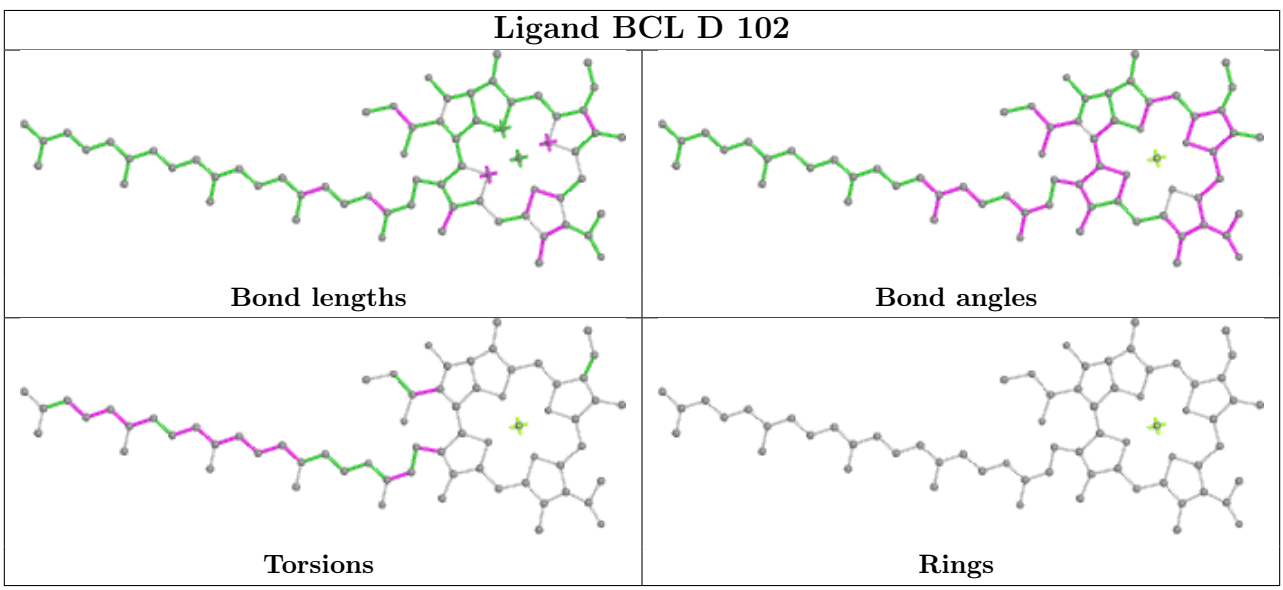
Ligand CRT 4 102



Ligand BCL 7 103



Ligand BCL D 102



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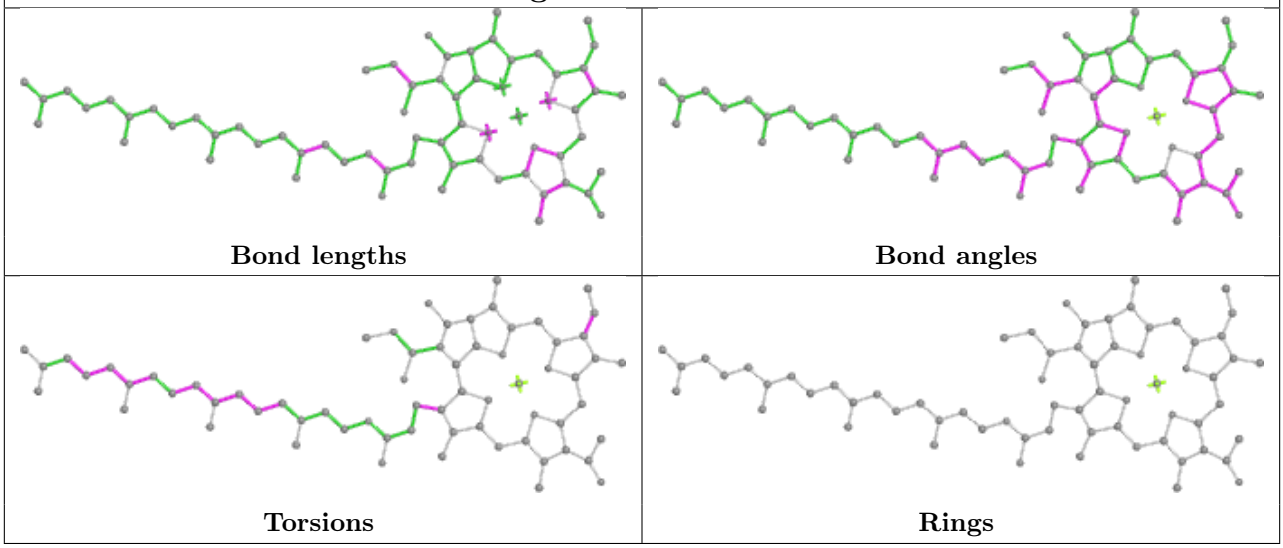

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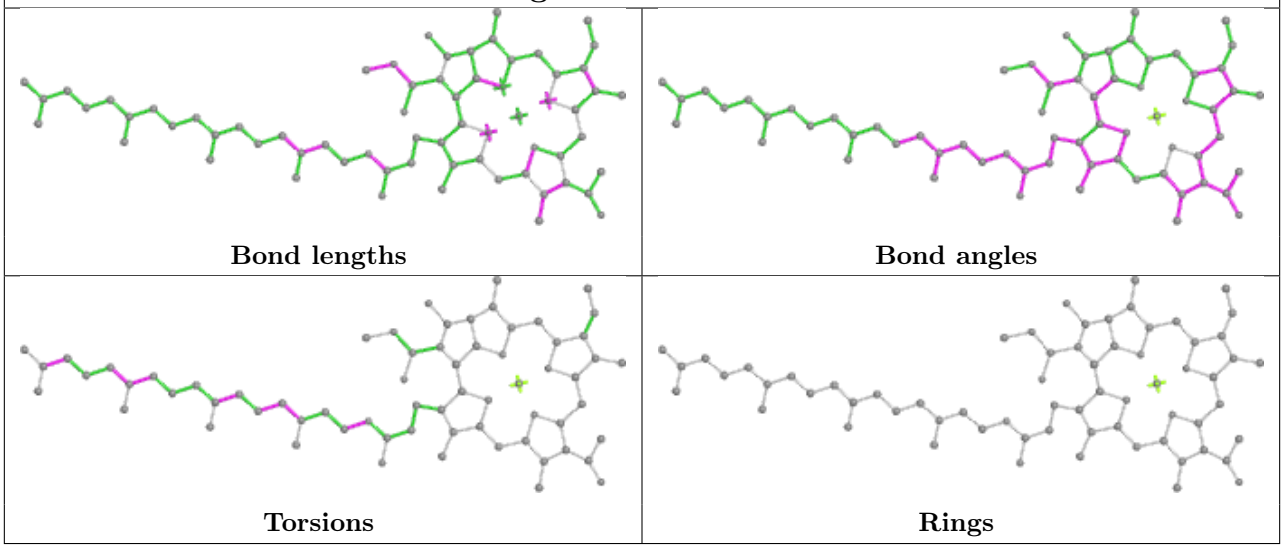
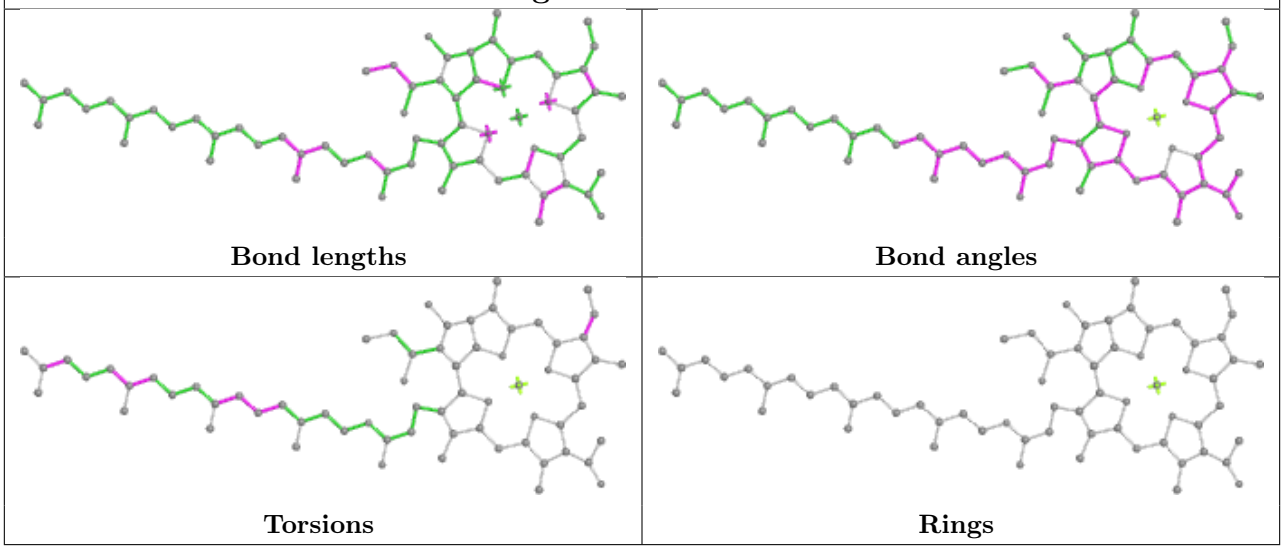
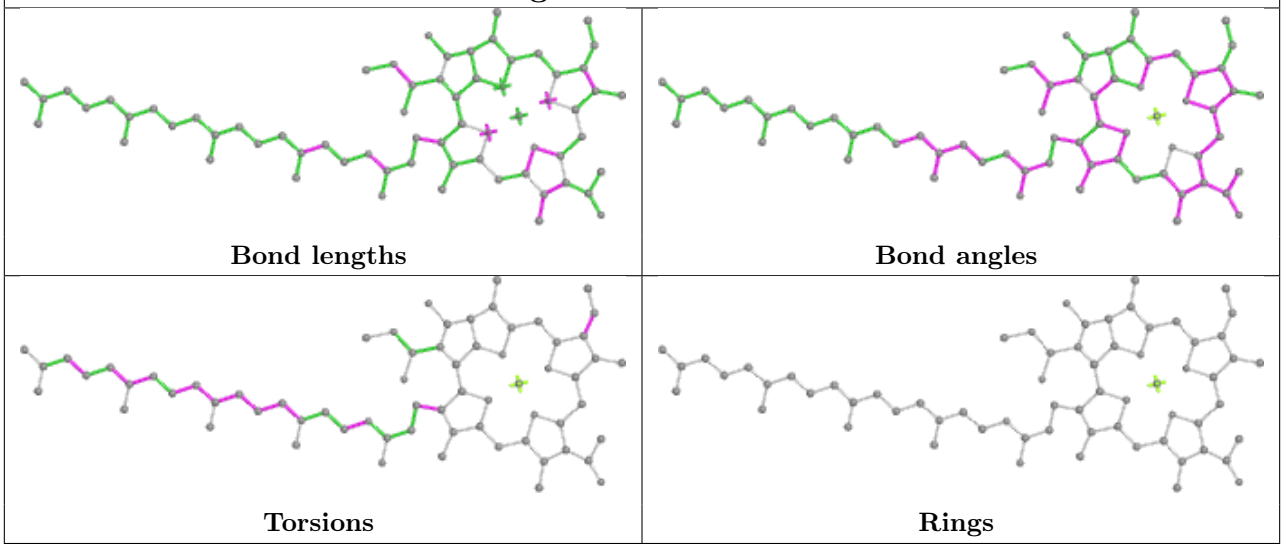


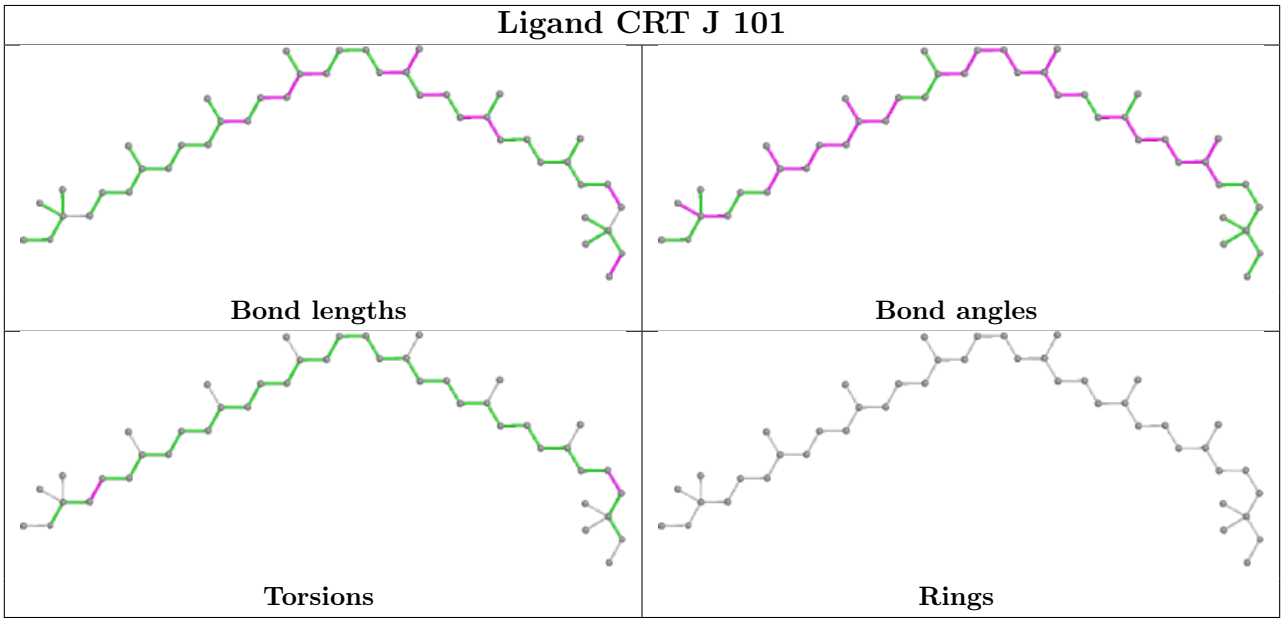
Ligand BCL I 103



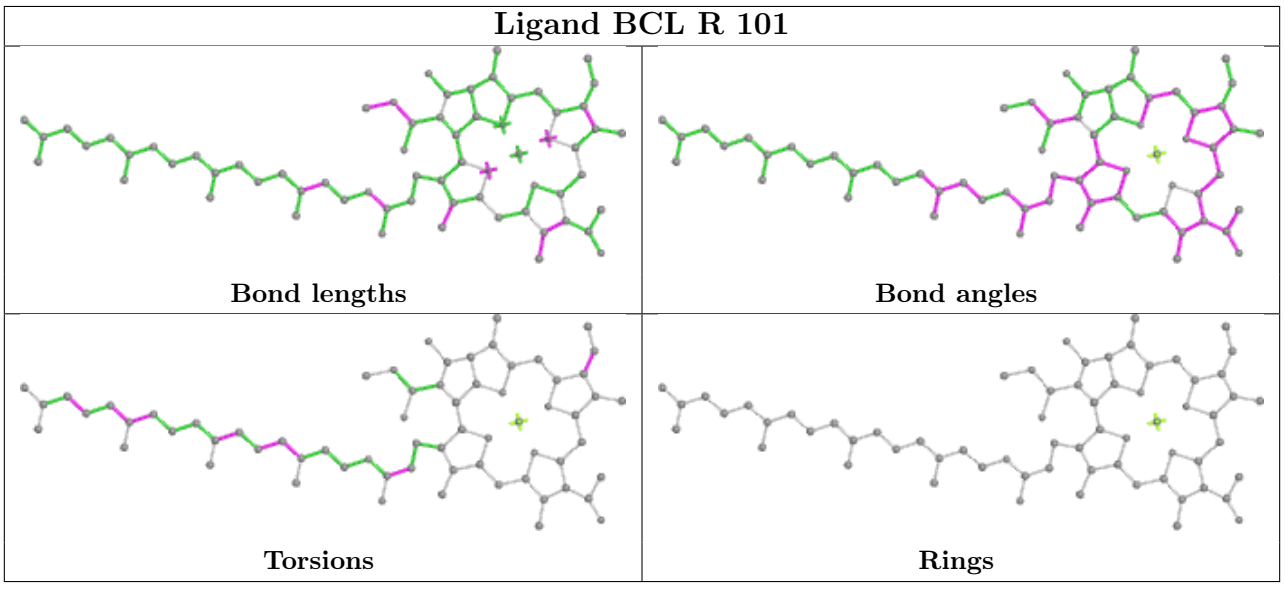
Ligand BCL 3 102



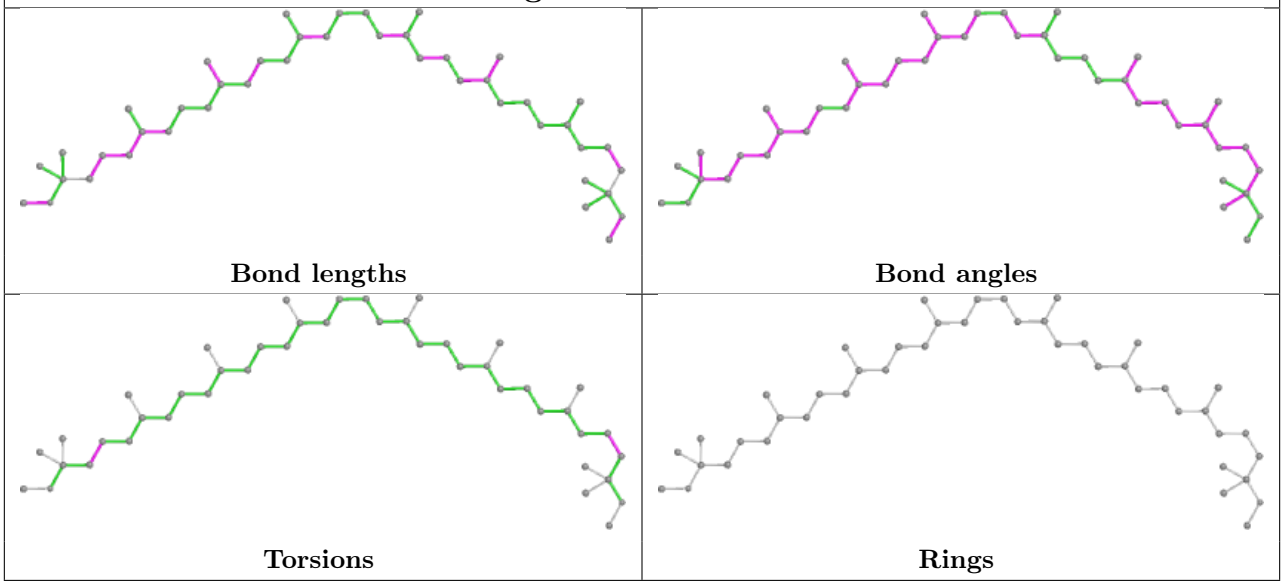
Ligand CRT J 101



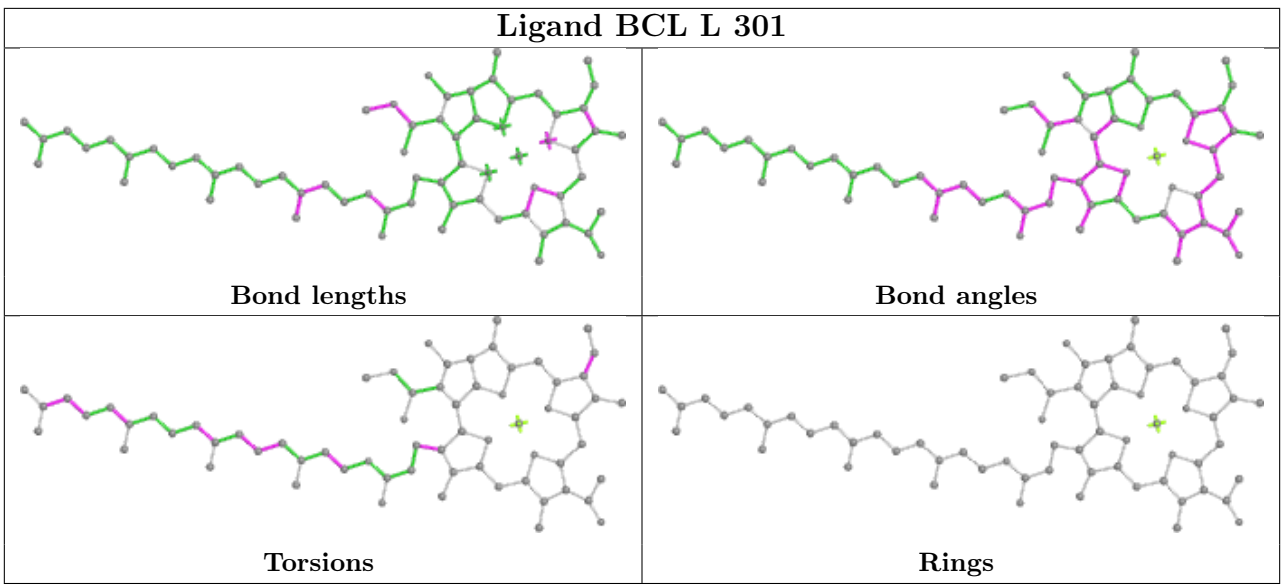
Ligand BCL R 101



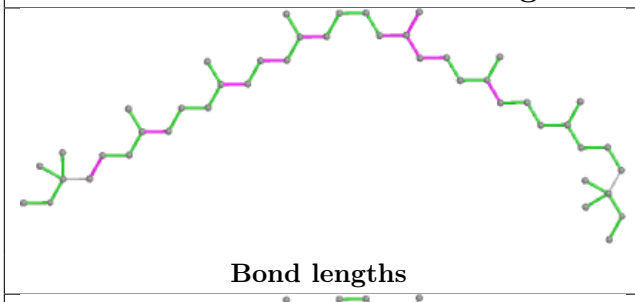
Ligand CRT A 101



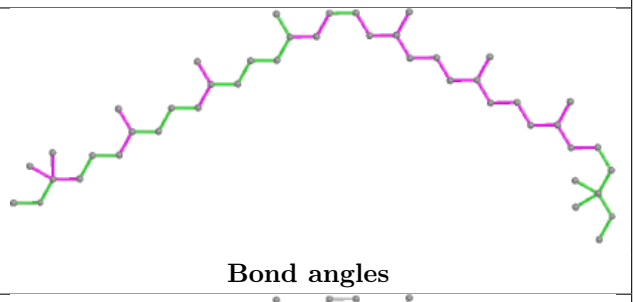
Ligand BCL L 301



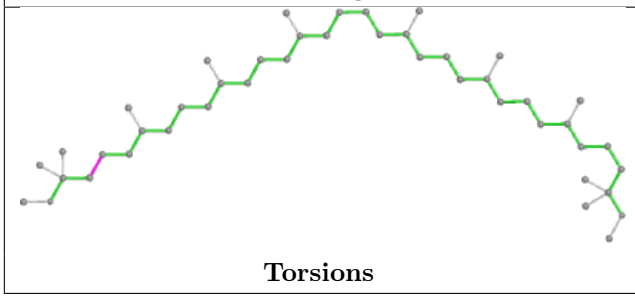
Ligand CRT W 103



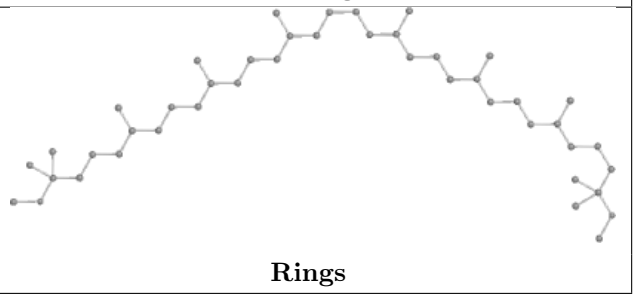
Bond lengths



Bond angles

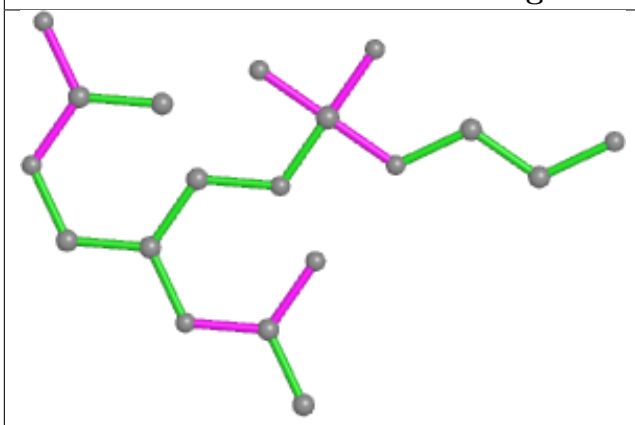


Torsions

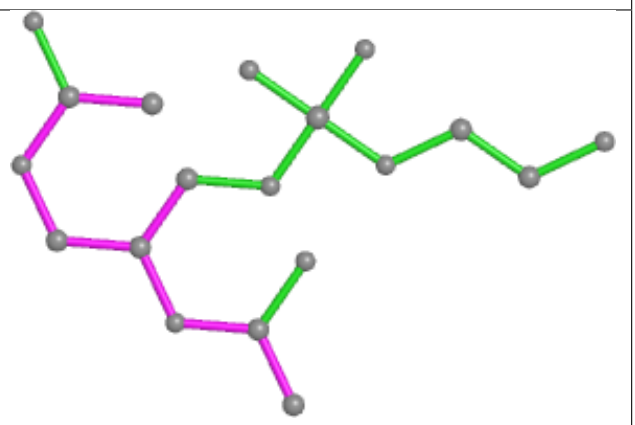


Rings

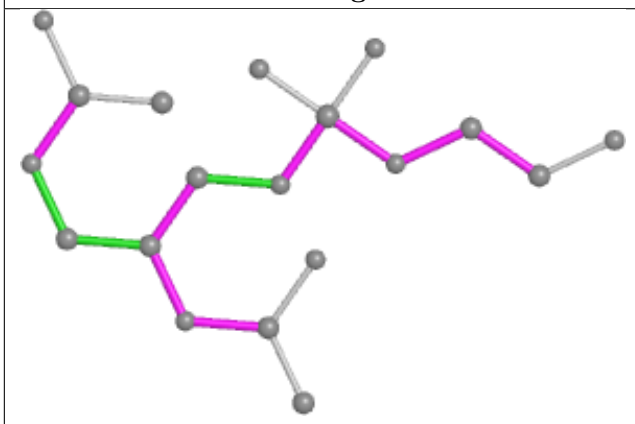
Ligand PEF H 301



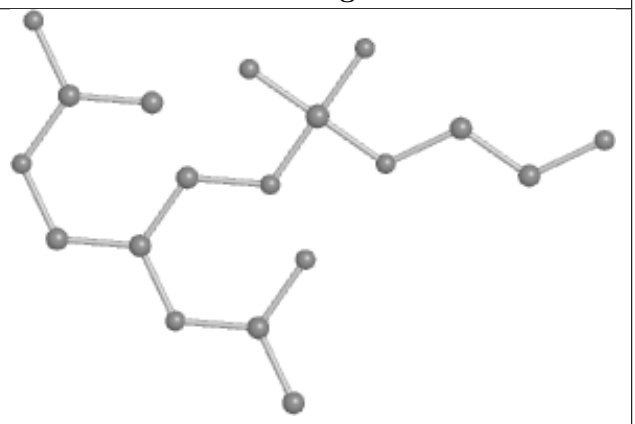
Bond lengths



Bond angles

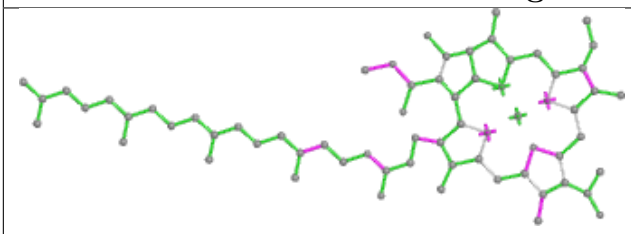


Torsions

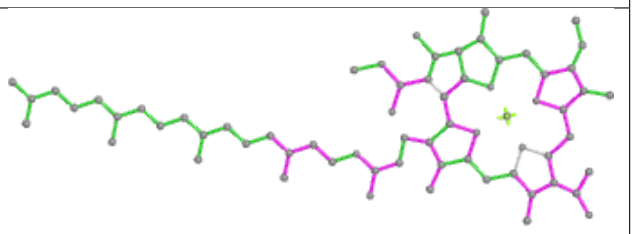


Rings

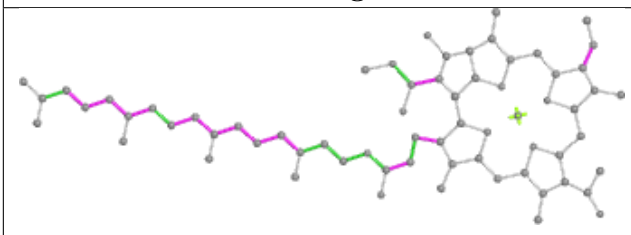
Ligand BCL F 102



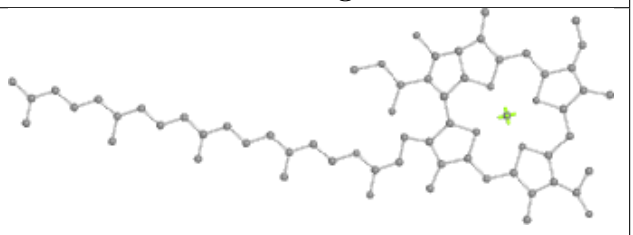
Bond lengths



Bond angles

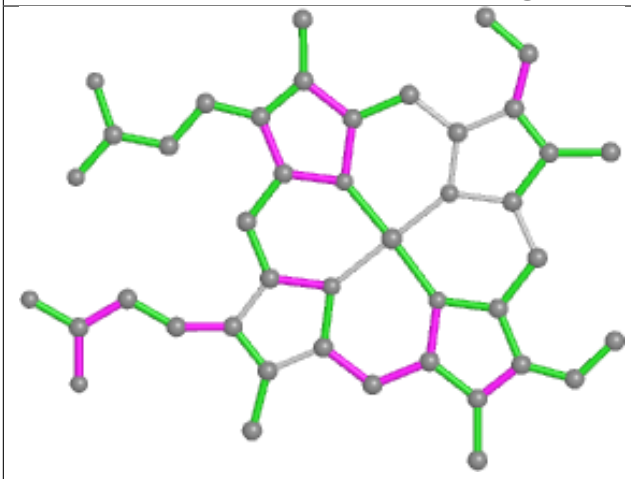


Torsions

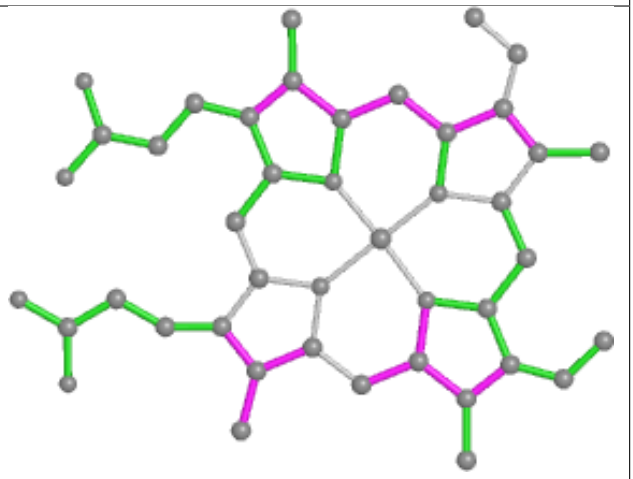


Rings

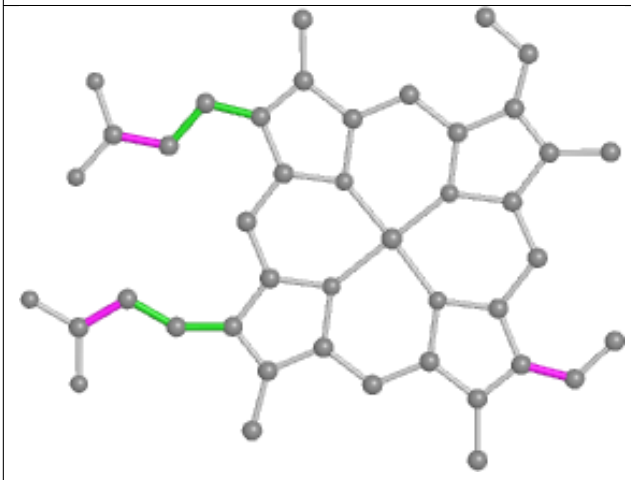
Ligand HEM C 503



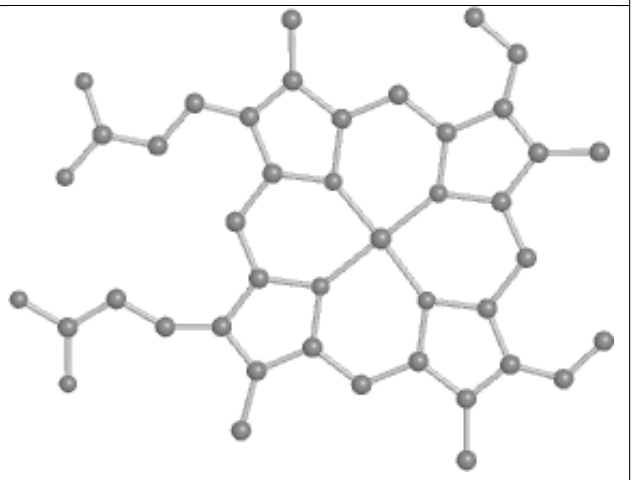
Bond lengths



Bond angles

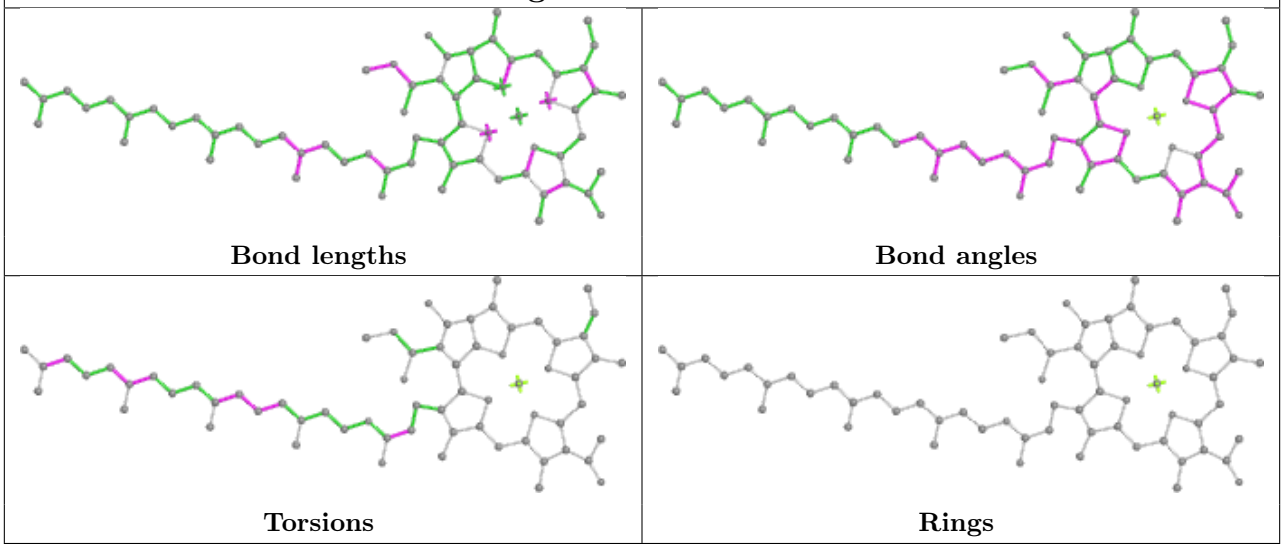


Torsions

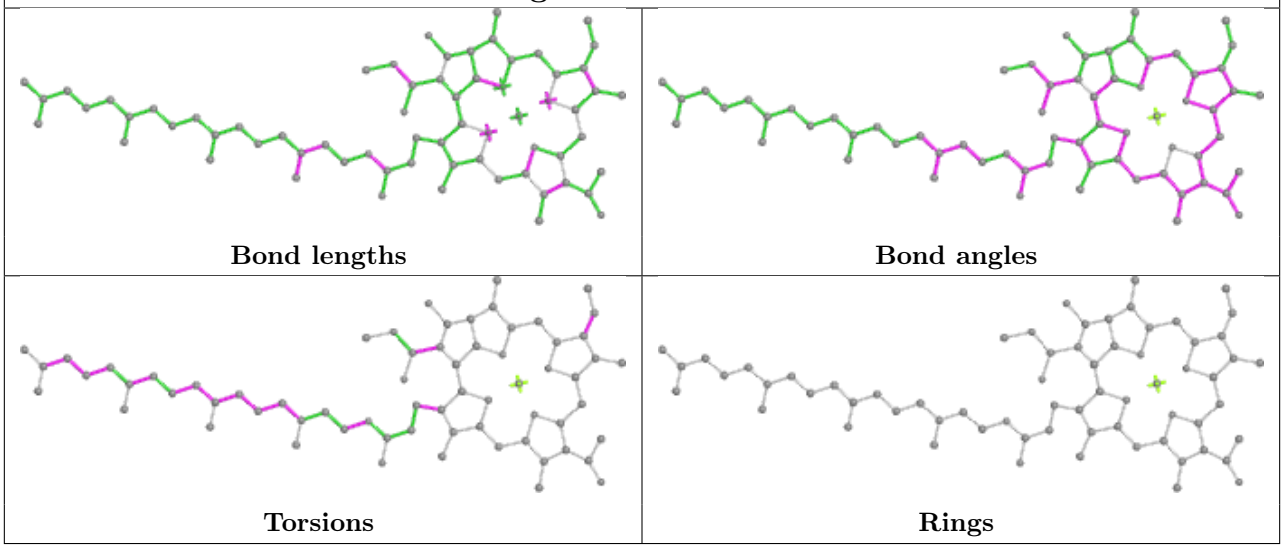


Rings

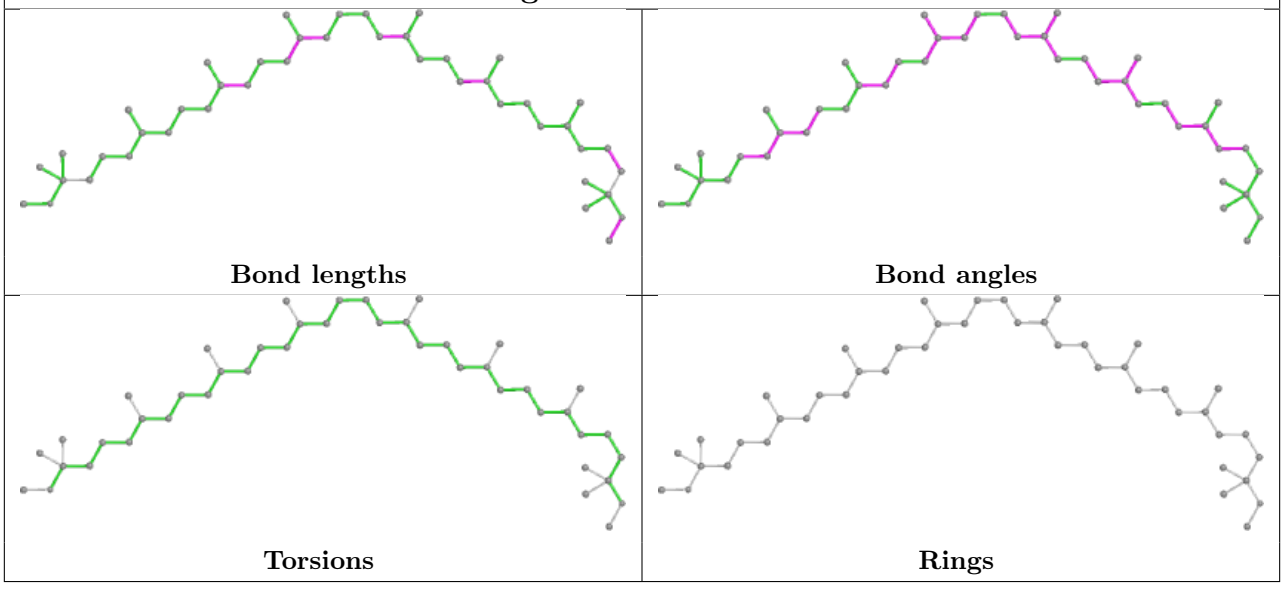
Ligand BCL Z 101



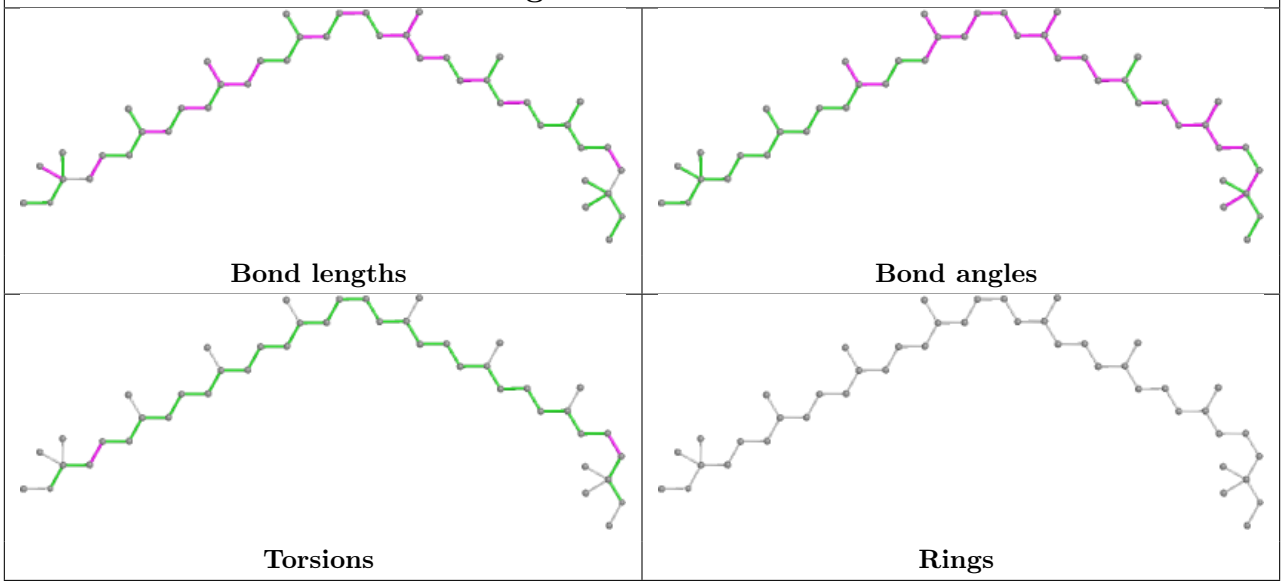
Ligand BCL 5 102



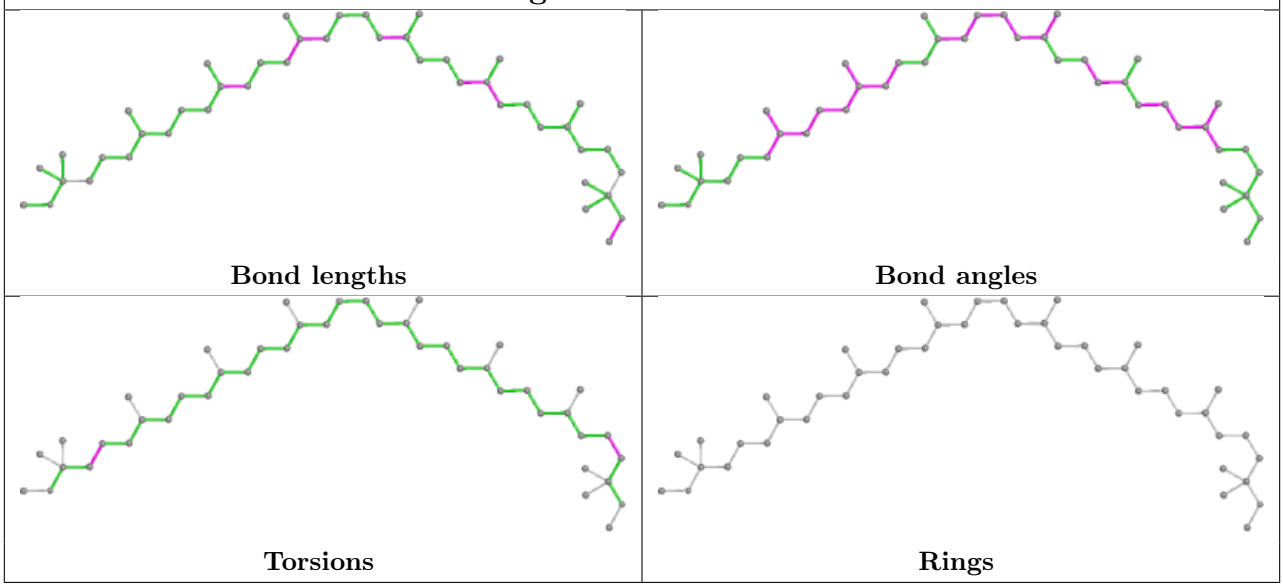
Ligand CRT M 406



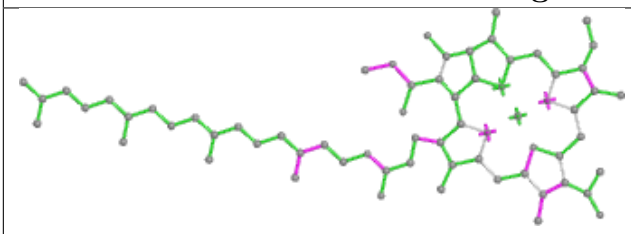
Ligand CRT P 102



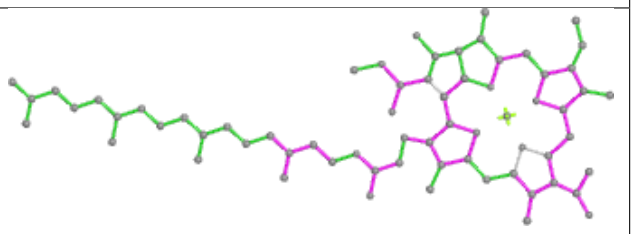
Ligand CRT 8 101



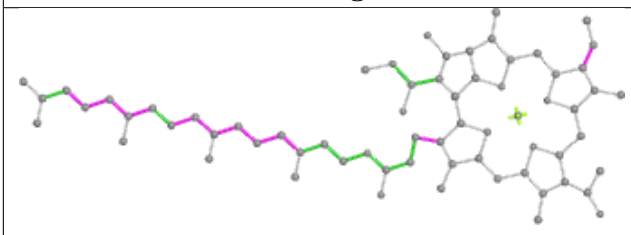
Ligand BCL I 102



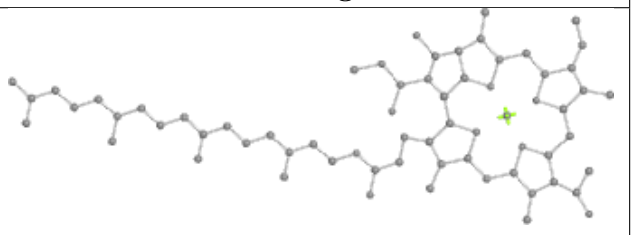
Bond lengths



Bond angles

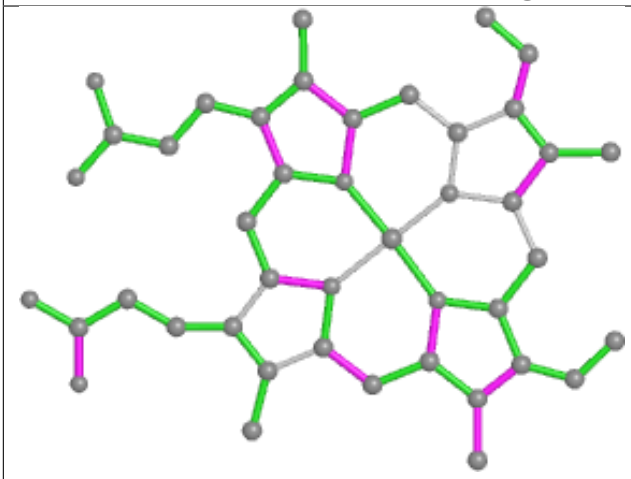


Torsions

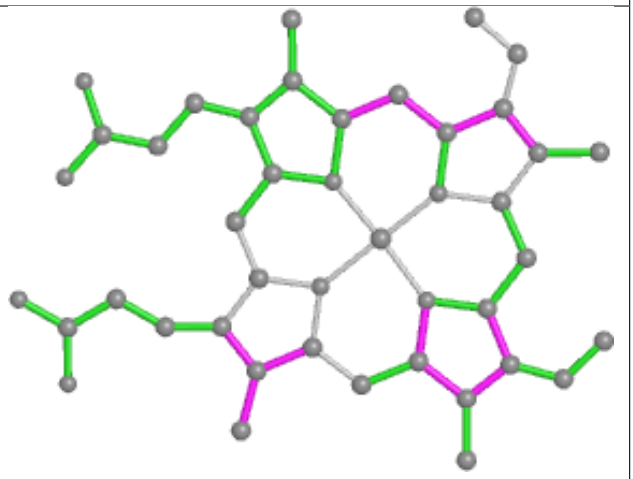


Rings

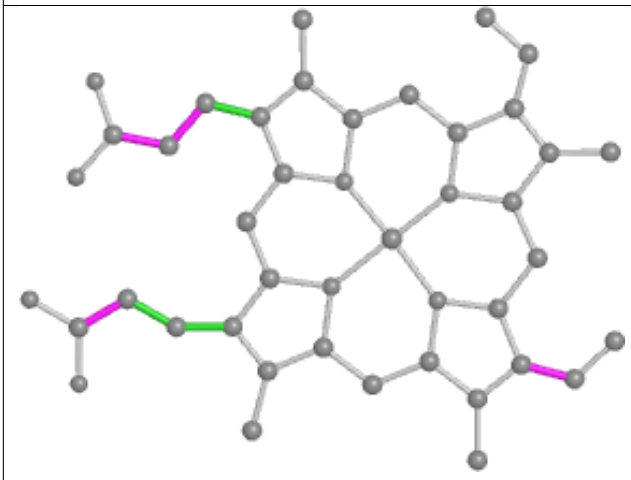
Ligand HEM C 504



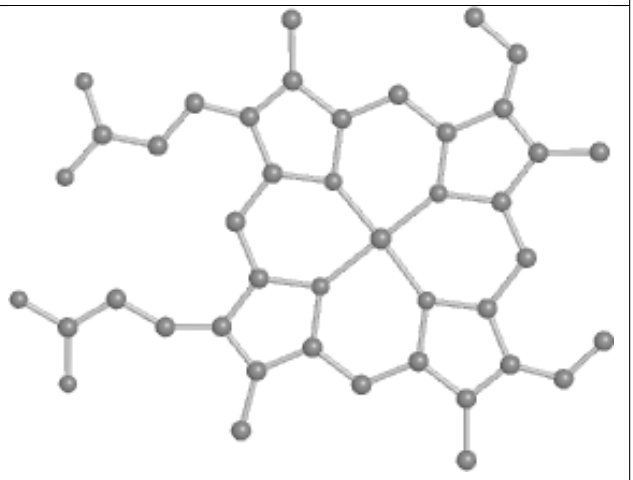
Bond lengths



Bond angles

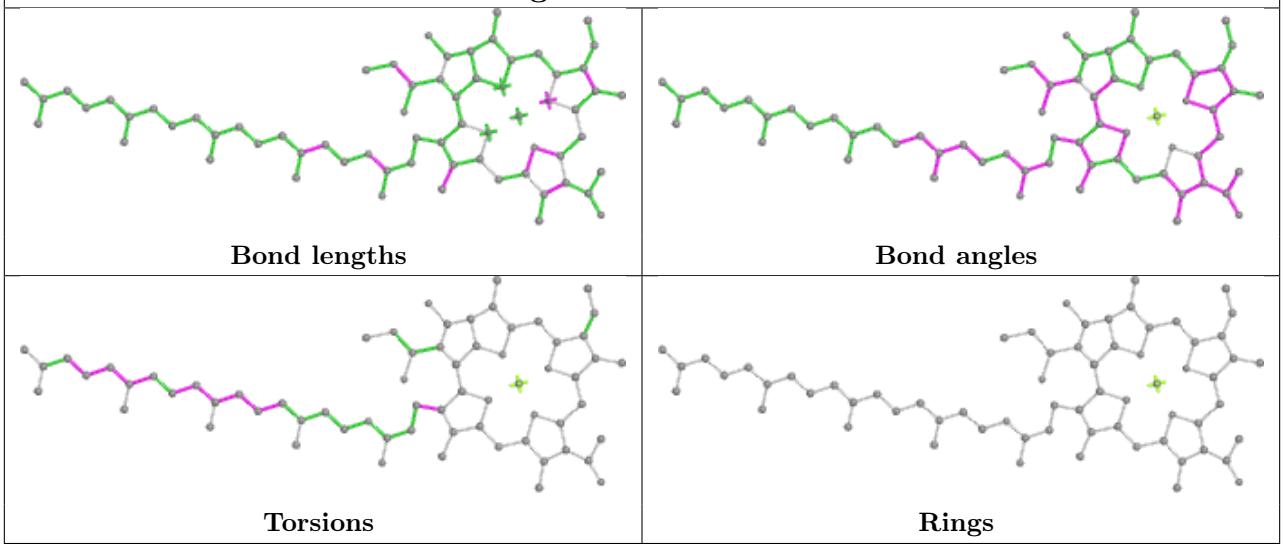


Torsions

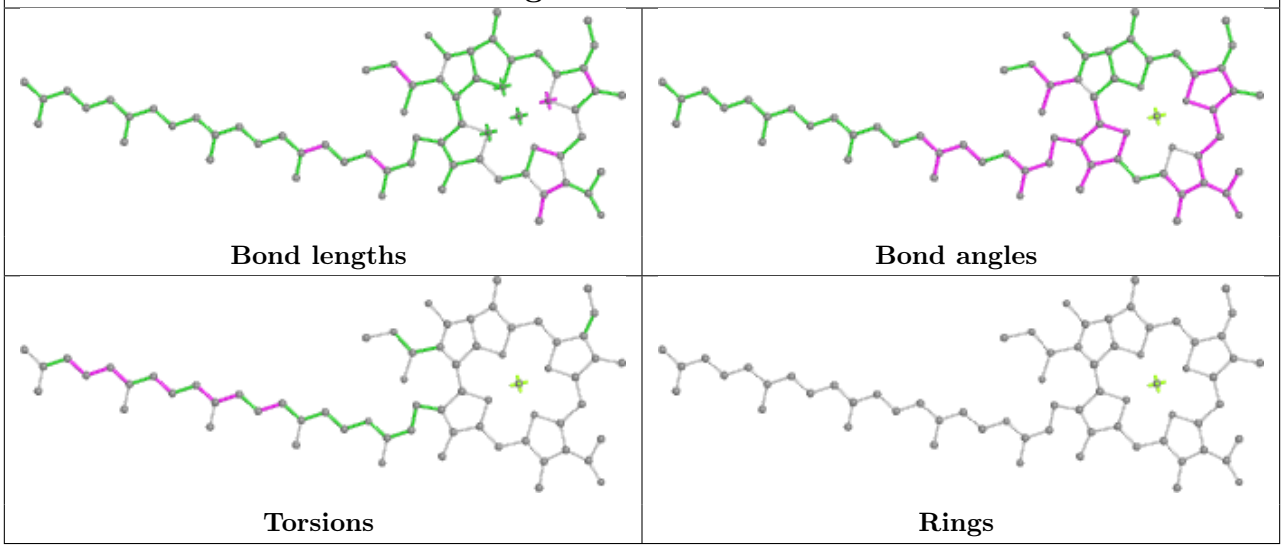


Rings

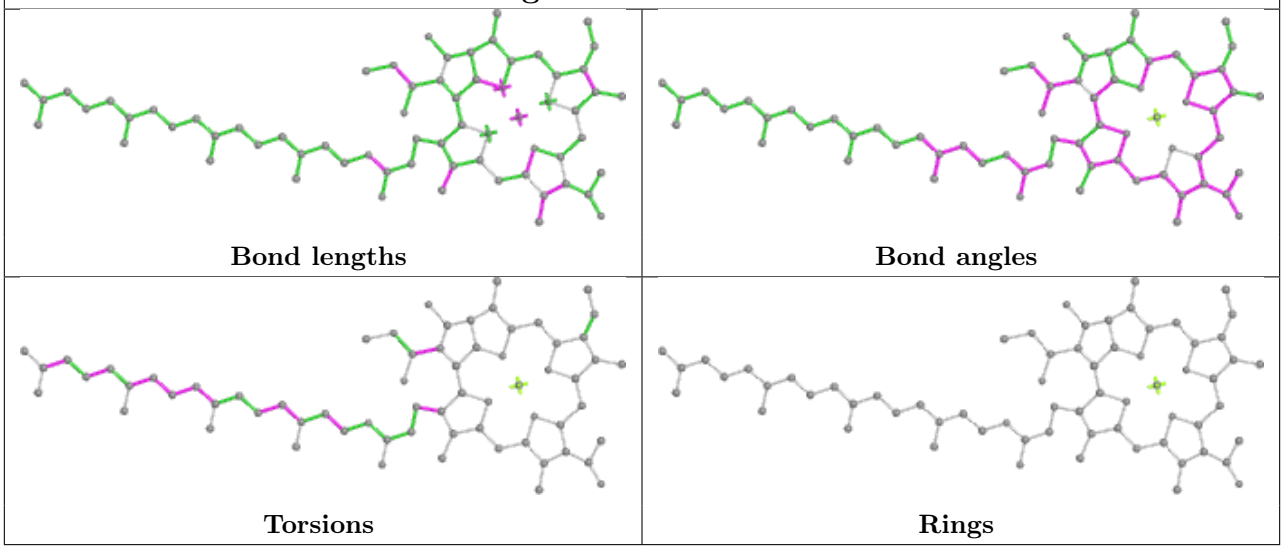
Ligand BCL 7 102



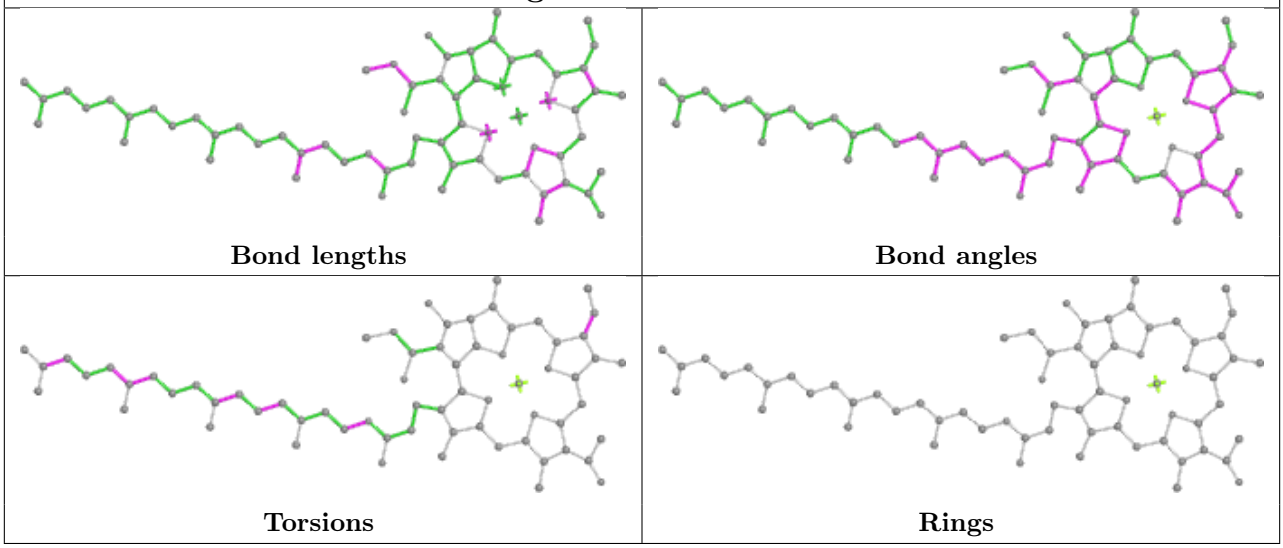
Ligand BCL G 101



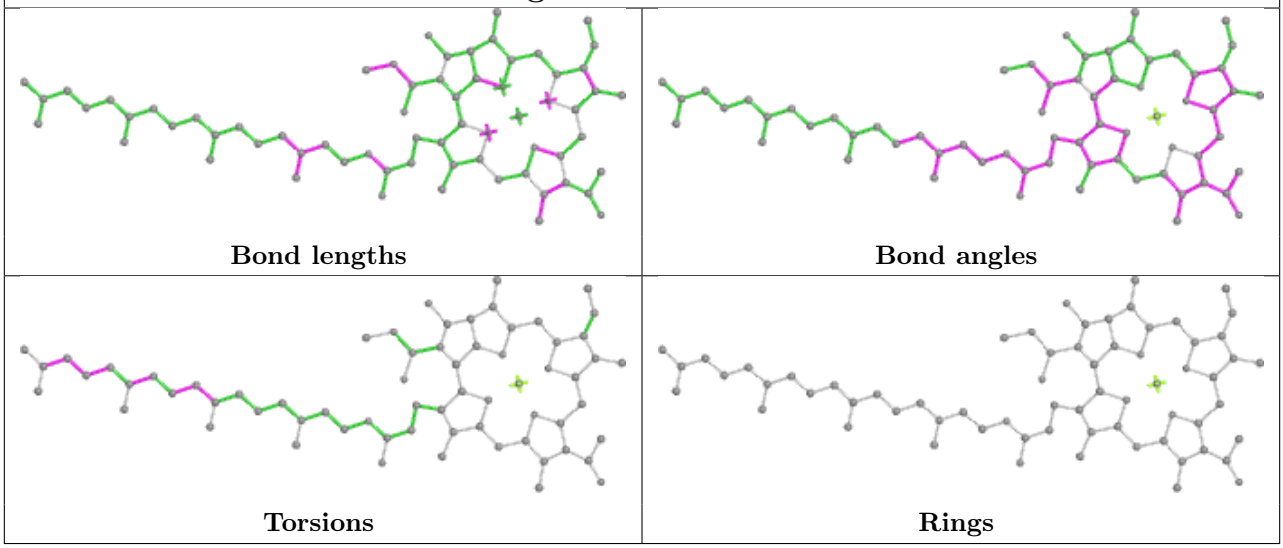
Ligand BCL M 402



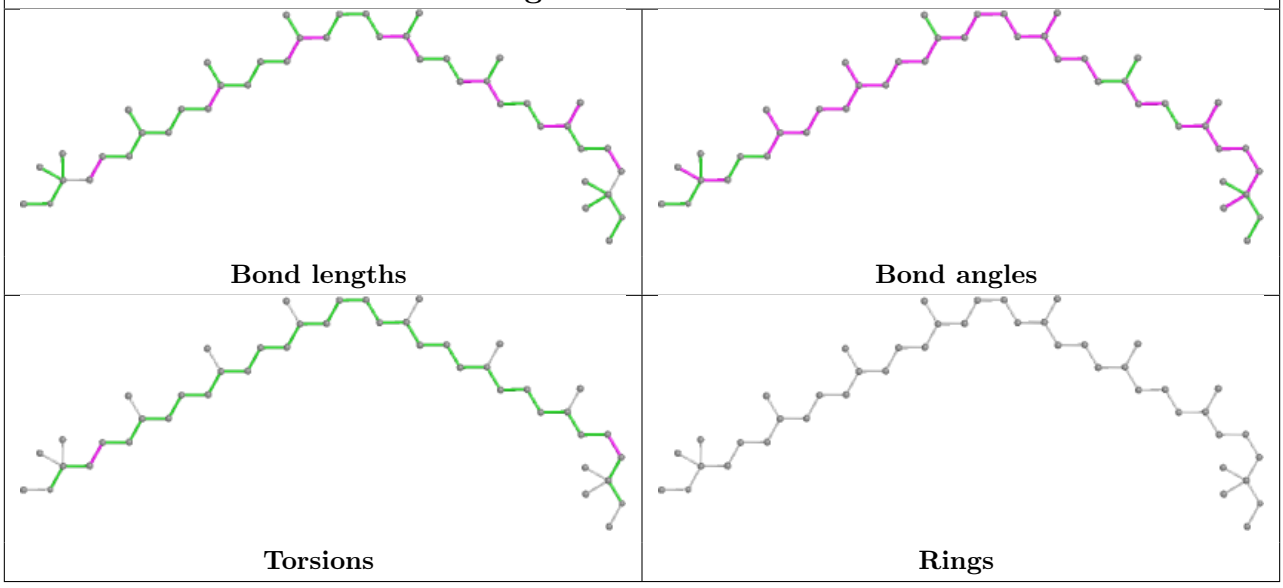
Ligand BCL P 101



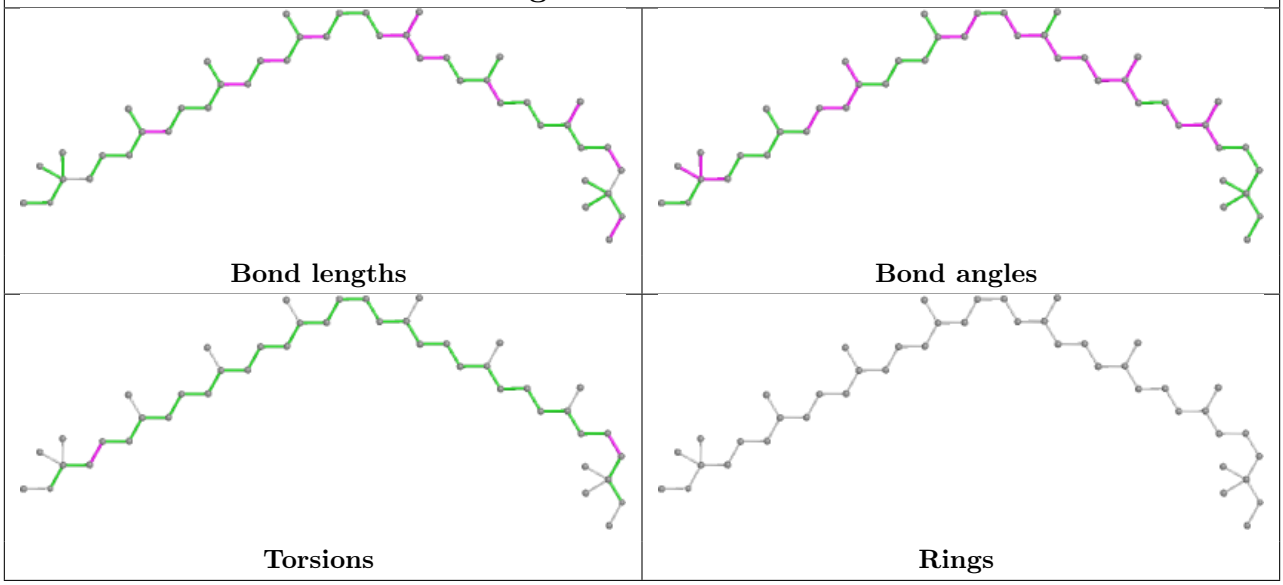
Ligand BCL E 101



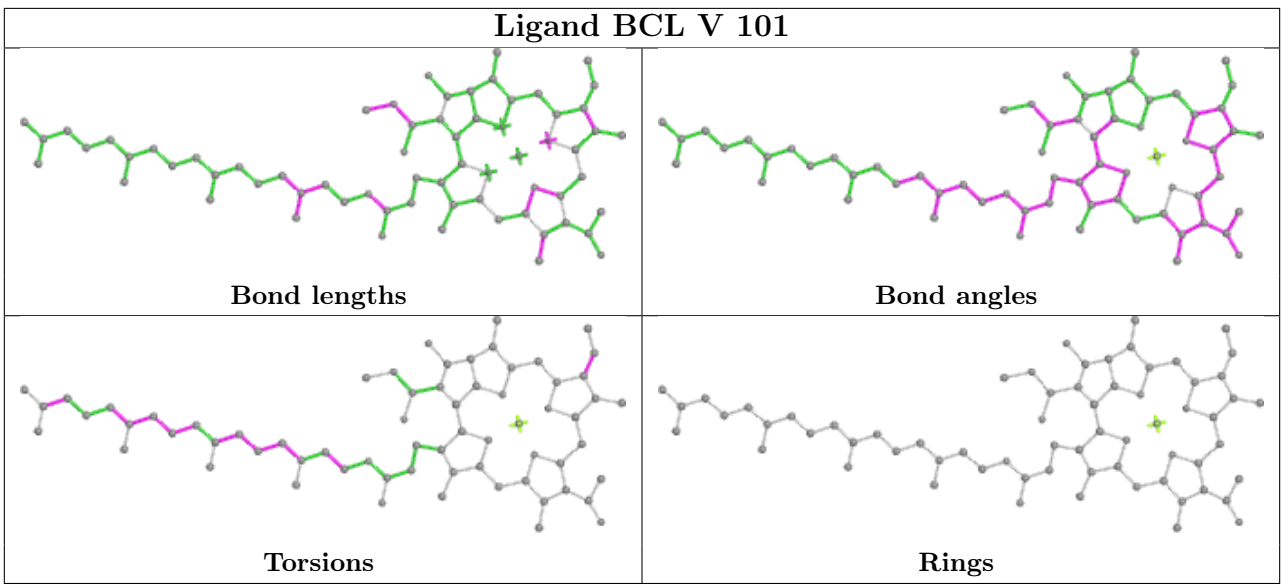
Ligand CRT R 102



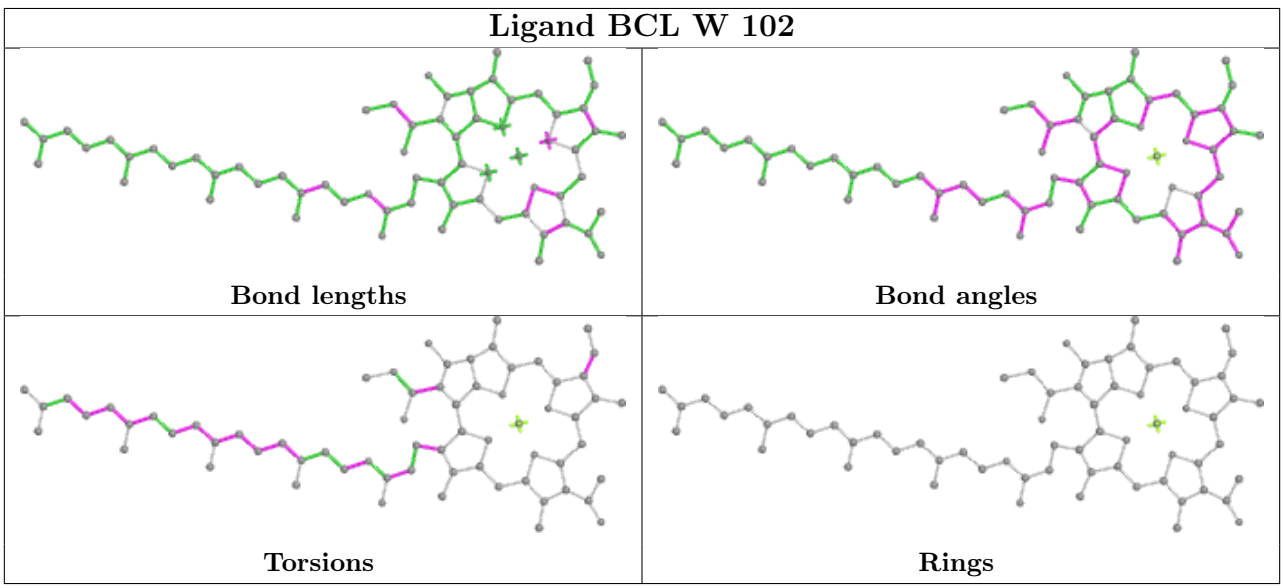
Ligand CRT 3 103



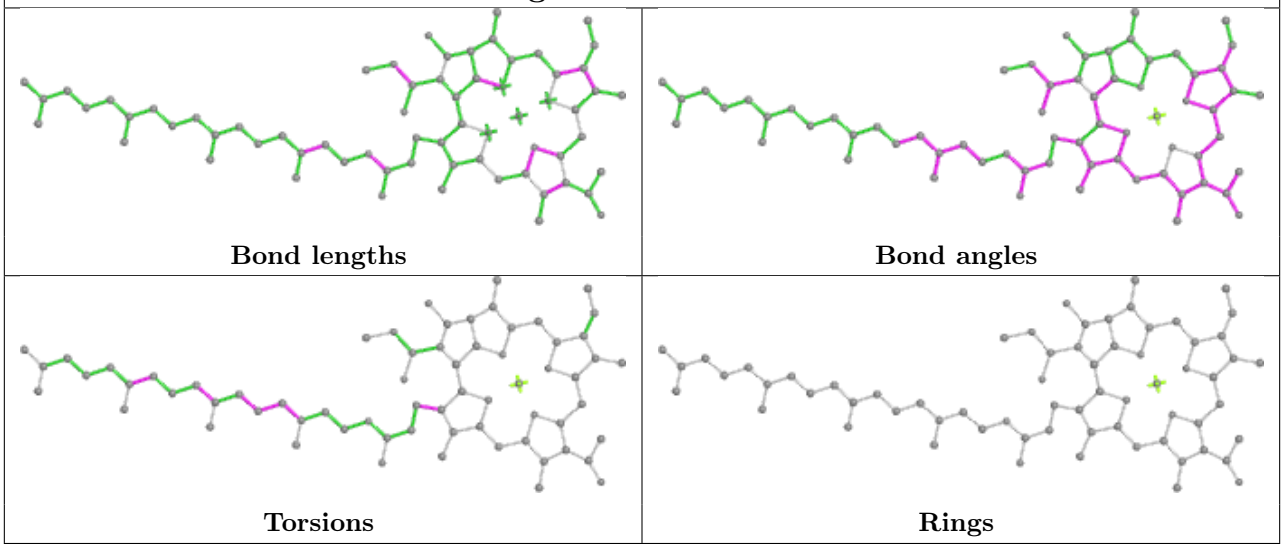
Ligand BCL V 101



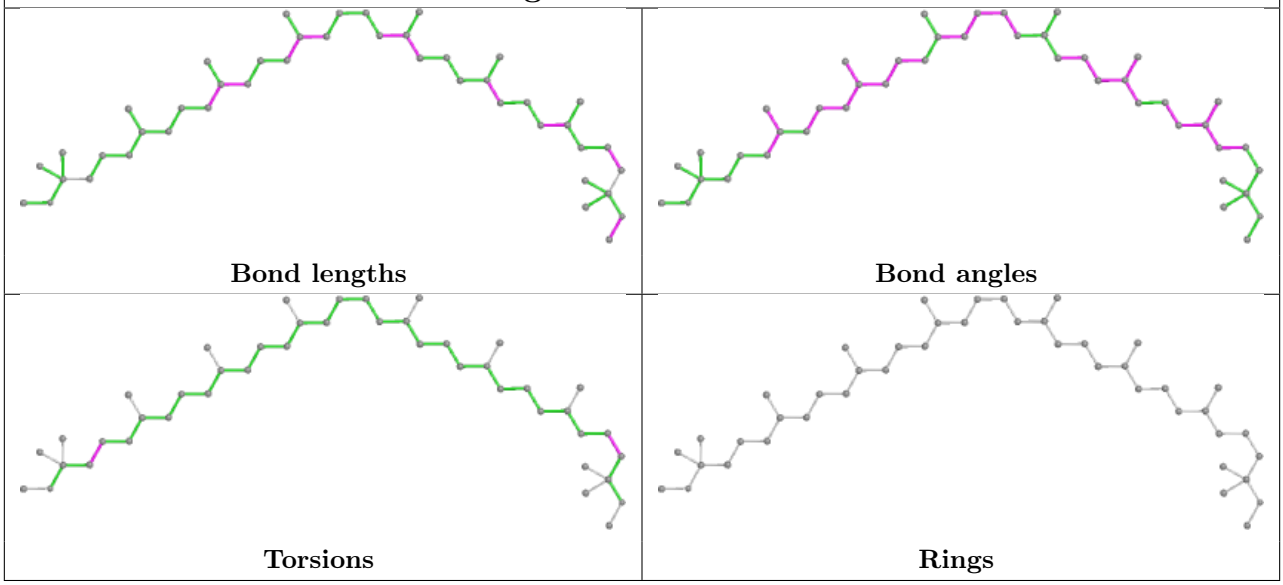
Ligand BCL W 102



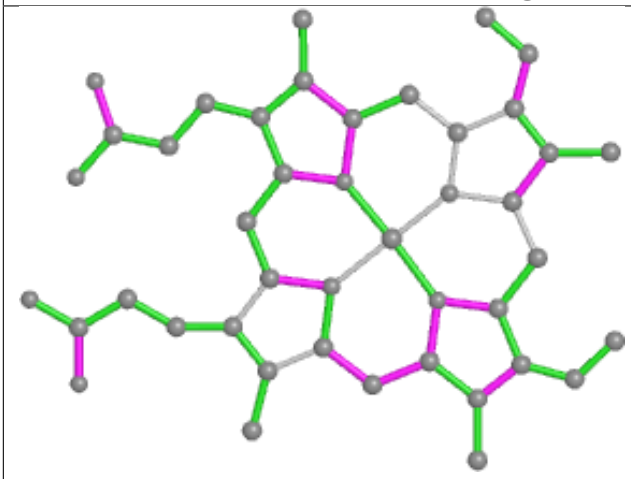
Ligand BCL L 303



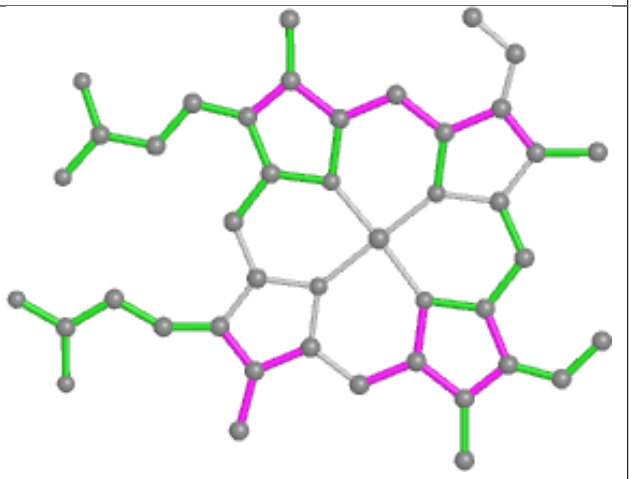
Ligand CRT N 102



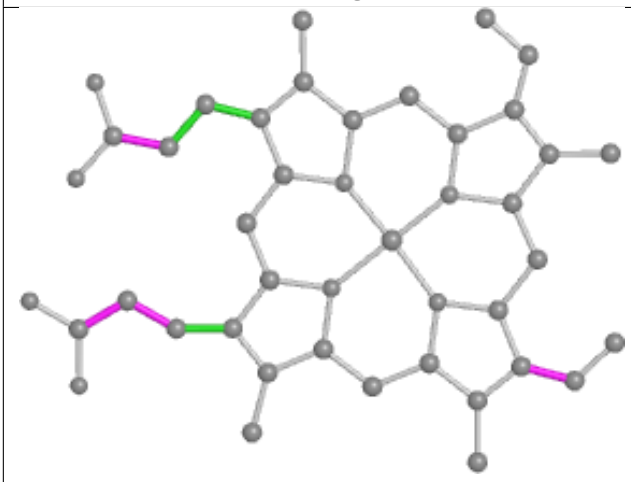
Ligand HEM C 501



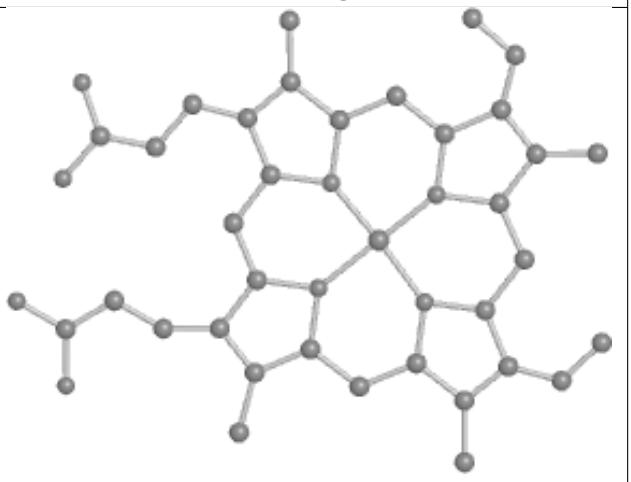
Bond lengths



Bond angles

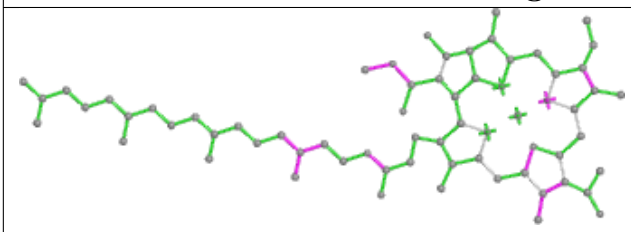


Torsions

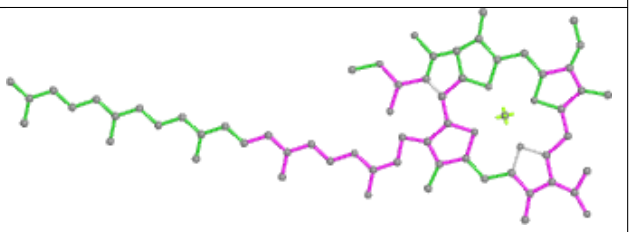


Rings

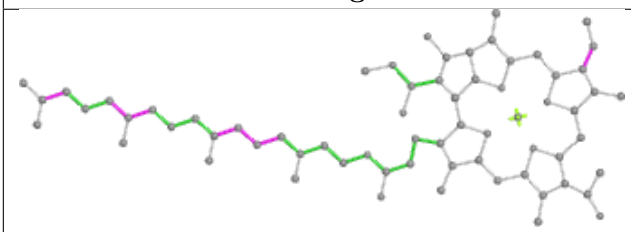
Ligand BCL T 101



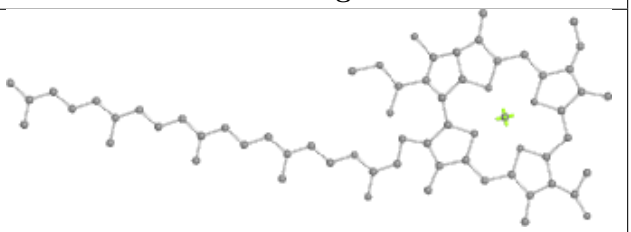
Bond lengths



Bond angles

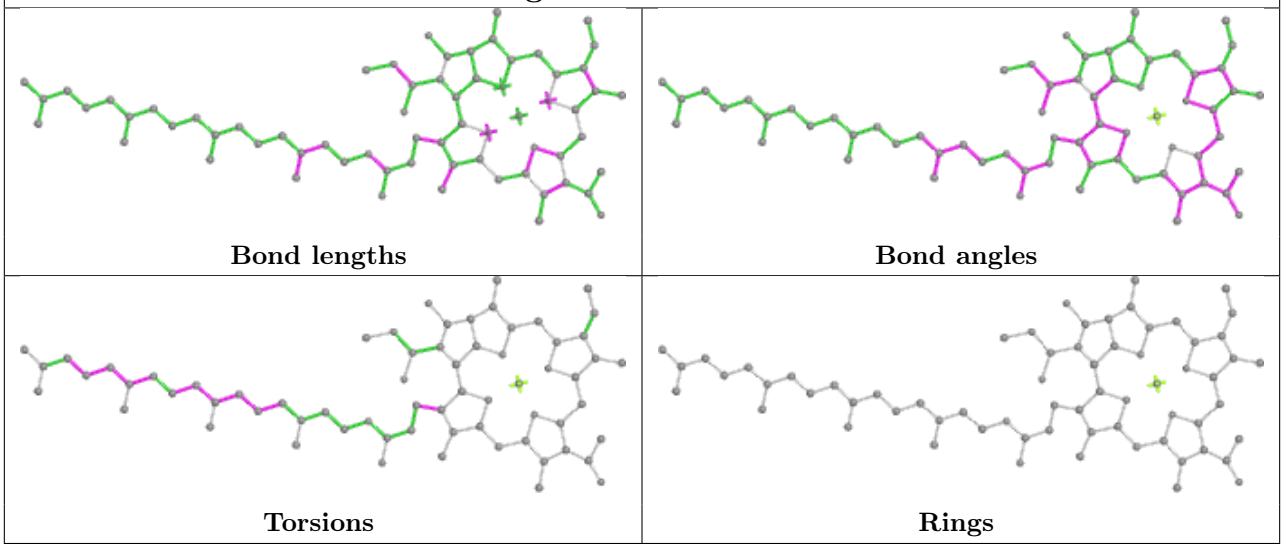


Torsions

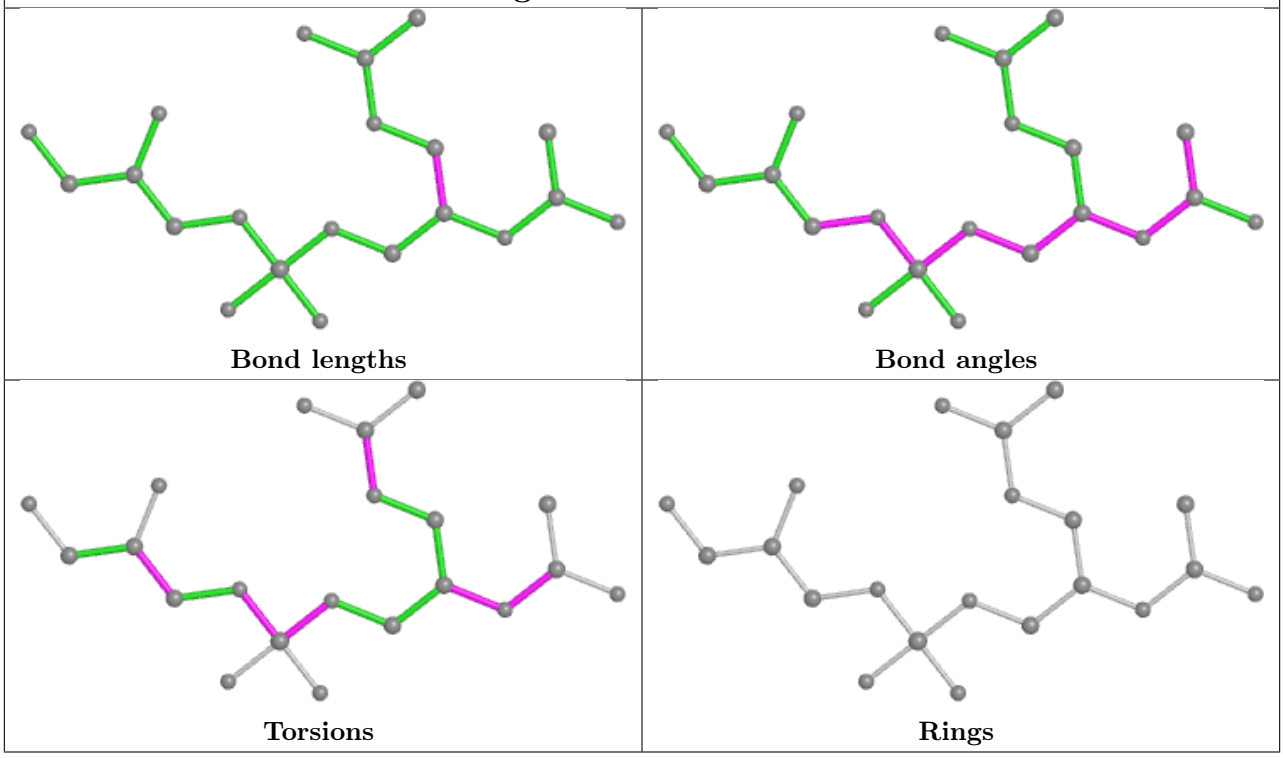


Rings

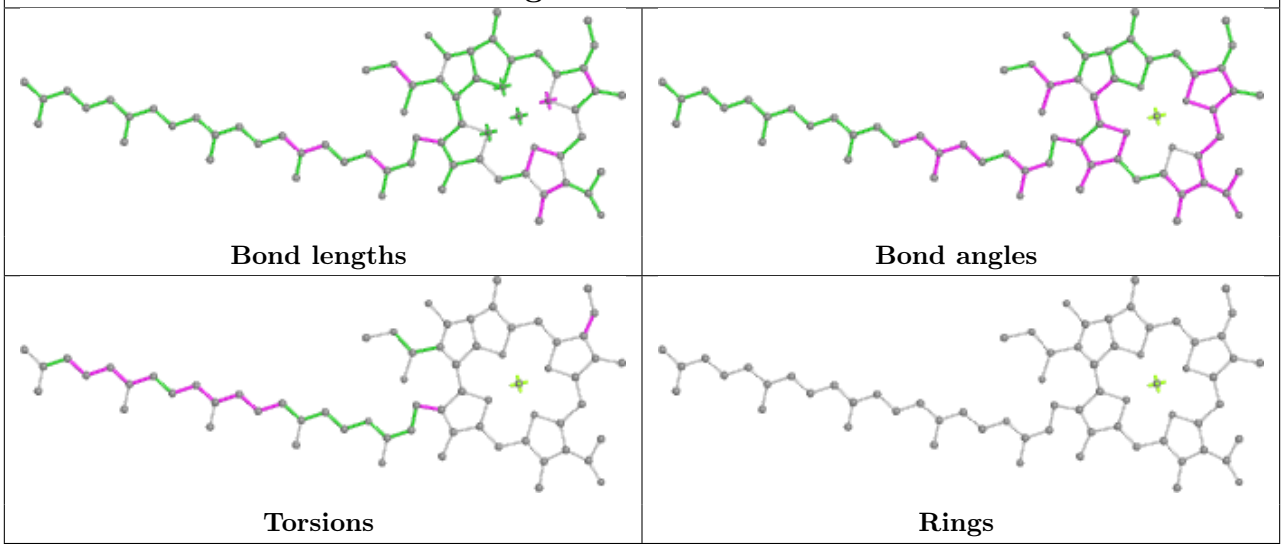
Ligand BCL U 102



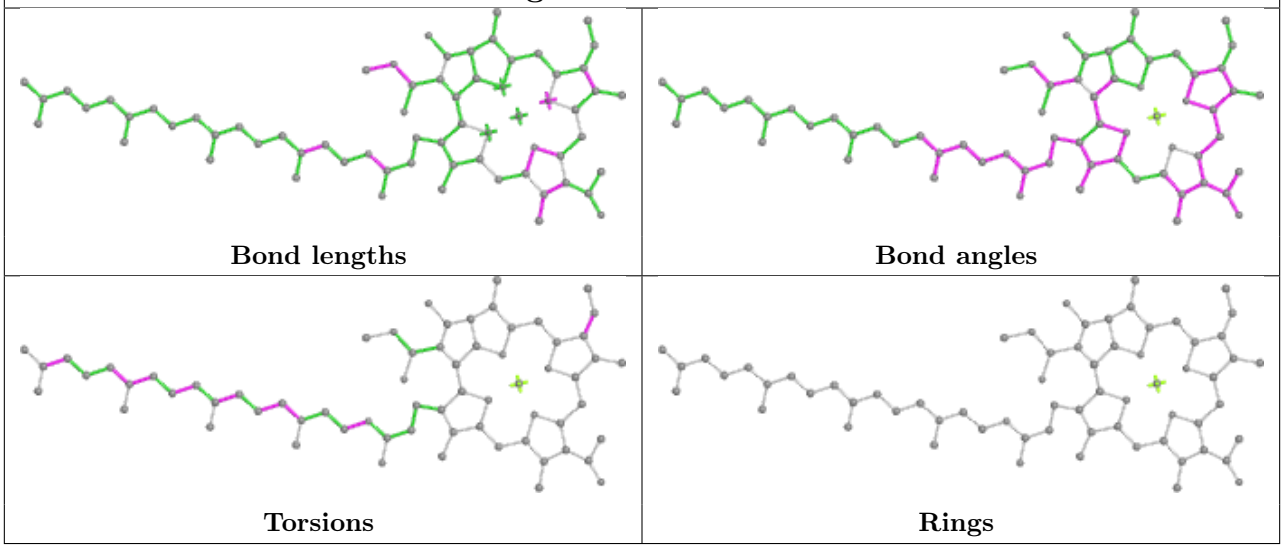
Ligand PGW M 407



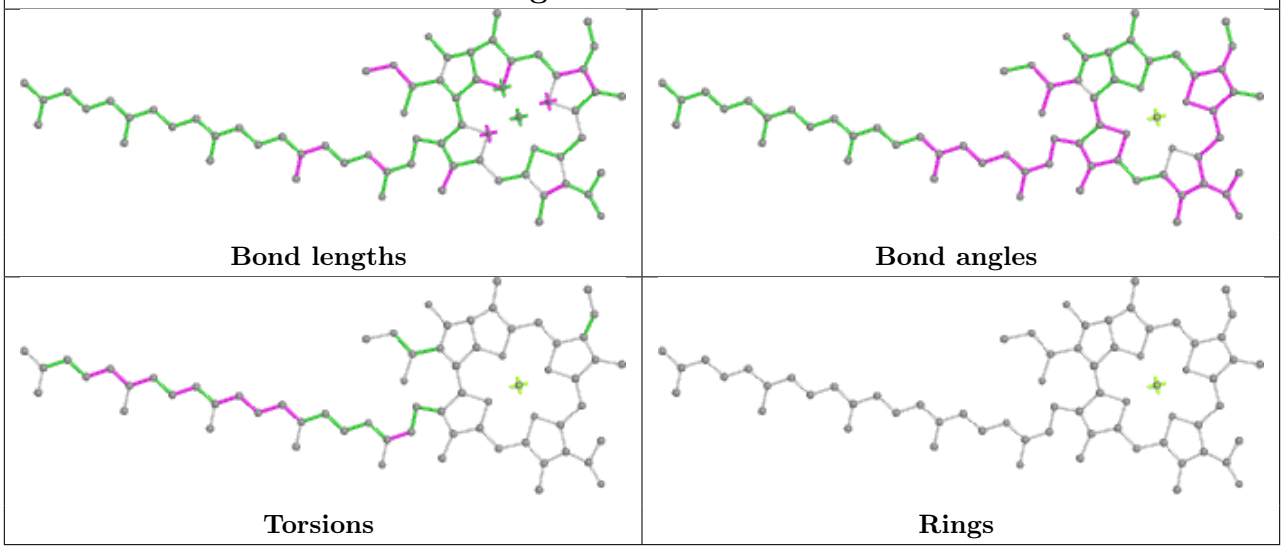
Ligand BCL K 102



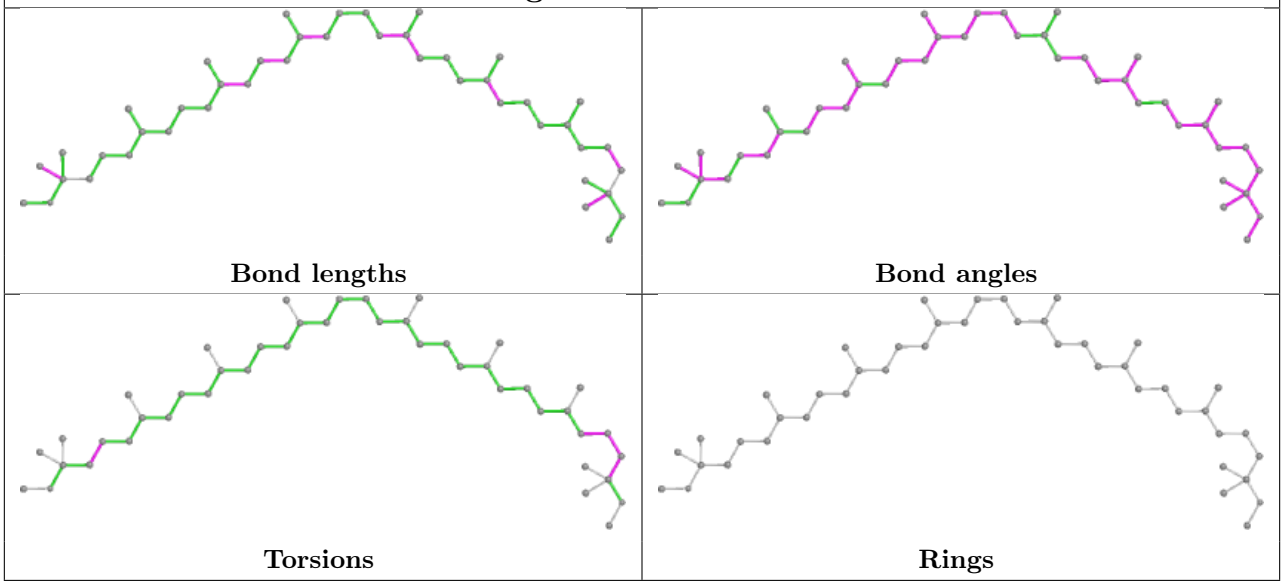
Ligand BCL B 101



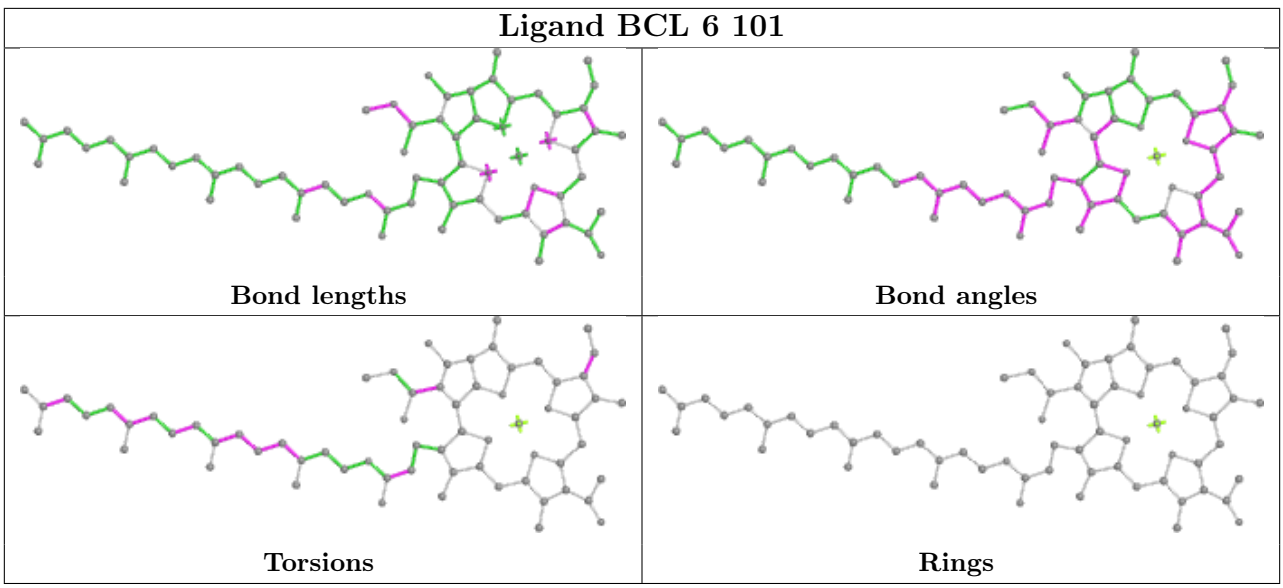
Ligand BCL 2 101



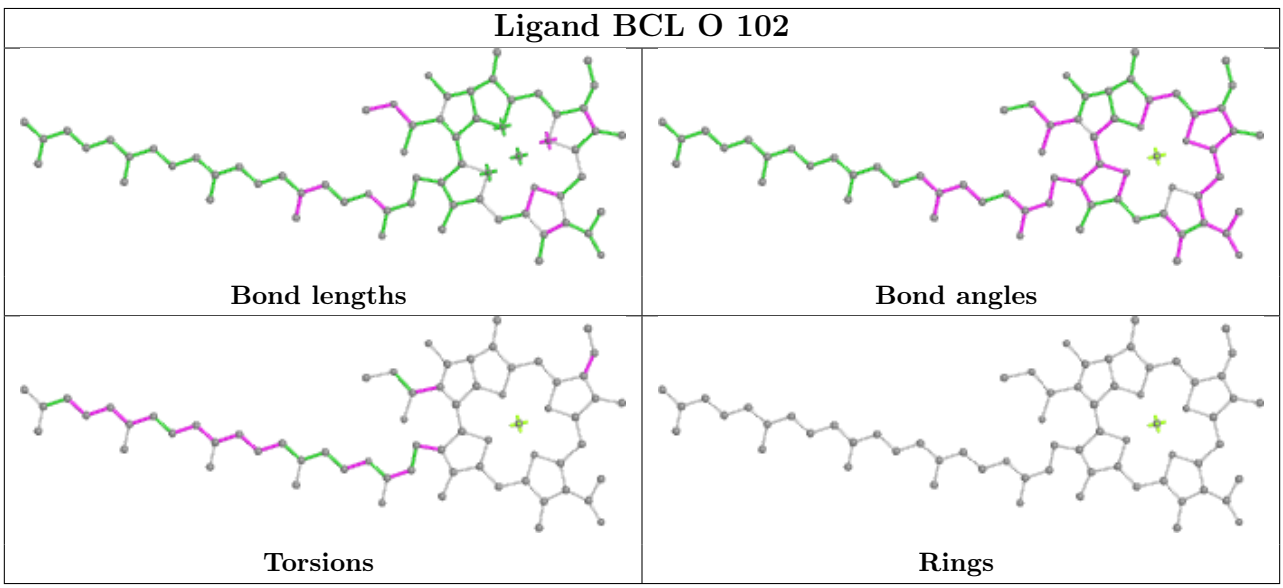
Ligand CRT T 102



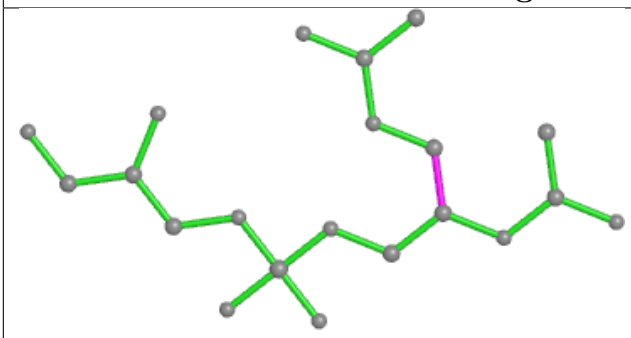
Ligand BCL 6 101



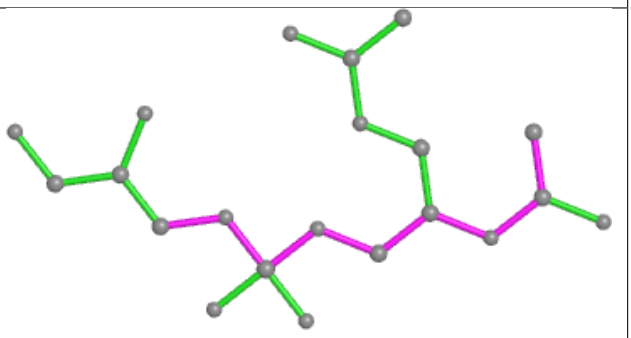
Ligand BCL O 102



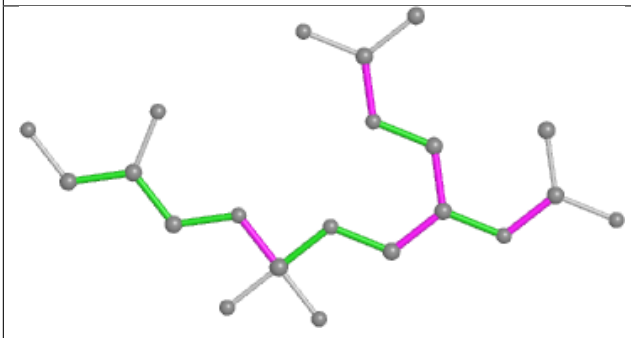
Ligand PGW H 302



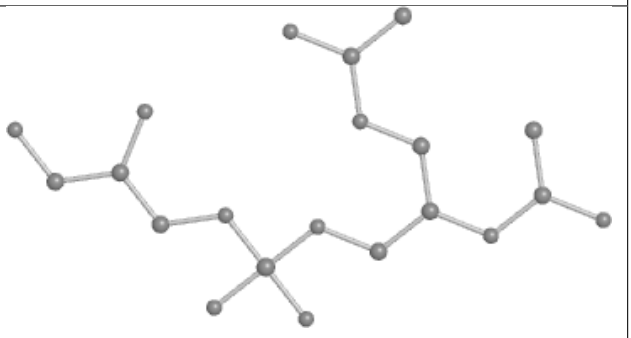
Bond lengths



Bond angles

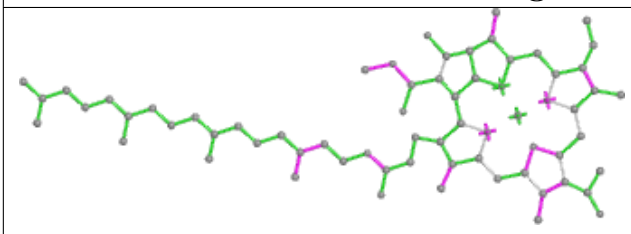


Torsions

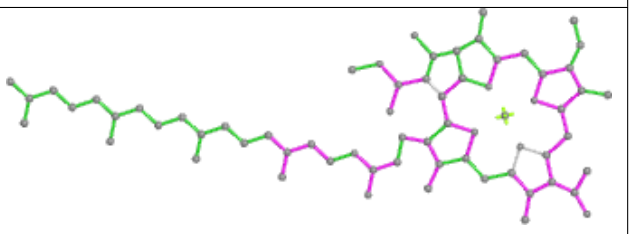


Rings

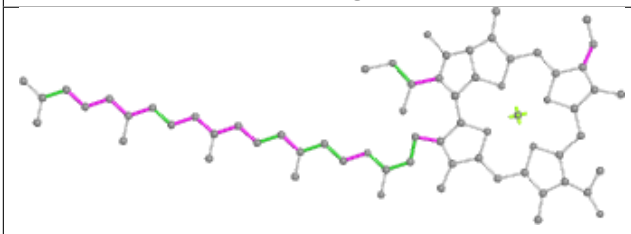
Ligand BCL S 102



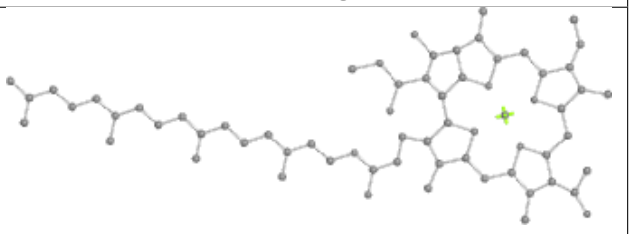
Bond lengths



Bond angles

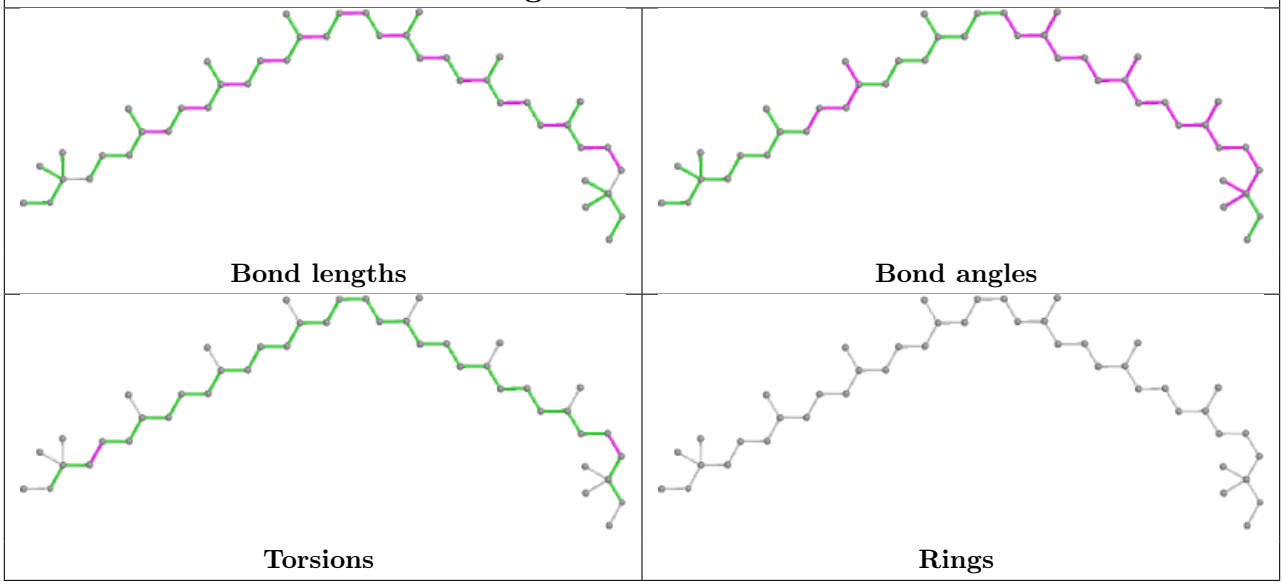


Torsions

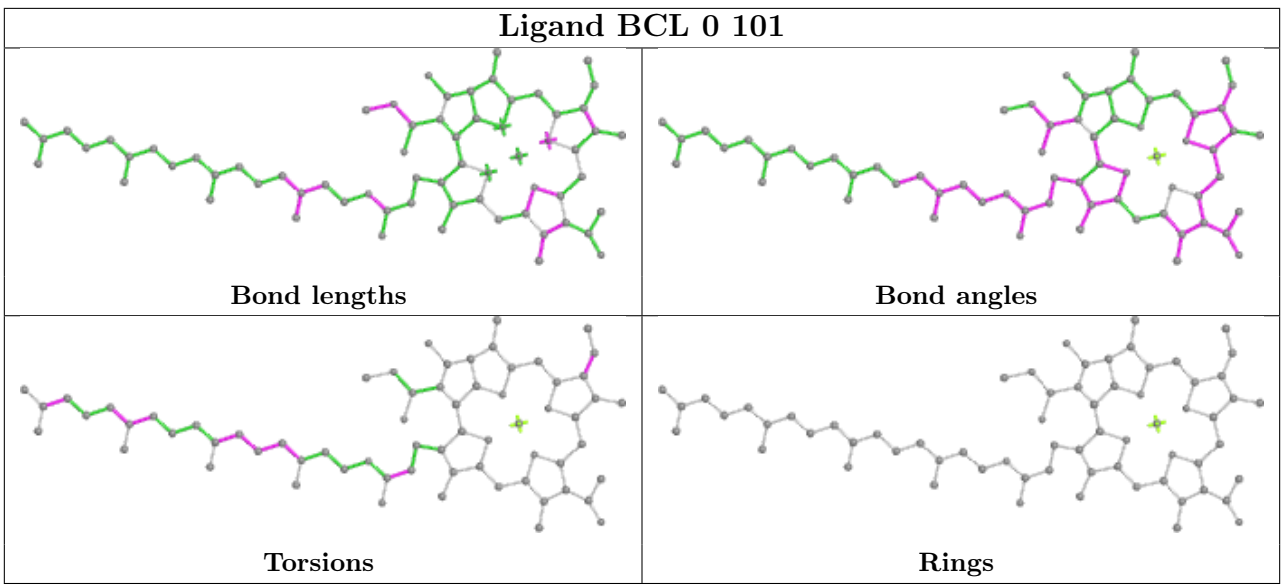


Rings

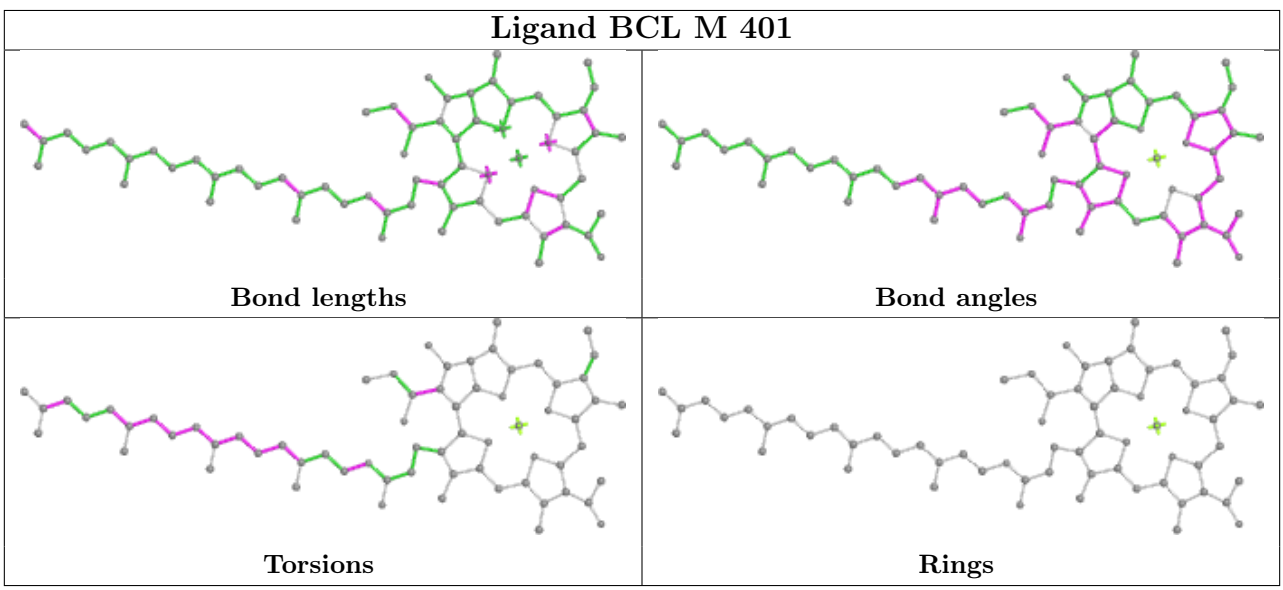
Ligand CRT X 102



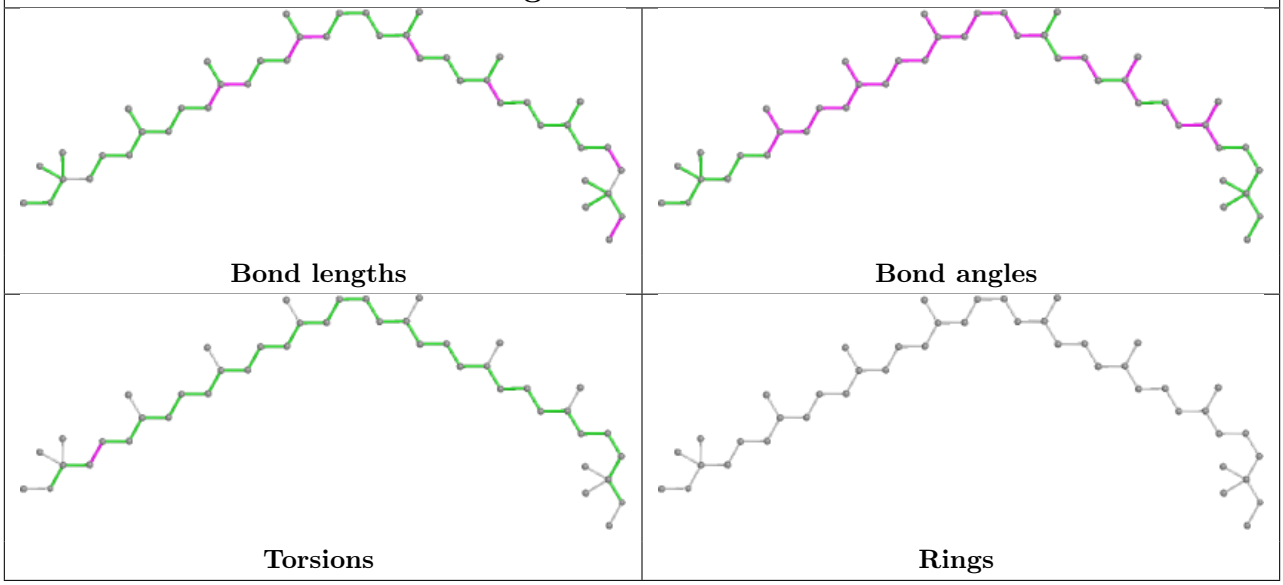
Ligand BCL 0 101



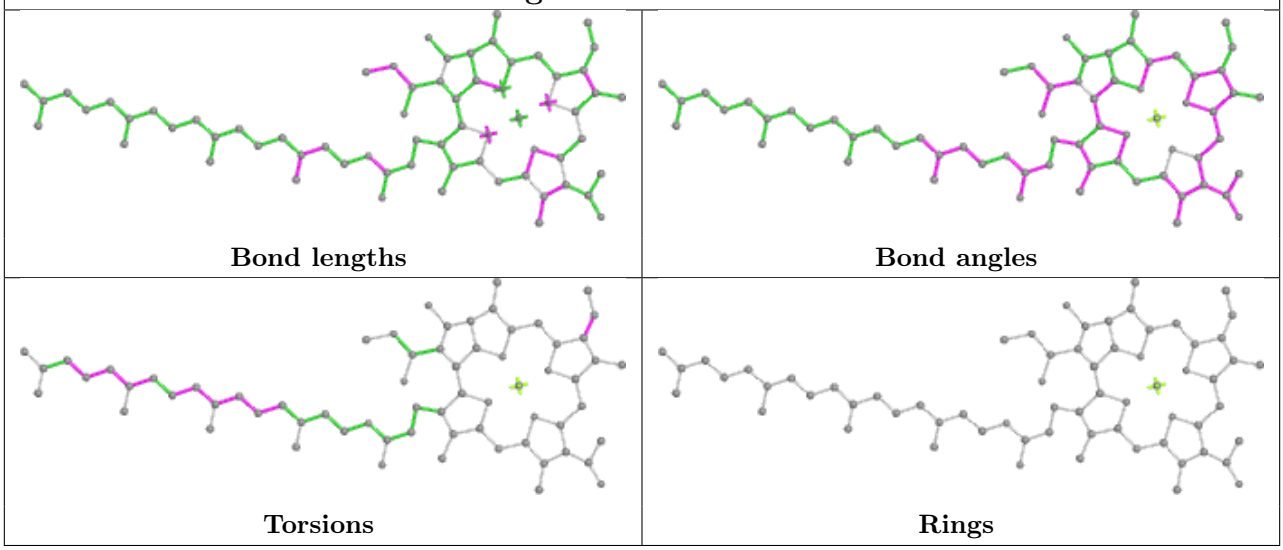
Ligand BCL M 401



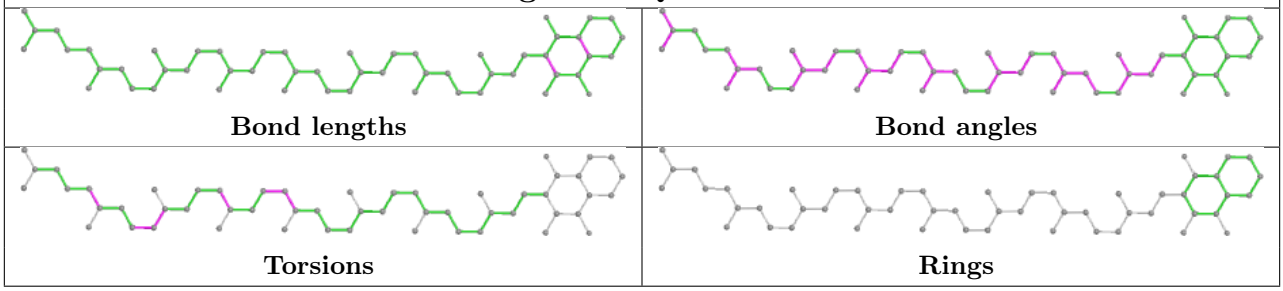
Ligand CRT G 102



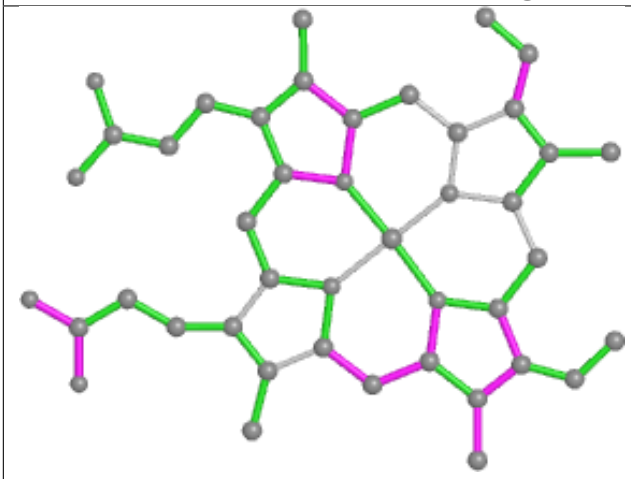
Ligand BCL Y 102



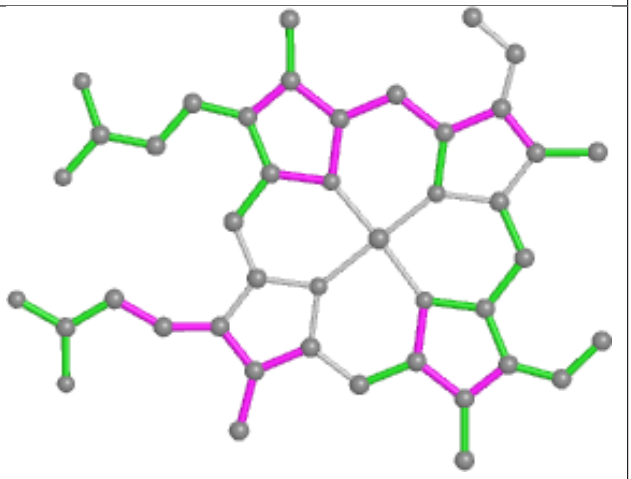
Ligand MQ8 M 405



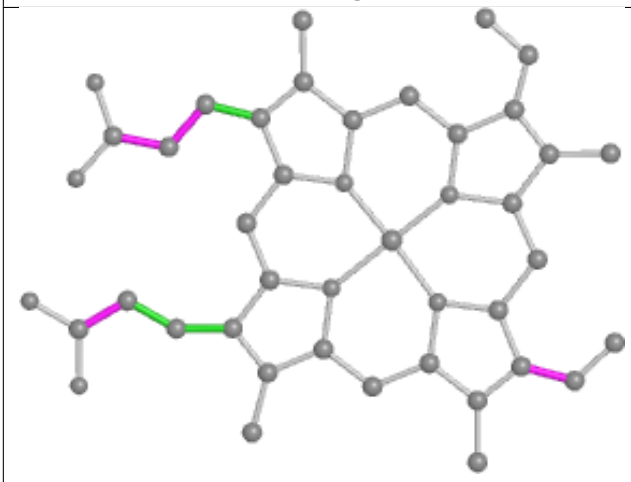
Ligand HEM C 502



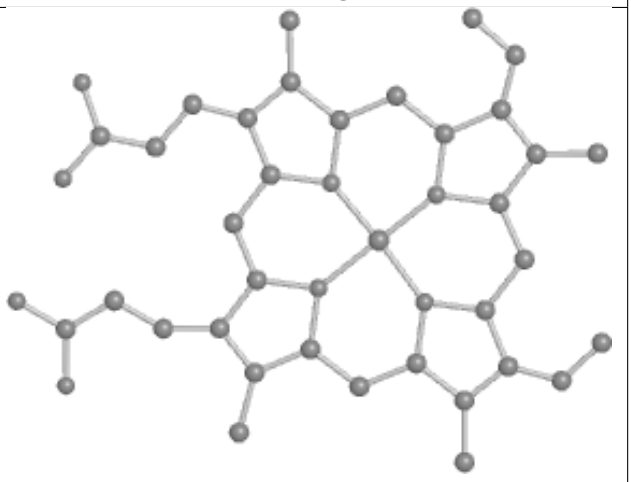
Bond lengths



Bond angles

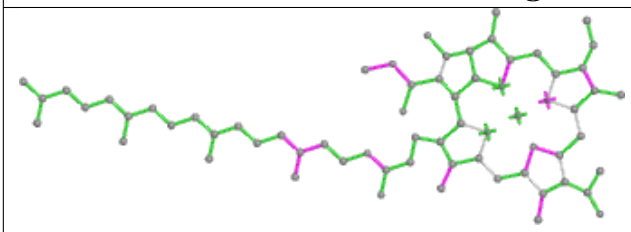


Torsions

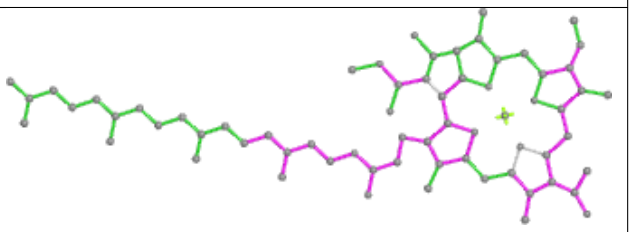


Rings

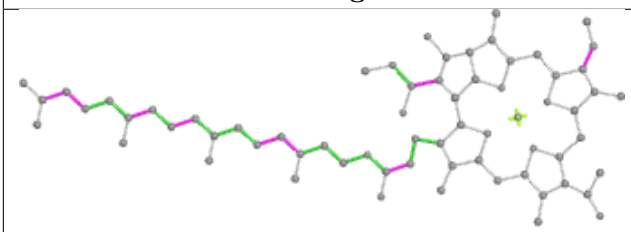
Ligand BCL X 101



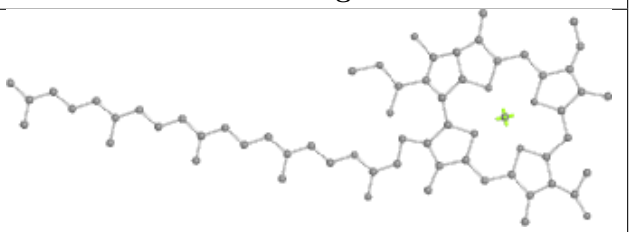
Bond lengths



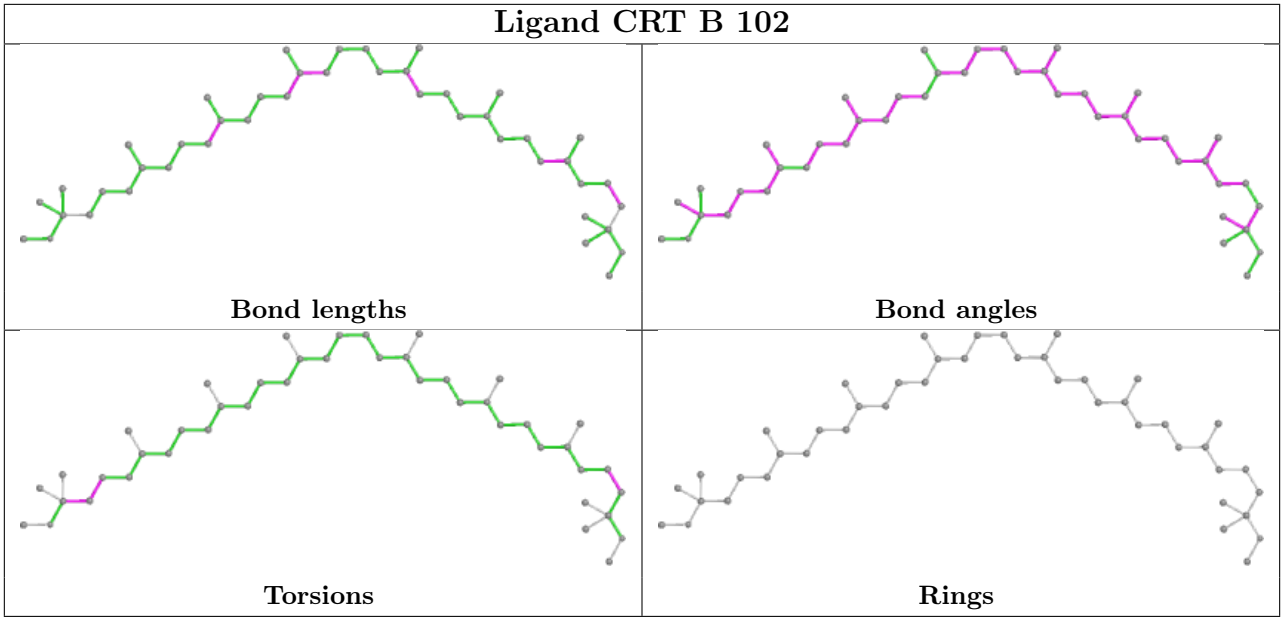
Bond angles

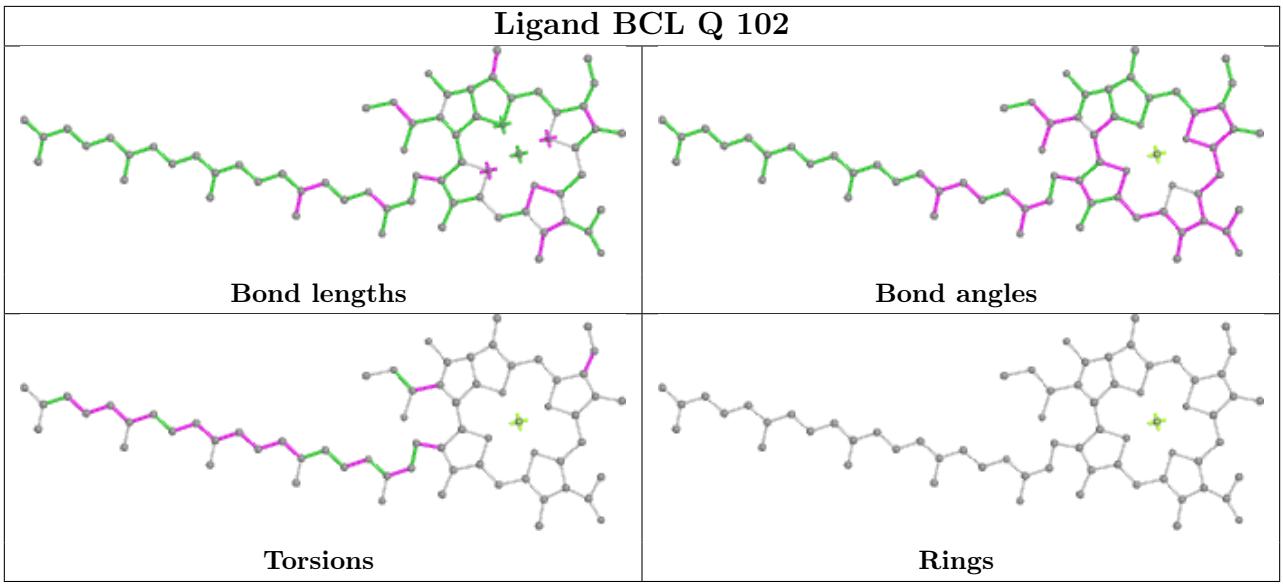


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	317/404 (78%)	0.03	16 (5%) 28 10	25, 67, 117, 142	1 (0%)
2	L	280/281 (99%)	-0.21	5 (1%) 68 40	15, 66, 102, 123	0
3	M	319/325 (98%)	-0.07	6 (1%) 66 37	32, 76, 115, 142	0
4	H	258/259 (99%)	0.21	19 (7%) 14 4	45, 89, 152, 198	0
5	1	60/61 (98%)	0.65	11 (18%) 1 0	62, 109, 257, 261	0
5	3	60/61 (98%)	0.45	6 (10%) 7 2	66, 137, 225, 231	0
5	5	60/61 (98%)	0.95	12 (20%) 1 0	82, 165, 250, 269	0
5	7	60/61 (98%)	0.87	12 (20%) 1 0	80, 149, 247, 254	0
5	9	60/61 (98%)	1.74	14 (23%) 0 0	74, 142, 282, 286	0
5	A	60/61 (98%)	1.18	15 (25%) 0 0	87, 147, 249, 250	0
5	D	60/61 (98%)	0.77	9 (15%) 2 1	86, 137, 260, 279	0
5	F	60/61 (98%)	1.17	12 (20%) 1 0	83, 178, 247, 256	0
5	I	60/61 (98%)	1.16	16 (26%) 0 0	81, 150, 244, 252	0
5	K	60/61 (98%)	1.32	20 (33%) 0 0	95, 155, 258, 259	0
5	O	60/61 (98%)	1.08	13 (21%) 0 0	84, 170, 249, 252	0
5	Q	60/61 (98%)	1.85	19 (31%) 0 0	105, 169, 257, 260	0
5	S	60/61 (98%)	1.20	14 (23%) 0 0	106, 167, 274, 278	0
5	U	60/61 (98%)	0.64	7 (11%) 4 1	80, 151, 265, 290	0
5	W	60/61 (98%)	0.47	6 (10%) 7 2	48, 114, 256, 264	0
5	Y	60/61 (98%)	1.07	10 (16%) 1 0	43, 105, 239, 258	0
6	0	40/47 (85%)	0.12	2 (5%) 28 10	112, 144, 199, 204	0
6	2	40/47 (85%)	0.19	3 (7%) 14 4	94, 117, 178, 181	0
6	4	40/47 (85%)	0.37	4 (10%) 7 2	100, 133, 177, 183	0
6	6	40/47 (85%)	-0.10	3 (7%) 14 4	104, 144, 171, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
6	8	40/47 (85%)	0.92	8 (20%) 1 0	107, 140, 180, 182	0
6	B	40/47 (85%)	0.34	5 (12%) 3 1	106, 141, 220, 242	0
6	E	40/47 (85%)	0.19	3 (7%) 14 4	108, 131, 156, 162	0
6	G	40/47 (85%)	0.38	6 (15%) 2 1	125, 155, 169, 179	0
6	J	40/47 (85%)	-0.19	0 100 100	124, 152, 204, 205	0
6	N	40/47 (85%)	0.37	4 (10%) 7 2	143, 160, 187, 195	0
6	P	40/47 (85%)	0.23	6 (15%) 2 1	136, 158, 179, 183	0
6	R	40/47 (85%)	0.47	6 (15%) 2 1	137, 176, 194, 197	0
6	T	40/47 (85%)	0.36	5 (12%) 3 1	141, 164, 209, 210	0
6	V	40/47 (85%)	0.04	3 (7%) 14 4	107, 141, 157, 160	0
6	X	40/47 (85%)	-0.18	0 100 100	80, 109, 154, 166	0
6	Z	40/47 (85%)	0.29	3 (7%) 14 4	60, 100, 182, 189	0
All	All	2774/2997 (92%)	0.41	303 (10%) 5 2	15, 109, 237, 290	1 (0%)

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	9	57	ALA	13.4
5	Y	5	ASN	11.9
5	Y	4	MET	11.6
5	Y	2	PHE	11.3
5	9	61	LYS	10.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} 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	O	101	1/1	0.13	0.40	167,167,167,167	0
15	CRT	A	101	44/44	0.28	0.91	100,120,180,182	0
8	CA	Q	101	1/1	0.33	0.16	159,159,159,159	0
8	CA	7	101	1/1	0.37	0.07	161,161,161,161	0
15	CRT	B	102	44/44	0.39	0.98	125,143,171,171	0
15	CRT	J	101	44/44	0.40	0.89	133,168,197,198	0
8	CA	U	101	1/1	0.41	0.08	125,125,125,125	0
15	CRT	8	101	44/44	0.41	0.84	138,179,215,216	0
15	CRT	2	102	44/44	0.43	1.11	110,160,199,221	0
8	CA	F	101	1/1	0.46	0.24	157,157,157,157	0
15	CRT	A	103	44/44	0.46	0.89	169,184,188,189	0
15	CRT	P	102	44/44	0.51	0.80	187,222,226,227	0
15	CRT	3	103	44/44	0.56	0.71	116,145,185,187	0
15	CRT	G	102	44/44	0.58	0.82	138,158,216,217	0
15	CRT	T	102	44/44	0.62	1.14	136,158,177,178	0
15	CRT	R	102	44/44	0.63	0.48	89,127,136,137	0
15	CRT	N	102	44/44	0.63	0.66	151,161,169,169	0
15	CRT	X	102	44/44	0.63	1.18	131,163,207,207	0
15	CRT	4	102	44/44	0.66	0.76	107,121,188,189	0
15	CRT	V	102	44/44	0.67	0.52	76,133,176,179	0
8	CA	W	101	1/1	0.67	0.09	118,118,118,118	0
8	CA	I	101	1/1	0.68	0.33	158,158,158,158	0
15	CRT	W	103	44/44	0.69	0.64	77,126,154,155	0
8	CA	K	101	1/1	0.73	0.18	152,152,152,152	0
11	UQ8	L	304	53/53	0.74	0.59	84,134,142,144	0
16	PGW	M	407	21/51	0.74	0.30	65,132,182,186	0
13	FE	M	404	1/1	0.75	0.15	127,127,127,127	0
8	CA	3	101	1/1	0.75	0.21	113,113,113,113	0
8	CA	5	101	1/1	0.77	0.34	141,141,141,141	0
9	BCL	6	101	66/66	0.80	0.39	105,119,198,199	0
14	MQ8	M	405	53/53	0.81	0.40	27,87,158,160	0
15	CRT	M	406	44/44	0.82	0.38	71,78,104,107	0
8	CA	D	101	1/1	0.82	0.12	142,142,142,142	0
16	PGW	H	302	21/51	0.83	0.32	64,102,145,160	0
9	BCL	R	101	66/66	0.84	0.36	115,128,228,230	0
9	BCL	D	102	66/66	0.85	0.33	120,130,197,203	0
9	BCL	7	102	66/66	0.85	0.34	86,93,190,193	0
9	BCL	B	101	66/66	0.85	0.37	104,120,212,217	0
12	PO4	H	303	5/5	0.86	0.19	112,113,126,128	0
9	BCL	9	102	66/66	0.87	0.27	122,129,145,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	G	101	66/66	0.87	0.29	110,123,217,218	0
9	BCL	A	102	66/66	0.87	0.35	123,129,202,205	0
9	BCL	E	101	66/66	0.88	0.31	95,109,168,172	0
9	BCL	K	102	66/66	0.89	0.32	120,127,226,229	0
9	BCL	7	103	66/66	0.89	0.32	76,89,176,183	0
9	BCL	O	102	66/66	0.89	0.33	81,93,159,165	0
10	BPH	L	302	65/65	0.89	0.26	55,64,75,82	0
9	BCL	F	102	66/66	0.89	0.32	102,112,154,155	0
9	BCL	X	101	66/66	0.89	0.33	68,86,200,202	0
9	BCL	2	101	66/66	0.89	0.32	81,102,191,196	0
9	BCL	3	102	66/66	0.89	0.27	71,81,147,153	0
9	BCL	I	102	66/66	0.89	0.26	79,89,147,149	0
17	PEF	H	301	19/47	0.89	0.31	75,105,128,134	0
9	BCL	P	101	66/66	0.90	0.27	69,83,204,210	0
9	BCL	I	103	66/66	0.90	0.32	96,117,201,205	0
9	BCL	V	101	66/66	0.90	0.28	80,97,189,205	0
8	CA	9	101	1/1	0.90	0.03	124,124,124,124	0
9	BCL	Y	102	66/66	0.90	0.32	48,61,172,173	0
9	BCL	Z	101	66/66	0.90	0.29	59,71,165,167	0
12	PO4	M	408	5/5	0.90	0.18	106,119,123,135	0
9	BCL	N	101	66/66	0.90	0.24	101,123,189,191	0
8	CA	A	104	1/1	0.90	0.34	185,185,185,185	0
9	BCL	4	101	66/66	0.90	0.27	72,101,222,225	0
9	BCL	Q	102	66/66	0.91	0.32	108,115,183,188	0
9	BCL	0	101	66/66	0.91	0.29	76,101,202,207	0
9	BCL	W	102	66/66	0.91	0.29	47,69,182,185	0
9	BCL	5	102	66/66	0.91	0.34	124,134,210,214	0
9	BCL	L	303	66/66	0.92	0.22	20,53,66,82	0
12	PO4	H	304	5/5	0.92	0.33	130,131,142,148	0
9	BCL	S	102	66/66	0.92	0.27	98,112,174,177	0
9	BCL	U	102	66/66	0.92	0.39	64,119,243,246	0
9	BCL	M	401	66/66	0.92	0.23	40,55,106,109	0
8	CA	S	101	1/1	0.92	0.15	154,154,154,154	0
10	BPH	M	403	65/65	0.93	0.20	43,59,137,144	0
9	BCL	T	101	66/66	0.93	0.25	53,88,229,234	0
9	BCL	1	102	66/66	0.93	0.32	62,74,153,162	0
7	HEM	C	503	43/43	0.94	0.28	56,67,85,91	0
7	HEM	C	504	43/43	0.94	0.22	43,52,64,74	0
12	PO4	L	305	5/5	0.94	0.14	84,104,111,116	0
9	BCL	M	402	66/66	0.94	0.22	28,43,60,64	0
7	HEM	C	501	43/43	0.94	0.19	54,64,73,75	0
8	CA	Y	101	1/1	0.94	0.10	79,79,79,79	0

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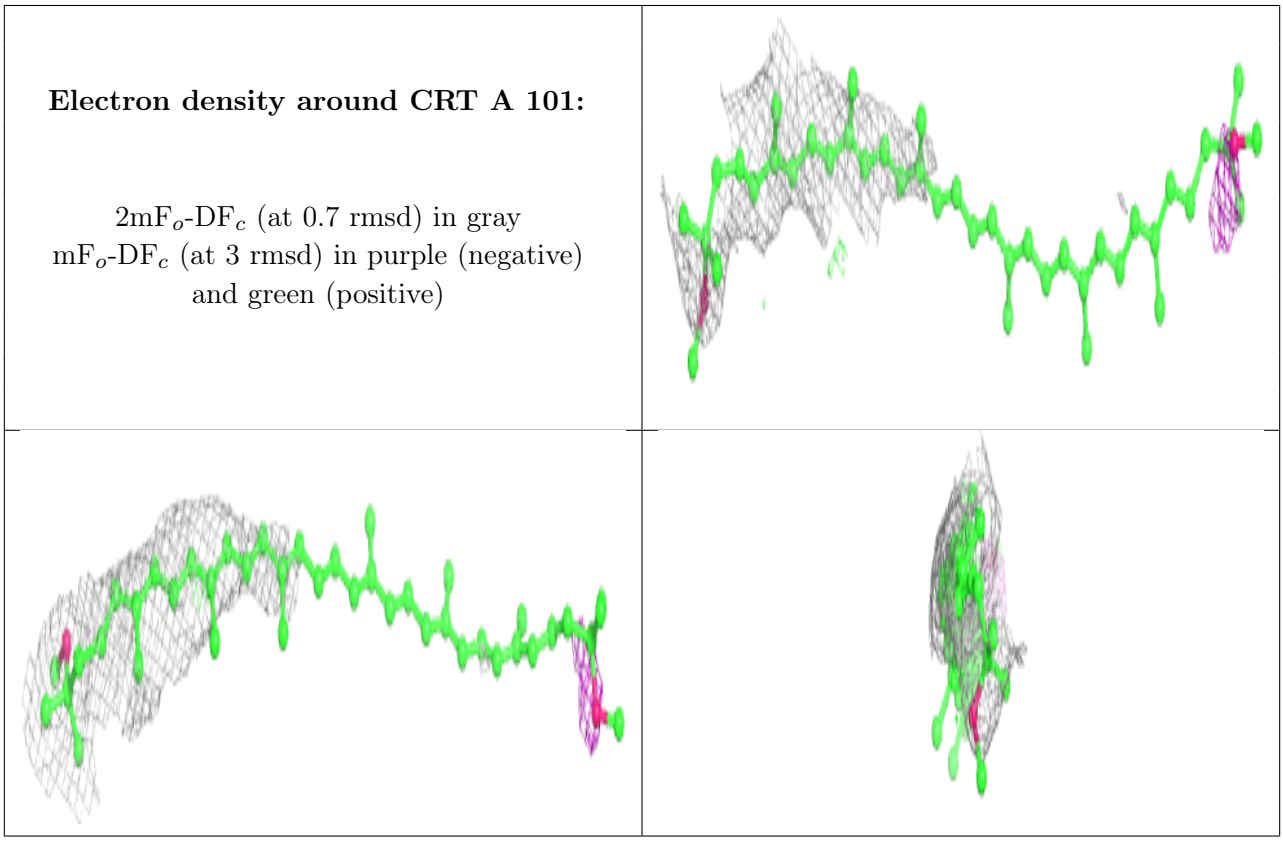
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	L	301	66/66	0.94	0.18	10,45,66,69	0
7	HEM	C	502	43/43	0.95	0.20	41,49,59,64	0
8	CA	C	505	1/1	0.95	0.23	93,93,93,93	0
8	CA	1	101	1/1	0.96	0.12	92,92,92,92	0

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.

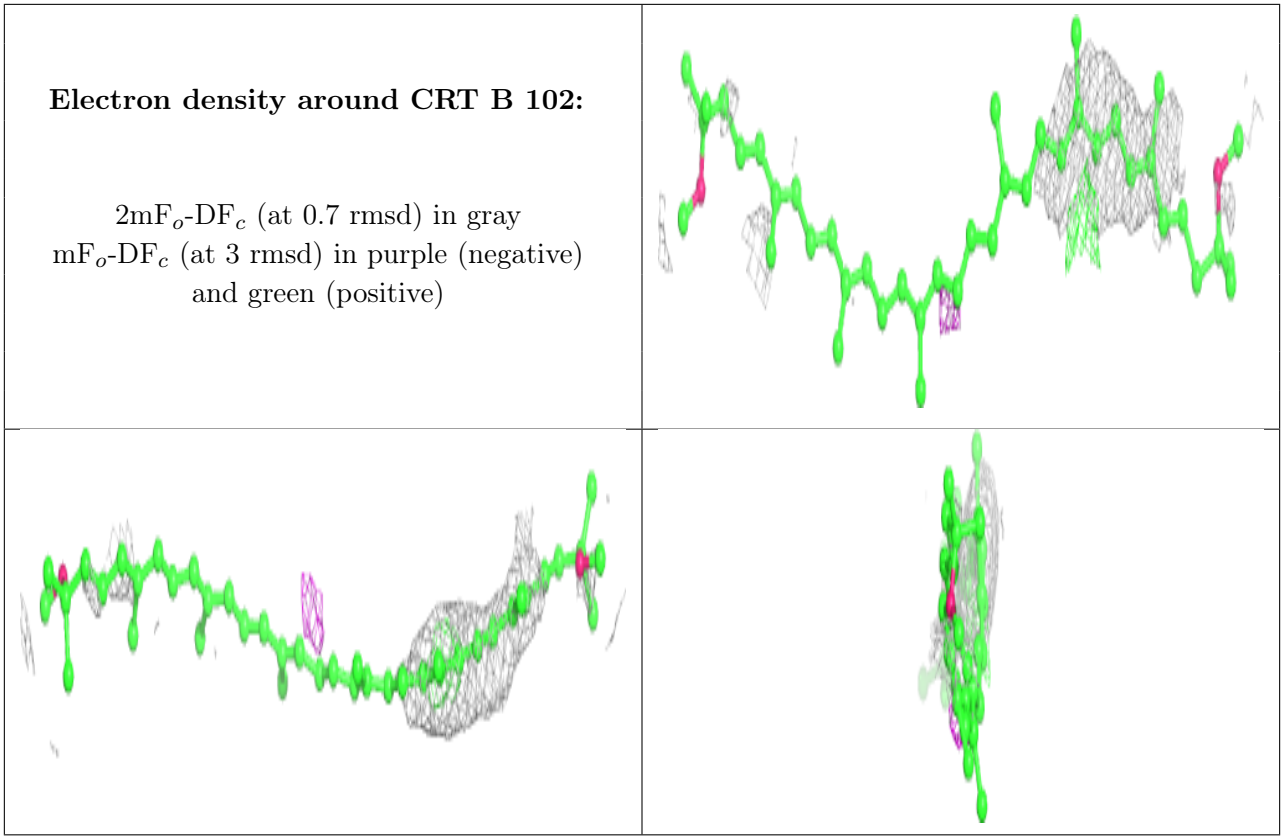
Electron density around CRT A 101:

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



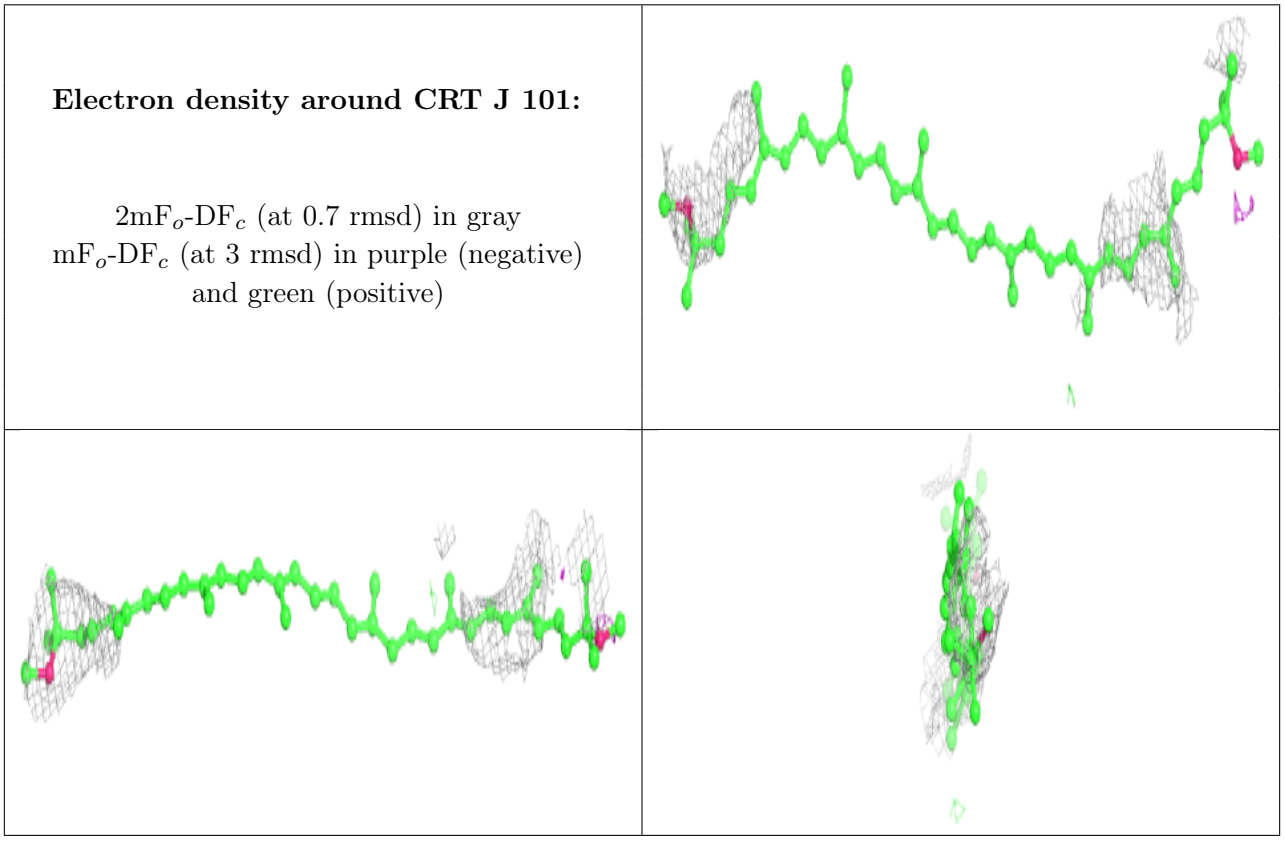
Electron density around CRT B 102:

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



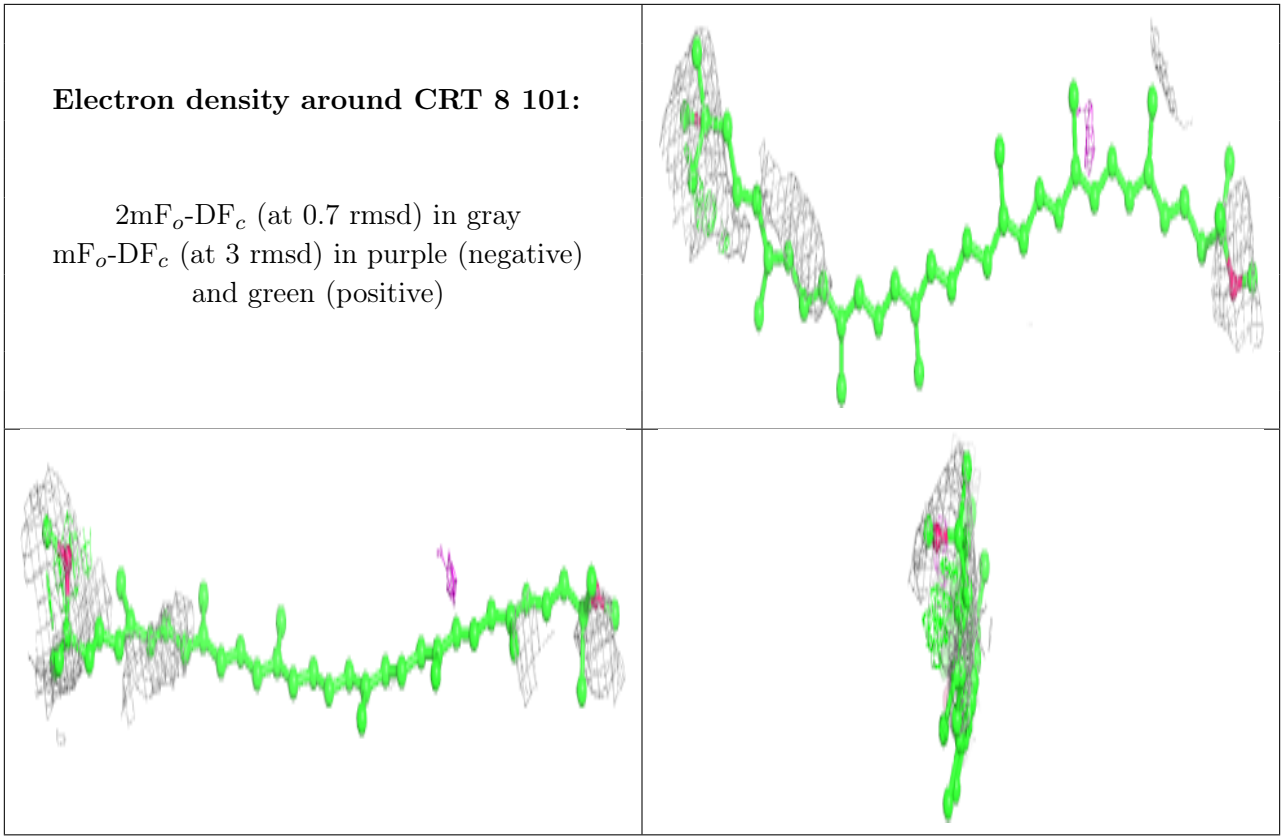
Electron density around CRT J 101:

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



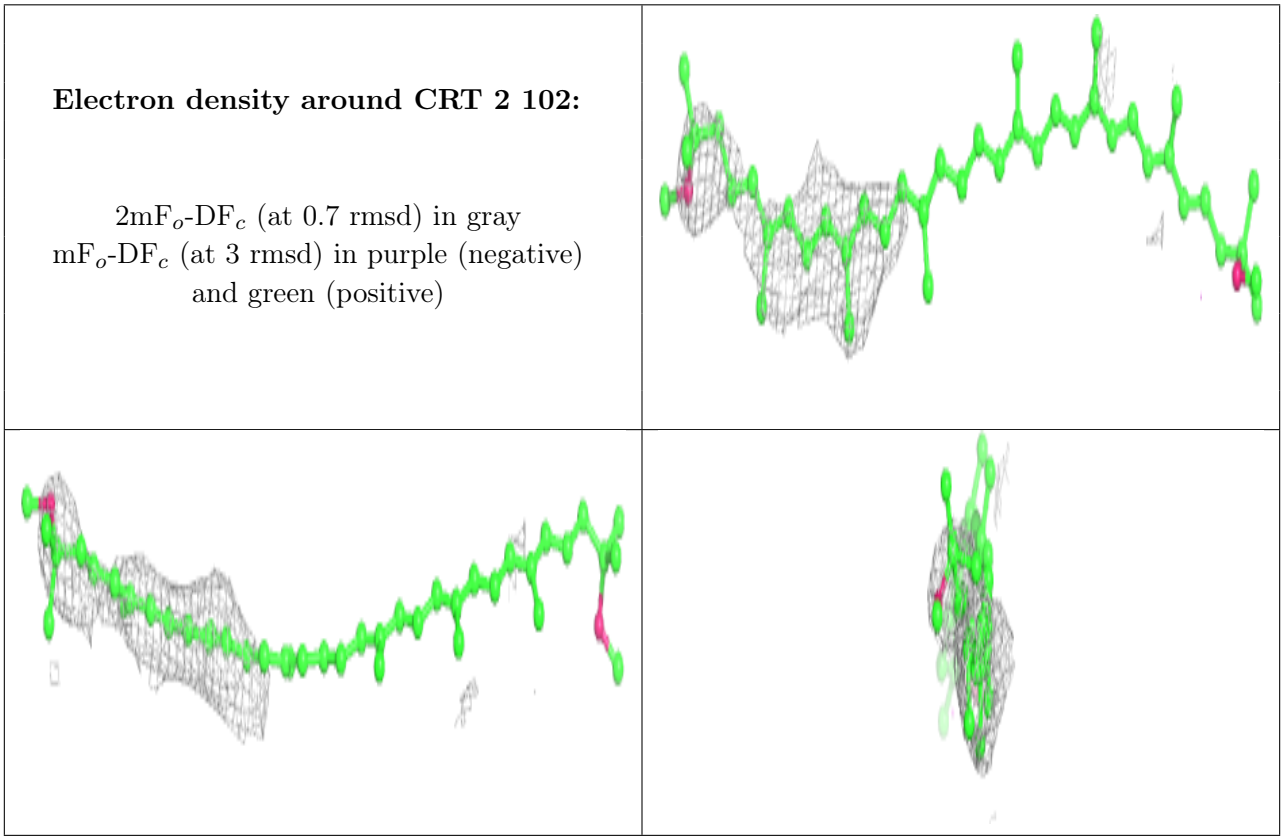
Electron density around CRT 8 101:

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



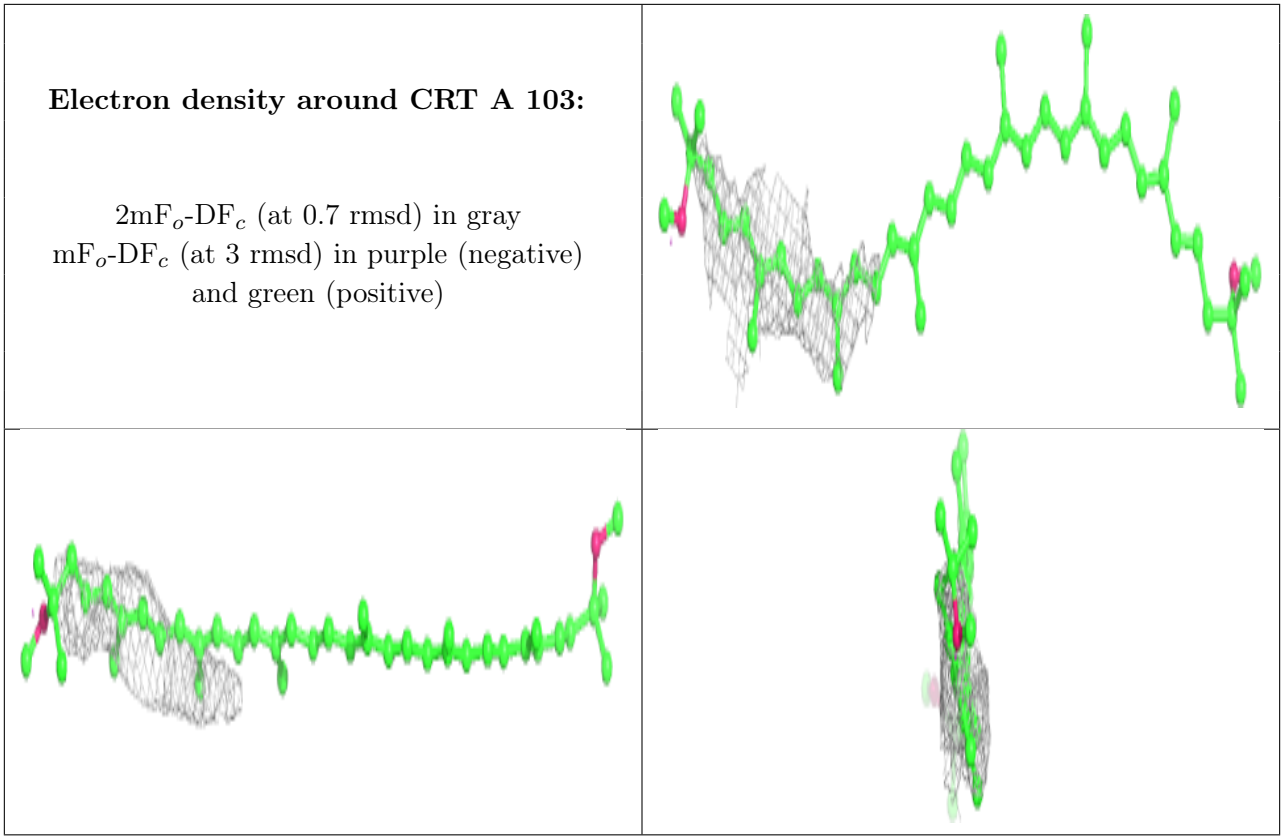
Electron density around CRT 2 102:

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



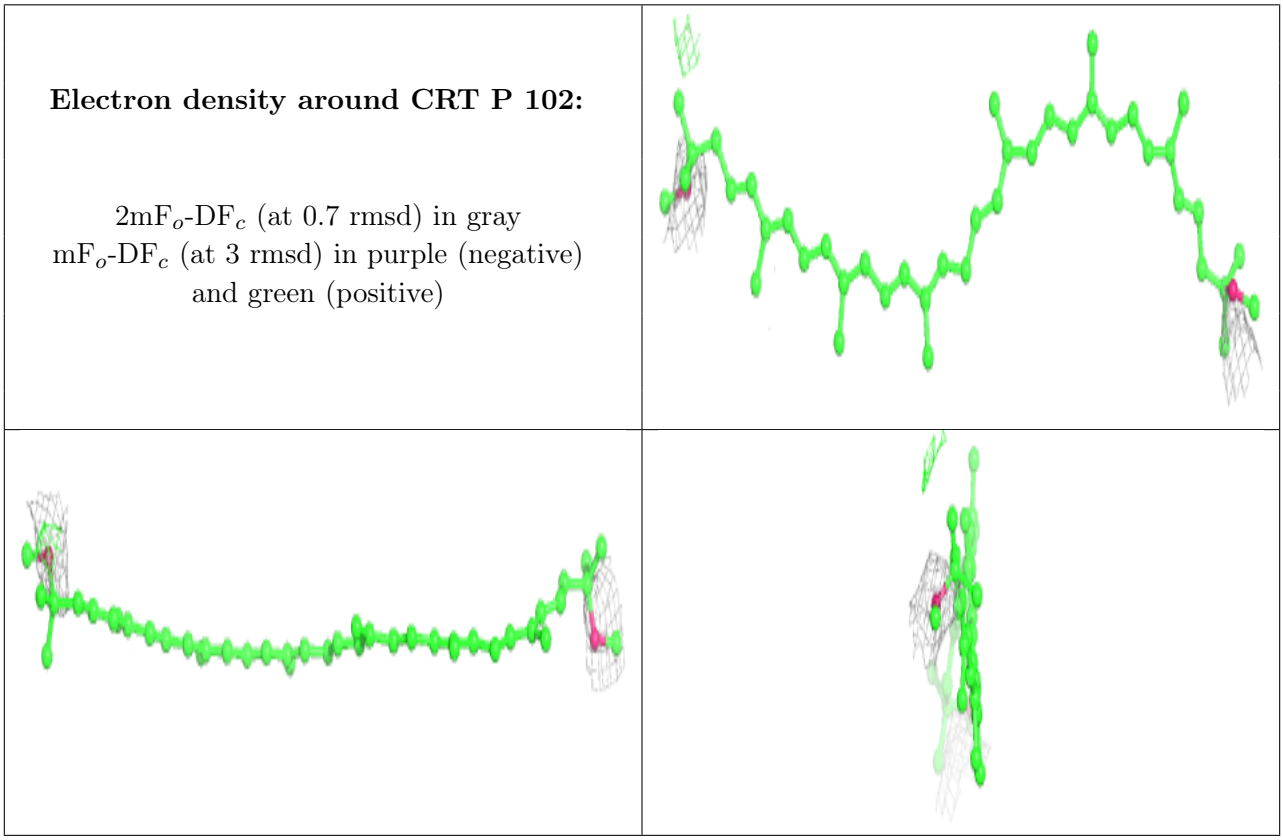
Electron density around CRT A 103:

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



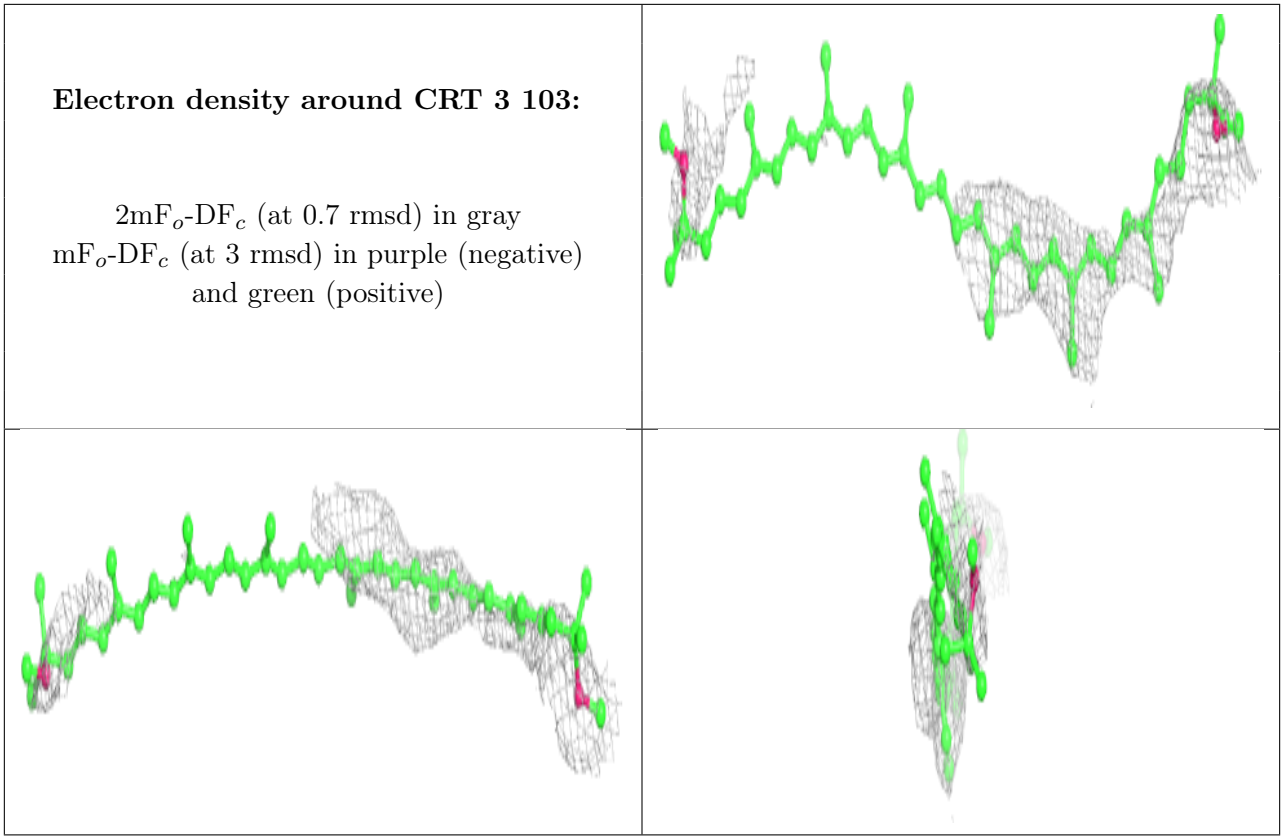
Electron density around CRT P 102:

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



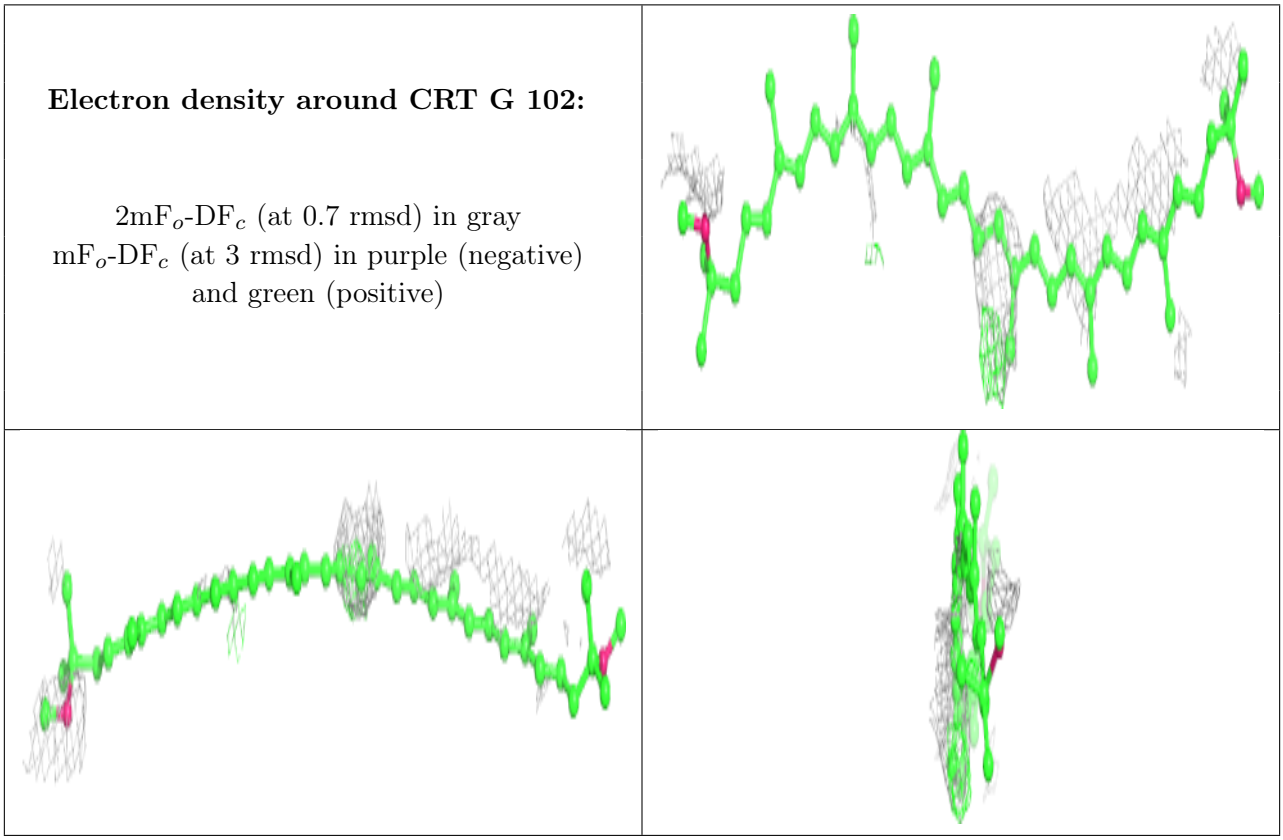
Electron density around CRT 3 103:

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



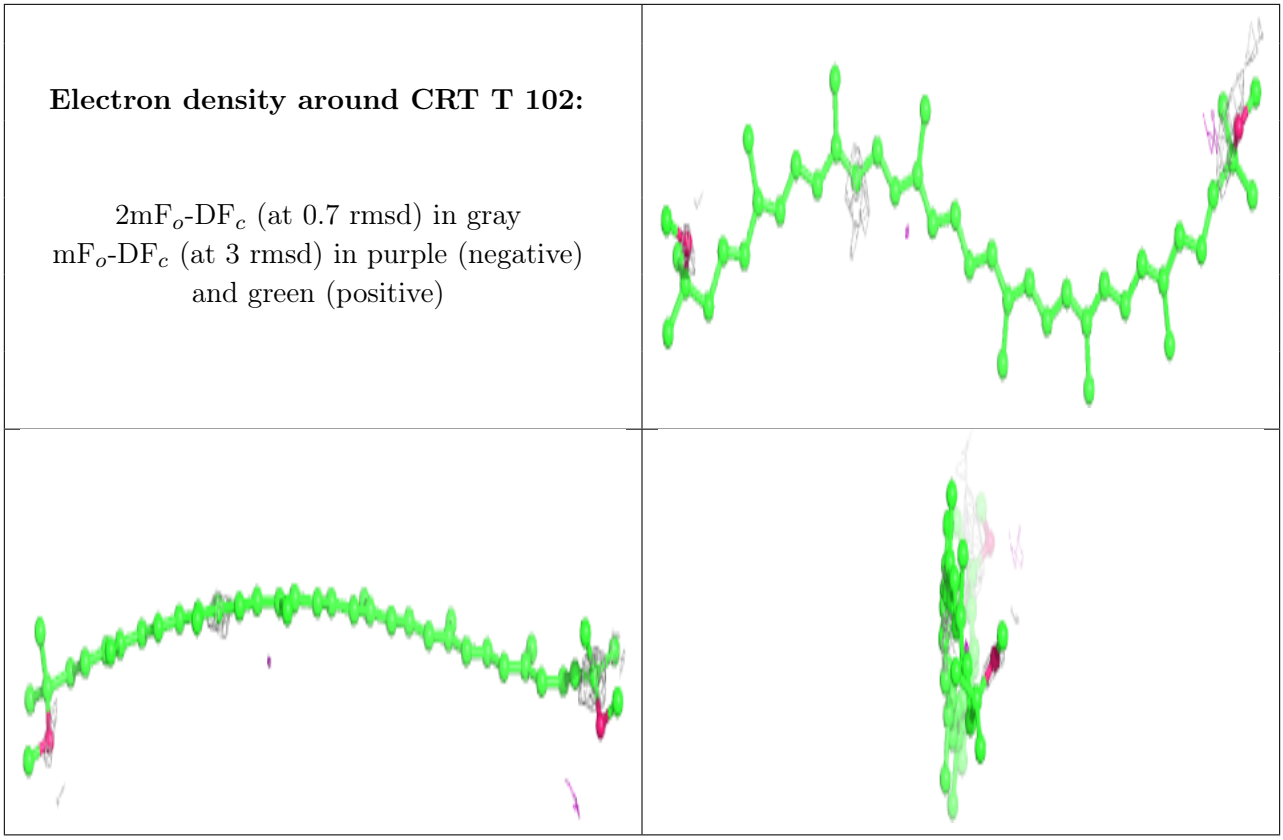
Electron density around CRT G 102:

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



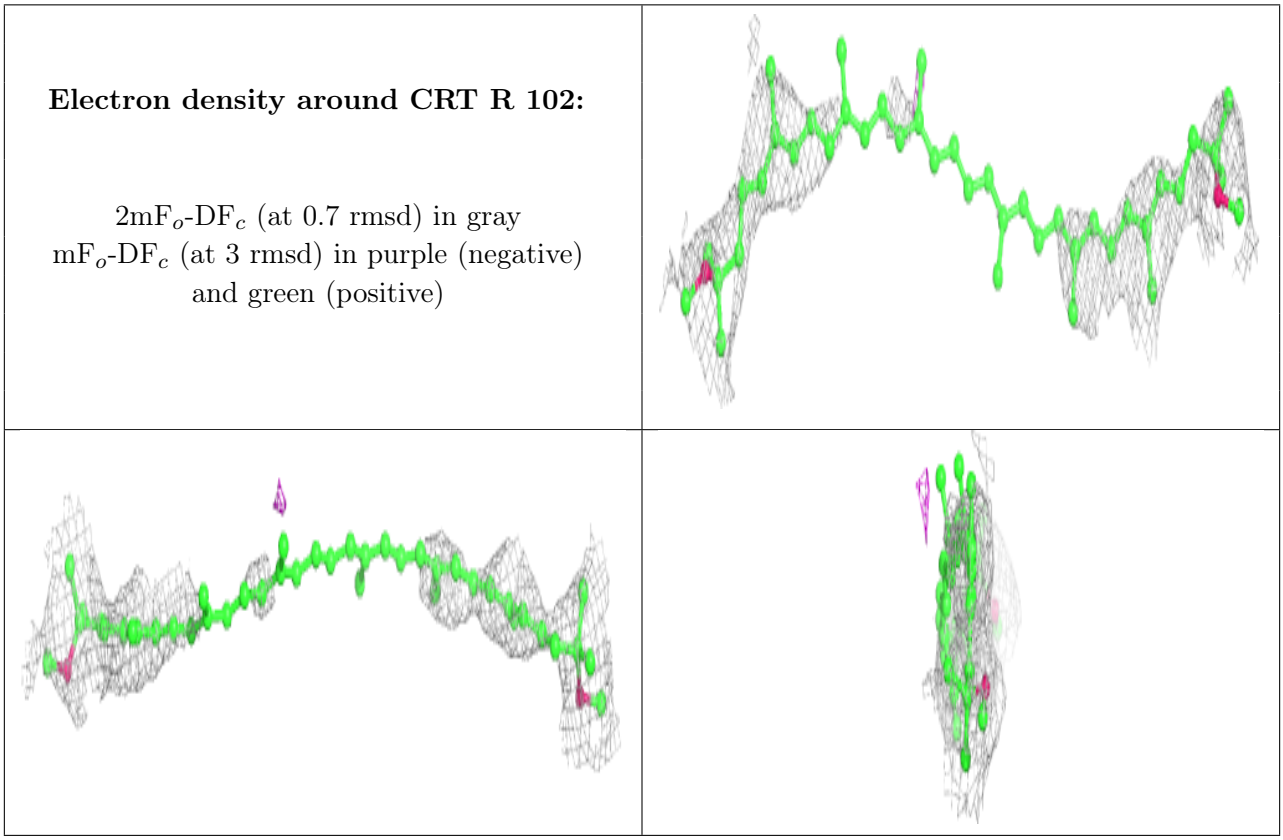
Electron density around CRT T 102:

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



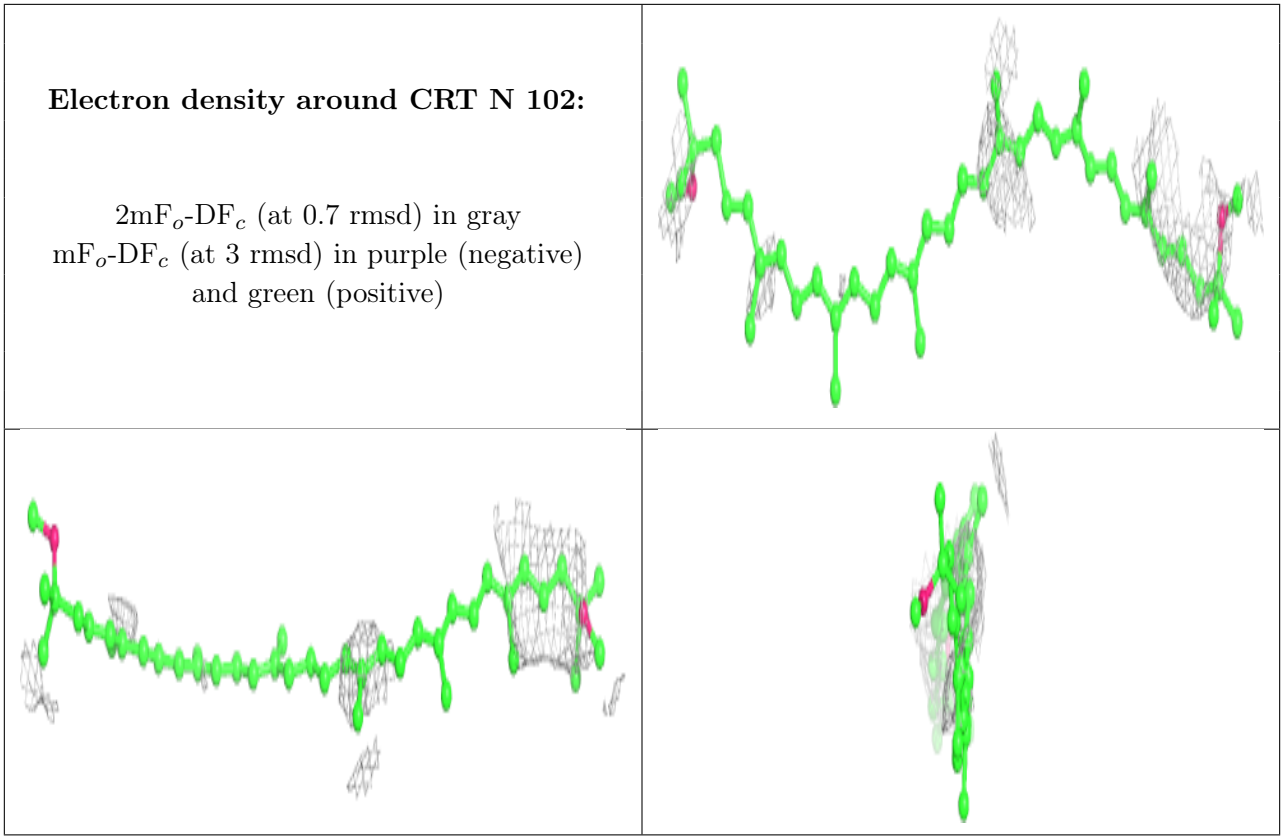
Electron density around CRT R 102:

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



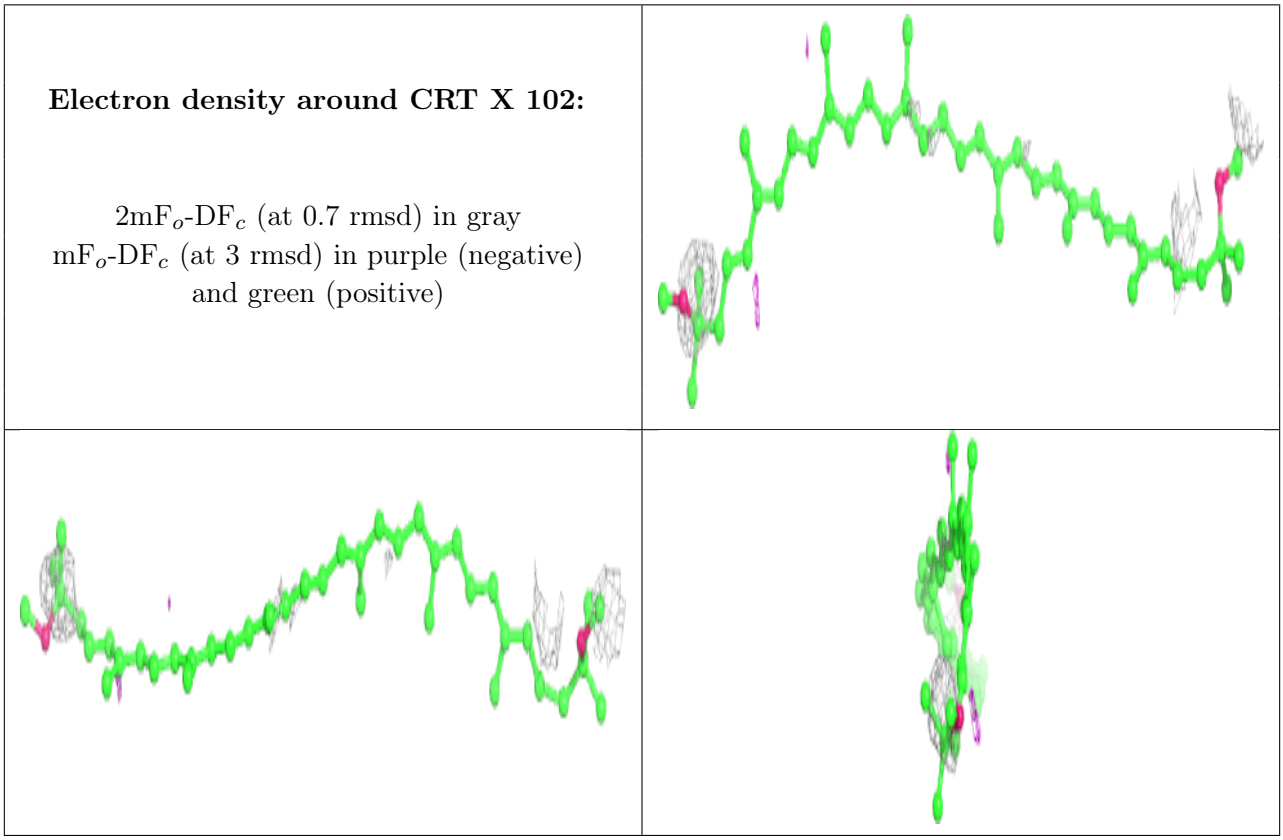
Electron density around CRT N 102:

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



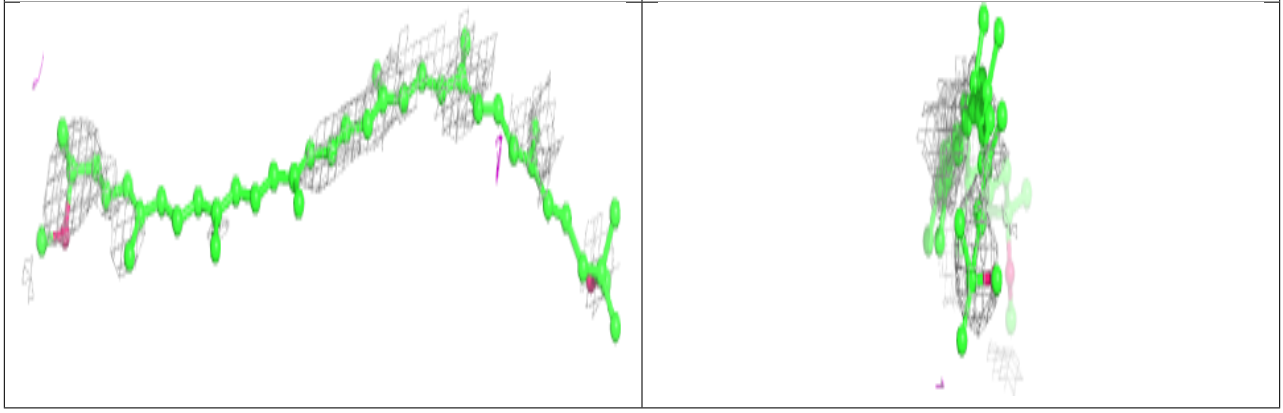
Electron density around CRT X 102:

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



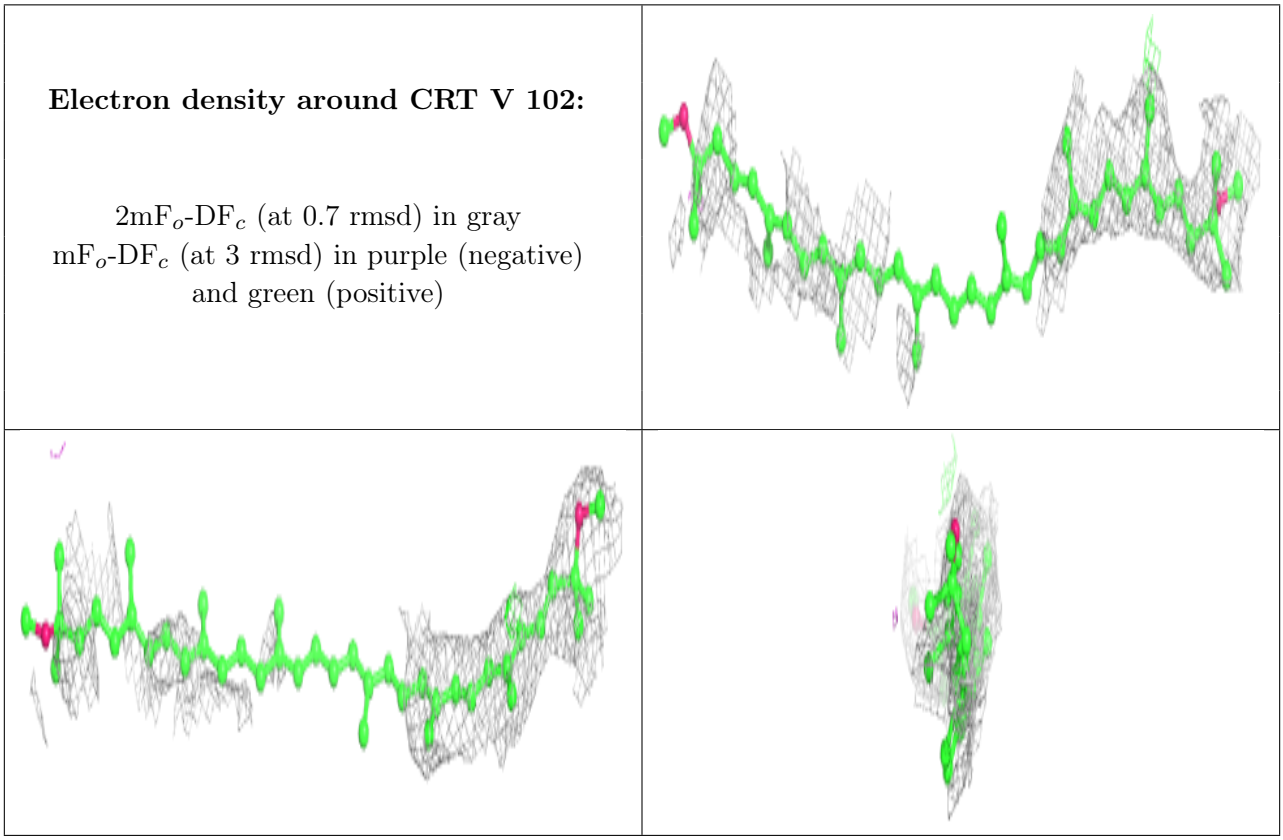
Electron density around CRT 4 102:

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



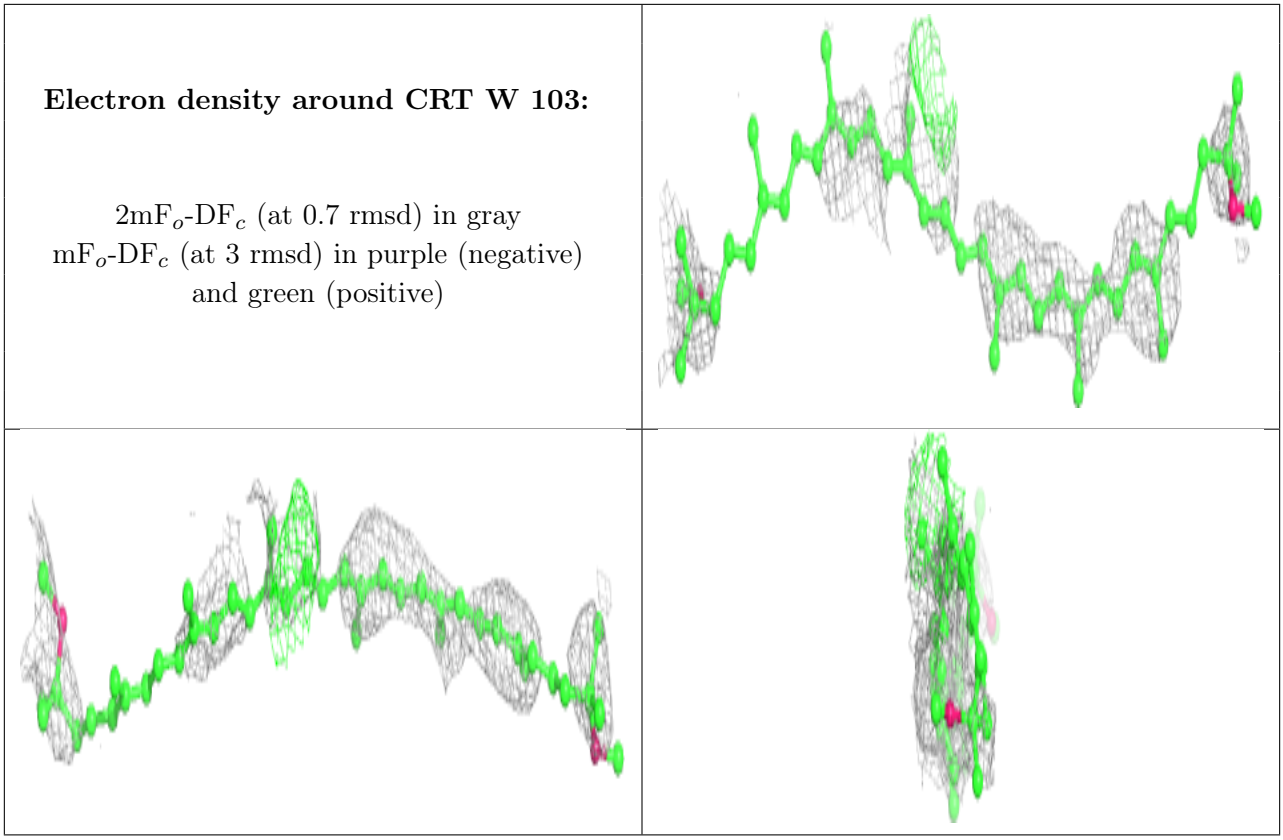
Electron density around CRT V 102:

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



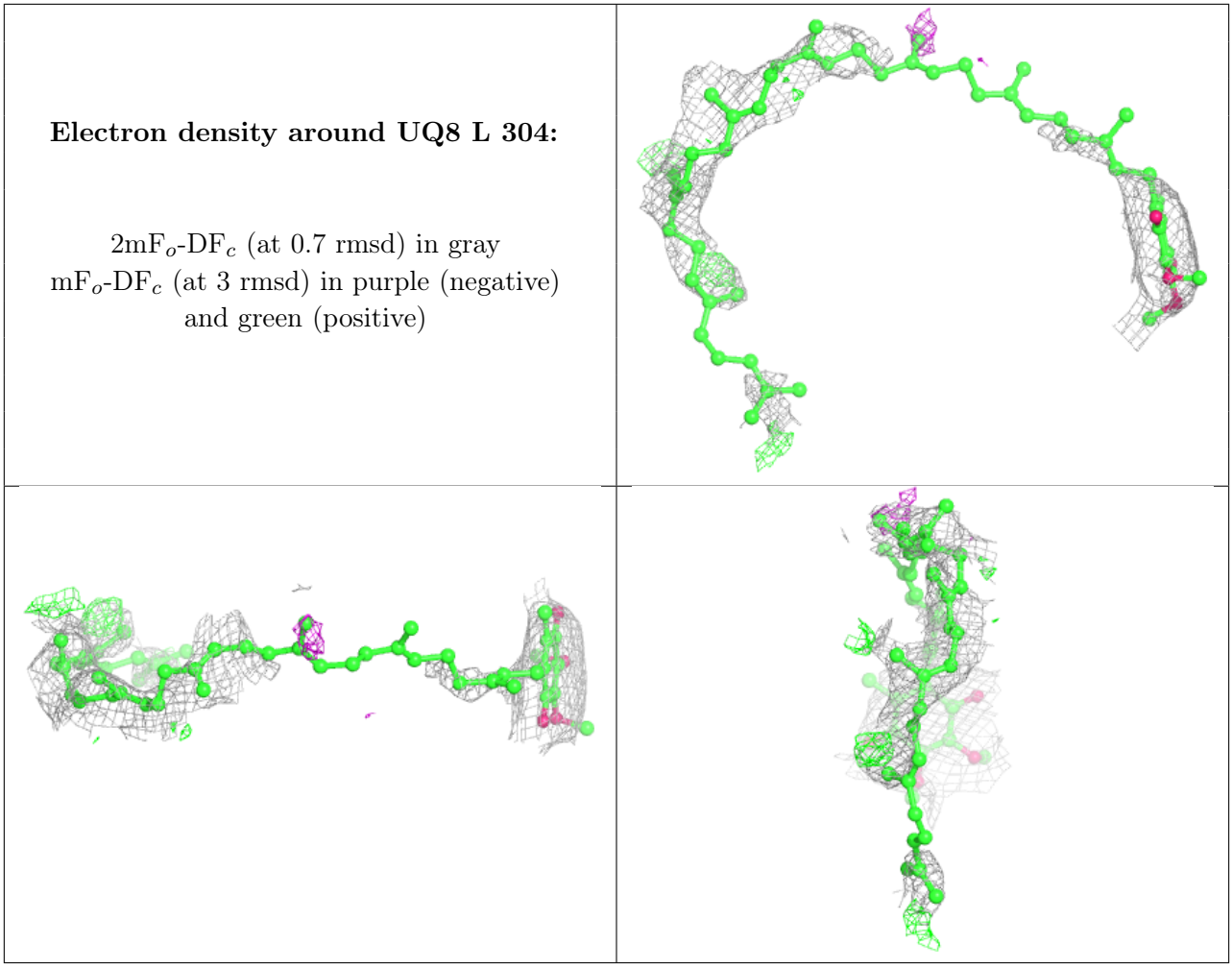
Electron density around CRT W 103:

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



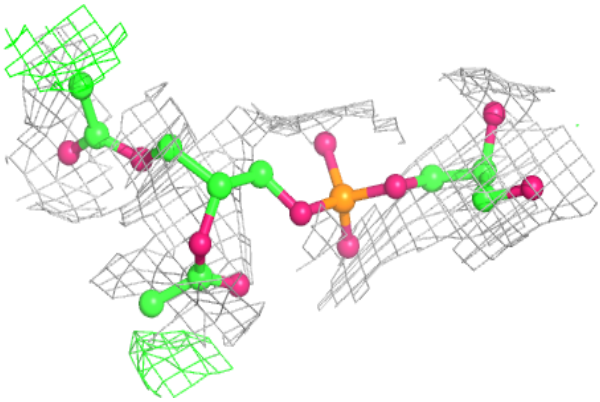
Electron density around UQ8 L 304:

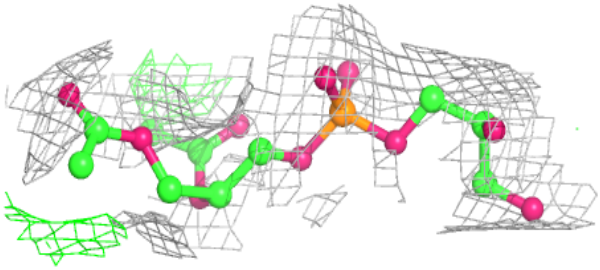
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

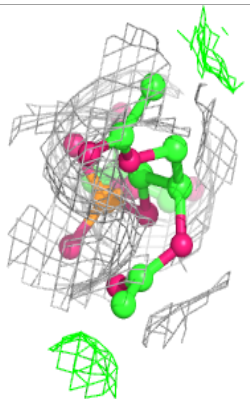


Electron density around PGW M 407:

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

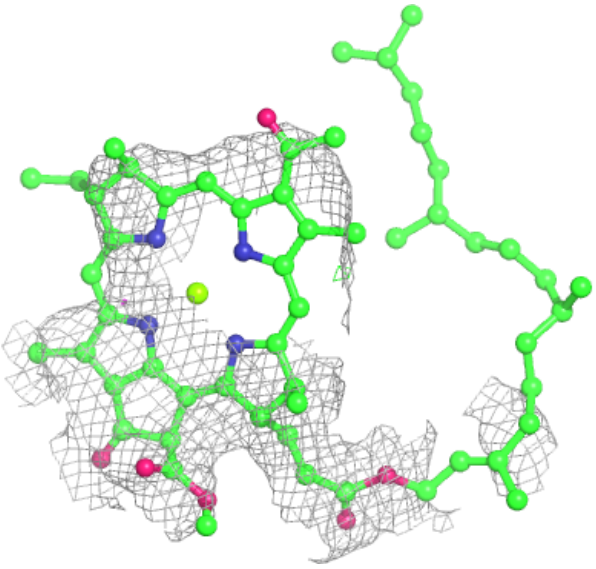


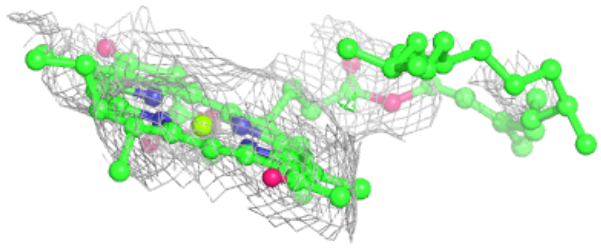


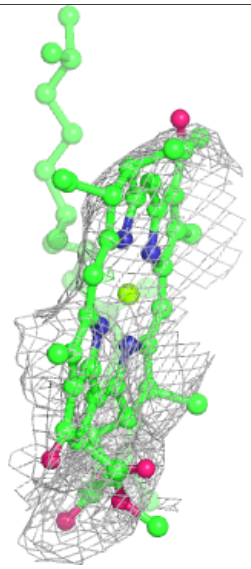


Electron density around BCL 6 101:

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

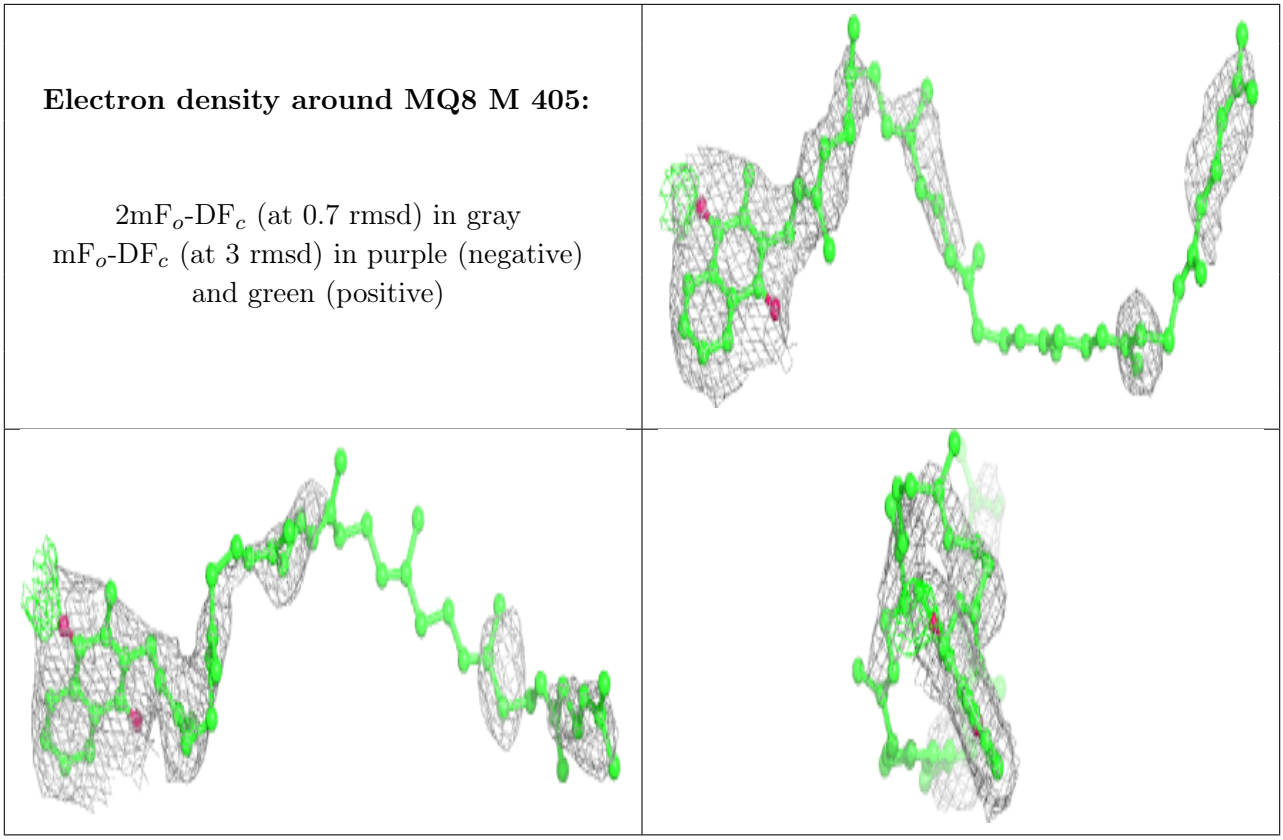






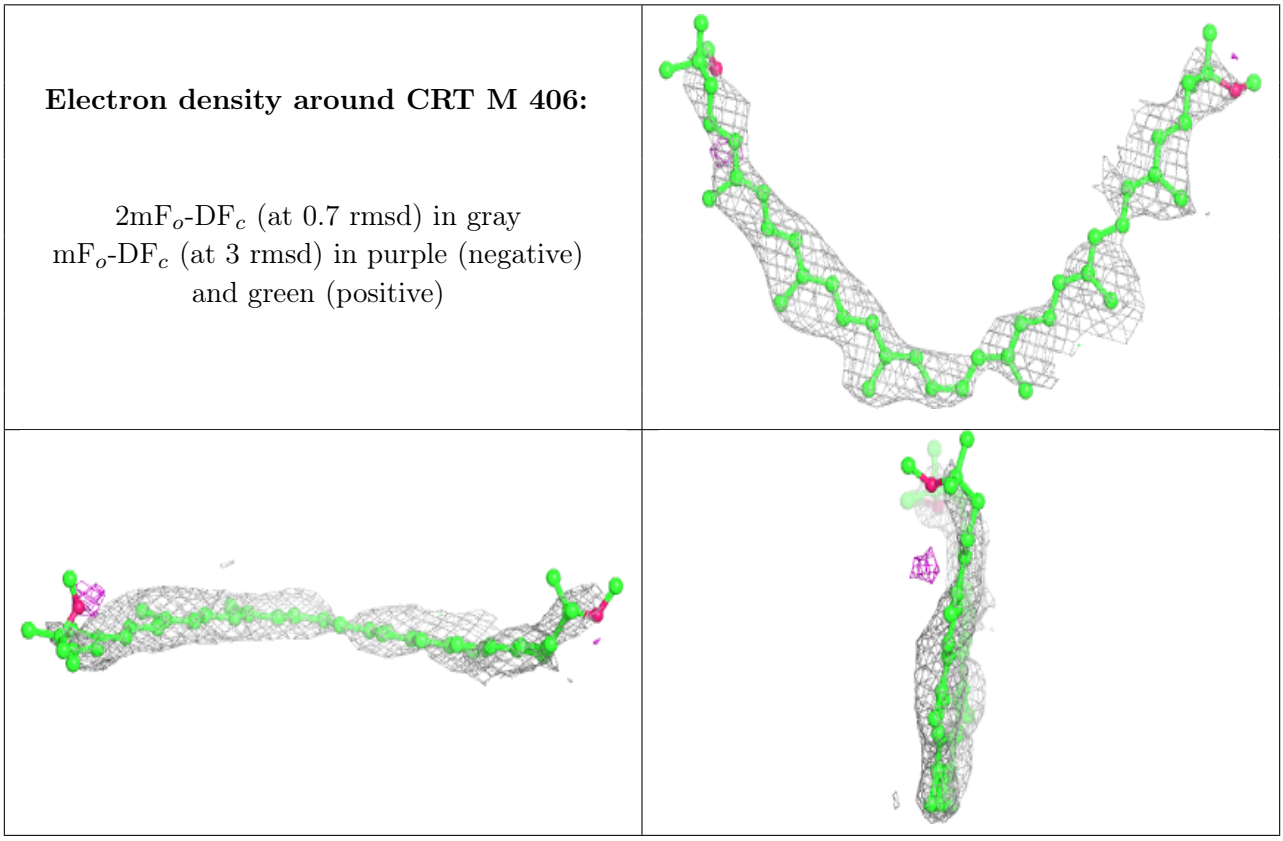
Electron density around MQ8 M 405:

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



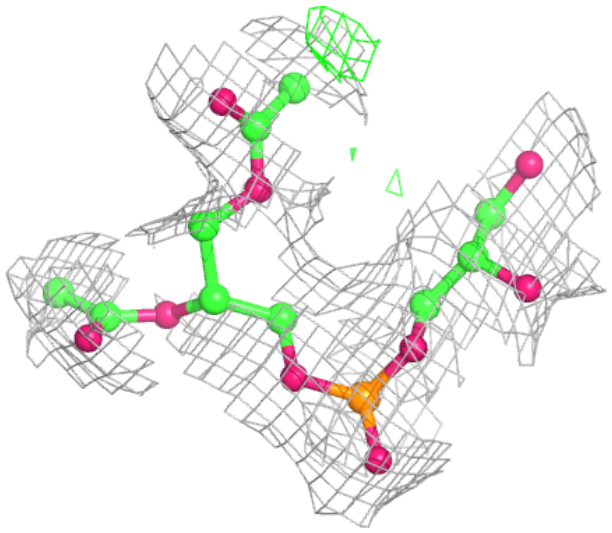
Electron density around CRT M 406:

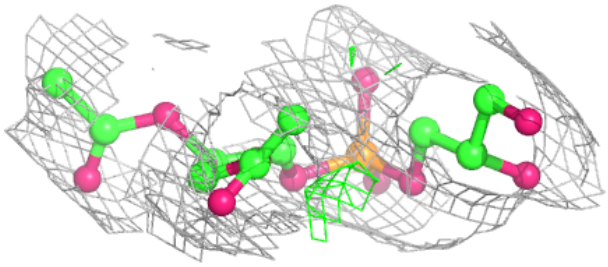
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

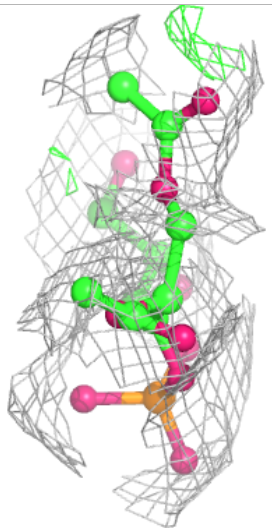


Electron density around PGW H 302:

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

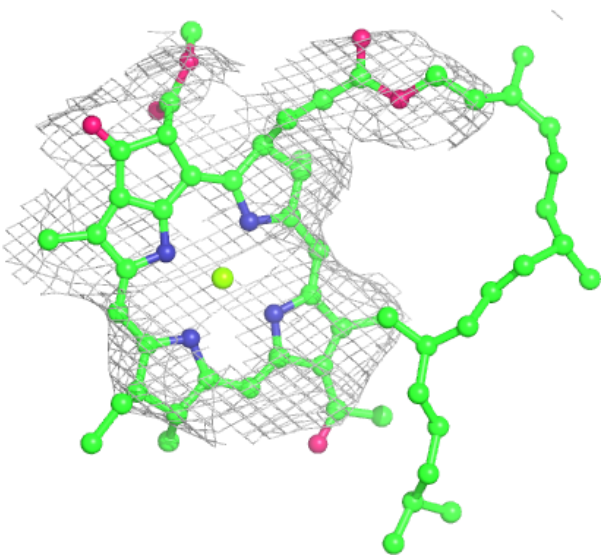


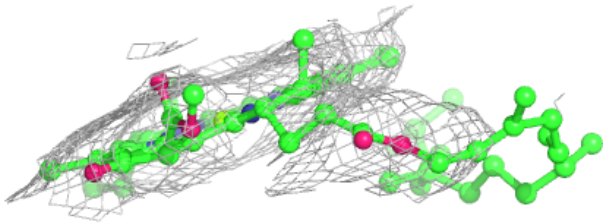


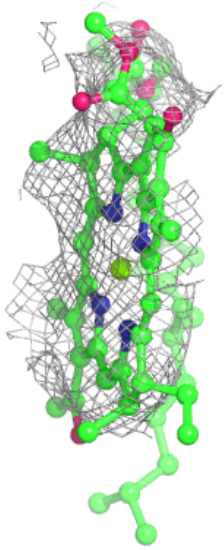


Electron density around BCL R 101:

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

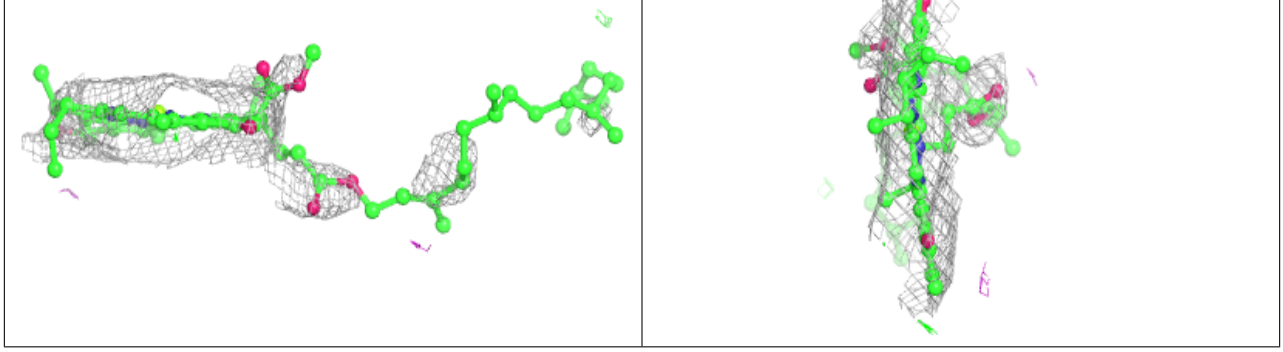






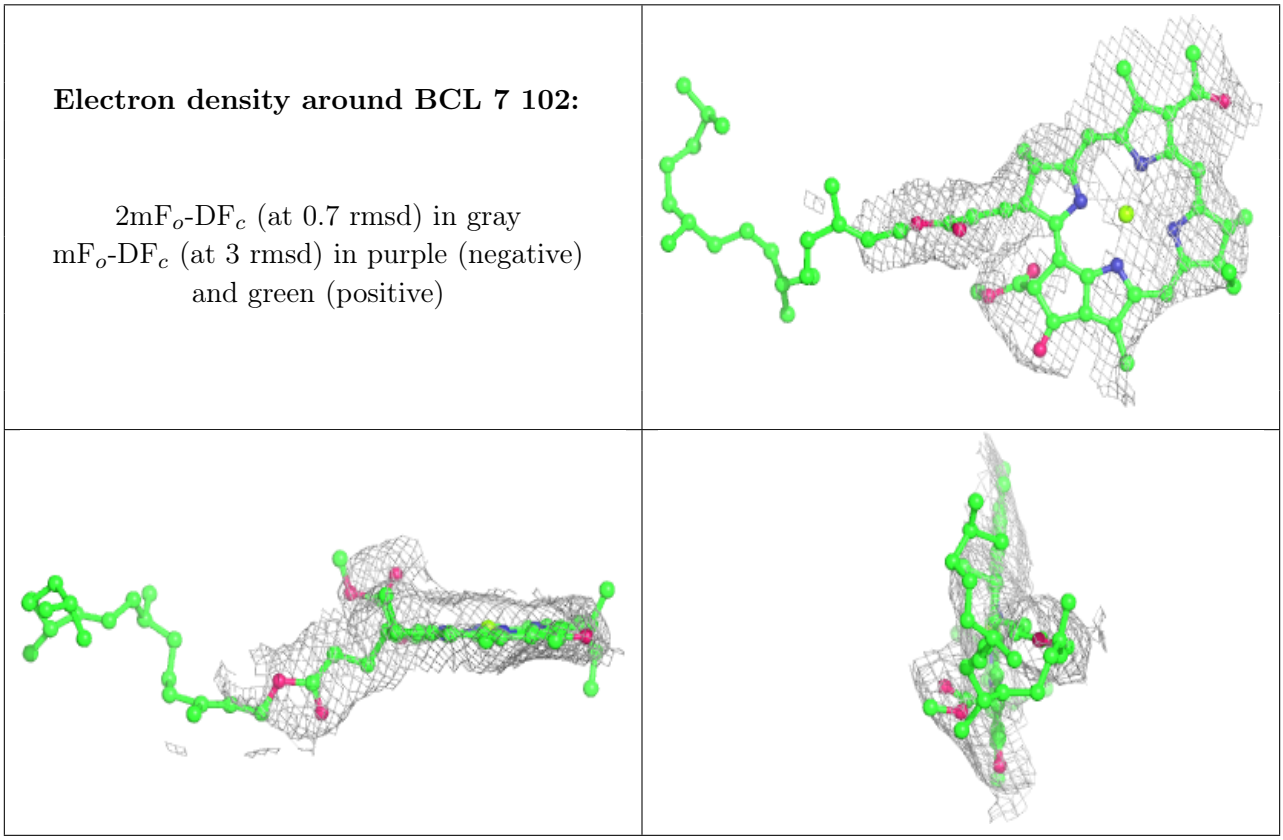
Electron density around BCL D 102:

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



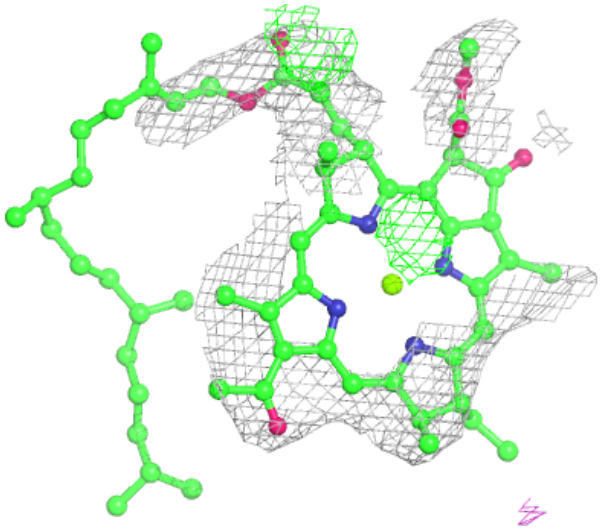
Electron density around BCL 7 102:

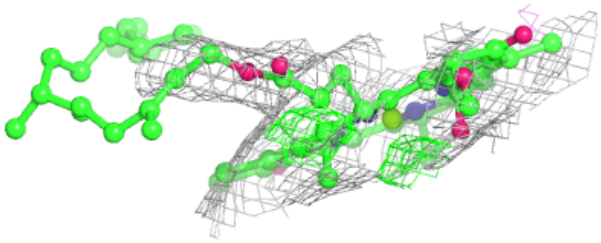
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

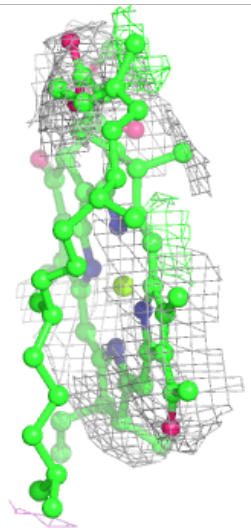


Electron density around BCL B 101:

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

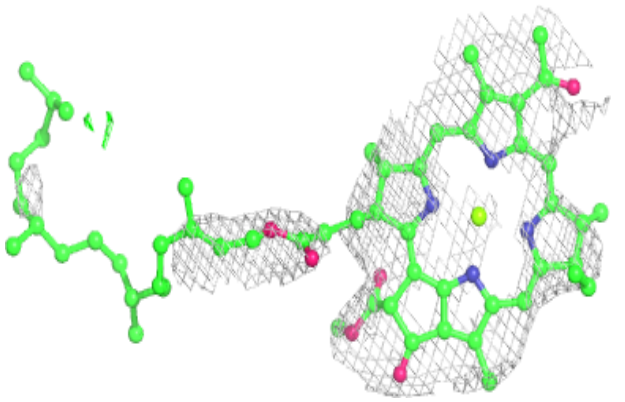


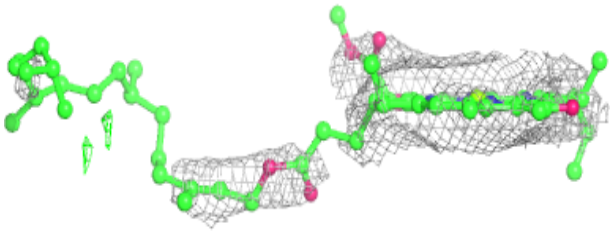


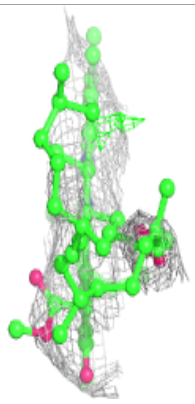


Electron density around BCL 9 102:

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

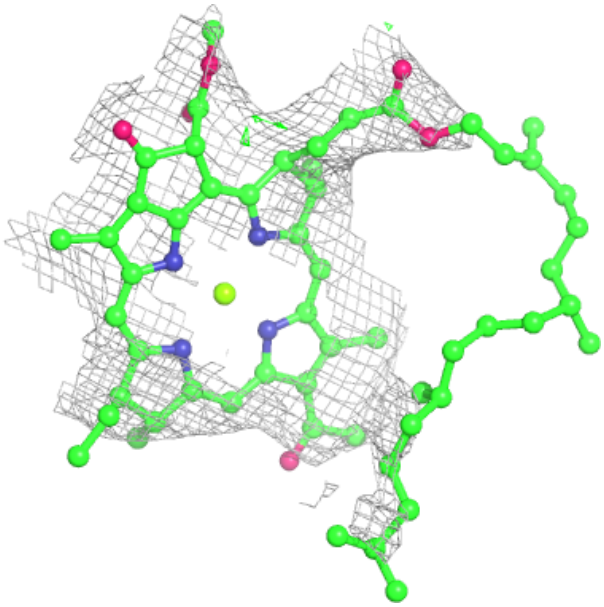


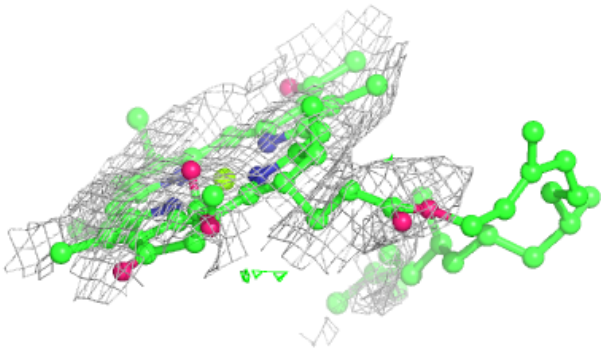


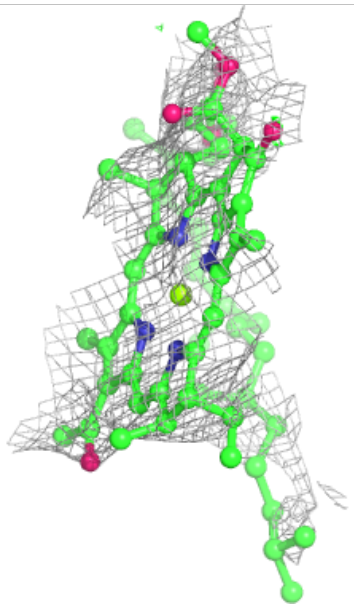


Electron density around BCL G 101:

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

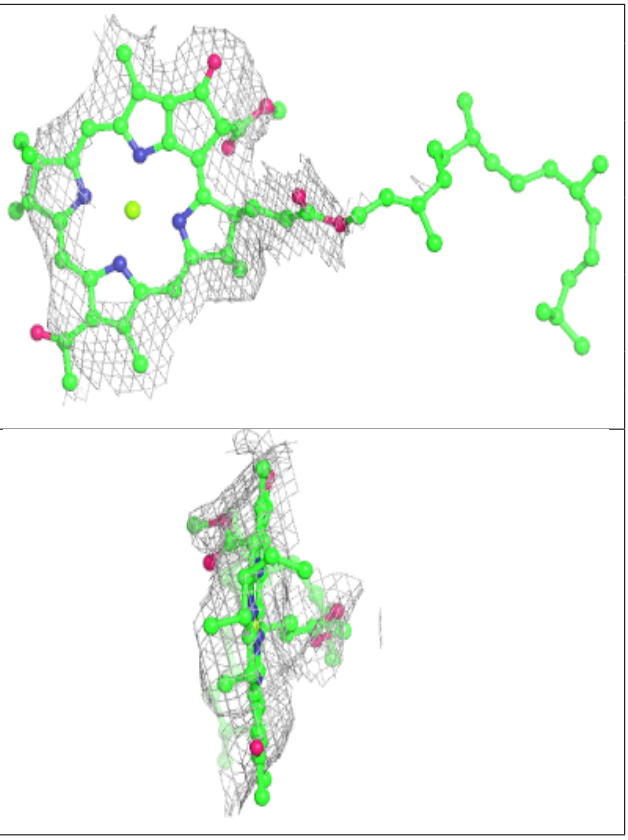






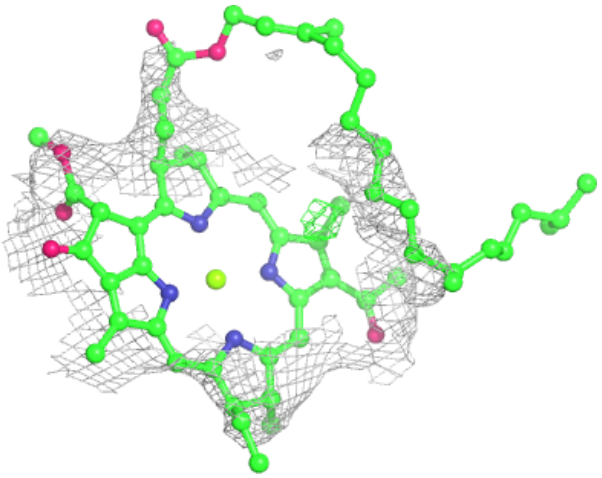
Electron density around BCL A 102:

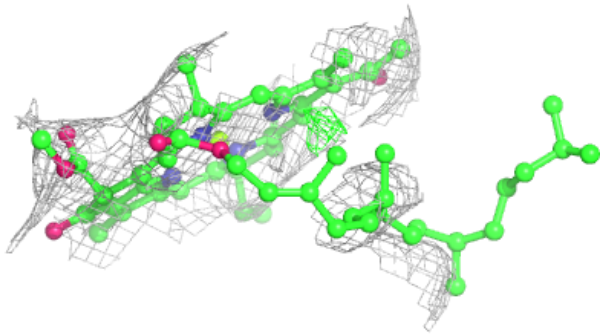
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

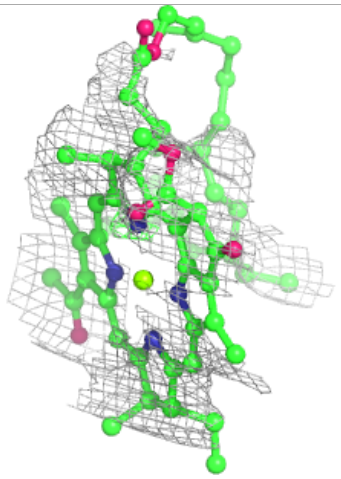


Electron density around BCL E 101:

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

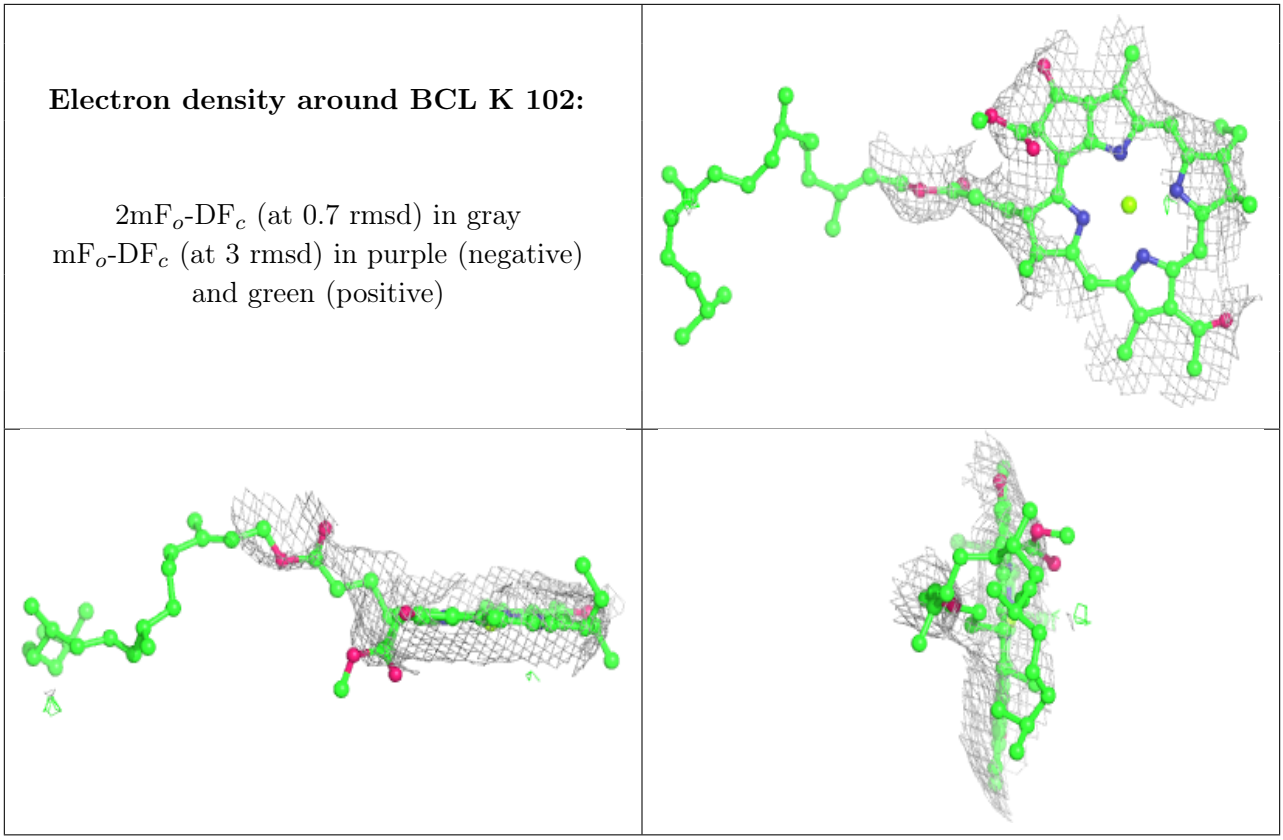






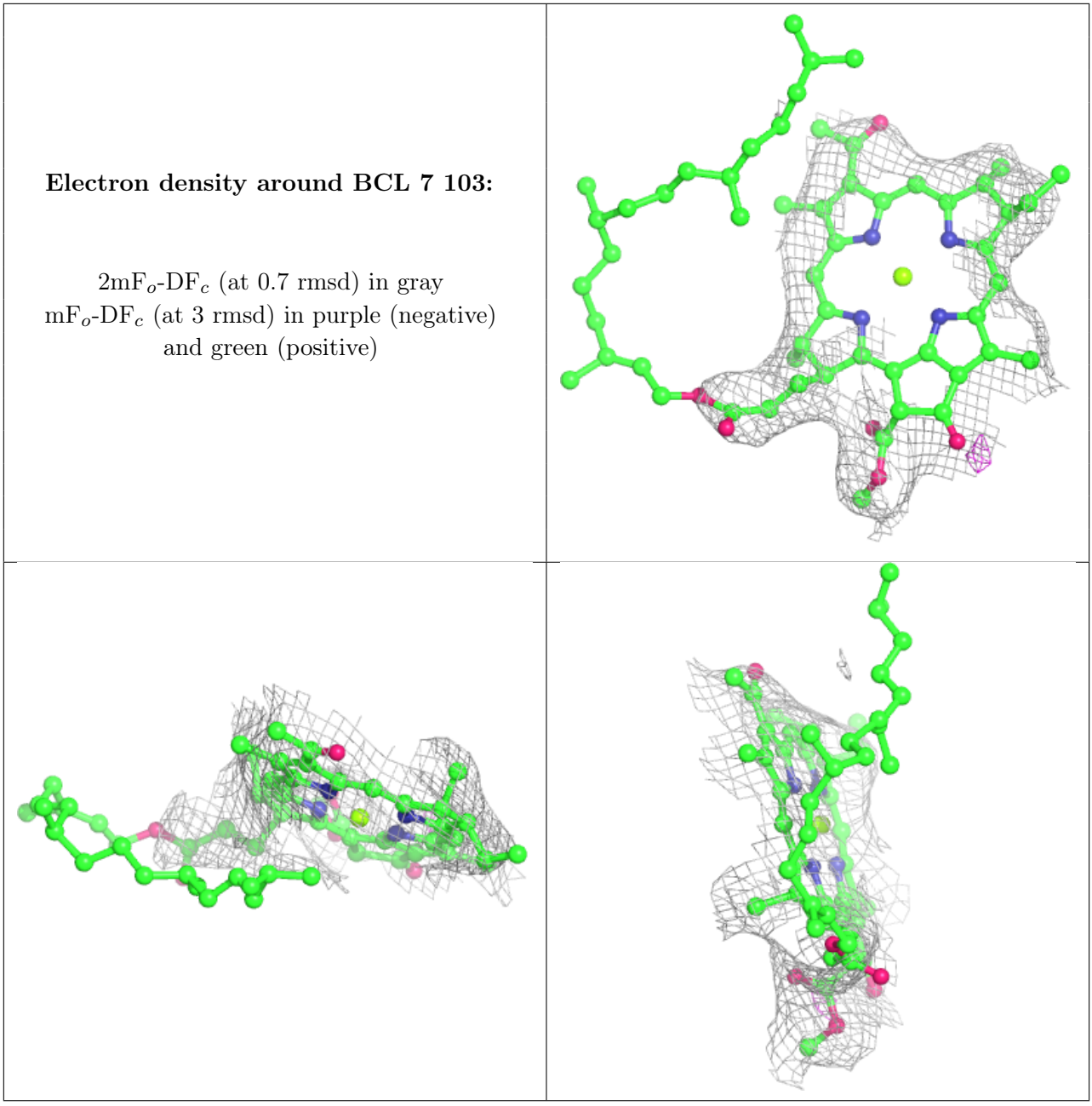
Electron density around BCL K 102:

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



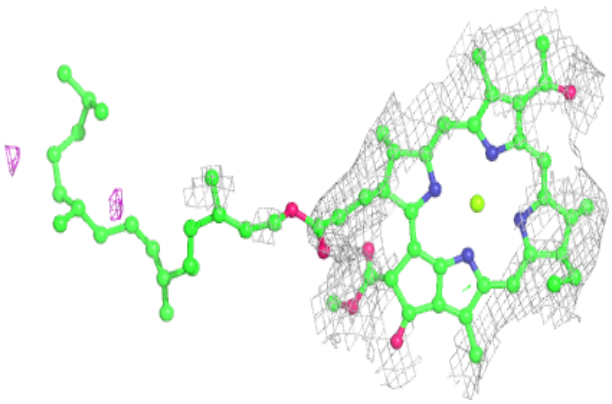
Electron density around BCL 7 103:

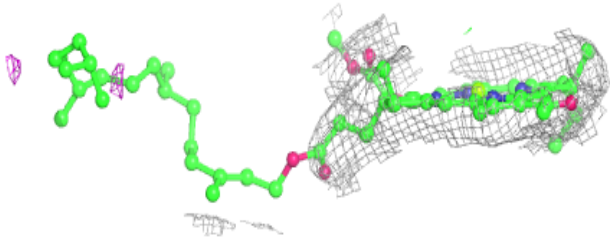
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

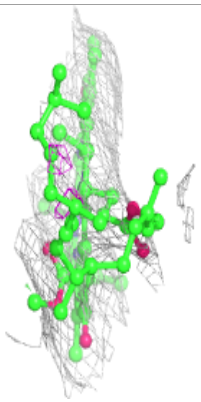


Electron density around BCL O 102:

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

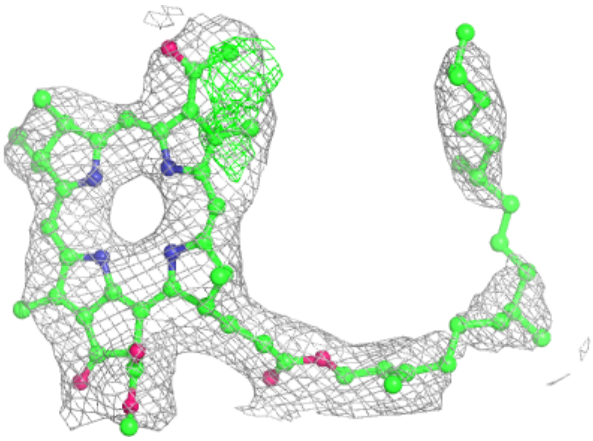


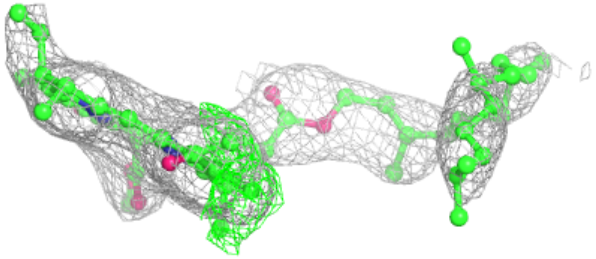


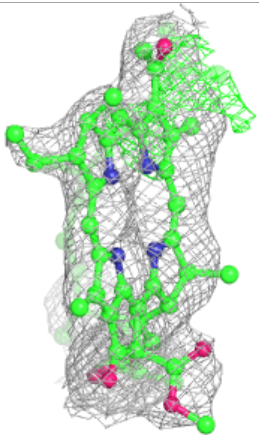


Electron density around BPH L 302:

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

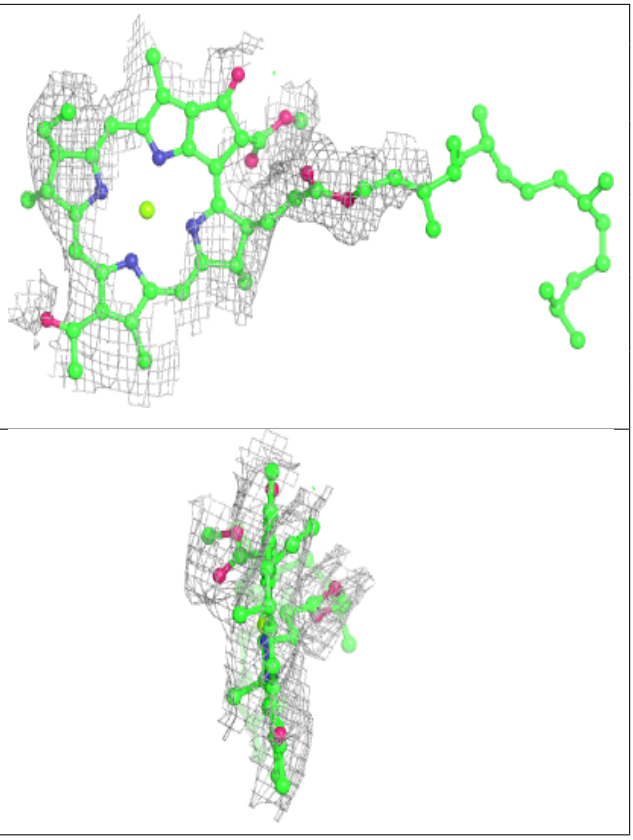


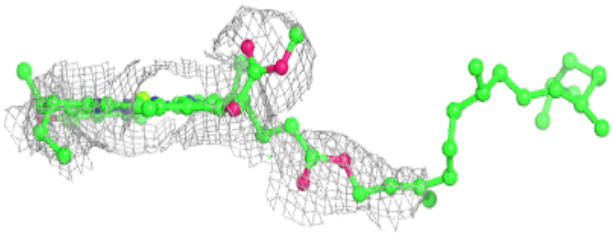




Electron density around BCL F 102:

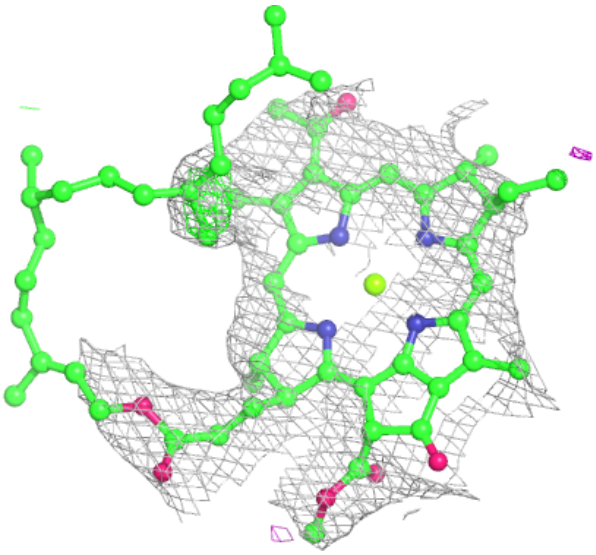
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

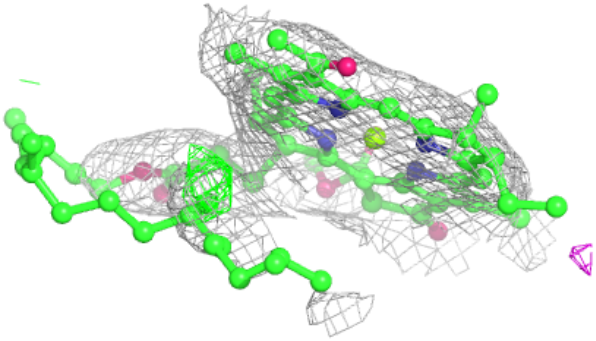


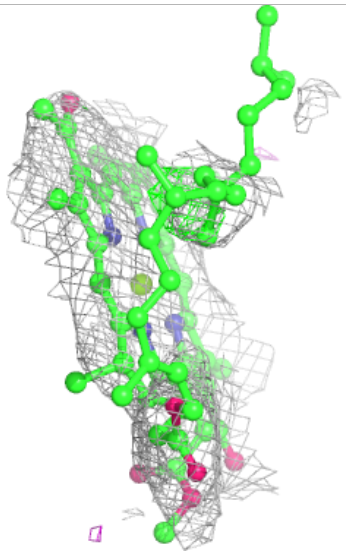


Electron density around BCL X 101:

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

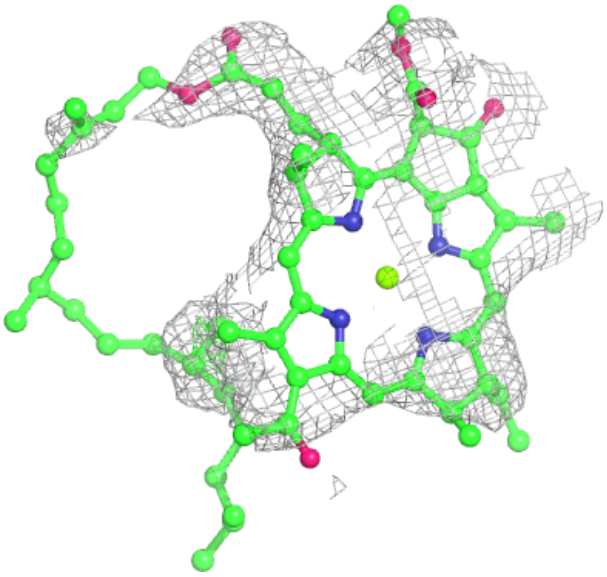


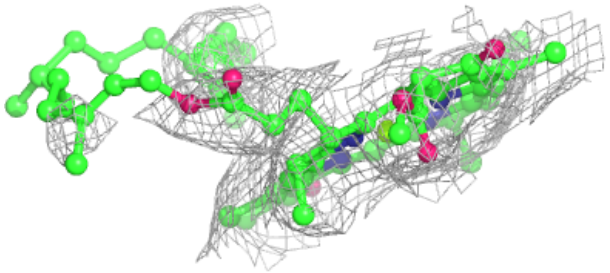


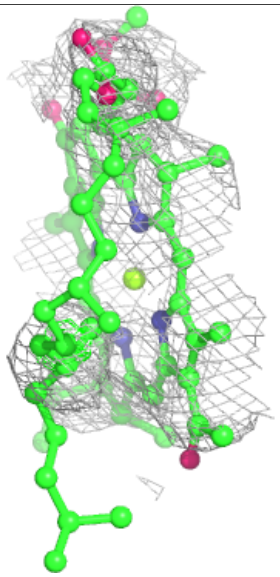


Electron density around BCL 2 101:

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

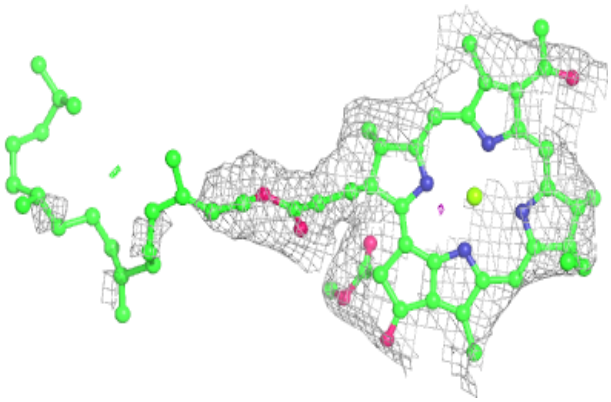


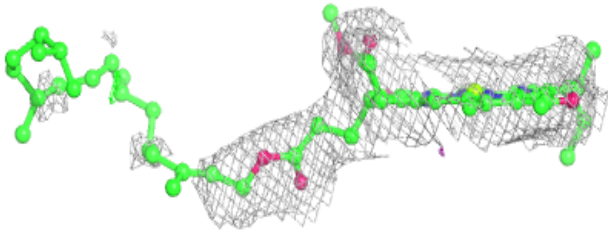


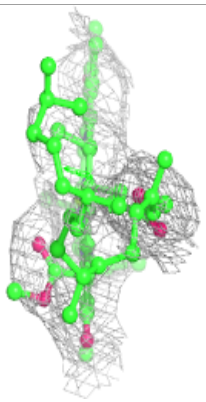


Electron density around BCL 3 102:

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

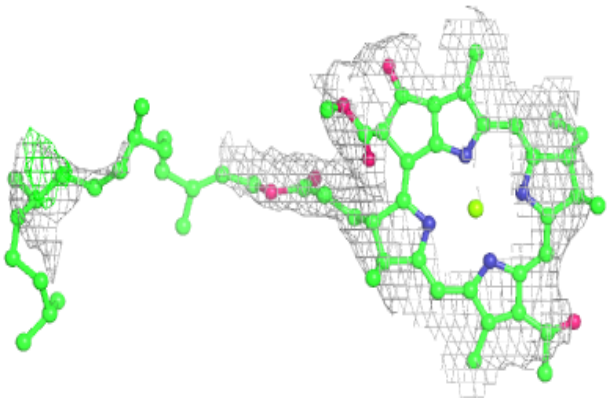


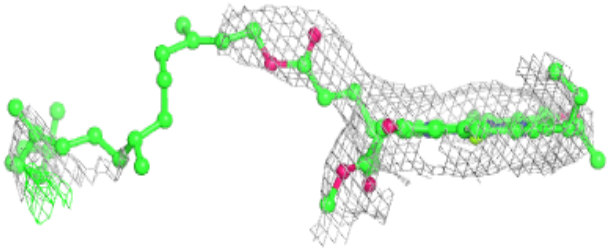


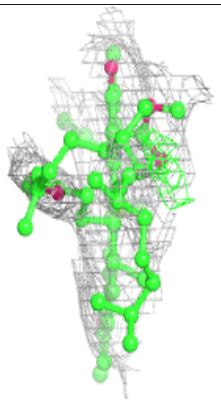


Electron density around BCL I 102:

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

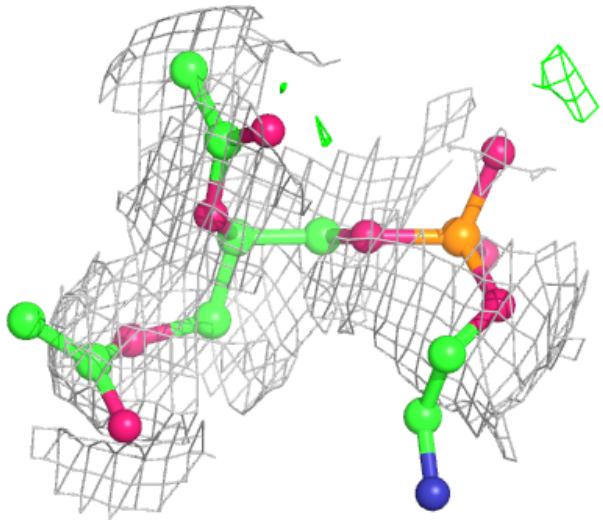


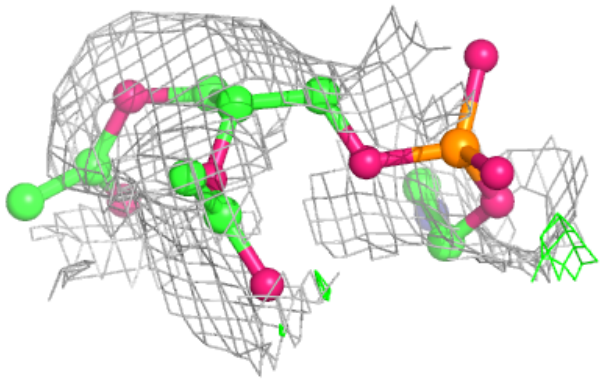


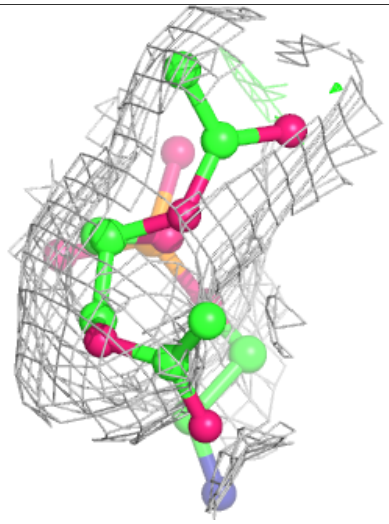


Electron density around PEF H 301:

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

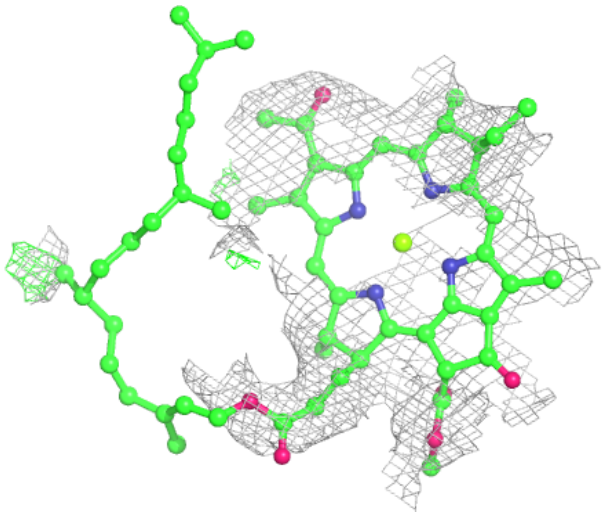


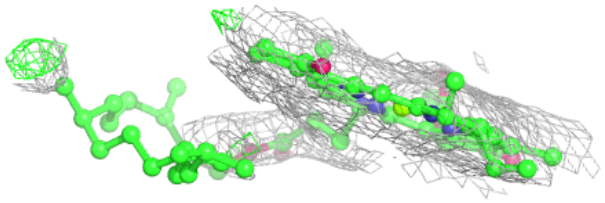


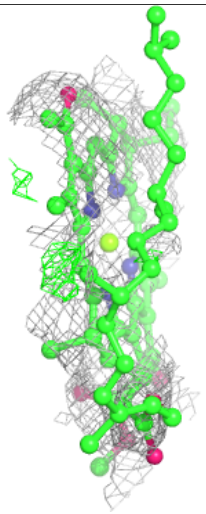


Electron density around BCL P 101:

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

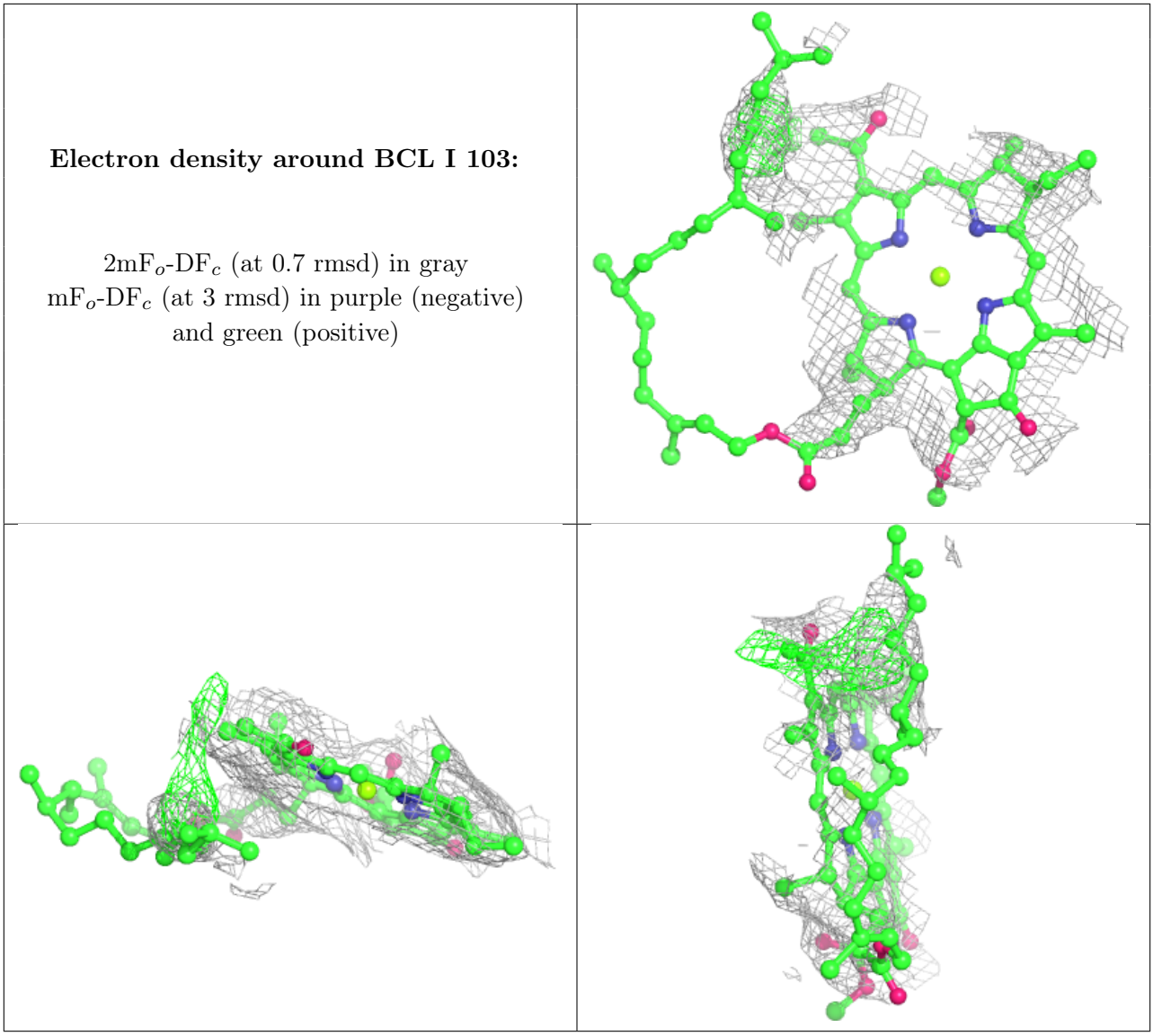






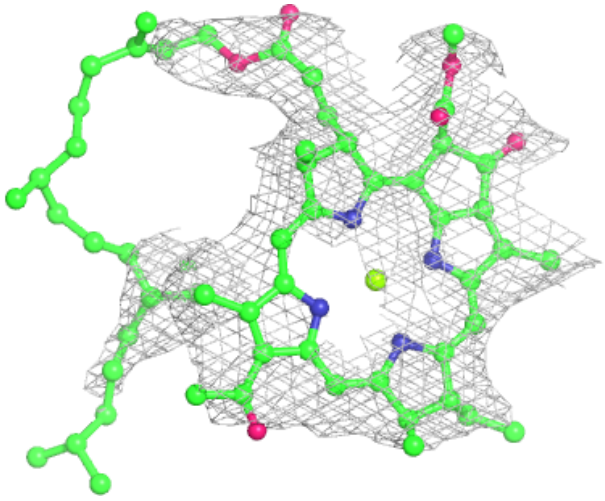
Electron density around BCL I 103:

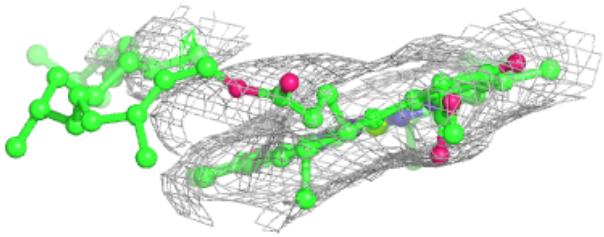
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

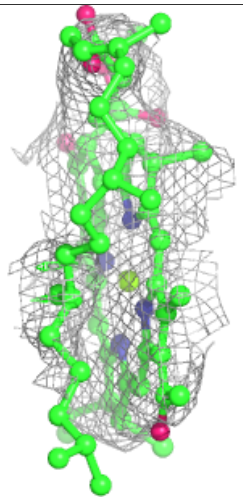


Electron density around BCL V 101:

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

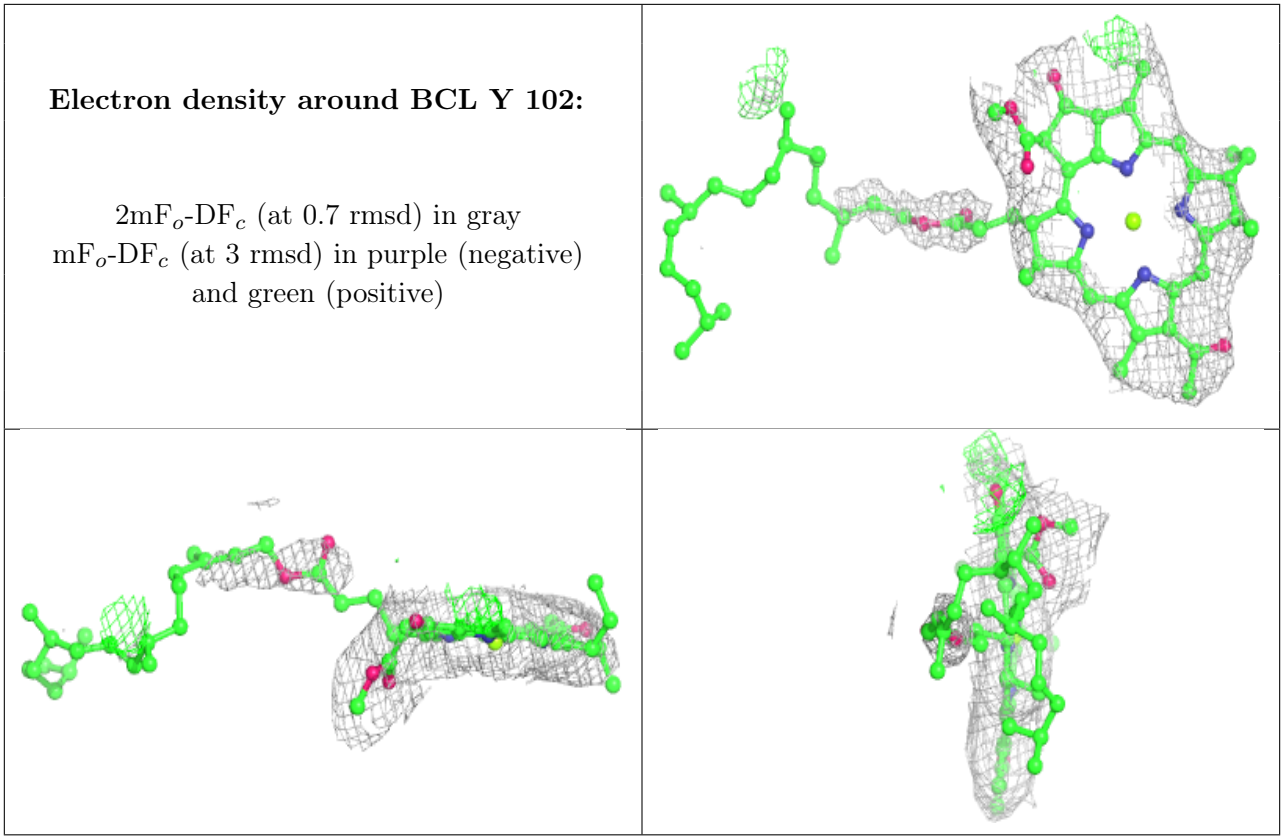






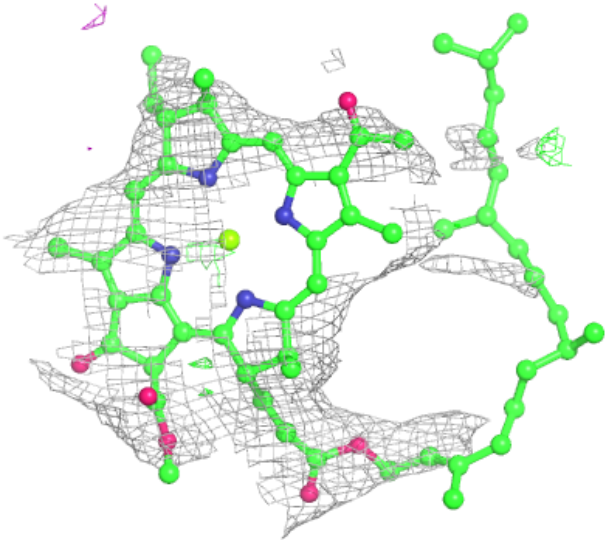
Electron density around BCL Y 102:

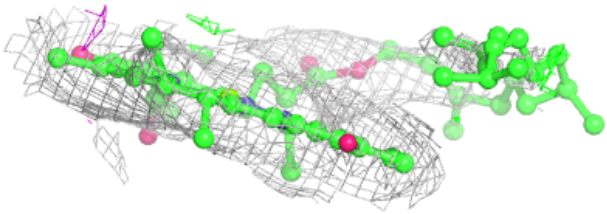
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

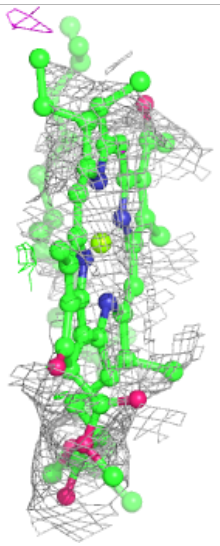


Electron density around BCL Z 101:

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

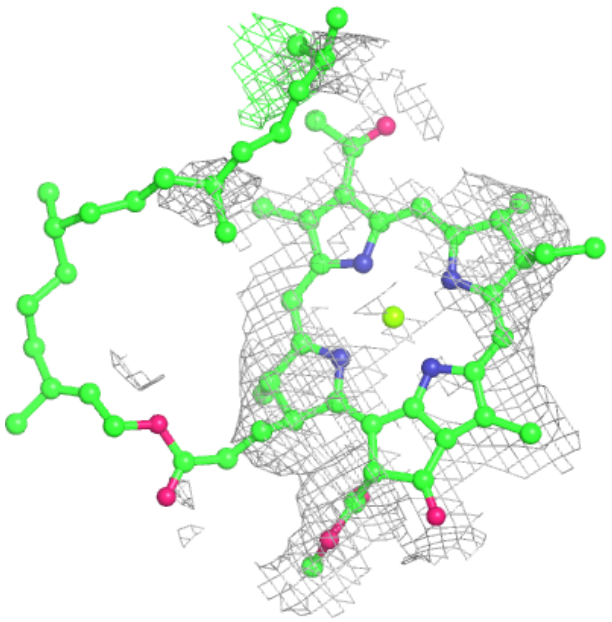


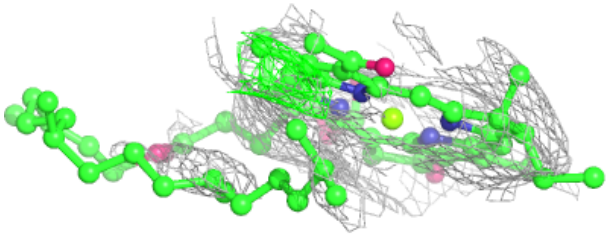


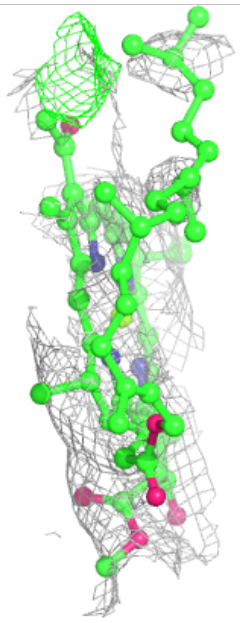


Electron density around BCL N 101:

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

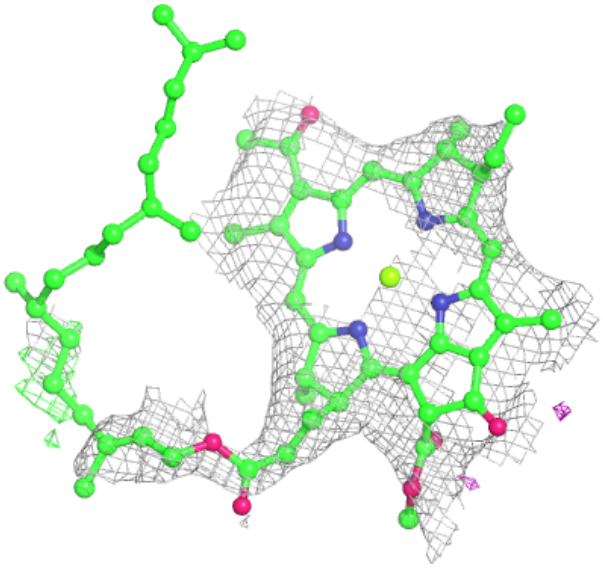


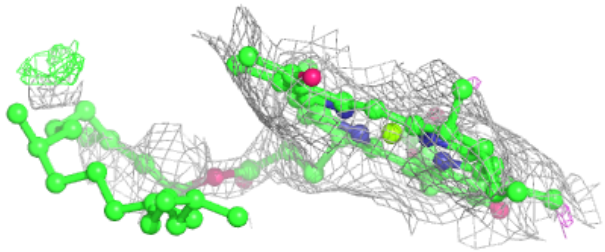


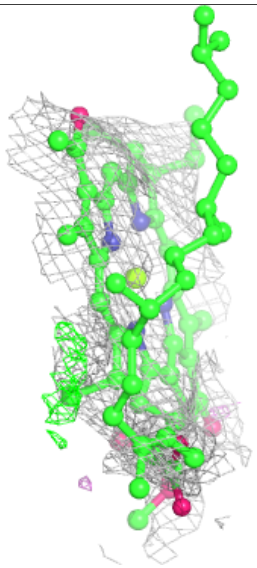


Electron density around BCL 4 101:

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

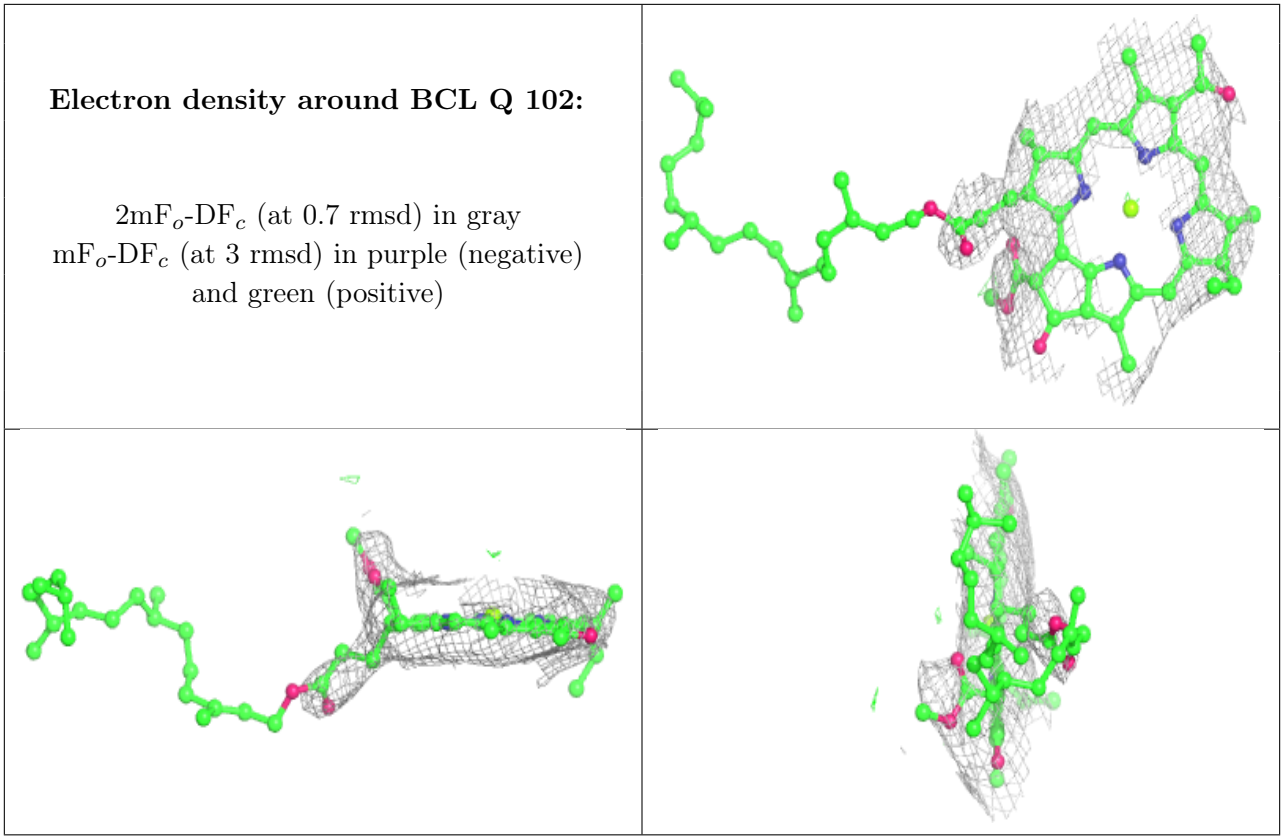






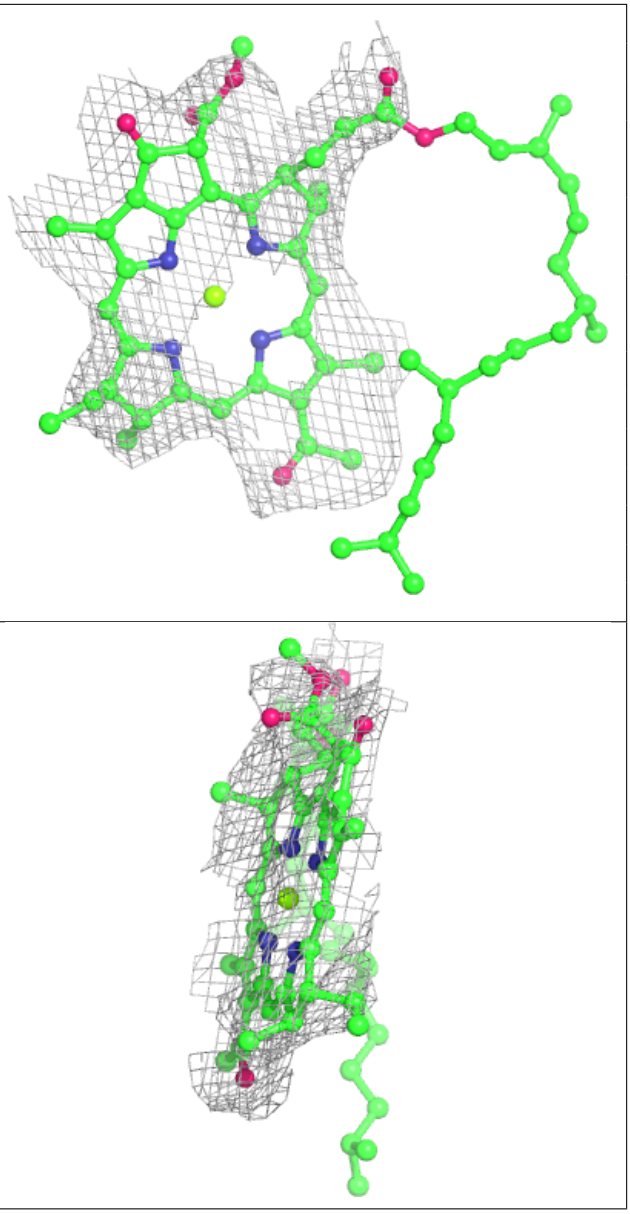
Electron density around BCL Q 102:

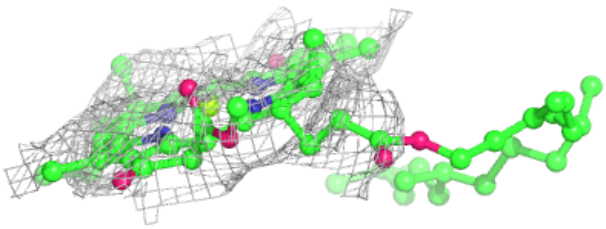
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BCL 0 101:

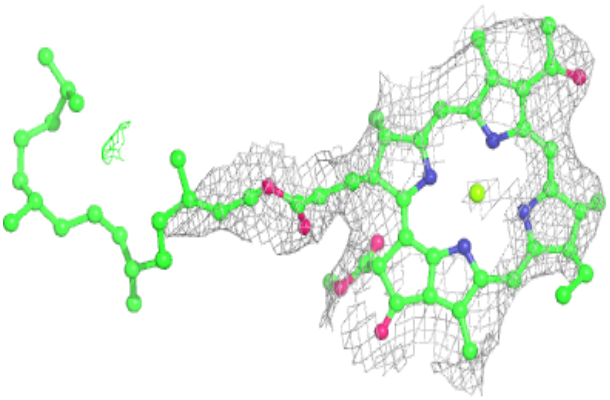
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

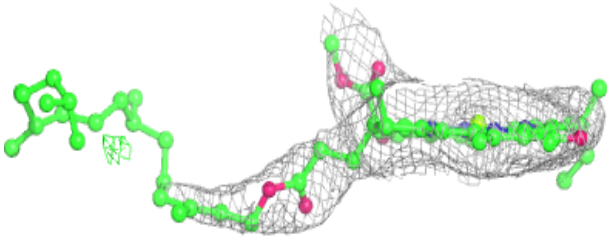


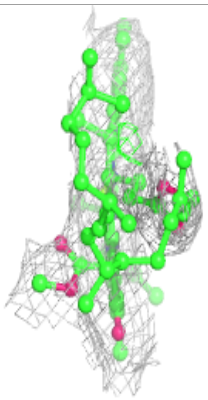


Electron density around BCL W 102:

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

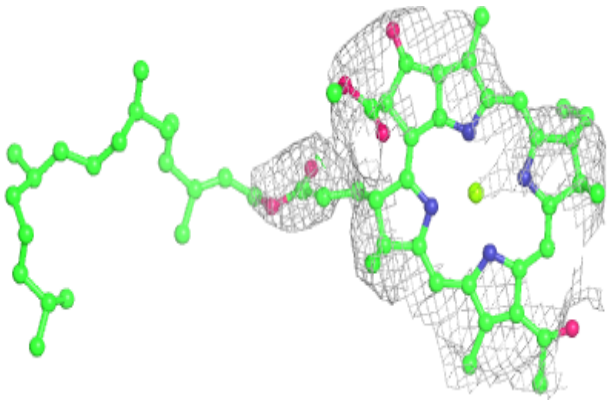


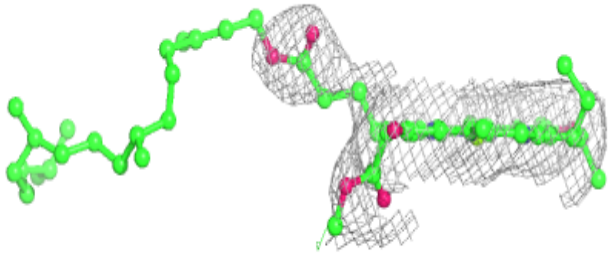


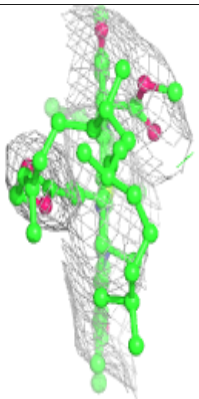


Electron density around BCL 5 102:

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

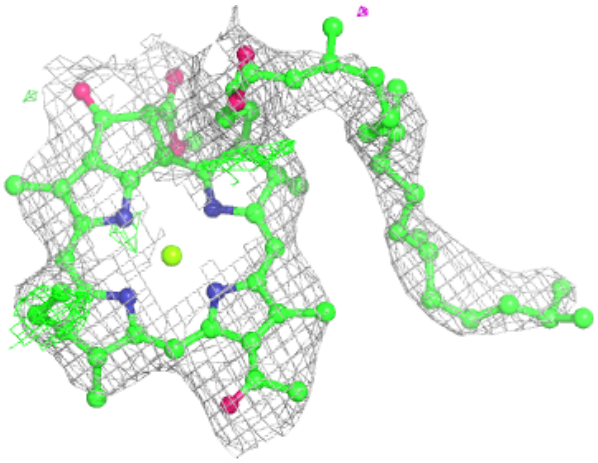


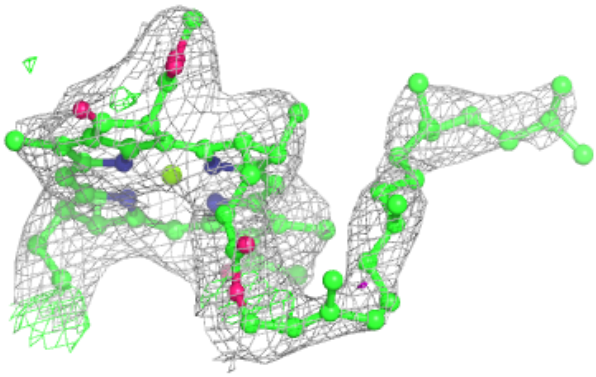


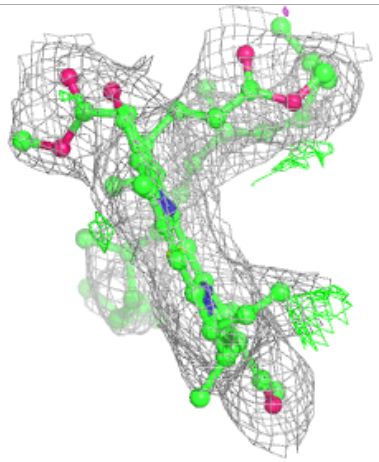


Electron density around BCL L 303:

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

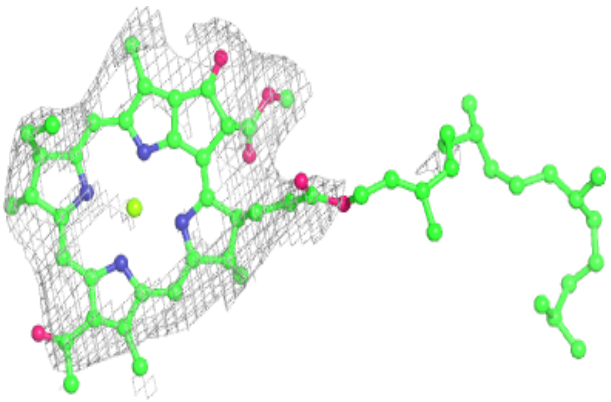


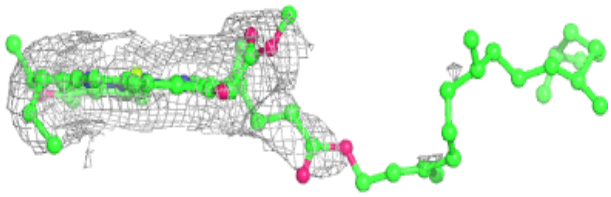


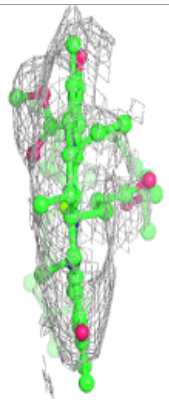


Electron density around BCL S 102:

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

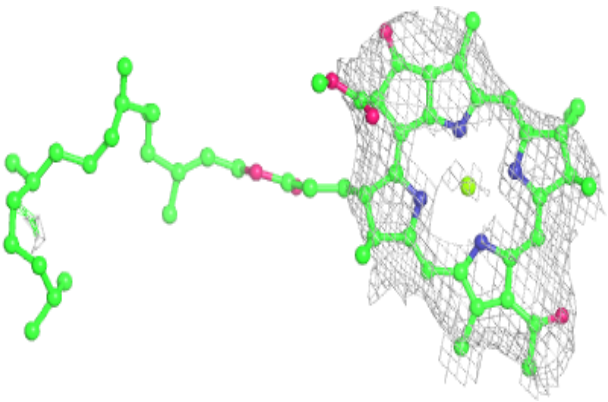


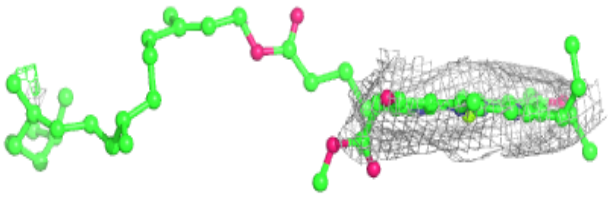


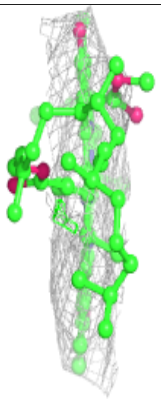


Electron density around BCL U 102:

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

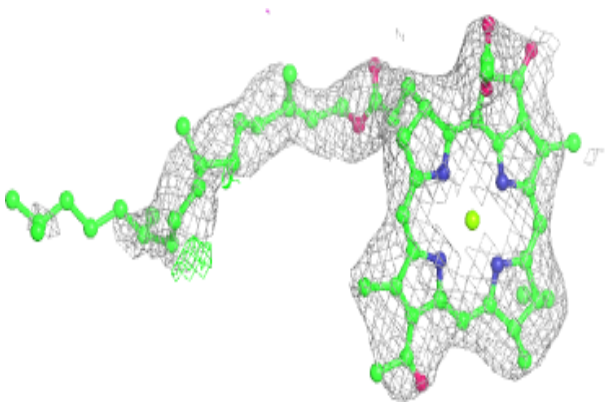


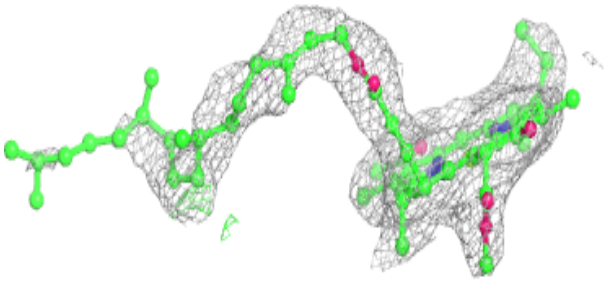


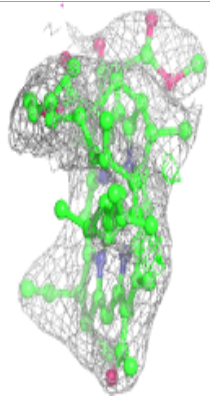


Electron density around BCL M 401:

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

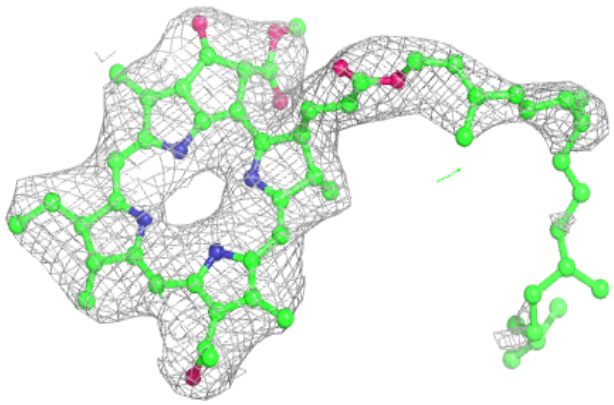


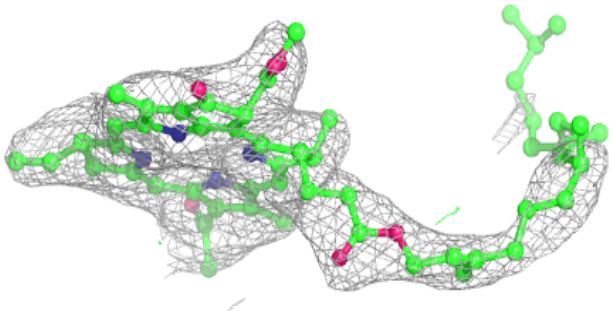


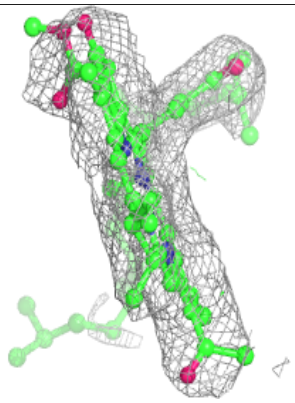


Electron density around BPH M 403:

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

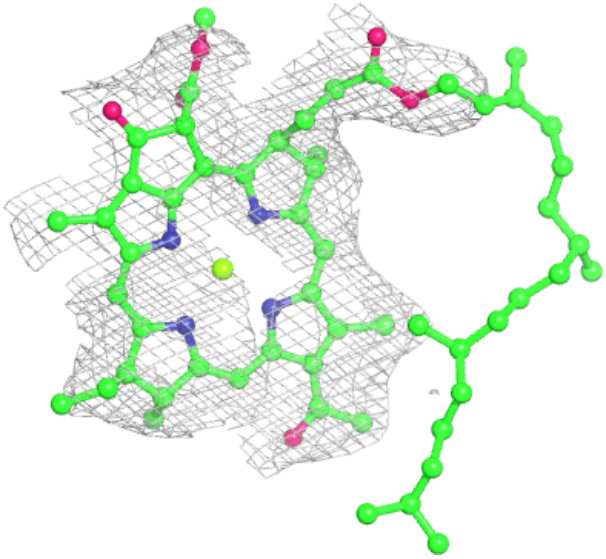


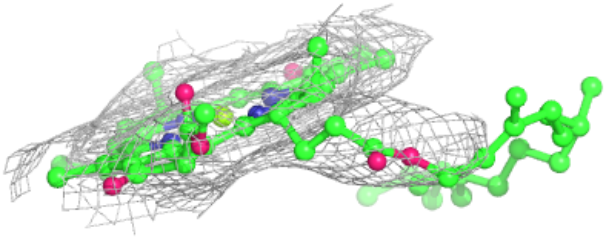


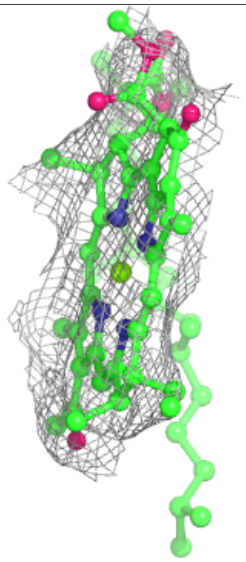


Electron density around BCL T 101:

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

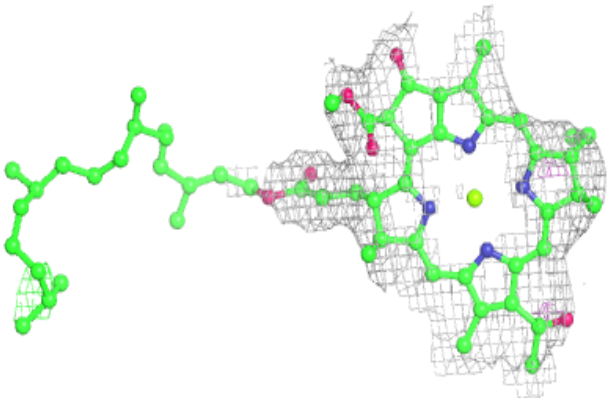


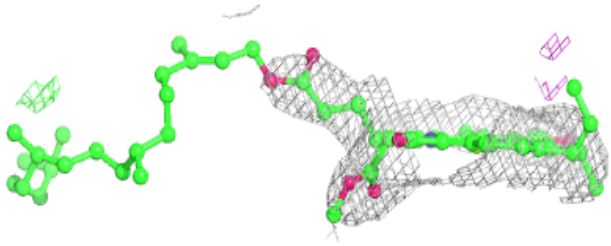


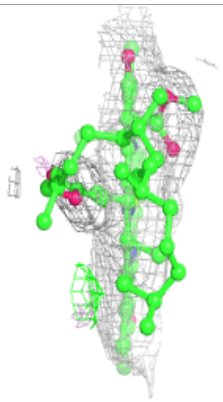


Electron density around BCL 1 102:

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

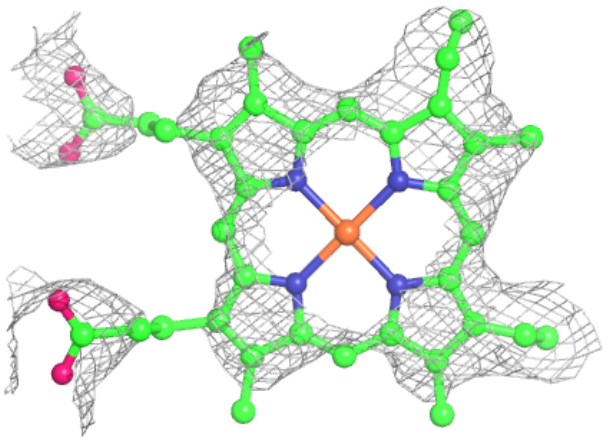


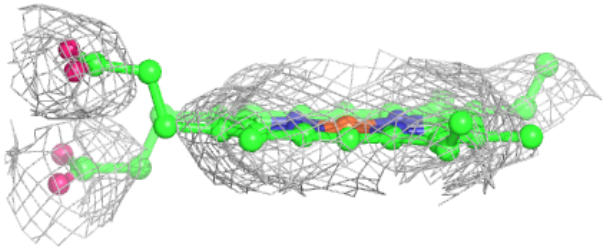


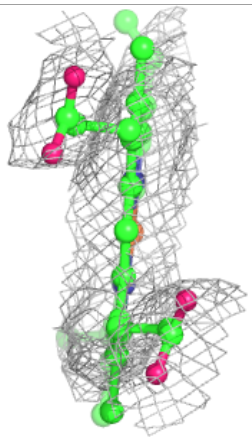


Electron density around HEM C 503:

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

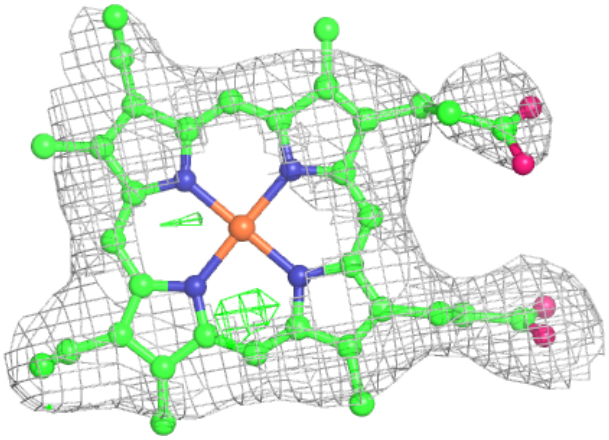


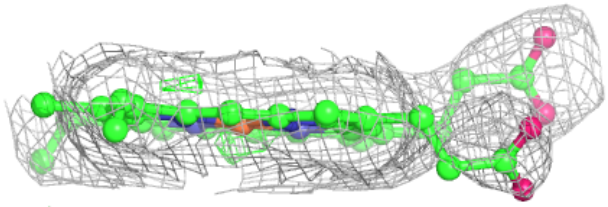


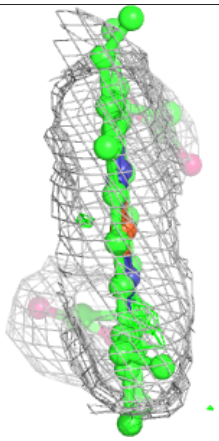


Electron density around HEM C 504:

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

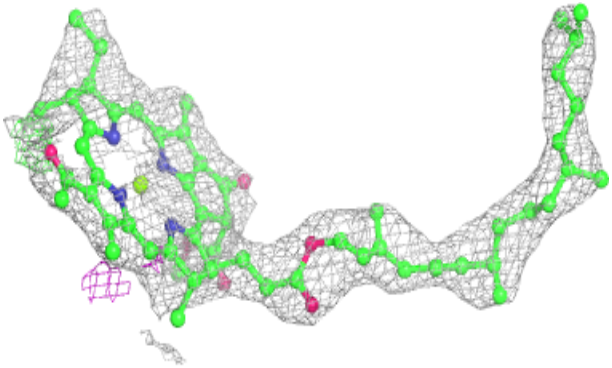


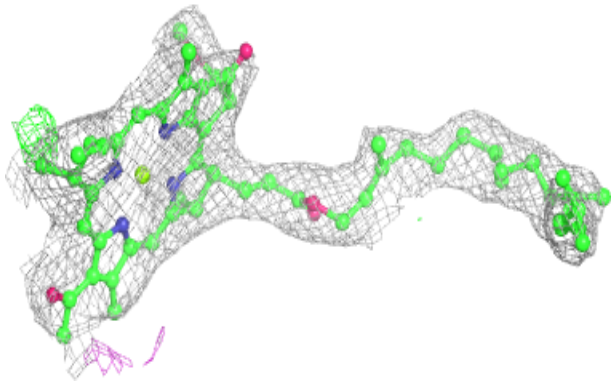


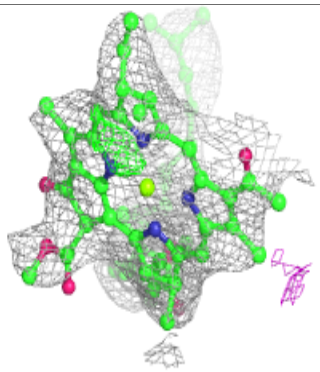


Electron density around BCL M 402:

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

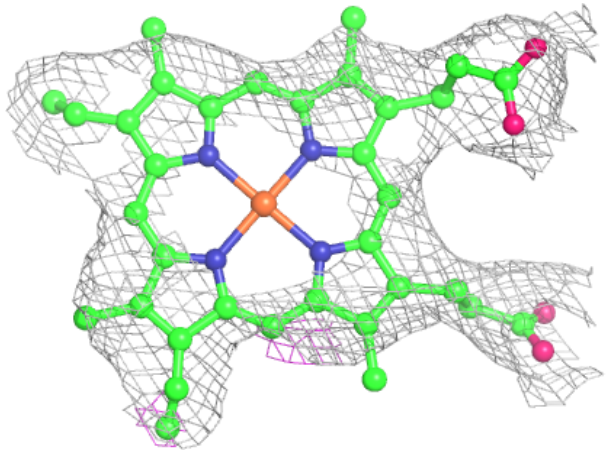


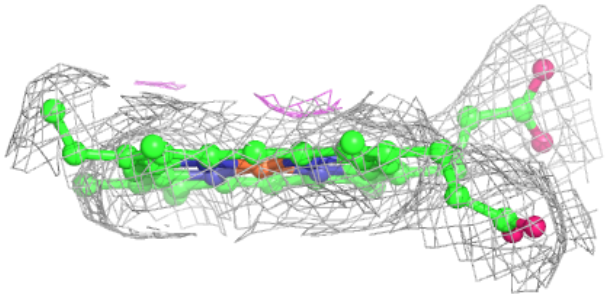


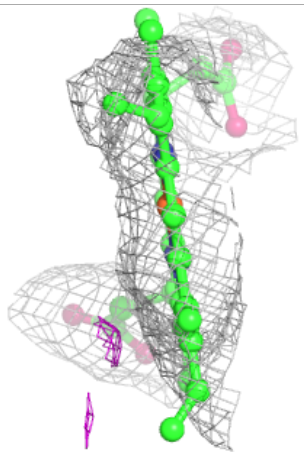


Electron density around HEM C 501:

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

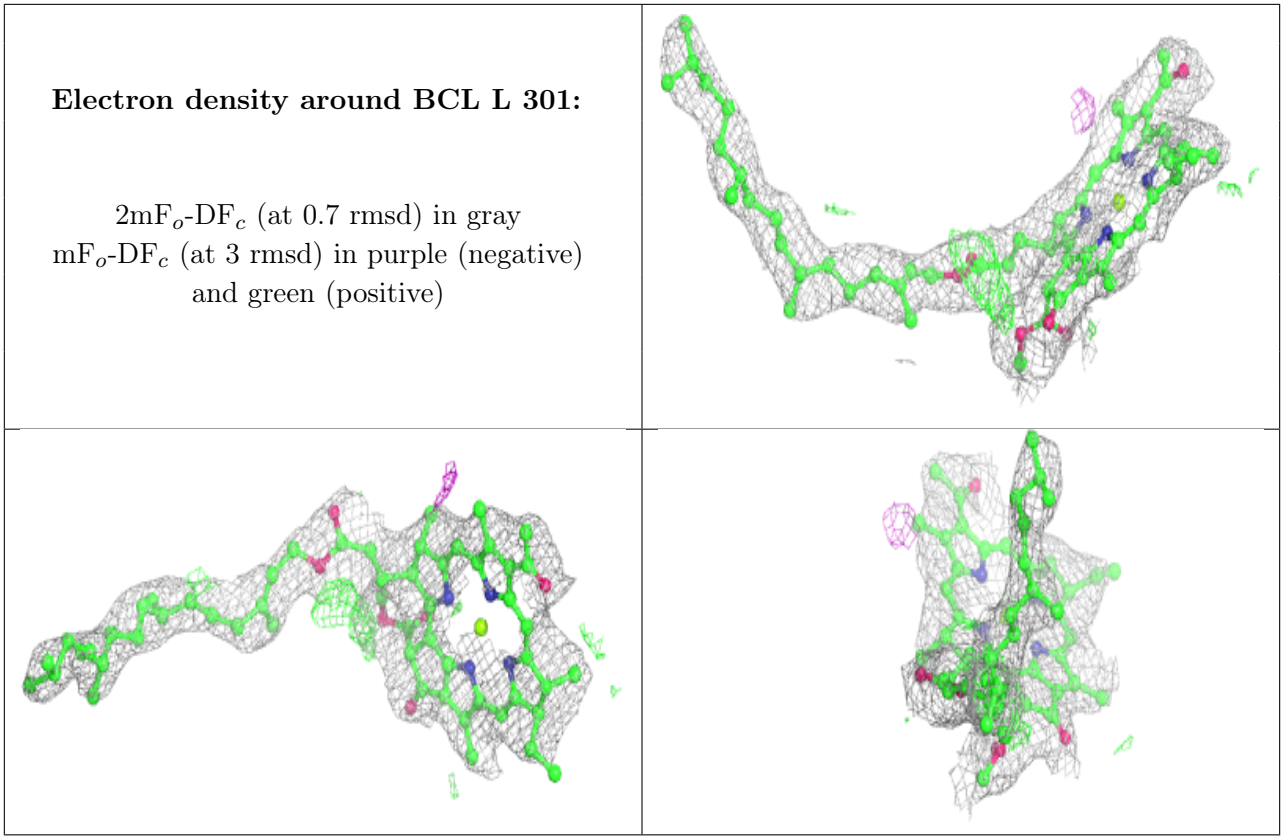






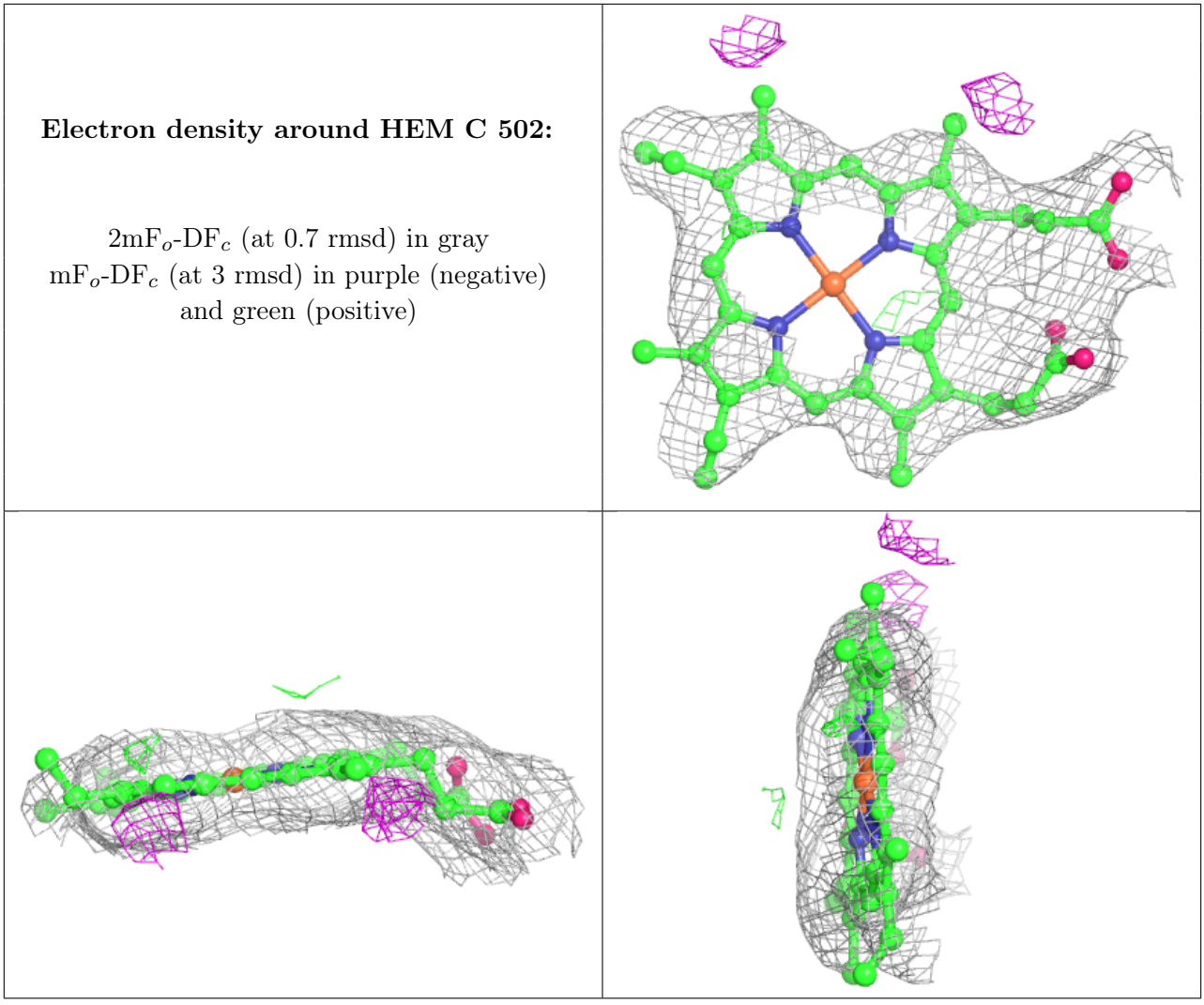
Electron density around BCL L 301:

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



Electron density around HEM C 502:

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



6.5 Other polymers (i)

There are no such residues in this entry.