



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:09 AM UTC

PDB ID : 4V9G / pdb_00004v9g
Title : RC-LH1-PufX dimer complex from Rhodobacter sphaeroides
Authors : Qian, P.; Papiz, M.Z.; Jackson, P.J.; Brindley, A.A.; Ng, I.W.; Olsen, J.D.;
Dickman, M.J.; Bullough, P.A.; Hunter, C.N.
Deposited on : 2013-02-21
Resolution : 7.78 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

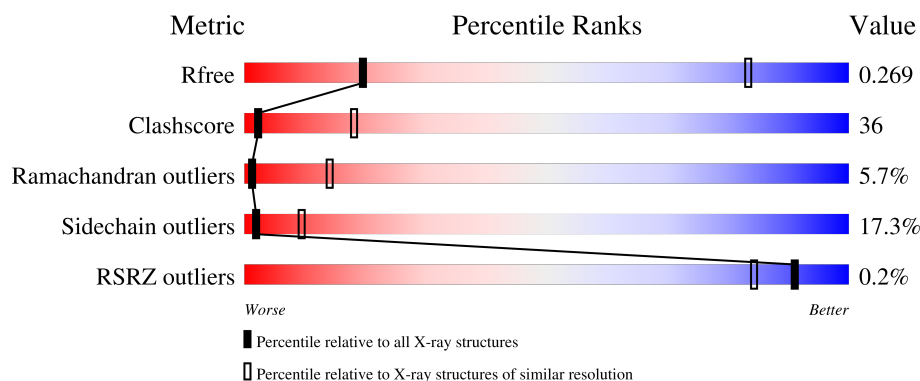
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.78 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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

Mol	Chain	Length	Quality of chain
1	A1	58	
1	A2	58	
1	A3	58	
1	A5	58	
1	A7	58	

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Mol	Chain	Length	Quality of chain
1	AD	58	
1	AF	58	
1	AJ	58	
1	AN	58	
1	AP	58	
1	AT	58	
1	AV	58	
1	AX	58	
1	AZ	58	
1	B1	58	
1	B2	58	
1	B3	58	
1	B5	58	
1	B7	58	
1	BD	58	
1	BF	58	
1	BJ	58	
1	BN	58	
1	BP	58	
1	BT	58	
1	BV	58	
1	BX	58	
1	BZ	58	
2	AB	82	
2	BB	82	

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Mol	Chain	Length	Quality of chain
3	A4	49	
3	A6	49	
3	A8	49	
3	A9	49	
3	AE	49	
3	AG	49	
3	AI	49	
3	AK	49	
3	AO	49	
3	AQ	49	
3	AS	49	
3	AU	49	
3	AW	49	
3	AY	49	
3	B4	49	
3	B6	49	
3	B8	49	
3	B9	49	
3	BE	49	
3	BG	49	
3	BI	49	
3	BK	49	
3	BO	49	
3	BQ	49	
3	BS	49	

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Mol	Chain	Length	Quality of chain
3	BU	49	
3	BW	49	
3	BY	49	
4	AH	260	
4	BH	260	
5	AL	282	
5	BL	282	
6	AM	308	
6	BM	308	

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
7	BCL	AL	301	-	-	X	-
7	BCL	AM	401	-	-	X	-
7	BCL	AM	402	-	-	X	-
7	BCL	BL	302	-	-	X	-
7	BCL	BL	303	-	-	X	-
7	BCL	BM	401	-	-	X	-
8	BPH	AL	303	-	-	X	-
8	BPH	BL	304	-	-	X	-
8	BPH	BM	402	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 38108 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 Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A5	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AT	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AV	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AX	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A3	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A7	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AD	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AF	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A1	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AJ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	A2	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AN	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AP	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	AZ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B5	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BT	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BV	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BX	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B3	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B7	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BD	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BF	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B1	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BJ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	B2	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BN	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BP	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			
1	BZ	42	Total	C	N	O	S	0	0	0
			345	236	54	53	2			

- Molecule 2 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	57	Total	C	N	O	S	0	0	0
			452	299	79	71	3			
2	BB	57	Total	C	N	O	S	0	0	0
			452	299	79	71	3			

- Molecule 3 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AS	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	A9	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AO	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AQ	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	A6	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AU	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AW	48	Total	C	N	O	S	0	0	0
			387	256	60	70	1			
3	AY	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	A4	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	A8	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AE	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AG	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AI	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	AK	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BS	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	B9	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BO	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BQ	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	B6	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BU	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BW	48	Total	C	N	O	S	0	0	0
			387	256	60	70	1			
3	BY	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	B4	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	B8	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	BE	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BG	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BI	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			
3	BK	48	Total	C	N	O	S	0	0	0
			388	256	61	70	1			

- Molecule 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AH	250	Total	C	N	O	S	0	0	0
			1901	1216	324	351	10			
4	BH	250	Total	C	N	O	S	0	0	0
			1901	1216	324	351	10			

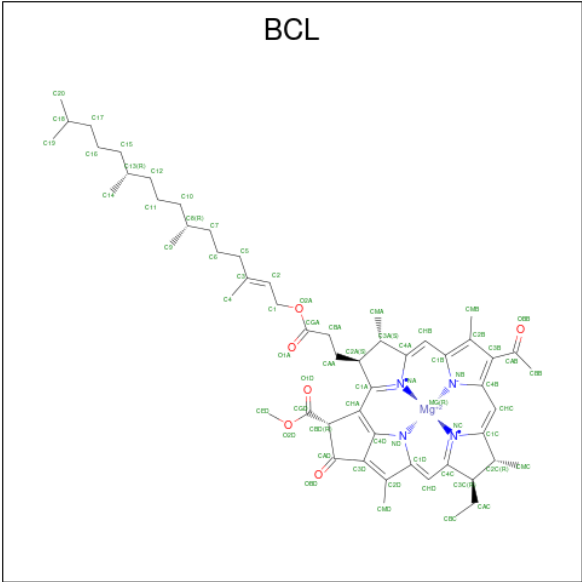
- Molecule 5 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AL	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			
5	BL	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 6 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AM	304	Total	C	N	O	S	0	1	0
			2427	1619	398	399	11			
6	BM	304	Total	C	N	O	S	0	1	0
			2427	1619	398	399	11			

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AT	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AT	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AV	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	A3	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	A7	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AD	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AD	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AF	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	A1	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AJ	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	A2	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AN	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AP	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	AP	1	Total 46	C 35	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AZ	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AS	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A9	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AO	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A6	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A6	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AW	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AY	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AY	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A4	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	A8	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AG	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AI	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AK	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	AL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	AL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	AM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	AM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	B5	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BT	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BV	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

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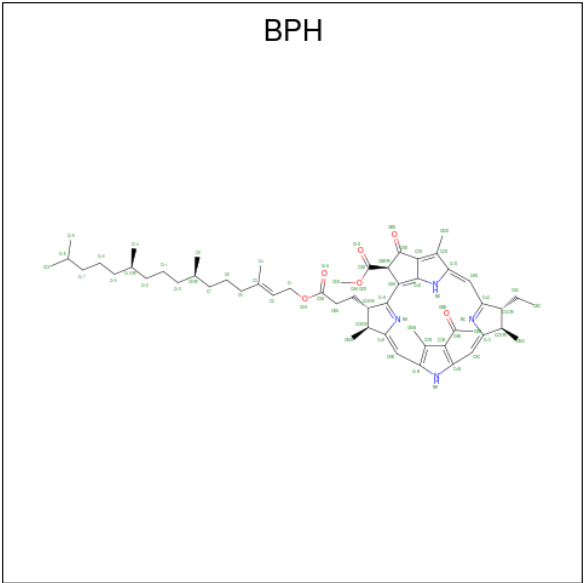
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	BV	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B3	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B7	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BD	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BD	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BF	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BF	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B1	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B2	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BP	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BP	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BZ	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BZ	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B9	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BO	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BO	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B6	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BU	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BY	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	BY	1	Total 46	C 35	Mg 1	N 4	O 6	0	0
7	B4	1	Total 46	C 35	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B8	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BI	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BK	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BK	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
7	BL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	BL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	BL	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	BM	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



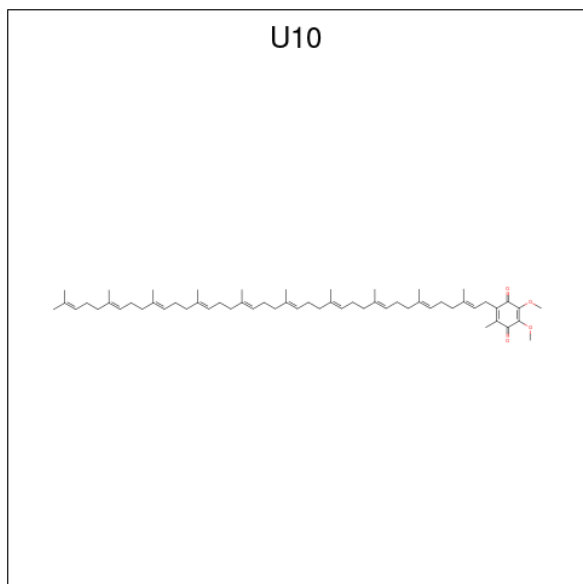
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	AL	1	Total	C	N	O		0	0
			65	55	4	6			
8	AM	1	Total	C	N	O		0	0
			65	55	4	6			
8	BL	1	Total	C	N	O		0	0
			65	55	4	6			

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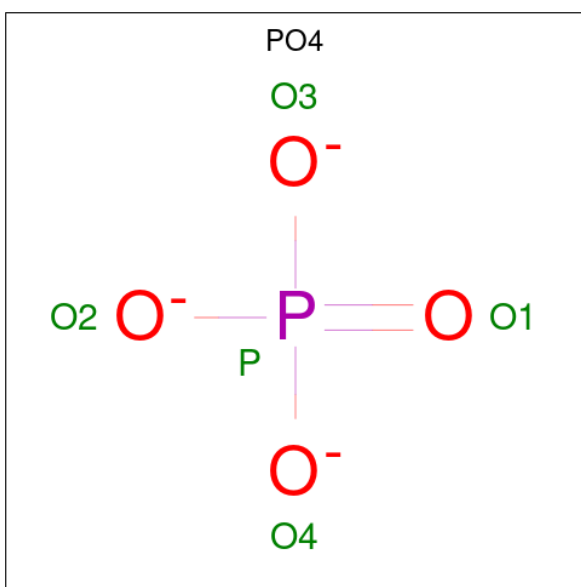
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	BM	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	AL	1	Total	C	O	0	0
			48	44	4		
9	AM	1	Total	C	O	0	0
			48	44	4		
9	BL	1	Total	C	O	0	0
			48	44	4		

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

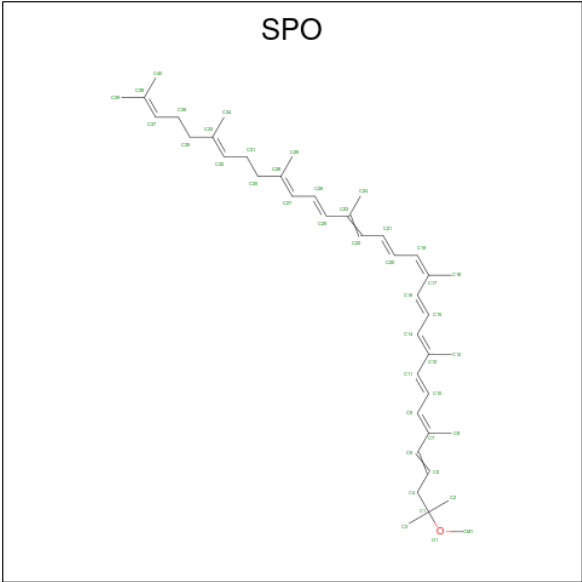


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	AL	1	Total	O	P	0	0
			5	4	1		
10	BL	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	AM	1	Total	Fe	0	0
			1	1		
11	BL	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).

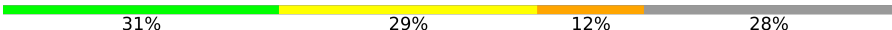


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	AM	1	Total	C	O	0	0
			42	41	1		

3 Residue-property plots [i](#)

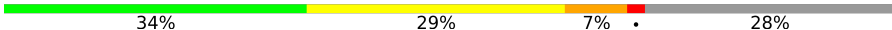
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Light-harvesting protein B-875 alpha chain

Chain A5: 

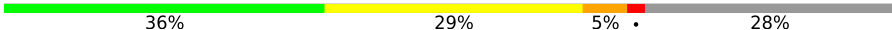


- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AT: 

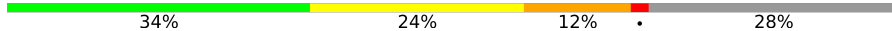


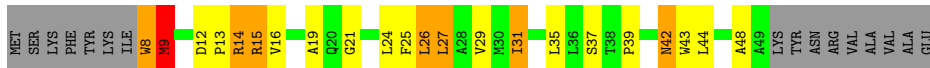
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AV: 

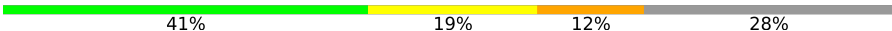


- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AX: 

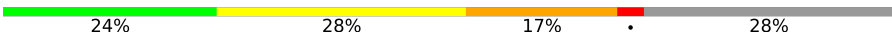


- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain A3: 

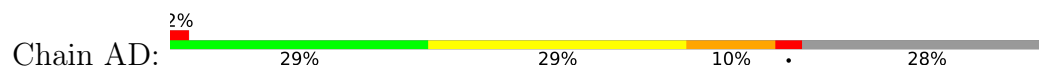


- Molecule 1: Light-harvesting protein B-875 alpha chain

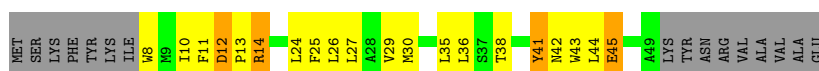
Chain A7: 



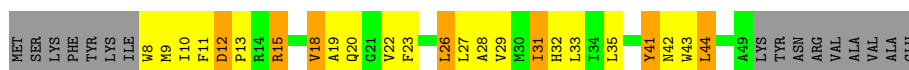
- Molecule 1: Light-harvesting protein B-875 alpha chain



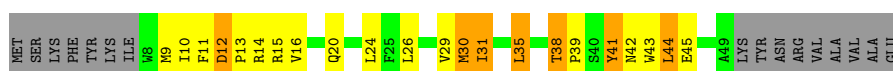
- Molecule 1: Light-harvesting protein B-875 alpha chain



- Molecule 1: Light-harvesting protein B-875 alpha chain



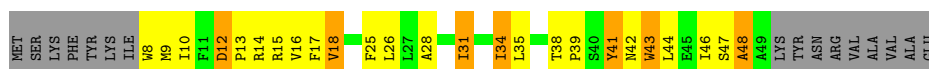
- Molecule 1: Light-harvesting protein B-875 alpha chain



- Molecule 1: Light-harvesting protein B-875 alpha chain



- Molecule 1: Light-harvesting protein B-875 alpha chain

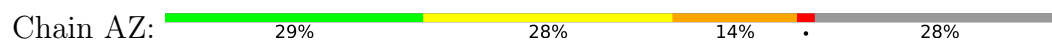


- Molecule 1: Light-harvesting protein B-875 alpha chain





- Molecule 1: Light-harvesting protein B-875 alpha chain



- Molecule 1: Light-harvesting protein B-875 alpha chain



- Molecule 1: Light-harvesting protein B-875 alpha chain



- Molecule 1: Light-harvesting protein B-875 alpha chain



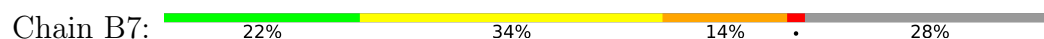
- Molecule 1: Light-harvesting protein B-875 alpha chain



- Molecule 1: Light-harvesting protein B-875 alpha chain

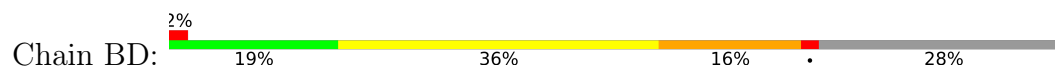


- Molecule 1: Light-harvesting protein B-875 alpha chain

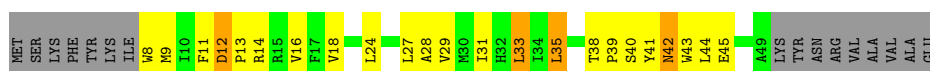




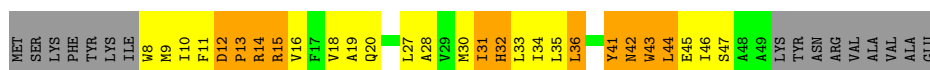
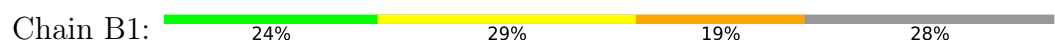
- Molecule 1: Light-harvesting protein B-875 alpha chain



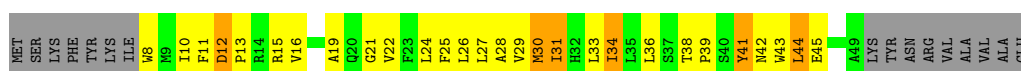
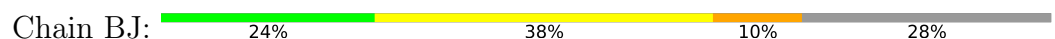
- Molecule 1: Light-harvesting protein B-875 alpha chain



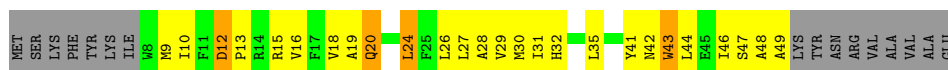
- Molecule 1: Light-harvesting protein B-875 alpha chain



- Molecule 1: Light-harvesting protein B-875 alpha chain



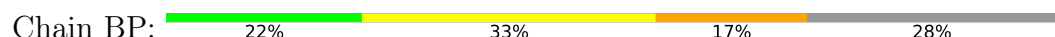
- Molecule 1: Light-harvesting protein B-875 alpha chain

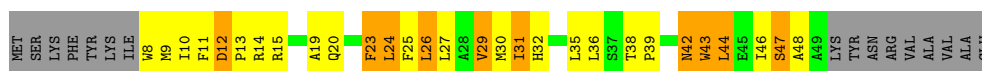


- Molecule 1: Light-harvesting protein B-875 alpha chain

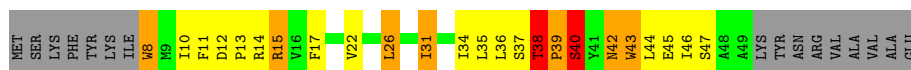
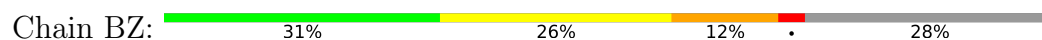


- Molecule 1: Light-harvesting protein B-875 alpha chain

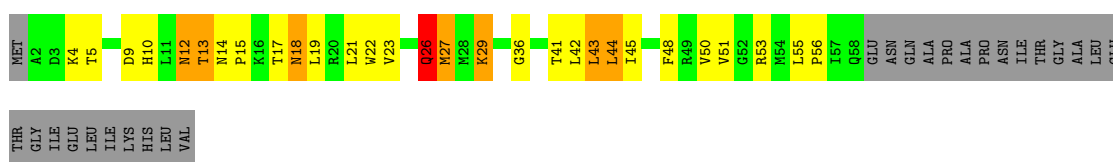




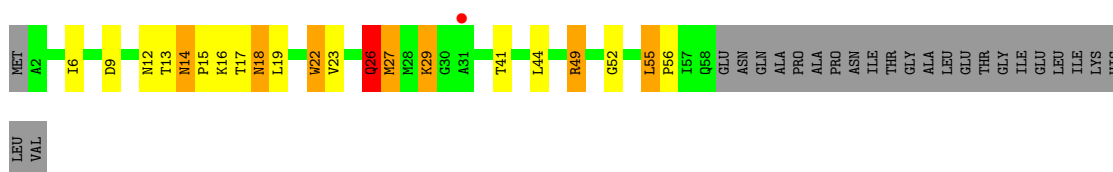
- Molecule 1: Light-harvesting protein B-875 alpha chain



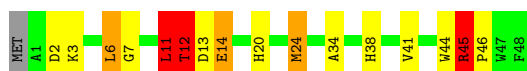
- Molecule 2: Intrinsic membrane protein PufX



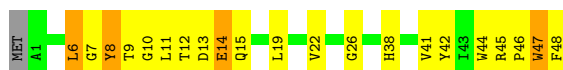
- Molecule 2: Intrinsic membrane protein PufX



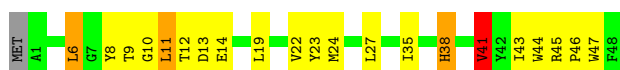
- Molecule 3: Light-harvesting protein B-875 beta chain



- Molecule 3: Light-harvesting protein B-875 beta chain

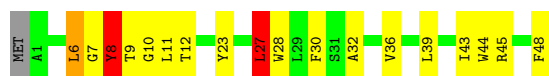


- Molecule 3: Light-harvesting protein B-875 beta chain



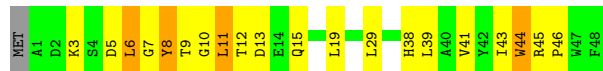
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AQ:  61% 31% . . .



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain A6:  57% 33% 8% .



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AU:  45% 45% 8% .

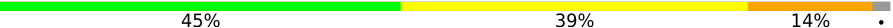


- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AW:  47% 45% . . .



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AY:  45% 39% 14% .



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain A4:  2% 41% 41% 14% . .



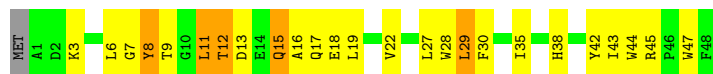
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain A8:  55% 31% 12% .



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AE:  47% 41% 10%



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AG:  45% 47% 6%



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AI:  47% 43% 8%



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain AK:  55% 33% 10%



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BS:  49% 37% 8%



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain B9:  53% 41% 6%



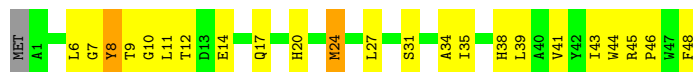
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BO:  61% 29% 6%



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BQ:  51% 43% ..



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain B6:  47% 39% 12% .



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BU:  55% 35% 6% ..



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BW:  57% 37% ...



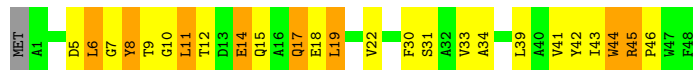
- Molecule 3: Light-harvesting protein B-875 beta chain

Chain BY:  65% 22% 10% .



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain B4:  47% 35% 16% .



- Molecule 3: Light-harvesting protein B-875 beta chain

Chain B8:  55% 33% 10% .



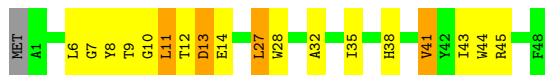
- Molecule 3: Light-harvesting protein B-875 beta chain



- Molecule 3: Light-harvesting protein B-875 beta chain



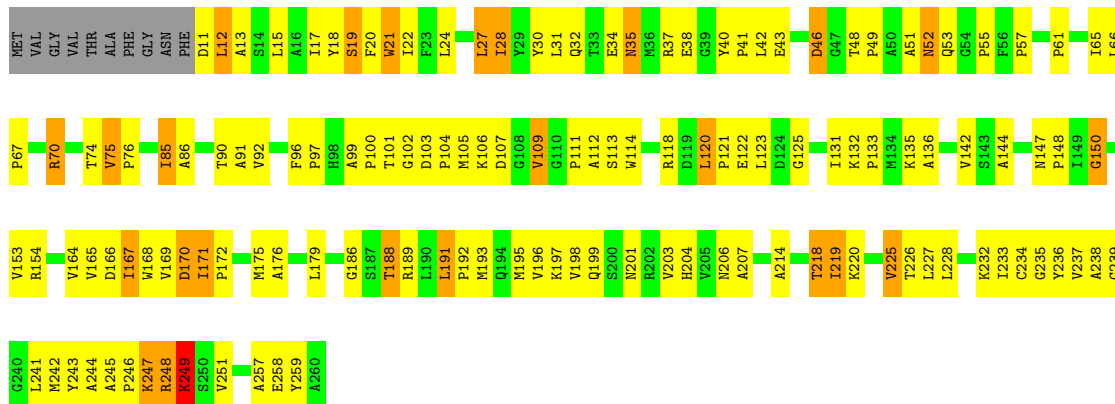
- Molecule 3: Light-harvesting protein B-875 beta chain



- Molecule 3: Light-harvesting protein B-875 beta chain



- Molecule 4: Reaction center protein H chain



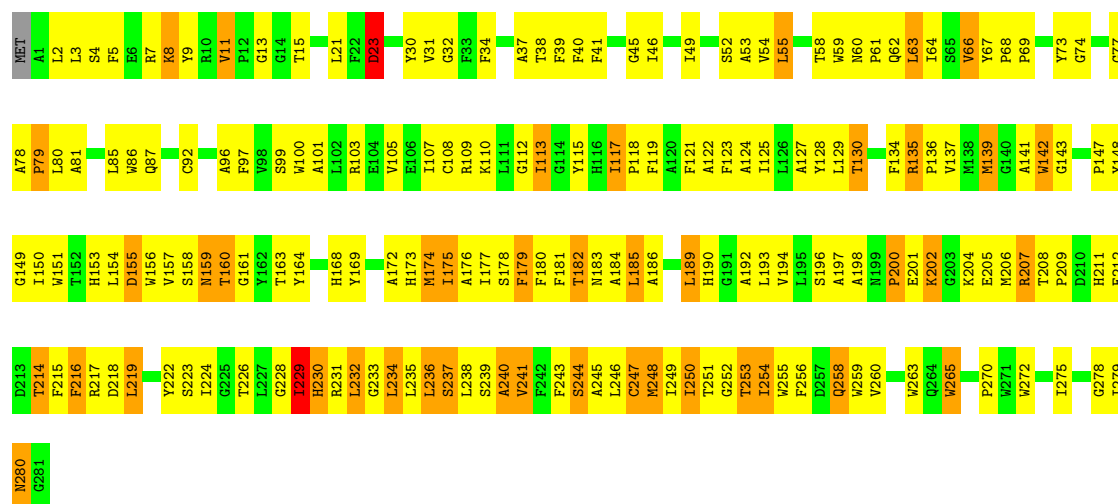
- Molecule 4: Reaction center protein H chain





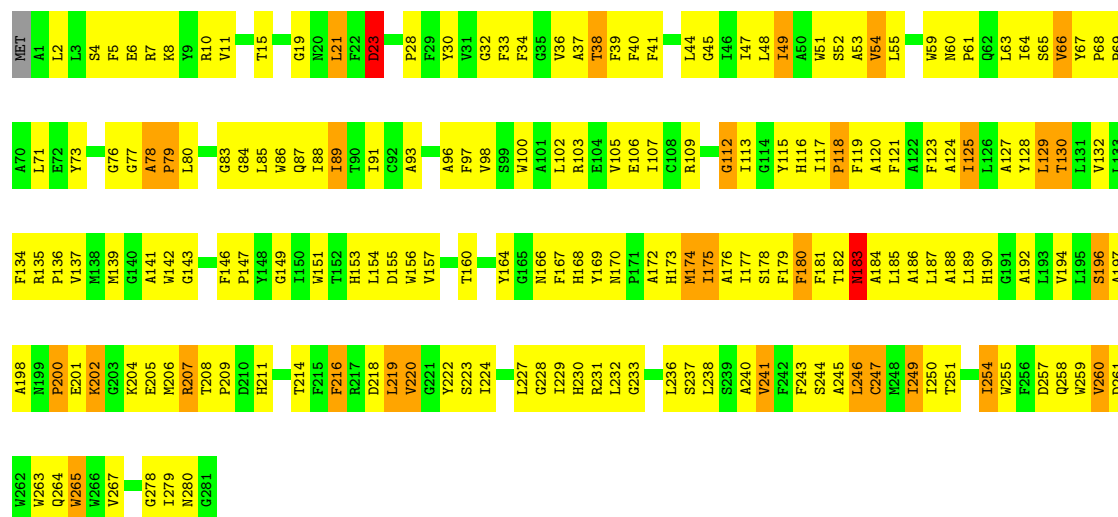
• Molecule 5: Reaction center protein L chain

Chain AL: 34% 50% 15%

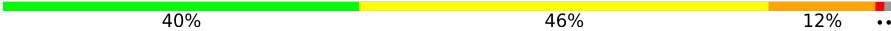


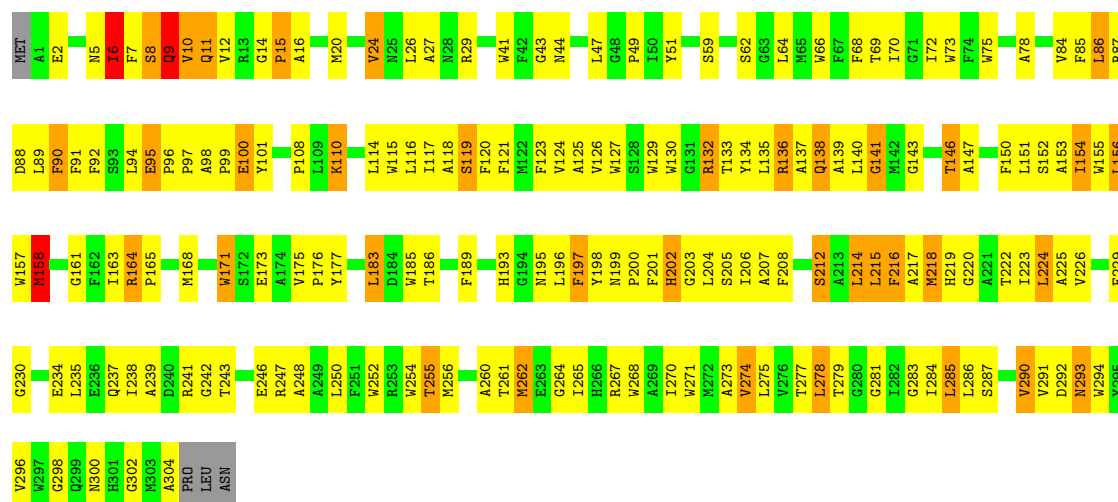
• Molecule 5: Reaction center protein L chain

Chain BL: 34% 55% 11%



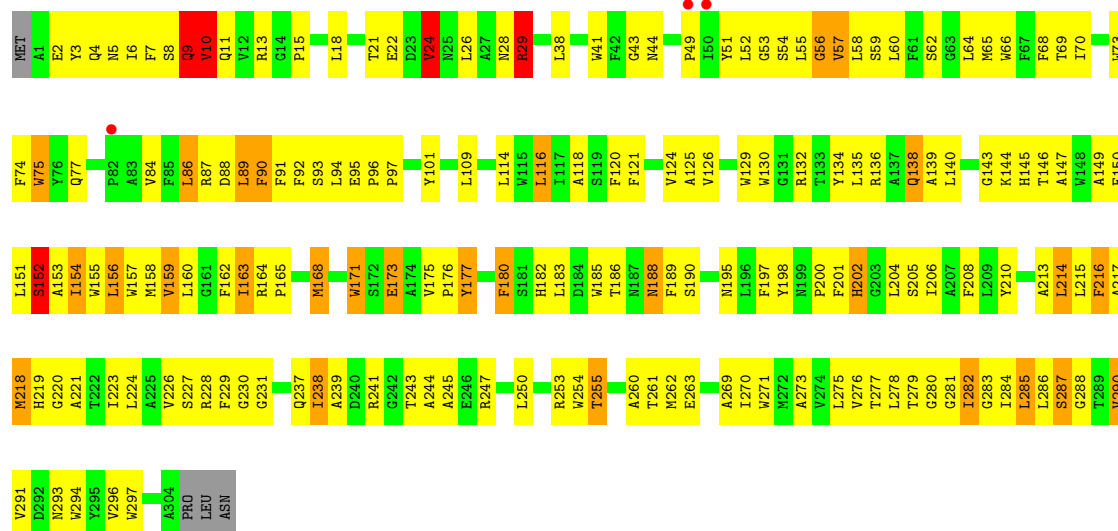
• Molecule 6: Reaction center protein M chain

Chain AM:  40% 46% 12% ..



• Molecule 6: Reaction center protein M chain

Chain BM:  40% 48% 9% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.08Å 415.07Å 129.82Å 90.00° 105.75° 90.00°	Depositor
Resolution (Å)	20.39 – 7.78 20.39 – 8.00	Depositor EDS
% Data completeness (in resolution range)	73.7 (20.39-7.78) 73.4 (20.39-8.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 7.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.228 , 0.258 0.236 , 0.269	Depositor DCC
R_{free} test set	319 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	430.3	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 392.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.178 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.883 for H, K, L 0.117 for -H, -K, H+L	Depositor
Outliers	0 of 6309 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	38108	wwPDB-VP
Average B, all atoms (Å ²)	258.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, FE2, PO4, BCL, U10, BPH

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	A1	0.30	0/356	0.62	0/486
1	A2	0.30	0/356	0.64	0/486
1	A3	0.33	0/356	0.56	0/486
1	A5	0.29	0/356	0.59	0/486
1	A7	0.32	0/356	0.61	1/486 (0.2%)
1	AD	0.32	0/356	0.58	0/486
1	AF	0.32	0/356	0.55	0/486
1	AJ	0.29	0/356	0.61	0/486
1	AN	0.32	0/356	0.67	0/486
1	AP	0.29	0/356	0.64	0/486
1	AT	0.32	0/356	0.58	0/486
1	AV	0.30	0/356	0.63	0/486
1	AX	0.31	0/356	0.58	0/486
1	AZ	0.33	0/356	0.59	0/486
1	B1	0.30	0/356	0.60	0/486
1	B2	0.31	0/356	0.64	0/486
1	B3	0.29	0/356	0.60	0/486
1	B5	0.29	0/356	0.60	0/486
1	B7	0.34	0/356	0.61	0/486
1	BD	0.33	0/356	0.61	0/486
1	BF	0.31	0/356	0.57	0/486
1	BJ	0.30	0/356	0.58	0/486
1	BN	0.31	0/356	0.64	0/486
1	BP	0.31	0/356	0.57	0/486
1	BT	0.31	0/356	0.65	0/486
1	BV	0.31	0/356	0.68	0/486
1	BX	0.37	0/356	0.66	0/486
1	BZ	0.32	0/356	0.58	0/486
2	AB	0.30	0/464	0.60	0/626
2	BB	0.30	0/464	0.58	0/626
3	A4	0.26	0/401	0.55	0/547
3	A6	0.28	0/401	0.66	0/547

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	A8	0.26	0/401	0.53	0/547
3	A9	0.27	0/401	0.57	0/547
3	AE	0.28	0/401	0.55	0/547
3	AG	0.28	0/401	0.67	0/547
3	AI	0.26	0/401	0.55	0/547
3	AK	0.27	0/401	0.55	0/547
3	AO	0.26	0/401	0.54	0/547
3	AQ	0.28	0/401	0.56	0/547
3	AS	0.29	0/401	0.58	0/547
3	AU	0.28	0/401	0.57	0/547
3	AW	0.25	0/400	0.55	0/545
3	AY	0.27	0/401	0.67	0/547
3	B4	0.28	0/401	0.50	0/547
3	B6	0.28	0/401	0.62	0/547
3	B8	0.25	0/401	0.58	0/547
3	B9	0.26	0/401	0.52	0/547
3	BE	0.27	0/401	0.53	0/547
3	BG	0.26	0/401	0.57	0/547
3	BI	0.27	0/401	0.63	0/547
3	BK	0.26	0/401	0.56	0/547
3	BO	0.27	0/401	0.60	0/547
3	BQ	0.28	0/401	0.55	0/547
3	BS	0.29	0/401	0.56	0/547
3	BU	0.27	0/401	0.64	0/547
3	BW	0.25	0/400	0.54	0/545
3	BY	0.26	0/401	0.52	0/547
4	AH	0.31	0/1950	0.67	1/2652 (0.0%)
4	BH	0.31	0/1950	0.67	0/2652
5	AL	0.61	7/2320 (0.3%)	0.67	1/3175 (0.0%)
5	BL	0.70	10/2320 (0.4%)	0.68	2/3175 (0.1%)
6	AM	0.55	5/2524 (0.2%)	0.61	0/3445
6	BM	0.48	1/2524 (0.0%)	0.63	0/3445
All	All	0.40	23/35710 (0.1%)	0.62	5/48716 (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
1	A7	0	1
1	AZ	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B1	0	1
1	B7	0	1
3	AQ	0	1
3	AS	0	2
3	BS	0	2
4	BH	0	1
5	AL	0	3
6	AM	0	3
6	BM	0	1
All	All	0	17

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	BM	152	SER	CB-OG	14.57	1.71	1.42
5	BL	196	SER	CB-OG	11.35	1.64	1.42
6	AM	158	MET	SD-CE	11.25	2.07	1.79
5	BL	155	ASP	CG-OD2	10.88	1.46	1.25
5	BL	155	ASP	CG-OD1	10.44	1.45	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AL	159	ASN	OD1-CG-ND2	7.61	130.21	122.60
5	BL	183	ASN	CB-CG-ND2	-7.19	105.61	116.40
5	BL	183	ASN	OD1-CG-ND2	5.71	128.31	122.60
4	AH	257	ALA	CB-CA-C	-5.22	110.58	116.63
1	A7	9	MET	CB-CA-C	-5.16	110.21	117.23

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A7	38	THR	Peptide
3	AQ	27	LEU	Peptide
3	AS	11	LEU	Peptide
3	AS	12	THR	Peptide
1	AZ	38	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	345	0	355	27	0
1	A2	345	0	355	39	0
1	A3	345	0	355	19	0
1	A5	345	0	355	25	0
1	A7	345	0	355	35	0
1	AD	345	0	355	29	0
1	AF	345	0	355	18	0
1	AJ	345	0	355	22	0
1	AN	345	0	355	26	0
1	AP	345	0	355	25	0
1	AT	345	0	355	20	0
1	AV	345	0	355	16	0
1	AX	345	0	355	17	0
1	AZ	345	0	355	25	0
1	B1	345	0	355	28	0
1	B2	345	0	355	25	0
1	B3	345	0	355	15	0
1	B5	345	0	355	21	0
1	B7	345	0	355	39	0
1	BD	345	0	355	37	0
1	BF	345	0	355	25	0
1	BJ	345	0	355	22	0
1	BN	345	0	355	25	0
1	BP	345	0	355	29	0
1	BT	345	0	355	18	0
1	BV	345	0	355	15	0
1	BX	345	0	355	16	0
1	BZ	345	0	355	32	0
2	AB	452	0	462	21	0
2	BB	452	0	462	21	0
3	A4	388	0	370	34	0
3	A6	388	0	370	24	0
3	A8	388	0	370	19	0
3	A9	388	0	370	25	0
3	AE	388	0	370	33	0
3	AG	388	0	370	22	0
3	AI	388	0	370	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AK	388	0	370	23	0
3	AO	388	0	370	22	0
3	AQ	388	0	370	18	0
3	AS	388	0	370	32	0
3	AU	388	0	370	24	0
3	AW	387	0	363	28	0
3	AY	388	0	370	21	0
3	B4	388	0	370	17	0
3	B6	388	0	370	30	0
3	B8	388	0	370	20	0
3	B9	388	0	370	20	0
3	BE	388	0	370	38	0
3	BG	388	0	370	12	0
3	BI	388	0	370	27	0
3	BK	388	0	370	23	0
3	BO	388	0	370	23	0
3	BQ	388	0	370	28	0
3	BS	388	0	370	37	0
3	BU	388	0	370	19	0
3	BW	387	0	363	23	0
3	BY	388	0	370	12	0
4	AH	1901	0	1909	125	0
4	BH	1901	0	1909	111	0
5	AL	2232	0	2187	261	0
5	BL	2232	0	2187	292	0
6	AM	2427	0	2338	246	0
6	BM	2427	0	2338	224	0
7	A1	46	0	35	2	0
7	A2	46	0	35	3	0
7	A3	46	0	35	5	0
7	A4	46	0	35	4	0
7	A6	92	0	70	15	0
7	A7	46	0	35	9	0
7	A8	46	0	35	9	0
7	A9	46	0	35	10	0
7	AD	92	0	70	21	0
7	AF	46	0	35	14	0
7	AG	46	0	35	2	0
7	AI	46	0	35	10	0
7	AJ	46	0	35	8	0
7	AK	46	0	35	5	0
7	AL	132	0	148	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AM	132	0	148	50	0
7	AN	46	0	35	4	0
7	AO	46	0	35	17	0
7	AP	92	0	70	22	0
7	AS	46	0	35	11	0
7	AT	92	0	70	14	0
7	AV	46	0	35	6	0
7	AW	46	0	35	1	0
7	AY	92	0	70	6	0
7	AZ	46	0	35	11	0
7	B1	46	0	35	2	0
7	B2	46	0	35	8	0
7	B3	46	0	35	5	0
7	B4	46	0	35	2	0
7	B5	46	0	35	1	0
7	B6	46	0	35	4	0
7	B7	46	0	35	2	0
7	B8	46	0	35	12	0
7	B9	46	0	35	7	0
7	BD	92	0	70	13	0
7	BF	92	0	70	12	0
7	BI	46	0	35	14	0
7	BK	92	0	70	17	0
7	BL	198	0	222	84	0
7	BM	66	0	74	27	0
7	BO	92	0	70	24	0
7	BP	92	0	70	27	0
7	BT	46	0	35	6	0
7	BU	46	0	35	7	0
7	BV	92	0	70	12	0
7	BY	92	0	70	7	0
7	BZ	92	0	70	24	0
8	AL	65	0	76	25	0
8	AM	65	0	76	17	0
8	BL	65	0	76	47	0
8	BM	65	0	76	27	0
9	AL	48	0	63	19	0
9	AM	48	0	63	11	0
9	BL	48	0	63	17	0
10	AL	5	0	0	0	0
10	BL	5	0	0	0	0
11	AM	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	BL	1	0	0	0	0
12	AM	42	0	60	9	0
All	All	38108	0	37183	2728	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 36.

The worst 5 of 2728 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)
3:BS:12:THR:CB	3:BS:13:ASP:HB2	1.15	1.62
5:BL:219:LEU:CD2	5:BL:219:LEU:CG	1.78	1.62
5:BL:219:LEU:CG	5:BL:219:LEU:CD1	1.75	1.58
6:AM:262:MET:CB	6:AM:262:MET:CG	1.75	1.57
5:BL:125:ILE:CG1	5:BL:125:ILE:CD1	1.75	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	A1	40/58 (69%)	29 (72%)	8 (20%)	3 (8%)	1	10
1	A2	40/58 (69%)	27 (68%)	7 (18%)	6 (15%)	0	3
1	A3	40/58 (69%)	24 (60%)	13 (32%)	3 (8%)	1	10
1	A5	40/58 (69%)	23 (58%)	12 (30%)	5 (12%)	0	4
1	A7	40/58 (69%)	23 (58%)	11 (28%)	6 (15%)	0	3
1	AD	40/58 (69%)	22 (55%)	13 (32%)	5 (12%)	0	4
1	AF	40/58 (69%)	26 (65%)	12 (30%)	2 (5%)	1	16
1	AJ	40/58 (69%)	29 (72%)	7 (18%)	4 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AN	40/58 (69%)	29 (72%)	6 (15%)	5 (12%)	0	4
1	AP	40/58 (69%)	28 (70%)	10 (25%)	2 (5%)	1	16
1	AT	40/58 (69%)	26 (65%)	9 (22%)	5 (12%)	0	4
1	AV	40/58 (69%)	28 (70%)	11 (28%)	1 (2%)	4	26
1	AX	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	0	7
1	AZ	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	0	7
1	B1	40/58 (69%)	28 (70%)	8 (20%)	4 (10%)	0	7
1	B2	40/58 (69%)	30 (75%)	7 (18%)	3 (8%)	1	10
1	B3	40/58 (69%)	27 (68%)	12 (30%)	1 (2%)	4	26
1	B5	40/58 (69%)	24 (60%)	12 (30%)	4 (10%)	0	7
1	B7	40/58 (69%)	23 (58%)	12 (30%)	5 (12%)	0	4
1	BD	40/58 (69%)	26 (65%)	11 (28%)	3 (8%)	1	10
1	BF	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	0	7
1	BJ	40/58 (69%)	27 (68%)	10 (25%)	3 (8%)	1	10
1	BN	40/58 (69%)	31 (78%)	8 (20%)	1 (2%)	4	26
1	BP	40/58 (69%)	26 (65%)	11 (28%)	3 (8%)	1	10
1	BT	40/58 (69%)	25 (62%)	13 (32%)	2 (5%)	1	16
1	BV	40/58 (69%)	29 (72%)	9 (22%)	2 (5%)	1	16
1	BX	40/58 (69%)	28 (70%)	11 (28%)	1 (2%)	4	26
1	BZ	40/58 (69%)	25 (62%)	11 (28%)	4 (10%)	0	7
2	AB	55/82 (67%)	24 (44%)	24 (44%)	7 (13%)	0	4
2	BB	55/82 (67%)	28 (51%)	22 (40%)	5 (9%)	0	8
3	A4	46/49 (94%)	30 (65%)	13 (28%)	3 (6%)	1	12
3	A6	46/49 (94%)	36 (78%)	9 (20%)	1 (2%)	5	29
3	A8	46/49 (94%)	30 (65%)	14 (30%)	2 (4%)	2	17
3	A9	46/49 (94%)	35 (76%)	8 (17%)	3 (6%)	1	12
3	AE	46/49 (94%)	34 (74%)	10 (22%)	2 (4%)	2	17
3	AG	46/49 (94%)	29 (63%)	16 (35%)	1 (2%)	5	29
3	AI	46/49 (94%)	34 (74%)	11 (24%)	1 (2%)	5	29
3	AK	46/49 (94%)	33 (72%)	10 (22%)	3 (6%)	1	12
3	AO	46/49 (94%)	33 (72%)	12 (26%)	1 (2%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AQ	46/49 (94%)	40 (87%)	5 (11%)	1 (2%)	5	29
3	AS	46/49 (94%)	32 (70%)	12 (26%)	2 (4%)	2	17
3	AU	46/49 (94%)	31 (67%)	10 (22%)	5 (11%)	0	6
3	AW	46/49 (94%)	33 (72%)	11 (24%)	2 (4%)	2	17
3	AY	46/49 (94%)	31 (67%)	13 (28%)	2 (4%)	2	17
3	B4	46/49 (94%)	27 (59%)	14 (30%)	5 (11%)	0	6
3	B6	46/49 (94%)	33 (72%)	12 (26%)	1 (2%)	5	29
3	B8	46/49 (94%)	30 (65%)	14 (30%)	2 (4%)	2	17
3	B9	46/49 (94%)	35 (76%)	8 (17%)	3 (6%)	1	12
3	BE	46/49 (94%)	33 (72%)	12 (26%)	1 (2%)	5	29
3	BG	46/49 (94%)	31 (67%)	15 (33%)	0	100	100
3	BI	46/49 (94%)	35 (76%)	11 (24%)	0	100	100
3	BK	46/49 (94%)	29 (63%)	15 (33%)	2 (4%)	2	17
3	BO	46/49 (94%)	33 (72%)	10 (22%)	3 (6%)	1	12
3	BQ	46/49 (94%)	38 (83%)	8 (17%)	0	100	100
3	BS	46/49 (94%)	31 (67%)	12 (26%)	3 (6%)	1	12
3	BU	46/49 (94%)	29 (63%)	13 (28%)	4 (9%)	0	9
3	BW	46/49 (94%)	32 (70%)	12 (26%)	2 (4%)	2	17
3	BY	46/49 (94%)	33 (72%)	11 (24%)	2 (4%)	2	17
4	AH	248/260 (95%)	178 (72%)	59 (24%)	11 (4%)	2	17
4	BH	248/260 (95%)	198 (80%)	43 (17%)	7 (3%)	4	24
5	AL	279/282 (99%)	203 (73%)	61 (22%)	15 (5%)	1	15
5	BL	279/282 (99%)	208 (75%)	61 (22%)	10 (4%)	2	20
6	AM	303/308 (98%)	223 (74%)	63 (21%)	17 (6%)	1	14
6	BM	303/308 (98%)	232 (77%)	56 (18%)	15 (5%)	1	16
All	All	4178/4860 (86%)	2942 (70%)	997 (24%)	239 (6%)	1	14

5 of 239 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A5	38	THR
1	A7	39	PRO
1	A7	41	TYR

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Mol	Chain	Res	Type
1	AD	10	ILE
1	A1	12	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	37/51 (72%)	31 (84%)	6 (16%)	2	11
1	A2	37/51 (72%)	31 (84%)	6 (16%)	2	11
1	A3	37/51 (72%)	29 (78%)	8 (22%)	1	6
1	A5	37/51 (72%)	32 (86%)	5 (14%)	4	14
1	A7	37/51 (72%)	27 (73%)	10 (27%)	0	3
1	AD	37/51 (72%)	30 (81%)	7 (19%)	1	8
1	AF	37/51 (72%)	32 (86%)	5 (14%)	4	14
1	AJ	37/51 (72%)	28 (76%)	9 (24%)	1	4
1	AN	37/51 (72%)	32 (86%)	5 (14%)	4	14
1	AP	37/51 (72%)	32 (86%)	5 (14%)	4	14
1	AT	37/51 (72%)	30 (81%)	7 (19%)	1	8
1	AV	37/51 (72%)	29 (78%)	8 (22%)	1	6
1	AX	37/51 (72%)	28 (76%)	9 (24%)	1	4
1	AZ	37/51 (72%)	29 (78%)	8 (22%)	1	6
1	B1	37/51 (72%)	28 (76%)	9 (24%)	1	4
1	B2	37/51 (72%)	32 (86%)	5 (14%)	4	14
1	B3	37/51 (72%)	28 (76%)	9 (24%)	1	4
1	B5	37/51 (72%)	33 (89%)	4 (11%)	6	21
1	B7	37/51 (72%)	29 (78%)	8 (22%)	1	6
1	BD	37/51 (72%)	25 (68%)	12 (32%)	0	2
1	BF	37/51 (72%)	32 (86%)	5 (14%)	4	14
1	BJ	37/51 (72%)	30 (81%)	7 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BN	37/51 (72%)	32 (86%)	5 (14%)	4	14
1	BP	37/51 (72%)	28 (76%)	9 (24%)	1	4
1	BT	37/51 (72%)	29 (78%)	8 (22%)	1	6
1	BV	37/51 (72%)	29 (78%)	8 (22%)	1	6
1	BX	37/51 (72%)	29 (78%)	8 (22%)	1	6
1	BZ	37/51 (72%)	29 (78%)	8 (22%)	1	6
2	AB	46/66 (70%)	35 (76%)	11 (24%)	1	4
2	BB	46/66 (70%)	37 (80%)	9 (20%)	1	7
3	A4	39/40 (98%)	28 (72%)	11 (28%)	0	3
3	A6	39/40 (98%)	34 (87%)	5 (13%)	4	15
3	A8	39/40 (98%)	32 (82%)	7 (18%)	2	9
3	A9	39/40 (98%)	35 (90%)	4 (10%)	7	23
3	AE	39/40 (98%)	32 (82%)	7 (18%)	2	9
3	AG	39/40 (98%)	32 (82%)	7 (18%)	2	9
3	AI	39/40 (98%)	33 (85%)	6 (15%)	2	12
3	AK	39/40 (98%)	36 (92%)	3 (8%)	12	32
3	AO	39/40 (98%)	32 (82%)	7 (18%)	2	9
3	AQ	39/40 (98%)	34 (87%)	5 (13%)	4	15
3	AS	39/40 (98%)	34 (87%)	5 (13%)	4	15
3	AU	39/40 (98%)	35 (90%)	4 (10%)	7	23
3	AW	39/40 (98%)	34 (87%)	5 (13%)	4	15
3	AY	39/40 (98%)	30 (77%)	9 (23%)	1	5
3	B4	39/40 (98%)	31 (80%)	8 (20%)	1	7
3	B6	39/40 (98%)	33 (85%)	6 (15%)	2	12
3	B8	39/40 (98%)	33 (85%)	6 (15%)	2	12
3	B9	39/40 (98%)	36 (92%)	3 (8%)	12	32
3	BE	39/40 (98%)	31 (80%)	8 (20%)	1	7
3	BG	39/40 (98%)	31 (80%)	8 (20%)	1	7
3	BI	39/40 (98%)	35 (90%)	4 (10%)	7	23
3	BK	39/40 (98%)	33 (85%)	6 (15%)	2	12
3	BO	39/40 (98%)	35 (90%)	4 (10%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BQ	39/40 (98%)	35 (90%)	4 (10%)	7	23
3	BS	39/40 (98%)	31 (80%)	8 (20%)	1	7
3	BU	39/40 (98%)	37 (95%)	2 (5%)	21	42
3	BW	39/40 (98%)	36 (92%)	3 (8%)	12	32
3	BY	39/40 (98%)	33 (85%)	6 (15%)	2	12
4	AH	201/208 (97%)	165 (82%)	36 (18%)	2	9
4	BH	201/208 (97%)	176 (88%)	25 (12%)	4	17
5	AL	220/221 (100%)	179 (81%)	41 (19%)	1	8
5	BL	220/221 (100%)	180 (82%)	40 (18%)	2	9
6	AM	238/241 (99%)	198 (83%)	40 (17%)	2	10
6	BM	238/241 (99%)	193 (81%)	45 (19%)	1	8
All	All	3538/4020 (88%)	2927 (83%)	611 (17%)	2	9

5 of 611 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B4	14	GLU
6	BM	29	ARG
3	BE	8	TYR
3	B4	11	LEU
4	BH	219	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
4	BH	201	ASN
6	BM	187	ASN
5	BL	153	HIS
5	BL	230	HIS
3	AI	38	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 76 ligands modelled in this entry, 2 are monoatomic - leaving 74 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	$\# Z > 2$
7	BCL	AS	101	-	49,54,74	2.31	13 (26%)	55,91,115	2.73	15 (27%)
7	BCL	AL	301	-	69,74,74	1.85	11 (15%)	79,115,115	2.29	20 (25%)
9	U10	AM	405	-	48,48,63	2.03	4 (8%)	60,61,79	1.71	17 (28%)
7	BCL	BF	102	-	49,54,74	2.39	15 (30%)	55,91,115	2.81	16 (29%)
7	BCL	A3	101	-	49,54,74	2.35	14 (28%)	55,91,115	2.78	16 (29%)
7	BCL	B4	101	-	49,54,74	2.37	14 (28%)	55,91,115	2.79	16 (29%)
7	BCL	BV	101	-	49,54,74	2.20	11 (22%)	55,91,115	2.59	17 (30%)
8	BPH	BL	304	-	59,70,70	2.95	16 (27%)	59,101,101	2.50	17 (28%)
7	BCL	A6	102	-	49,54,74	2.42	15 (30%)	55,91,115	2.82	16 (29%)
7	BCL	BD	101	-	49,54,74	2.27	11 (22%)	55,91,115	2.67	17 (30%)
7	BCL	AZ	101	-	49,54,74	2.35	14 (28%)	55,91,115	2.76	16 (29%)
7	BCL	BL	303	-	69,74,74	2.05	16 (23%)	79,115,115	2.41	20 (25%)
7	BCL	BY	101	-	49,54,74	2.37	15 (30%)	55,91,115	2.81	16 (29%)
7	BCL	AL	302	-	69,74,74	2.04	16 (23%)	79,115,115	2.46	20 (25%)
7	BCL	A9	101	-	49,54,74	2.37	14 (28%)	55,91,115	2.78	16 (29%)
7	BCL	BO	101	-	49,54,74	2.33	14 (28%)	55,91,115	2.75	16 (29%)
7	BCL	B6	101	-	49,54,74	2.40	15 (30%)	55,91,115	2.80	16 (29%)
7	BCL	B2	101	-	49,54,74	2.20	11 (22%)	55,91,115	2.62	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	BP	101	-	49,54,74	2.20	11 (22%)	55,91,115	2.62	18 (32%)
7	BCL	B7	101	-	49,54,74	2.26	14 (28%)	55,91,115	2.70	18 (32%)
7	BCL	BK	102	-	49,54,74	2.37	14 (28%)	55,91,115	2.80	16 (29%)
7	BCL	AK	101	-	49,54,74	2.23	11 (22%)	55,91,115	2.62	16 (29%)
7	BCL	A6	101	-	49,54,74	2.24	14 (28%)	55,91,115	2.66	18 (32%)
7	BCL	BI	101	-	49,54,74	2.40	15 (30%)	55,91,115	2.81	17 (30%)
7	BCL	BO	102	-	49,54,74	2.35	15 (30%)	55,91,115	2.74	16 (29%)
7	BCL	BV	102	-	49,54,74	2.22	14 (28%)	55,91,115	2.66	18 (32%)
7	BCL	AG	101	-	49,54,74	2.39	14 (28%)	55,91,115	2.82	16 (29%)
7	BCL	AY	101	-	49,54,74	2.35	14 (28%)	55,91,115	2.77	16 (29%)
7	BCL	BF	101	-	49,54,74	2.21	11 (22%)	55,91,115	2.63	17 (30%)
7	BCL	A4	101	-	49,54,74	2.39	14 (28%)	55,91,115	2.80	16 (29%)
7	BCL	AN	101	-	49,54,74	2.34	14 (28%)	55,91,115	2.77	16 (29%)
7	BCL	AM	401	-	69,74,74	1.84	11 (15%)	79,115,115	2.30	21 (26%)
10	PO4	BL	307	-	4,4,4	0.94	0	6,6,6	0.46	0
7	BCL	BZ	101	-	49,54,74	2.34	14 (28%)	55,91,115	2.76	16 (29%)
7	BCL	A2	101	-	49,54,74	2.24	14 (28%)	55,91,115	2.67	17 (30%)
7	BCL	BP	102	-	49,54,74	2.40	15 (30%)	55,91,115	2.79	16 (29%)
7	BCL	AI	101	-	49,54,74	2.38	15 (30%)	55,91,115	2.79	16 (29%)
7	BCL	B1	101	-	49,54,74	2.35	15 (30%)	55,91,115	2.79	15 (27%)
7	BCL	AO	101	-	49,54,74	2.34	15 (30%)	55,91,115	2.75	16 (29%)
7	BCL	AV	101	-	49,54,74	2.23	11 (22%)	55,91,115	2.61	18 (32%)
7	BCL	A7	101	-	49,54,74	2.23	13 (26%)	55,91,115	2.64	18 (32%)
7	BCL	A8	101	-	49,54,74	2.21	12 (24%)	55,91,115	2.63	18 (32%)
7	BCL	B9	101	-	49,54,74	2.36	14 (28%)	55,91,115	2.77	16 (29%)
7	BCL	B8	101	-	49,54,74	2.23	14 (28%)	55,91,115	2.66	18 (32%)
7	BCL	A1	101	-	49,54,74	2.36	14 (28%)	55,91,115	2.79	15 (27%)
7	BCL	AM	402	-	69,74,74	2.07	15 (21%)	79,115,115	2.43	19 (24%)
7	BCL	B5	101	-	49,54,74	2.25	14 (28%)	55,91,115	2.68	18 (32%)
7	BCL	BK	101	-	49,54,74	2.20	11 (22%)	55,91,115	2.59	18 (32%)
7	BCL	BL	301	-	69,74,74	1.90	12 (17%)	79,115,115	2.32	23 (29%)
7	BCL	BL	302	-	69,74,74	1.92	11 (15%)	79,115,115	2.31	19 (24%)
12	SPO	AM	406	-	41,41,41	1.14	2 (4%)	47,50,50	2.21	15 (31%)
9	U10	AL	304	-	48,48,63	1.37	2 (4%)	60,61,79	1.66	16 (26%)
7	BCL	AD	101	-	49,54,74	2.25	11 (22%)	55,91,115	2.65	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	BT	101	-	49,54,74	2.24	14 (28%)	55,91,115	2.65	18 (32%)
8	BPH	BM	402	-	59,70,70	2.94	14 (23%)	59,101,101	2.46	17 (28%)
7	BCL	AP	102	-	49,54,74	2.41	15 (30%)	55,91,115	2.82	17 (30%)
7	BCL	BM	401	-	69,74,74	2.36	18 (26%)	79,115,115	2.54	22 (27%)
7	BCL	BZ	102	-	49,54,74	2.37	14 (28%)	55,91,115	2.79	16 (29%)
8	BPH	AL	303	-	59,70,70	2.94	16 (27%)	59,101,101	2.50	17 (28%)
7	BCL	BD	102	-	49,54,74	2.38	15 (30%)	55,91,115	2.79	16 (29%)
9	U10	BL	306	-	48,48,63	1.44	3 (6%)	60,61,79	1.66	16 (26%)
7	BCL	BU	101	-	49,54,74	2.41	15 (30%)	55,91,115	2.82	16 (29%)
7	BCL	AT	102	-	49,54,74	2.42	15 (30%)	55,91,115	2.83	16 (29%)
7	BCL	AP	101	-	49,54,74	2.22	13 (26%)	55,91,115	2.65	19 (34%)
7	BCL	AY	102	-	49,54,74	2.40	15 (30%)	55,91,115	2.81	16 (29%)
7	BCL	B3	101	-	49,54,74	2.35	14 (28%)	55,91,115	2.78	15 (27%)
7	BCL	BY	102	-	49,54,74	2.40	15 (30%)	55,91,115	2.80	16 (29%)
7	BCL	AD	102	-	49,54,74	2.37	15 (30%)	55,91,115	2.78	16 (29%)
10	PO4	AL	305	-	4,4,4	0.96	0	6,6,6	0.47	0
7	BCL	AF	101	-	49,54,74	2.21	11 (22%)	55,91,115	2.65	18 (32%)
7	BCL	AJ	101	-	49,54,74	2.38	14 (28%)	55,91,115	2.80	16 (29%)
7	BCL	AW	101	-	49,54,74	2.24	14 (28%)	55,91,115	2.66	17 (30%)
8	BPH	AM	403	-	59,70,70	2.94	14 (23%)	59,101,101	2.47	17 (28%)
7	BCL	AT	101	-	49,54,74	2.25	14 (28%)	55,91,115	2.68	18 (32%)

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
7	BCL	AS	101	-	-	11/17/113/137	-
7	BCL	AL	301	-	-	18/41/137/137	-
9	U10	AM	405	-	-	8/45/69/87	0/1/1/1
7	BCL	BF	102	-	-	10/17/113/137	-
7	BCL	A3	101	-	-	10/17/113/137	-
7	BCL	B4	101	-	-	8/17/113/137	-
7	BCL	BV	101	-	-	11/17/113/137	-
8	BPH	BL	304	-	-	15/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	A6	102	-	-	10/17/113/137	-
7	BCL	BD	101	-	-	12/17/113/137	-
7	BCL	AZ	101	-	-	11/17/113/137	-
7	BCL	BL	303	-	-	18/41/137/137	-
7	BCL	BY	101	-	-	10/17/113/137	-
7	BCL	AL	302	-	-	21/41/137/137	-
7	BCL	A9	101	-	-	11/17/113/137	-
7	BCL	BO	101	-	-	15/17/113/137	-
7	BCL	B6	101	-	-	6/17/113/137	-
7	BCL	B2	101	-	-	12/17/113/137	-
7	BCL	BP	101	-	-	7/17/113/137	-
7	BCL	B7	101	-	-	7/17/113/137	-
7	BCL	BK	102	-	-	7/17/113/137	-
7	BCL	AK	101	-	-	13/17/113/137	-
7	BCL	A6	101	-	-	9/17/113/137	-
7	BCL	BI	101	-	-	12/17/113/137	-
7	BCL	BO	102	-	-	7/17/113/137	-
7	BCL	BV	102	-	-	12/17/113/137	-
7	BCL	AG	101	-	-	12/17/113/137	-
7	BCL	AY	101	-	-	13/17/113/137	-
7	BCL	BF	101	-	-	13/17/113/137	-
7	BCL	A4	101	-	-	8/17/113/137	-
7	BCL	AN	101	-	-	12/17/113/137	-
7	BCL	AM	401	-	-	23/41/137/137	-
7	BCL	BZ	101	-	-	11/17/113/137	-
7	BCL	A2	101	-	-	11/17/113/137	-
7	BCL	BP	102	-	-	6/17/113/137	-
7	BCL	AI	101	-	-	11/17/113/137	-
7	BCL	B1	101	-	-	9/17/113/137	-
7	BCL	AO	101	-	-	8/17/113/137	-
7	BCL	AV	101	-	-	13/17/113/137	-
7	BCL	A7	101	-	-	9/17/113/137	-
7	BCL	A8	101	-	-	8/17/113/137	-
7	BCL	B9	101	-	-	13/17/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	B8	101	-	-	9/17/113/137	-
7	BCL	A1	101	-	-	10/17/113/137	-
7	BCL	AM	402	-	-	22/41/137/137	-
7	BCL	B5	101	-	-	8/17/113/137	-
7	BCL	BK	101	-	-	13/17/113/137	-
7	BCL	BL	301	-	-	24/41/137/137	-
7	BCL	BL	302	-	-	17/41/137/137	-
12	SPO	AM	406	-	-	15/47/47/47	-
9	U10	AL	304	-	-	7/45/69/87	0/1/1/1
7	BCL	AD	101	-	-	13/17/113/137	-
7	BCL	BT	101	-	-	8/17/113/137	-
8	BPH	BM	402	-	-	22/37/105/105	0/5/6/6
7	BCL	AP	102	-	-	8/17/113/137	-
7	BCL	BM	401	-	-	19/41/137/137	-
7	BCL	BZ	102	-	-	12/17/113/137	-
8	BPH	AL	303	-	-	15/37/105/105	0/5/6/6
7	BCL	BD	102	-	-	10/17/113/137	-
9	U10	BL	306	-	-	9/45/69/87	0/1/1/1
7	BCL	BU	101	-	-	8/17/113/137	-
7	BCL	AT	102	-	-	9/17/113/137	-
7	BCL	AP	101	-	-	12/17/113/137	-
7	BCL	AY	102	-	-	13/17/113/137	-
7	BCL	B3	101	-	-	11/17/113/137	-
7	BCL	BY	102	-	-	9/17/113/137	-
7	BCL	AD	102	-	-	10/17/113/137	-
7	BCL	AF	101	-	-	14/17/113/137	-
7	BCL	AJ	101	-	-	7/17/113/137	-
7	BCL	AW	101	-	-	9/17/113/137	-
8	BPH	AM	403	-	-	22/37/105/105	0/5/6/6
7	BCL	AT	101	-	-	9/17/113/137	-

The worst 5 of 947 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BL	304	BPH	C3D-C4D	-12.16	1.24	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AL	303	BPH	C3D-C4D	-12.10	1.24	1.41
8	BM	402	BPH	C3D-C4D	-12.07	1.24	1.41
8	AM	403	BPH	C3D-C4D	-12.04	1.24	1.41
8	BM	402	BPH	C1D-C2D	10.88	1.51	1.39

The worst 5 of 1226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AT	102	BCL	C4A-NA-C1A	9.75	111.13	106.68
7	AM	402	BCL	C4A-NA-C1A	9.71	111.11	106.68
7	AG	101	BCL	C4A-NA-C1A	9.69	111.10	106.68
7	BU	101	BCL	C4A-NA-C1A	9.67	111.09	106.68
7	AP	102	BCL	C4A-NA-C1A	9.63	111.07	106.68

There are no chirality outliers.

5 of 845 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	AT	101	BCL	C1A-C2A-CAA-CBA
7	AT	101	BCL	C3A-C2A-CAA-CBA
7	AT	101	BCL	CAD-CBD-CGD-O1D
7	AT	101	BCL	CAD-CBD-CGD-O2D
7	AT	101	BCL	CBD-CGD-O2D-CED

There are no ring outliers.

72 monomers are involved in 652 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AS	101	BCL	11	0
7	AL	301	BCL	31	0
9	AM	405	U10	11	0
7	BF	102	BCL	1	0
7	A3	101	BCL	5	0
7	B4	101	BCL	2	0
7	BV	101	BCL	8	0
8	BL	304	BPH	47	0
7	A6	102	BCL	14	0
7	BD	101	BCL	8	0
7	AZ	101	BCL	11	0
7	BL	303	BCL	28	0
7	BY	101	BCL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AL	302	BCL	19	0
7	A9	101	BCL	10	0
7	BO	101	BCL	5	0
7	B6	101	BCL	4	0
7	B2	101	BCL	8	0
7	BP	101	BCL	15	0
7	B7	101	BCL	2	0
7	BK	102	BCL	7	0
7	AK	101	BCL	5	0
7	A6	101	BCL	1	0
7	BI	101	BCL	14	0
7	BO	102	BCL	19	0
7	BV	102	BCL	5	0
7	AG	101	BCL	2	0
7	AY	101	BCL	2	0
7	BF	101	BCL	11	0
7	A4	101	BCL	4	0
7	AN	101	BCL	4	0
7	AM	401	BCL	29	0
7	BZ	101	BCL	11	0
7	A2	101	BCL	3	0
7	BP	102	BCL	12	0
7	AI	101	BCL	10	0
7	B1	101	BCL	2	0
7	AO	101	BCL	17	0
7	AV	101	BCL	6	0
7	A7	101	BCL	9	0
7	A8	101	BCL	9	0
7	B9	101	BCL	7	0
7	B8	101	BCL	12	0
7	A1	101	BCL	2	0
7	AM	402	BCL	22	0
7	B5	101	BCL	1	0
7	BK	101	BCL	10	0
7	BL	301	BCL	15	0
7	BL	302	BCL	46	0
12	AM	406	SPO	9	0
9	AL	304	U10	19	0
7	AD	101	BCL	8	0
7	BT	101	BCL	6	0
8	BM	402	BPH	27	0
7	AP	102	BCL	8	0

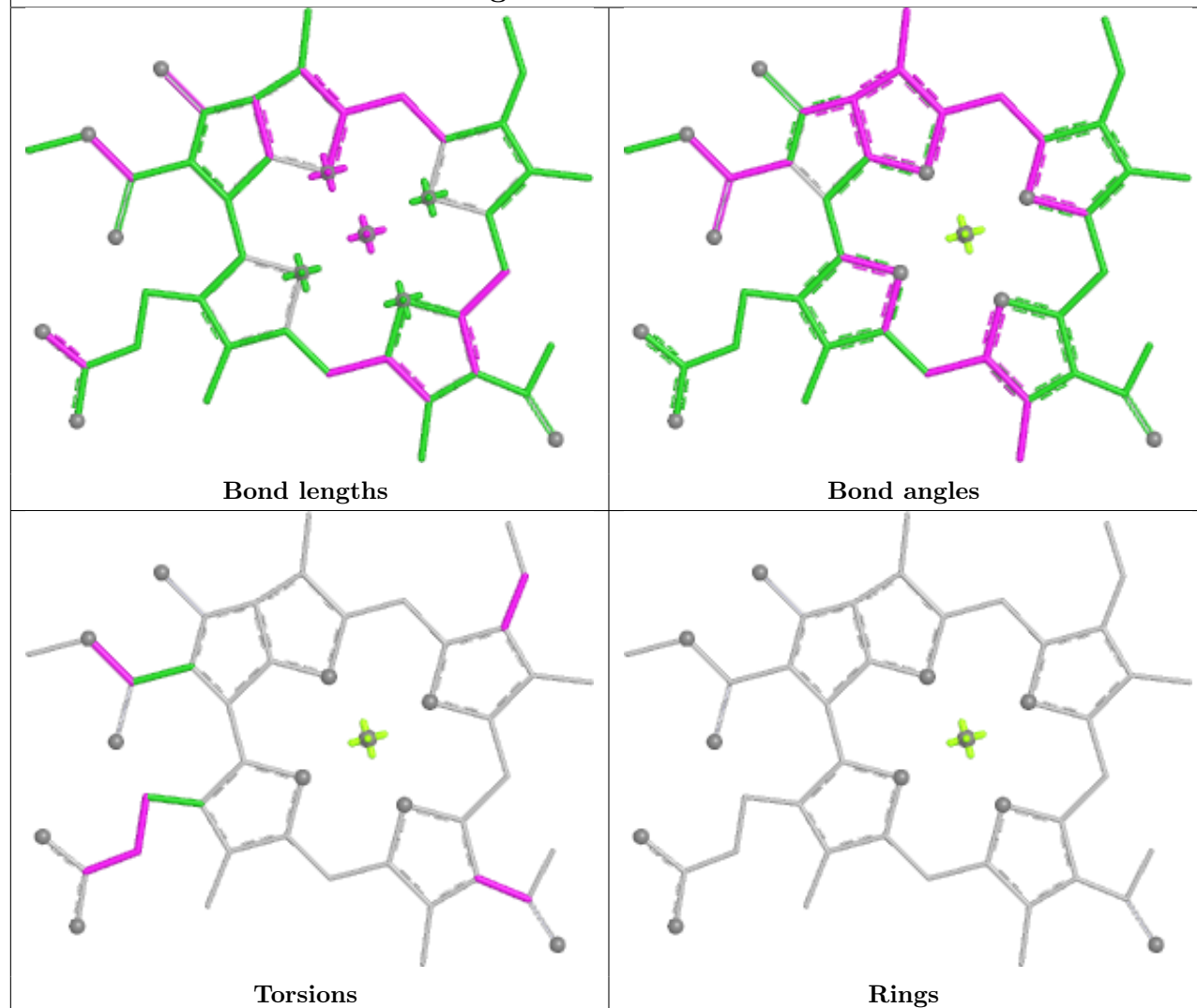
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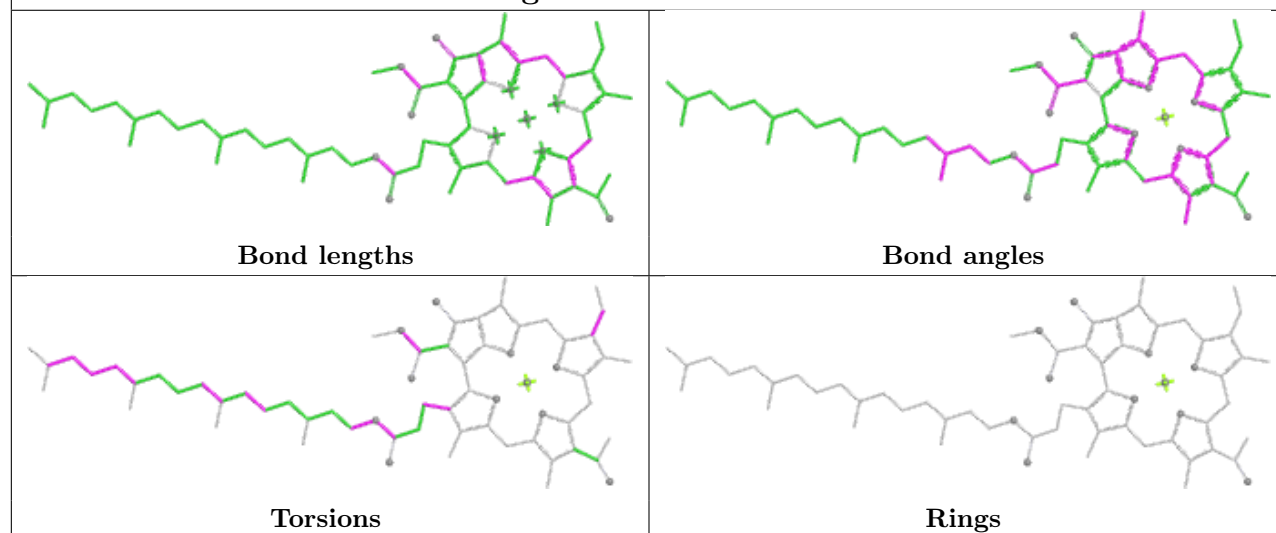
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	BM	401	BCL	27	0
7	BZ	102	BCL	13	0
8	AL	303	BPH	25	0
7	BD	102	BCL	5	0
9	BL	306	U10	17	0
7	BU	101	BCL	7	0
7	AT	102	BCL	13	0
7	AP	101	BCL	14	0
7	AY	102	BCL	4	0
7	B3	101	BCL	5	0
7	BY	102	BCL	5	0
7	AD	102	BCL	14	0
7	AF	101	BCL	14	0
7	AJ	101	BCL	8	0
7	AW	101	BCL	1	0
8	AM	403	BPH	17	0
7	AT	101	BCL	6	0

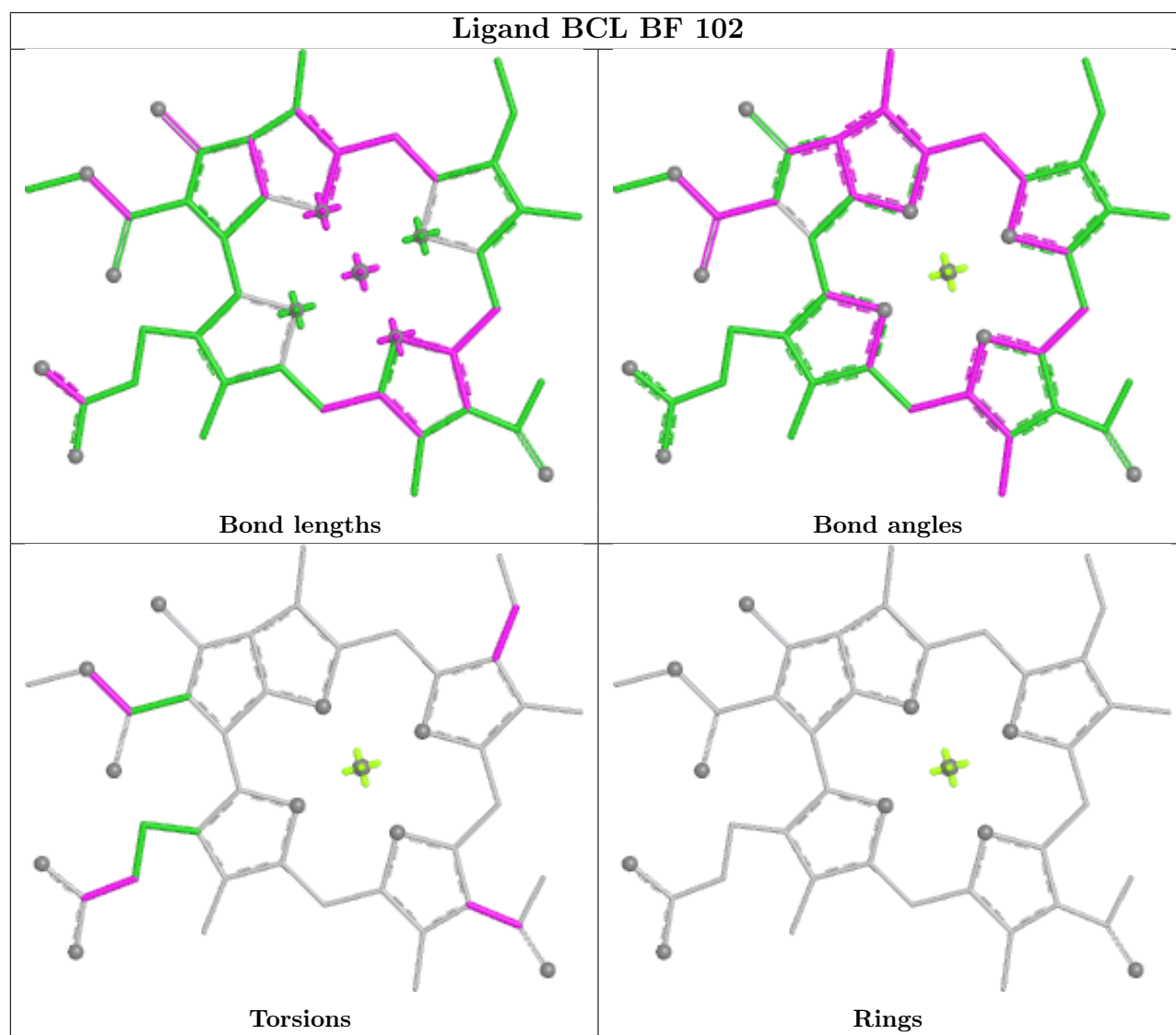
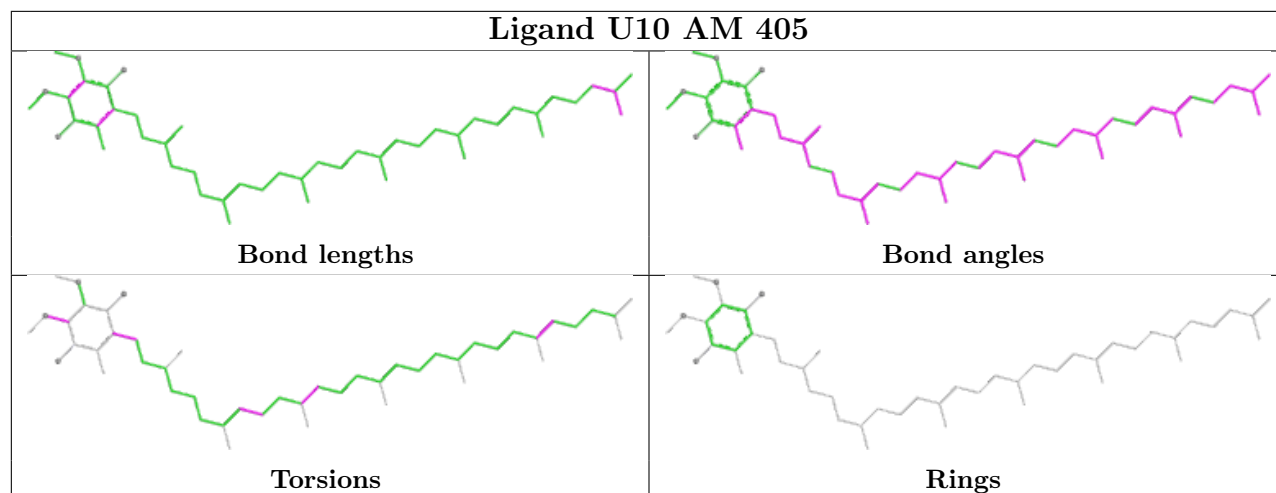
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand BCL AS 101

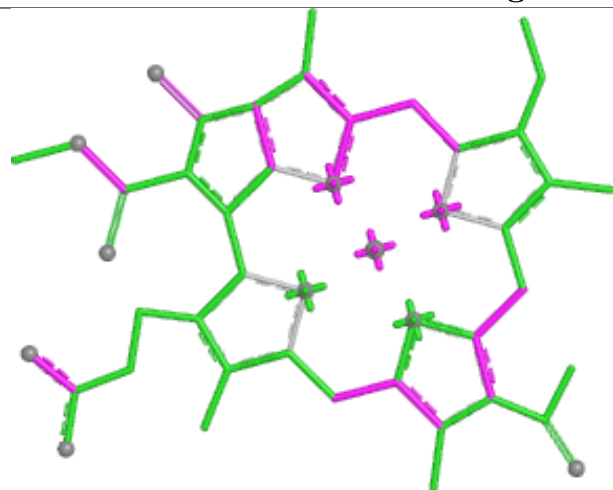


Ligand BCL AL 301

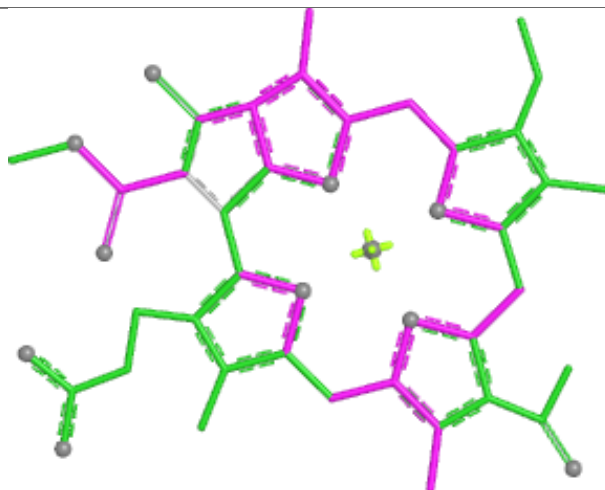




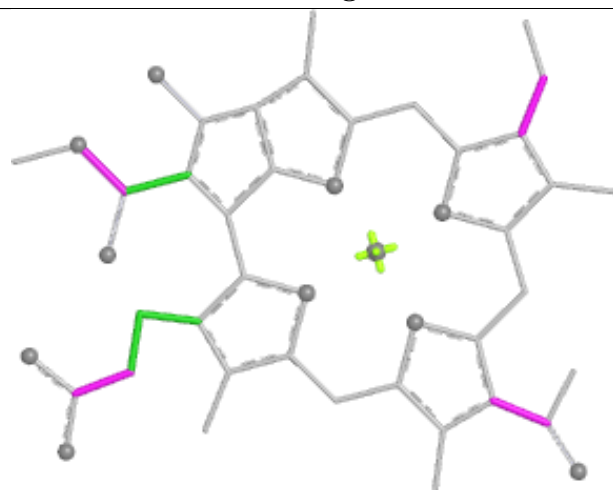
Ligand BCL A3 101



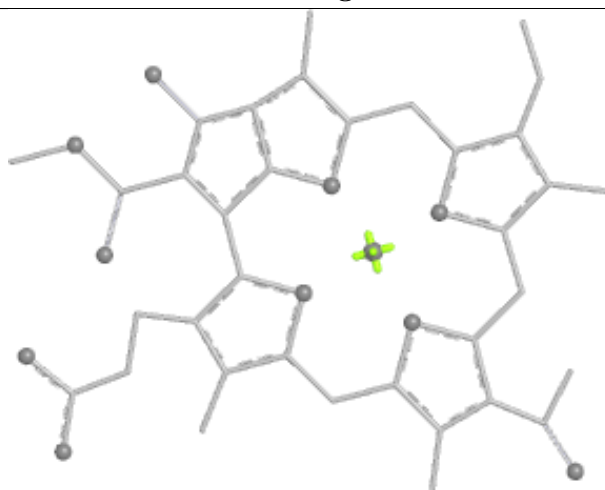
Bond lengths



Bond angles

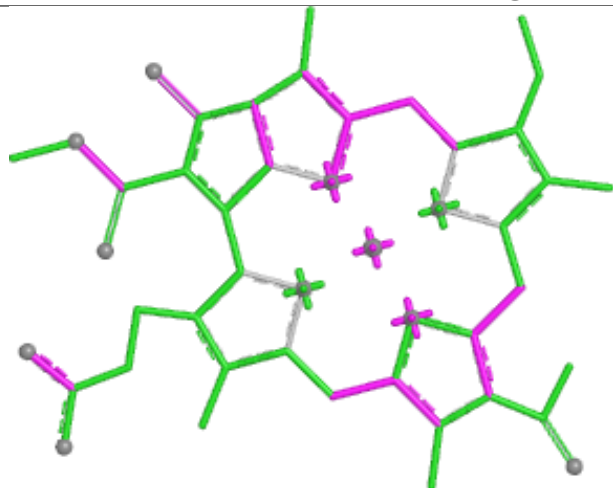


Torsions

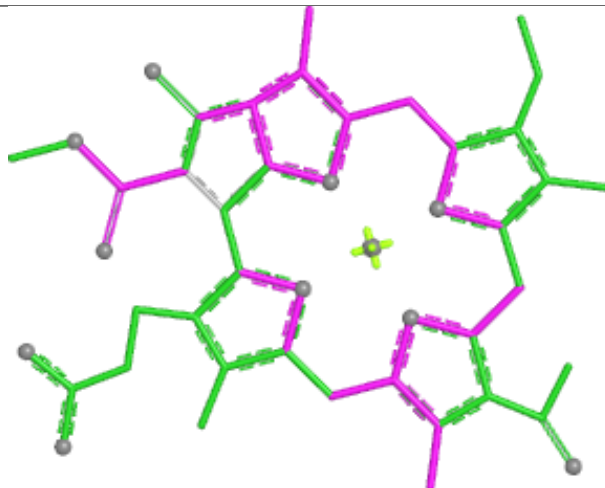


Rings

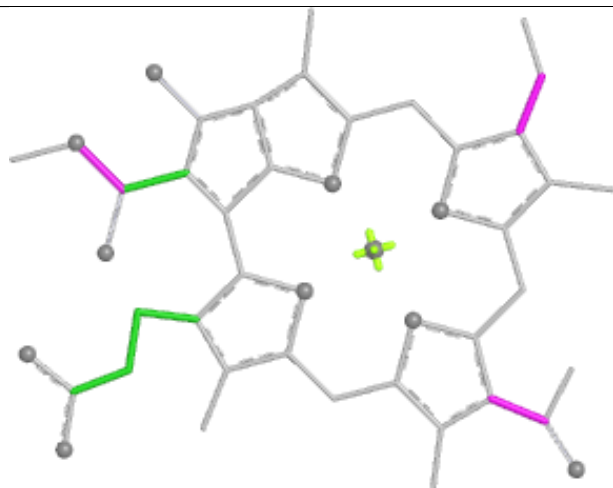
Ligand BCL B4 101



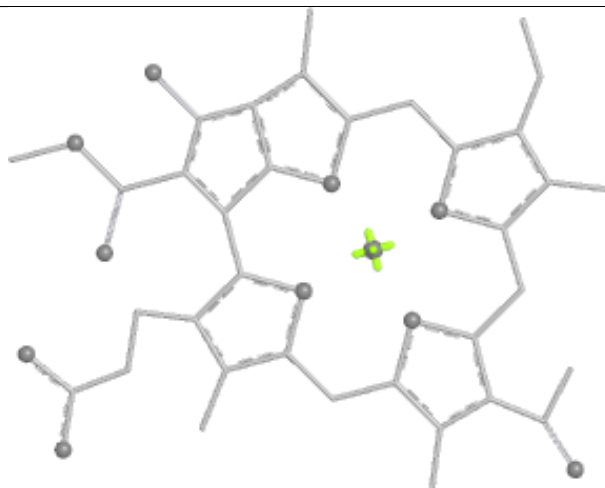
Bond lengths



Bond angles

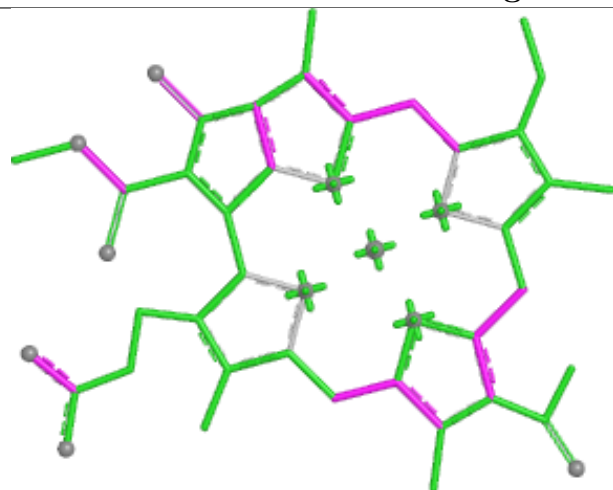


Torsions

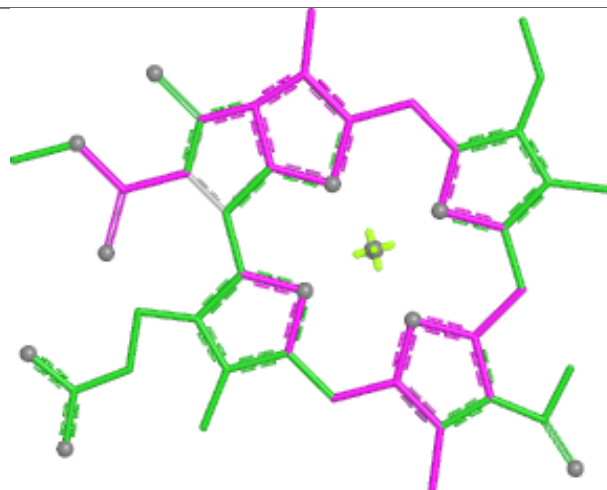


Rings

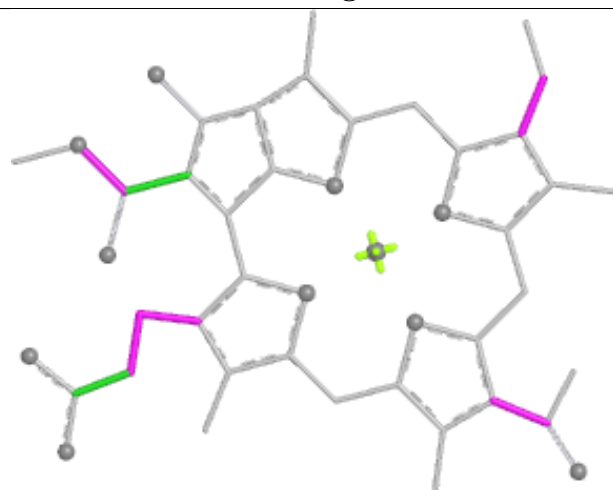
Ligand BCL BV 101



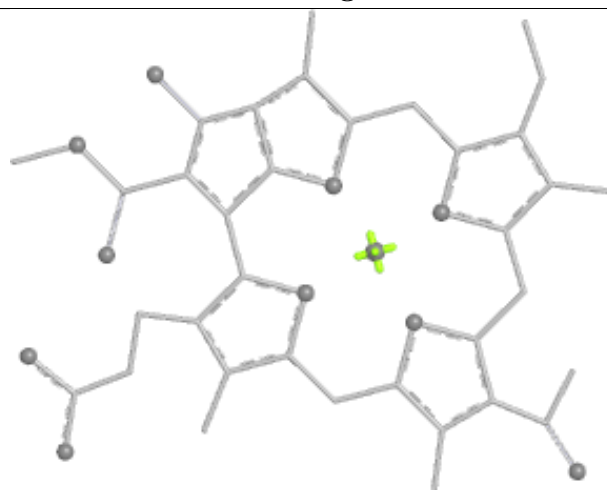
Bond lengths



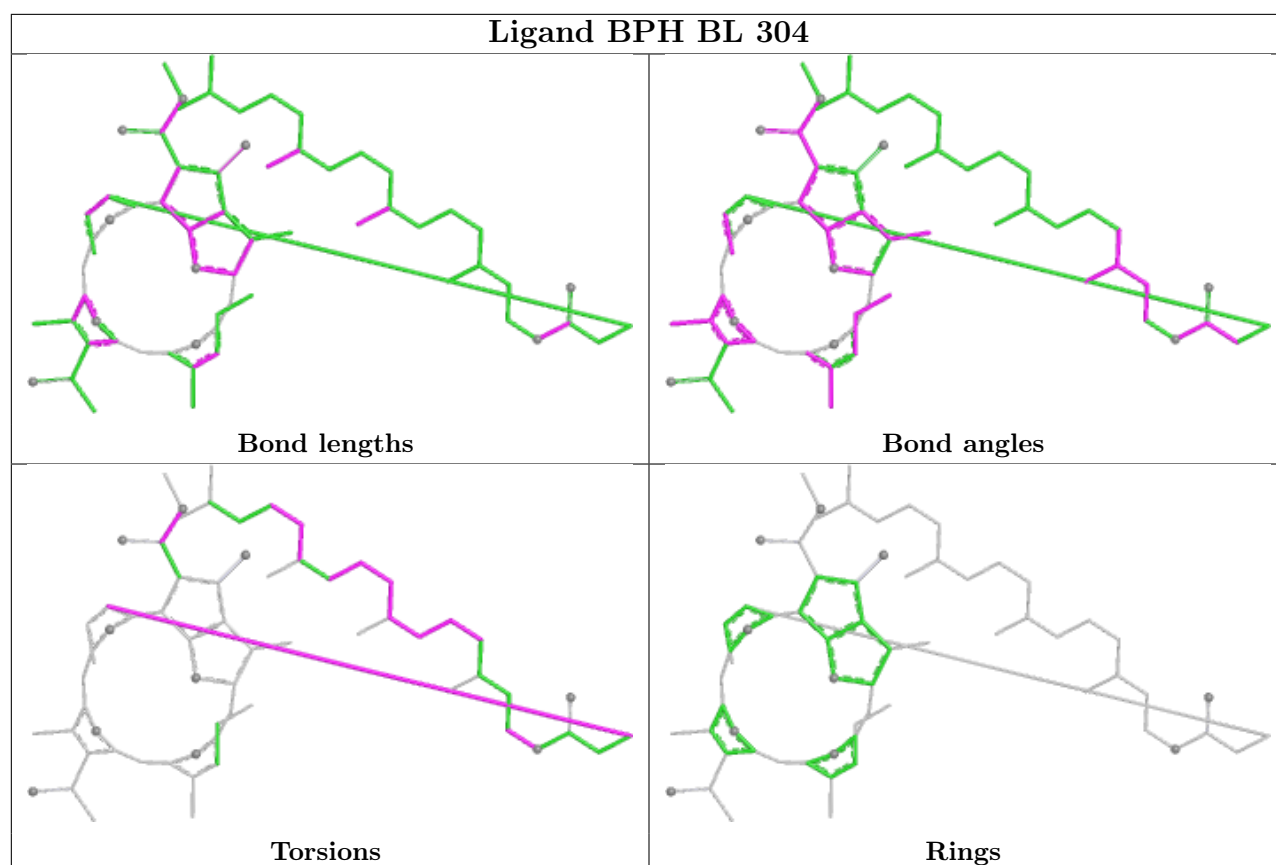
Bond angles



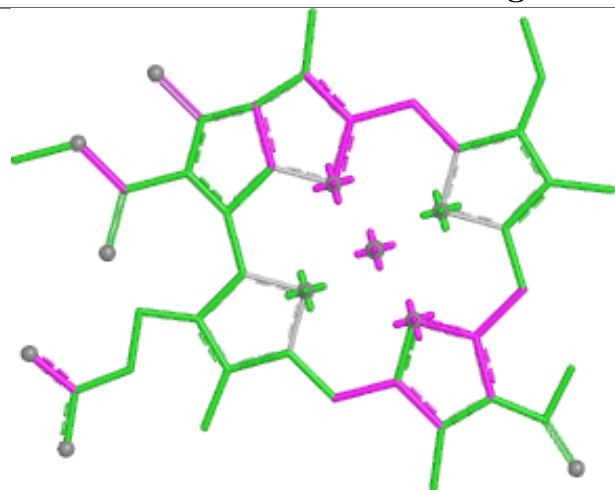
Torsions



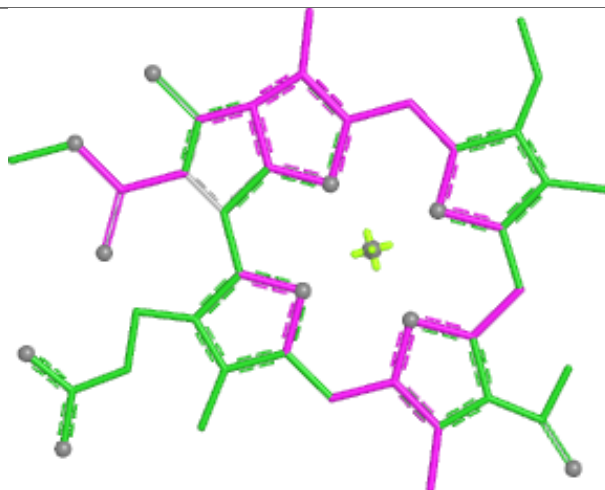
Rings



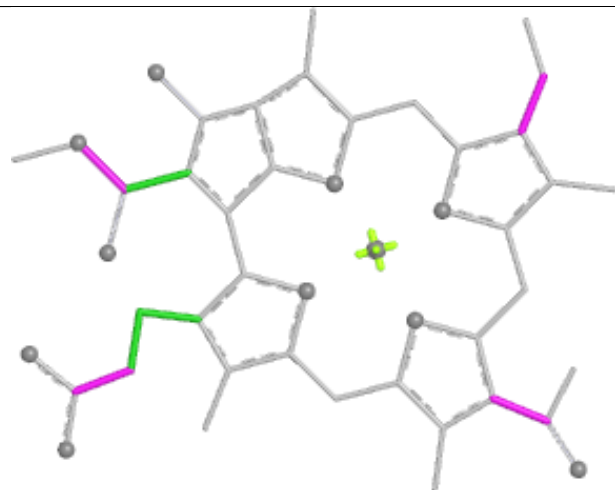
Ligand BCL A6 102



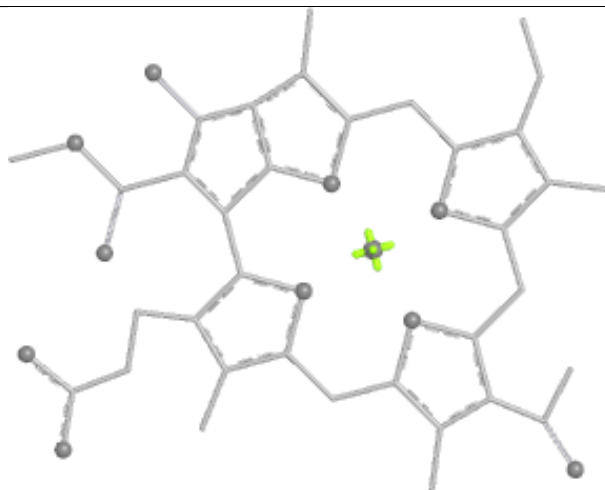
Bond lengths



Bond angles

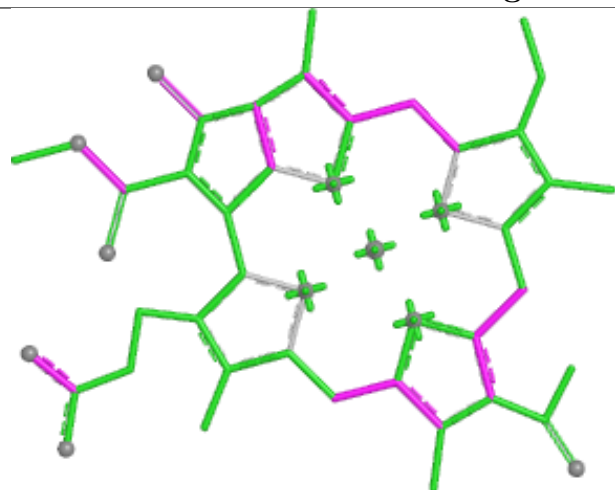


Torsions

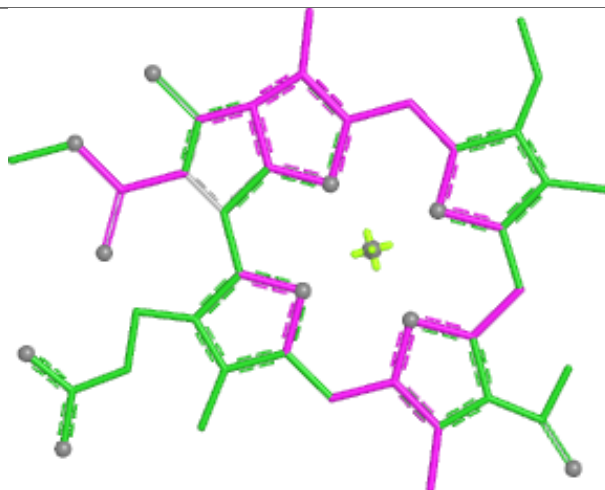


Rings

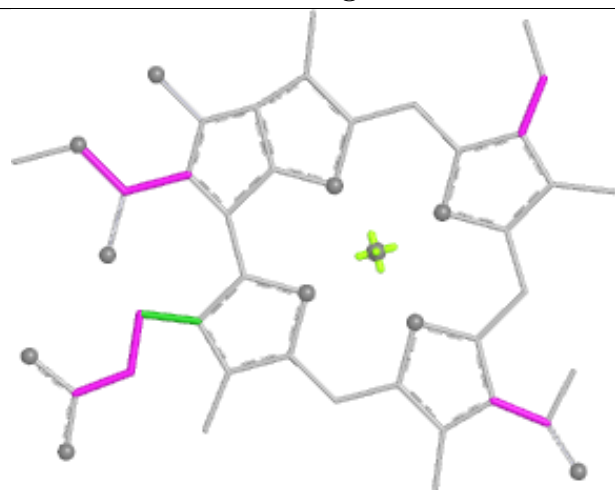
Ligand BCL BD 101



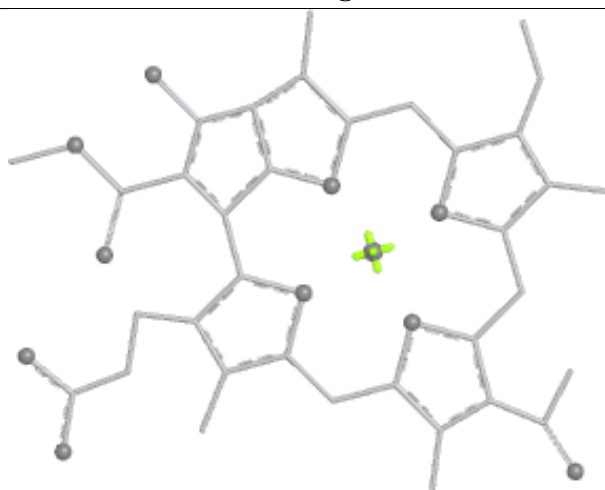
Bond lengths



Bond angles

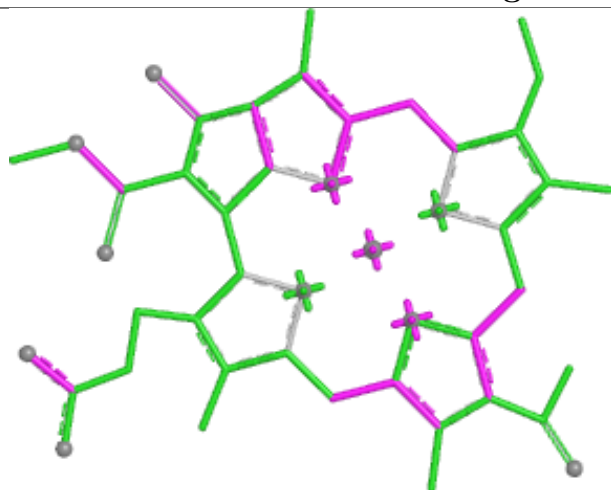


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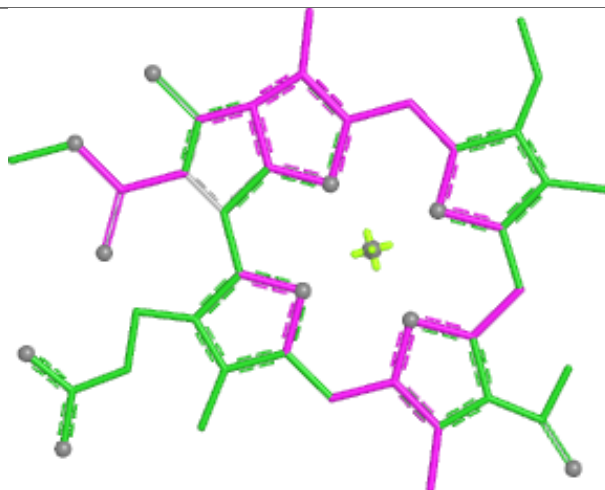


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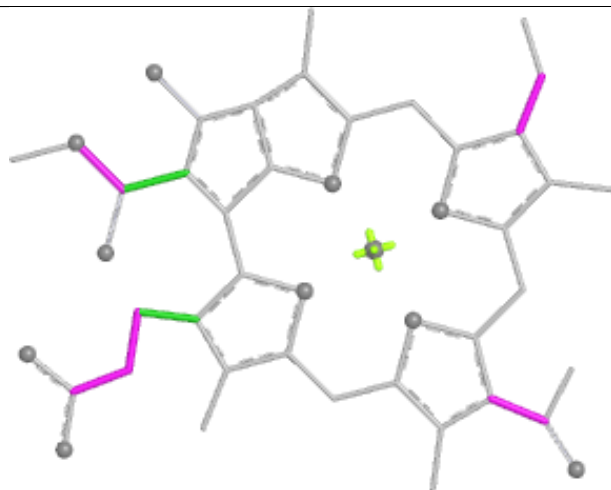
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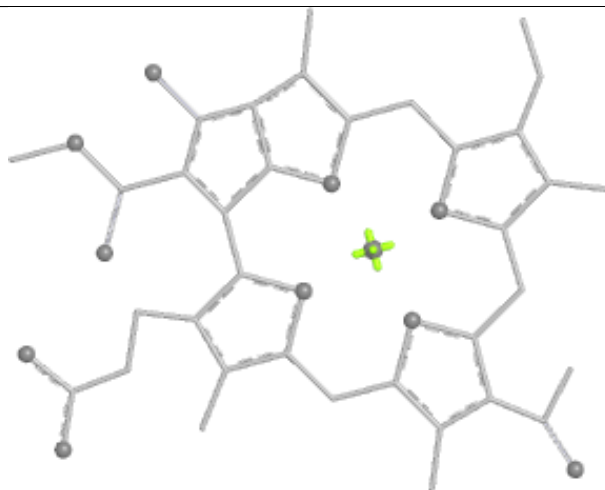
Bond lengths



Bond angles

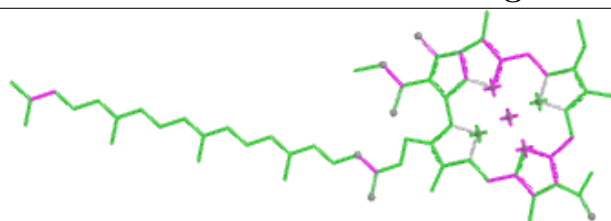


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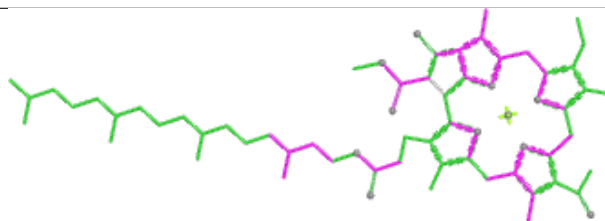


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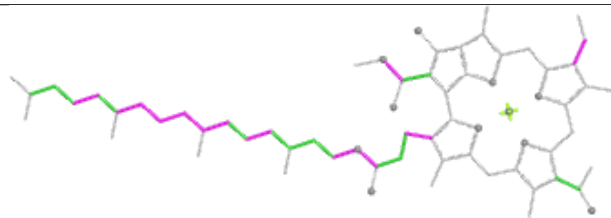
Ligand BCL BL 303



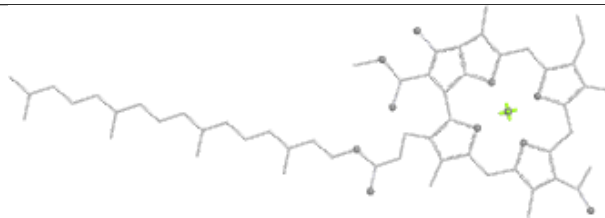
Bond lengths



Bond angles

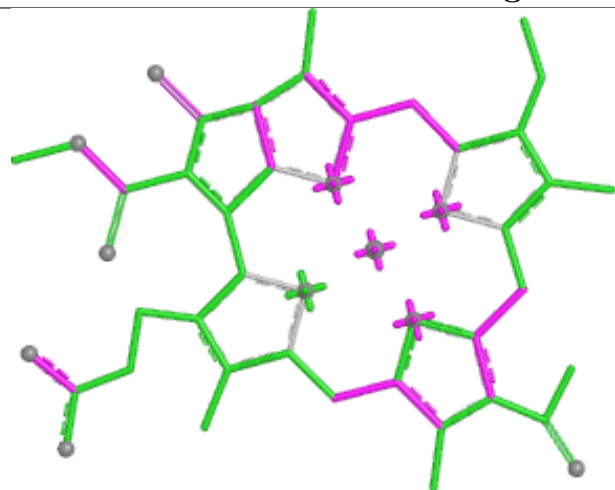


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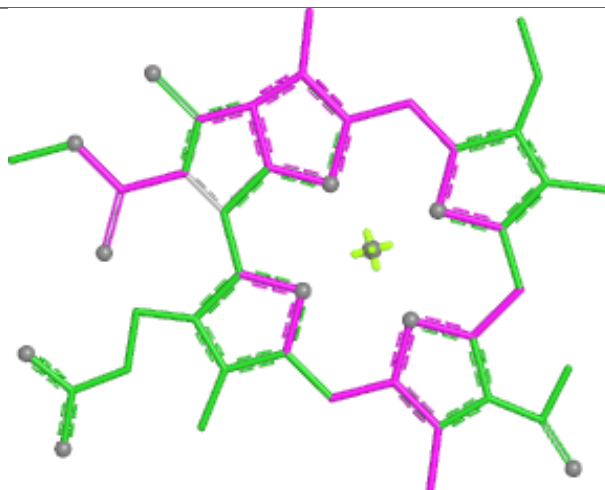


Rings

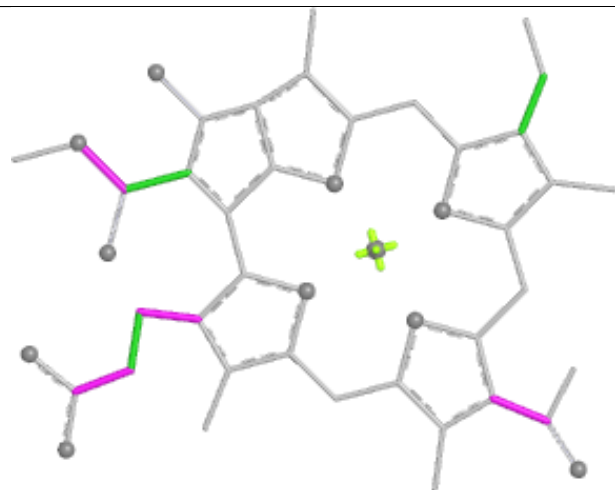
Ligand BCL BY 101



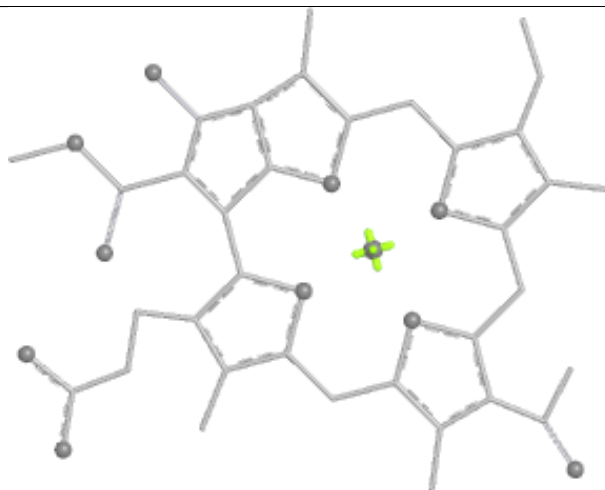
Bond lengths



Bond angles

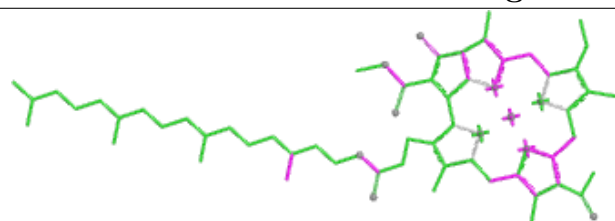


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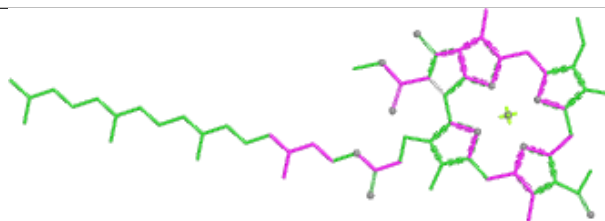


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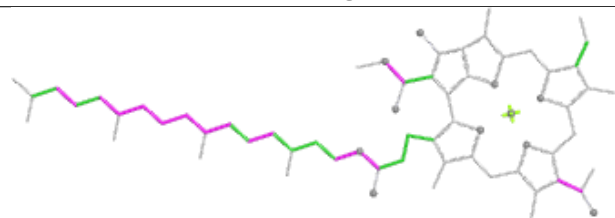
Ligand BCL AL 302



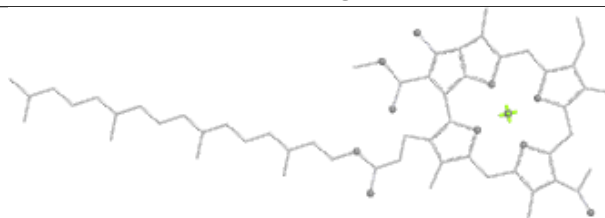
Bond lengths



Bond angles

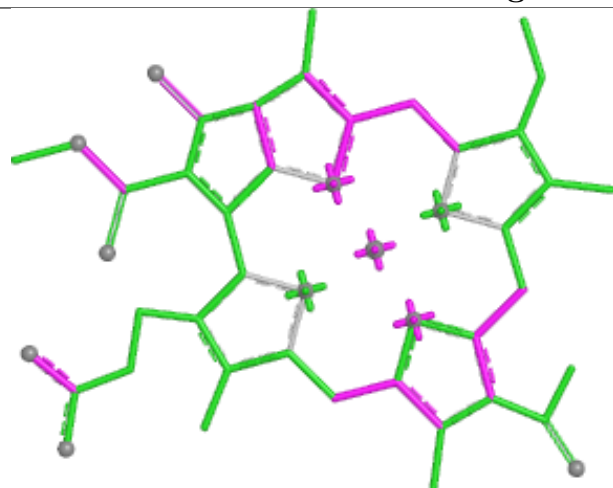


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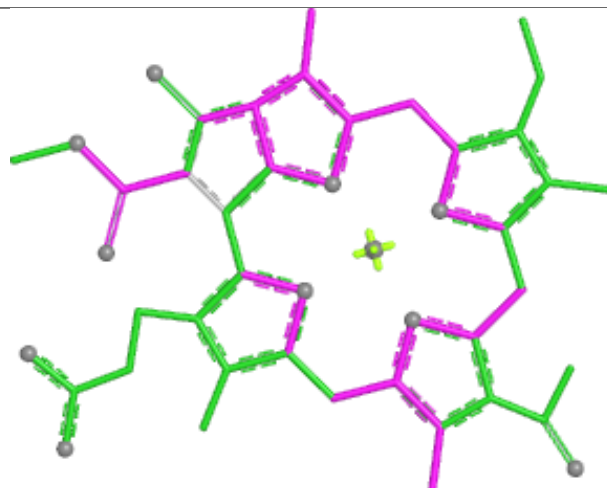


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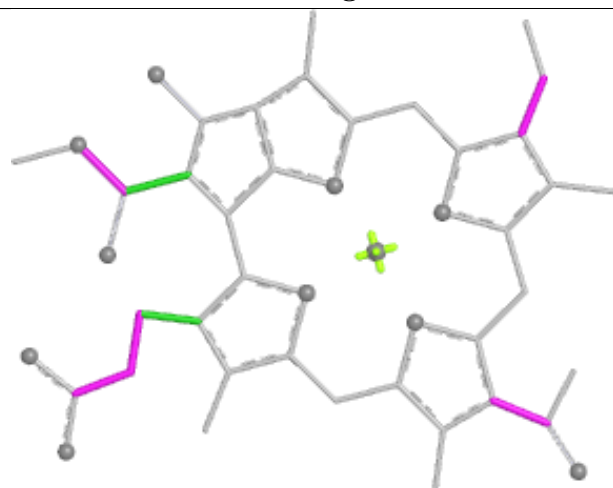
Ligand BCL A9 101



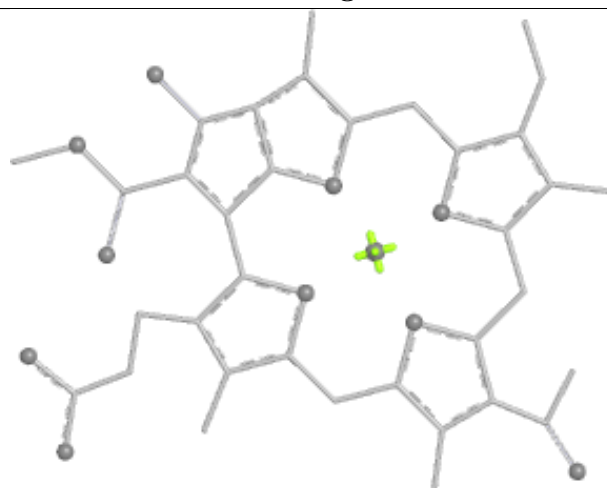
Bond lengths



Bond angles

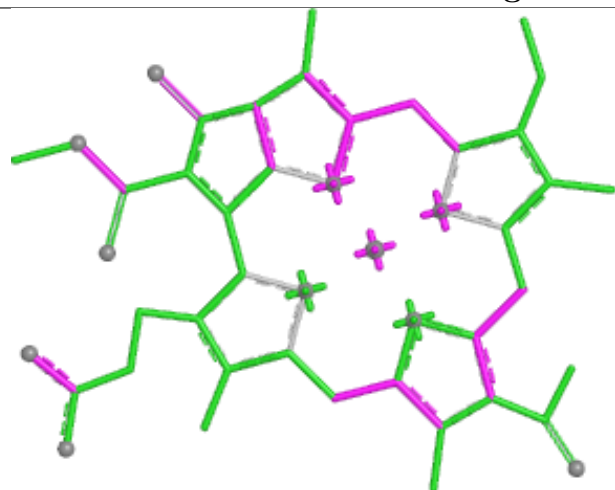


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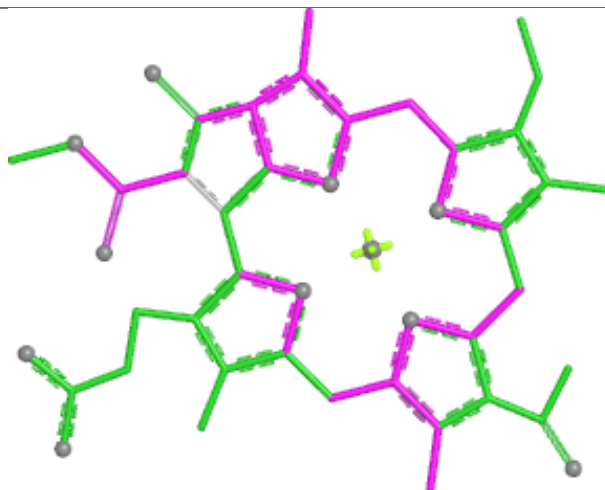


Rings

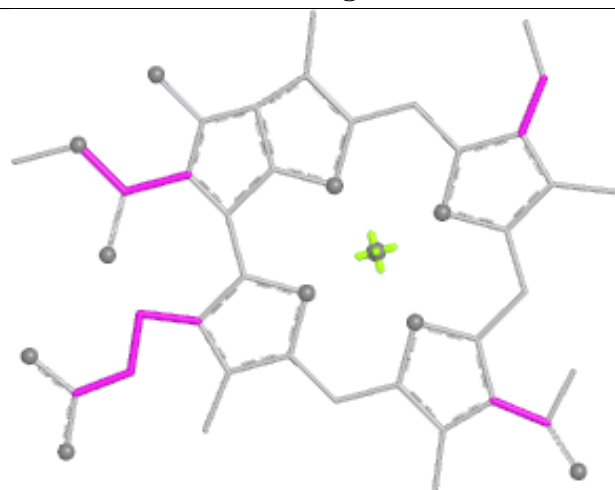
Ligand BCL BO 101



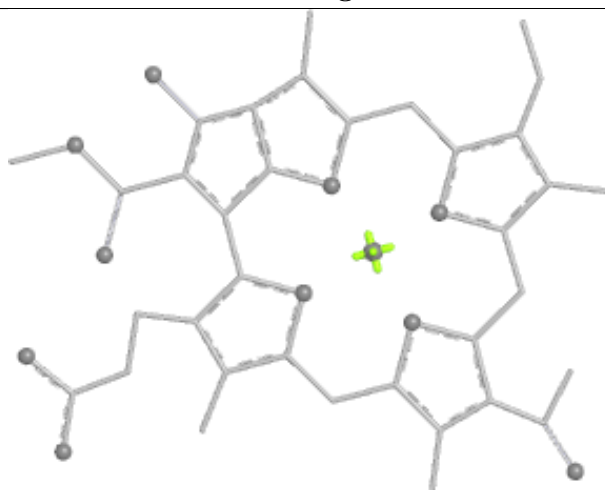
Bond lengths



Bond angles

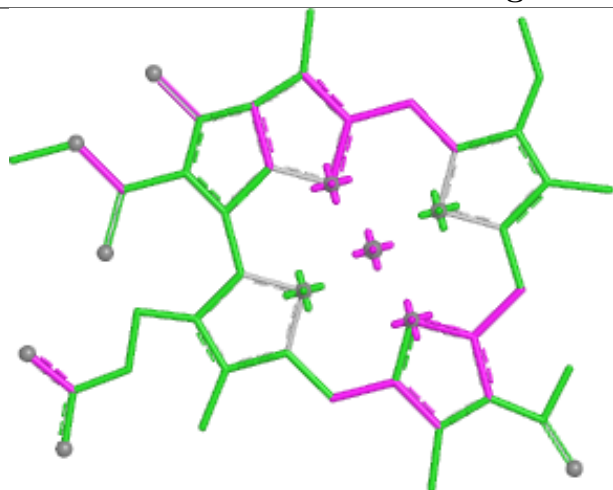


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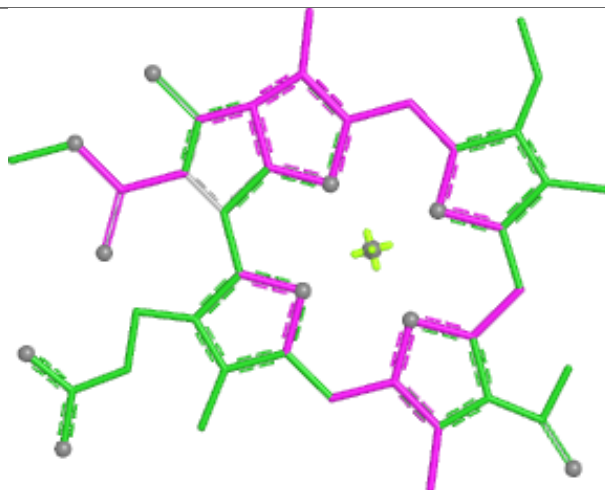


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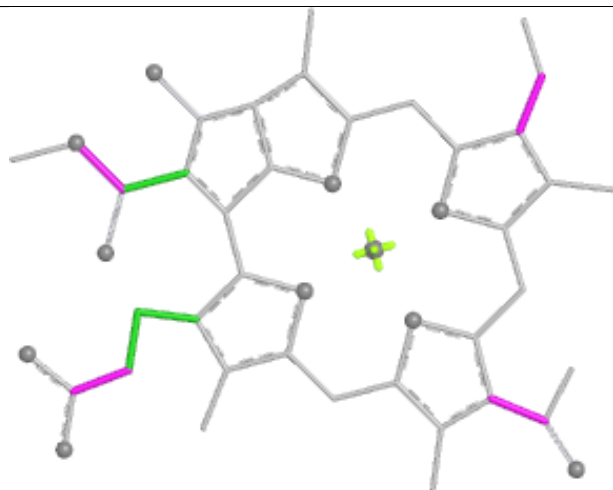
Ligand BCL B6 101



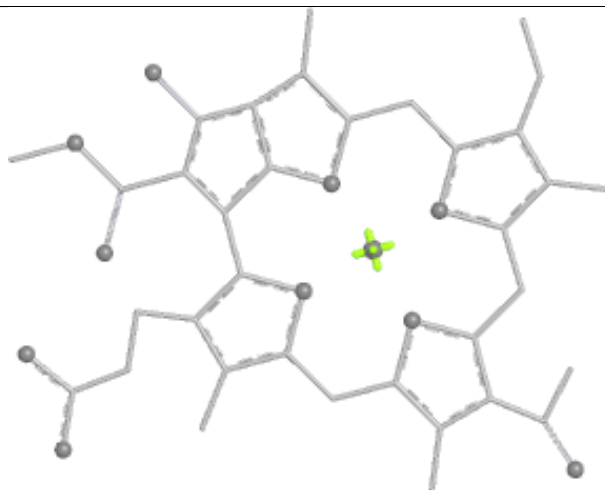
Bond lengths



Bond angles

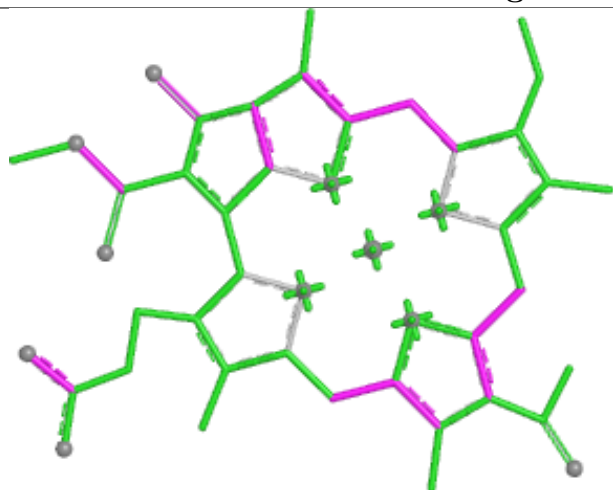


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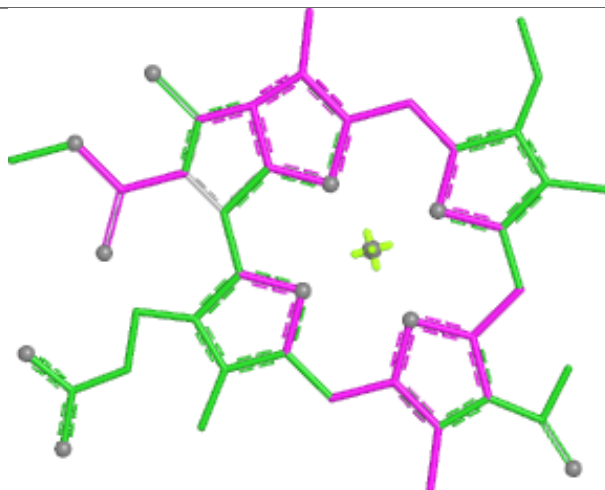


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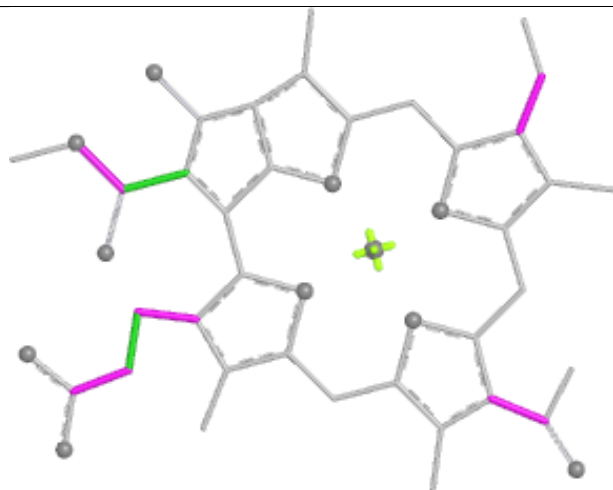
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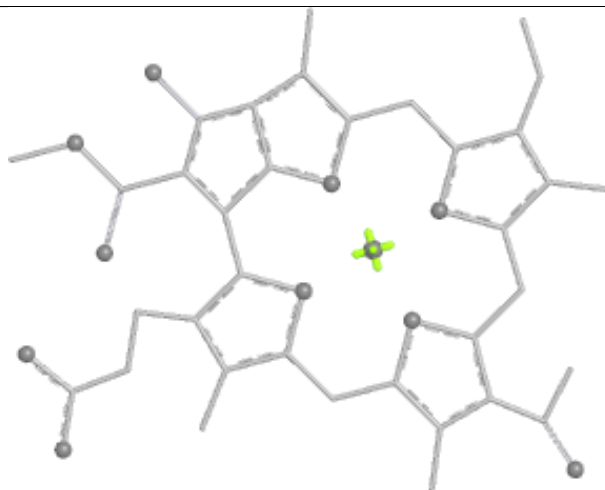
Bond lengths



Bond angles

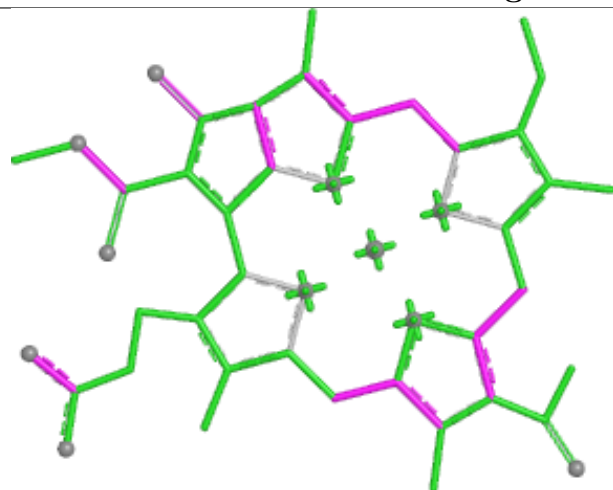


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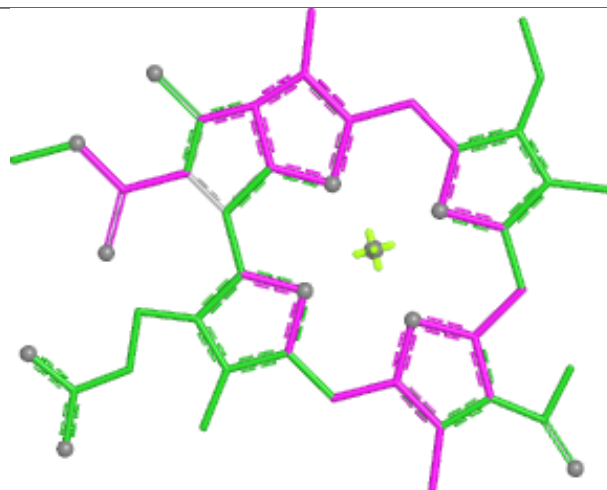


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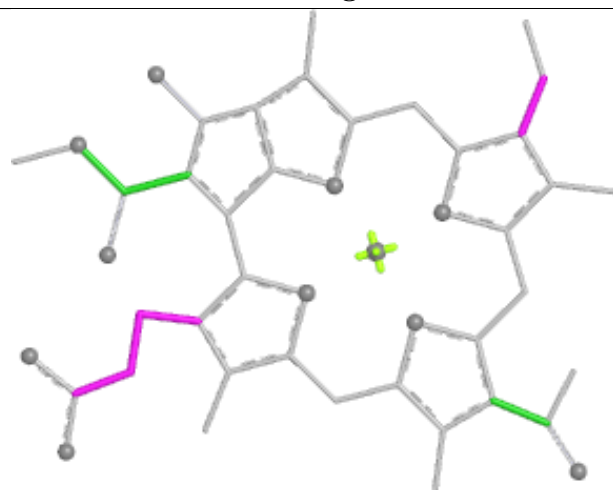
Ligand BCL BP 101



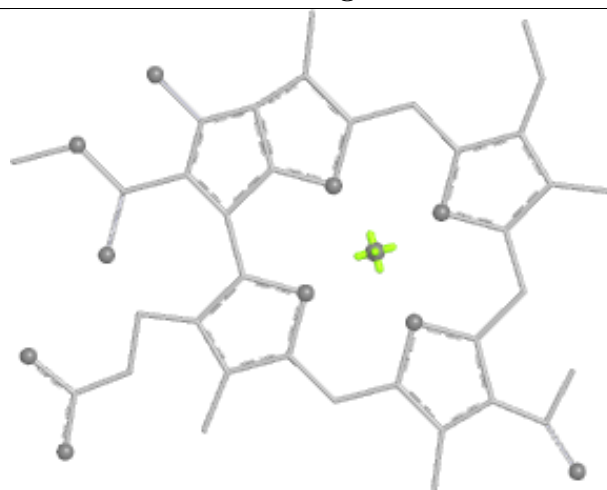
Bond lengths



Bond angles

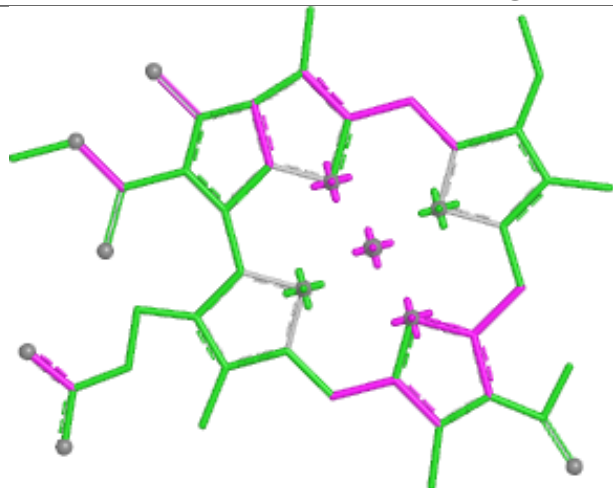


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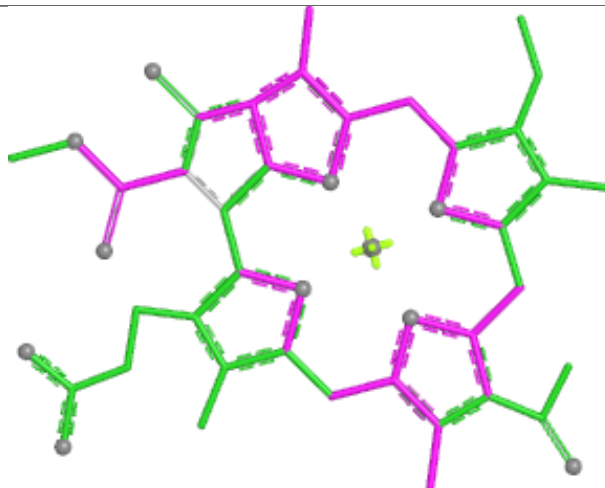


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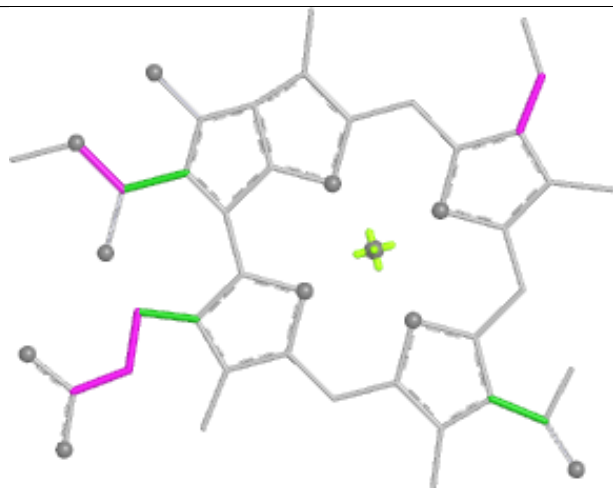
Ligand BCL B7 101



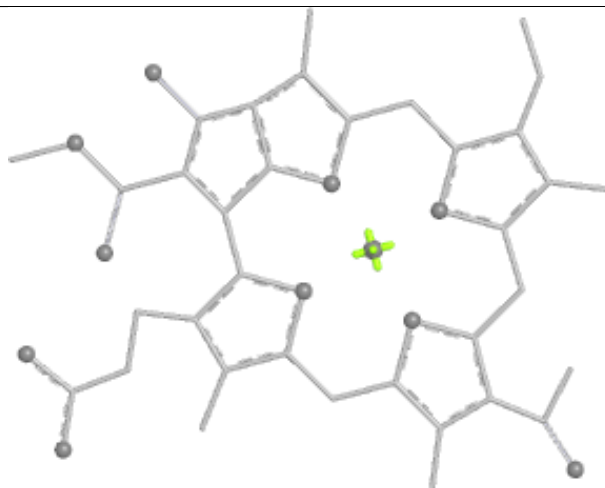
Bond lengths



Bond angles

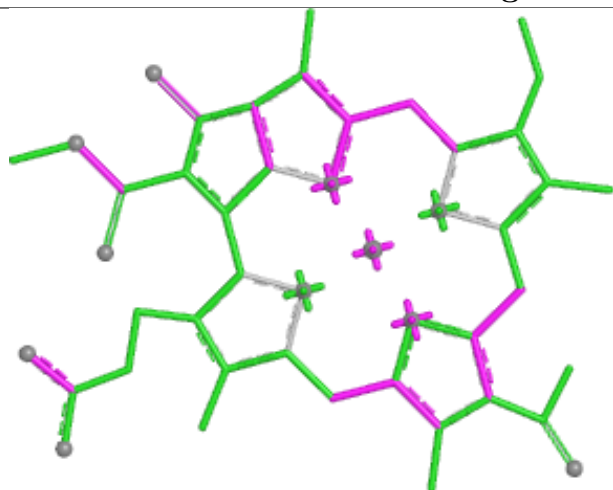


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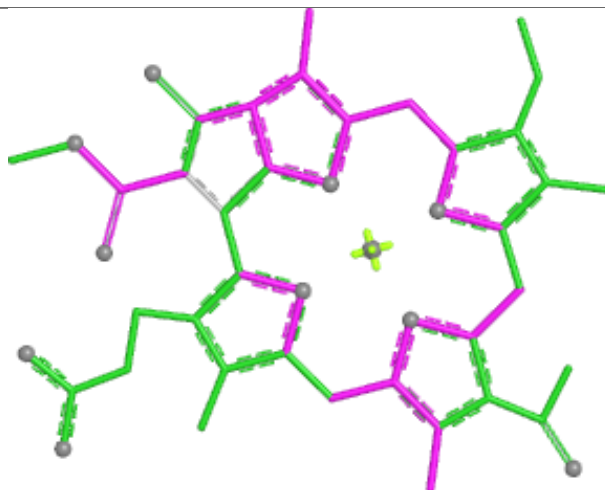


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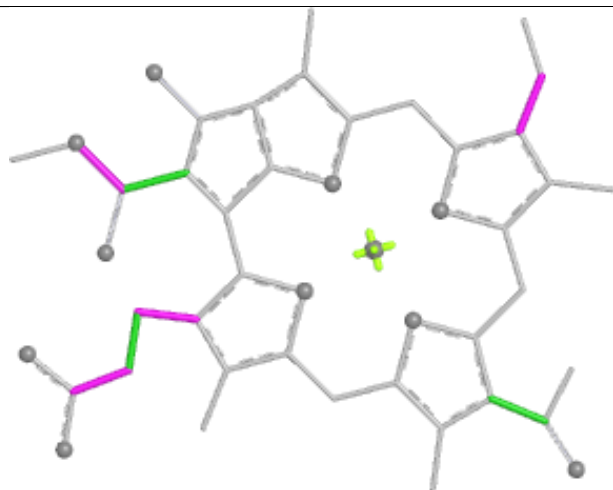
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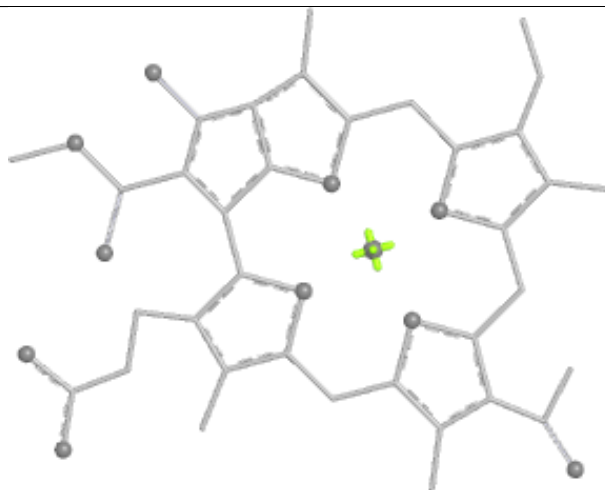
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Bond angles

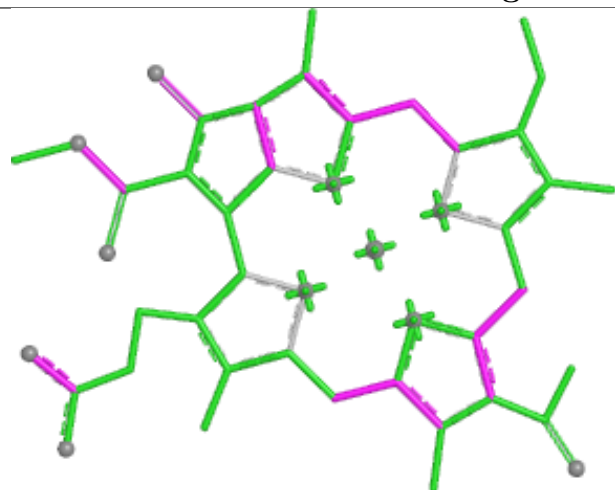


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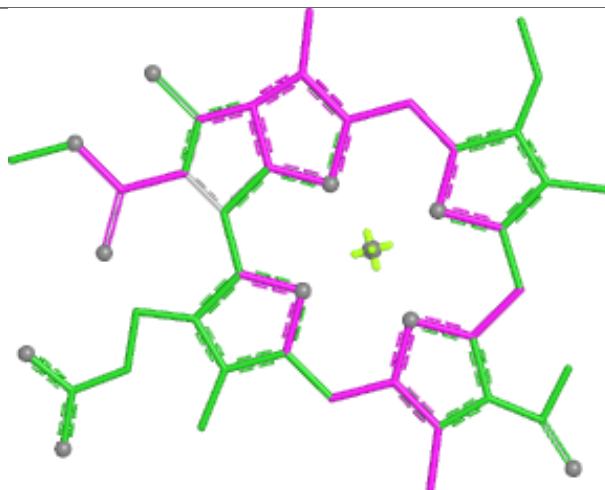


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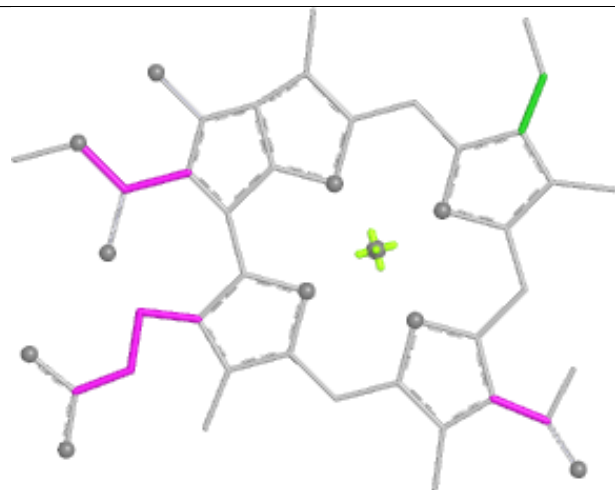
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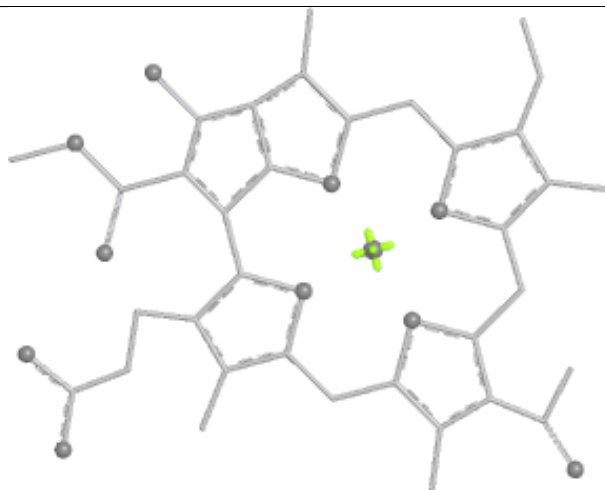
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Bond angles

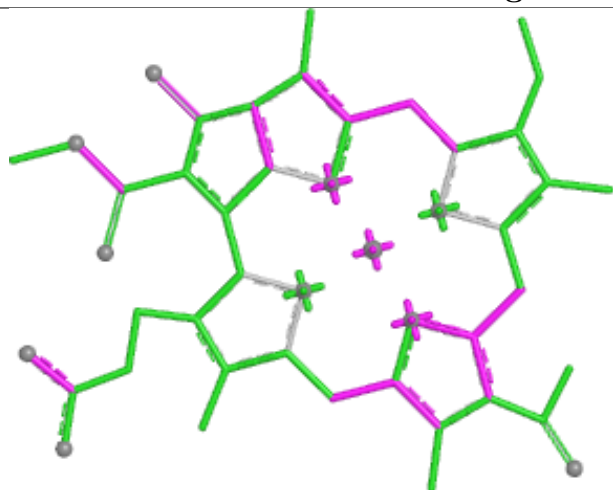


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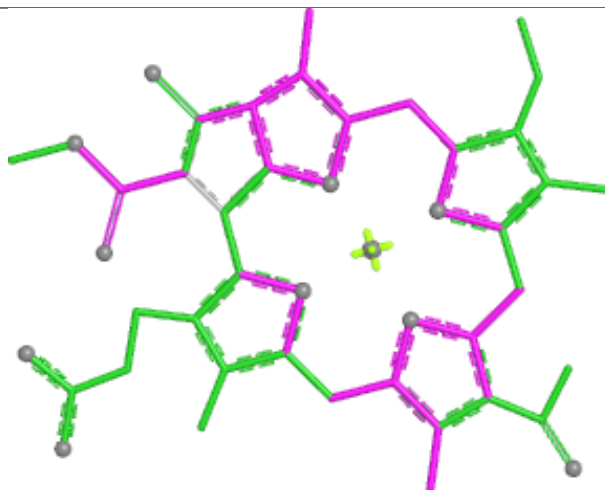


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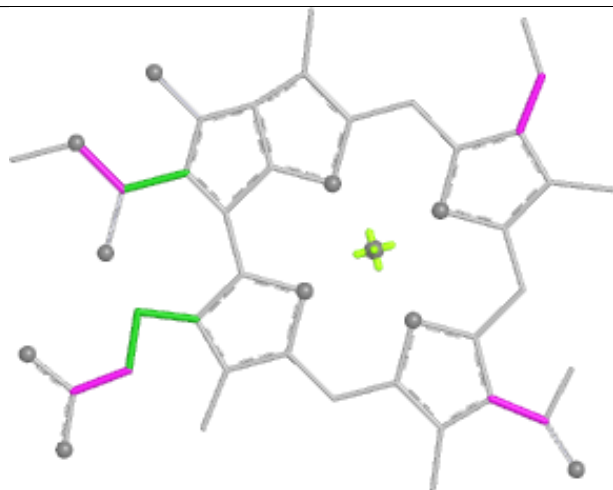
Ligand BCL A6 101



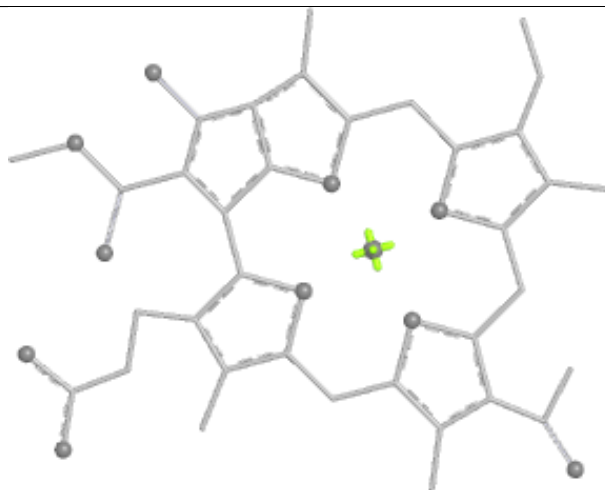
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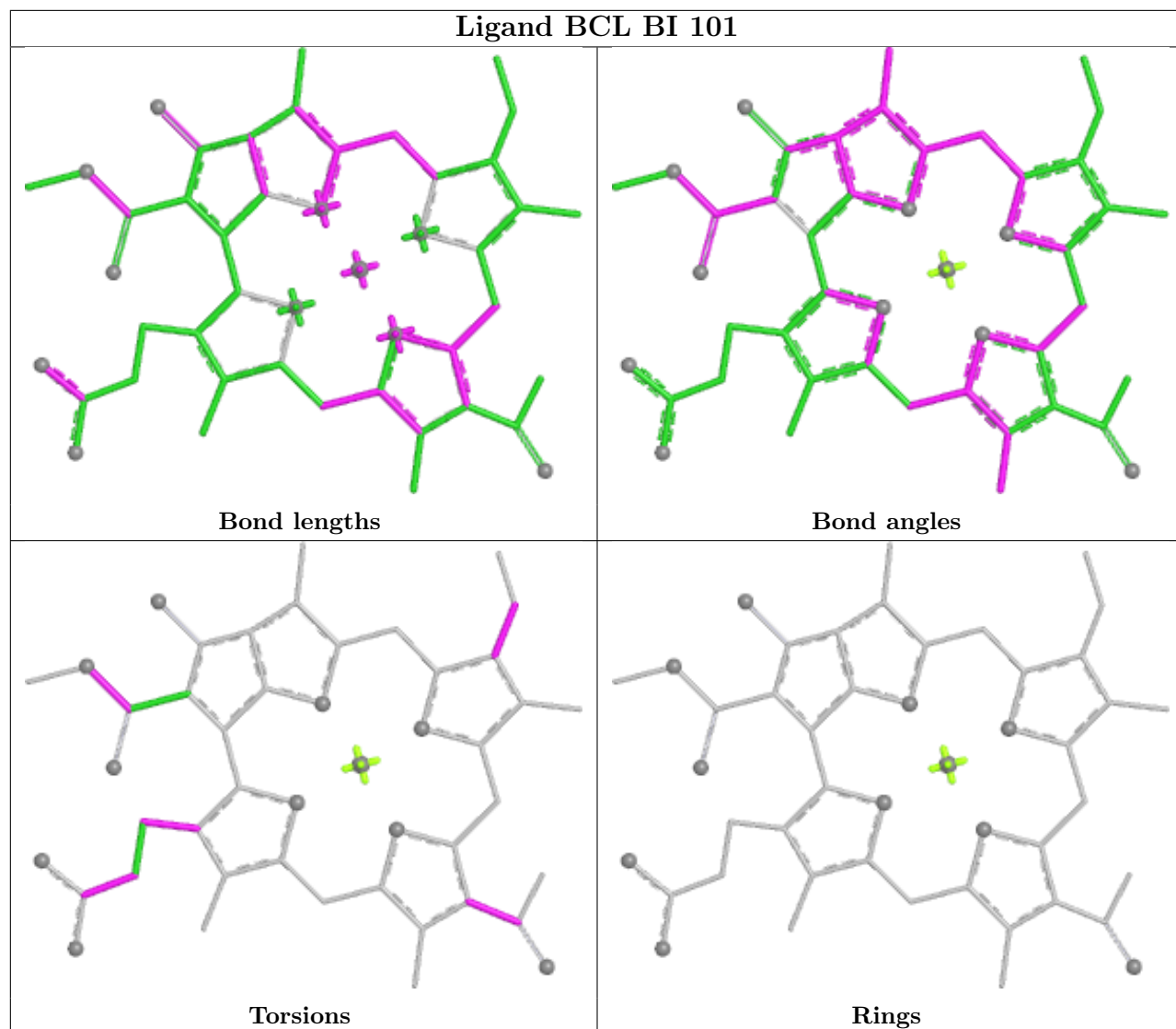
Bond angles



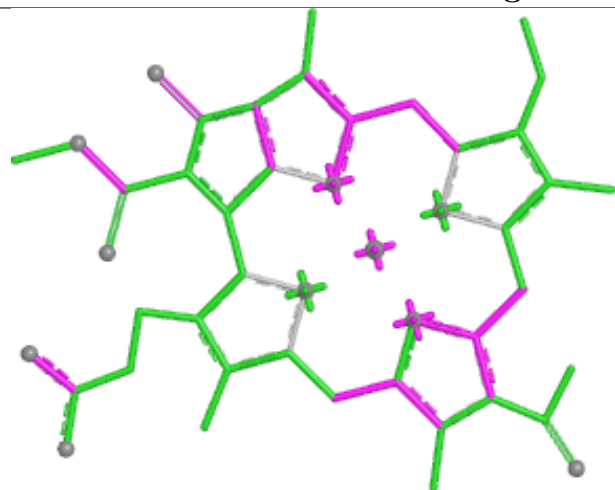
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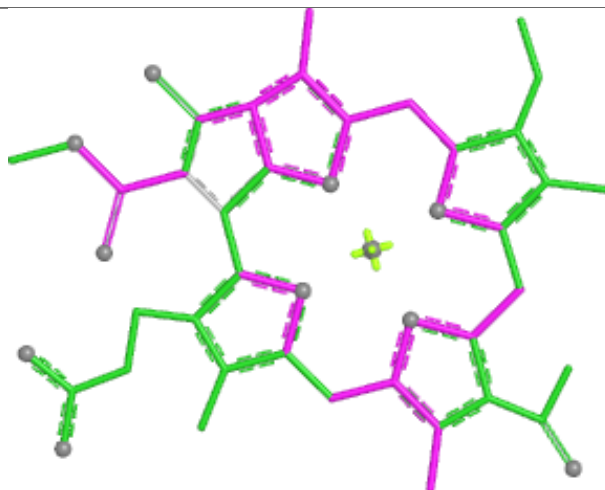
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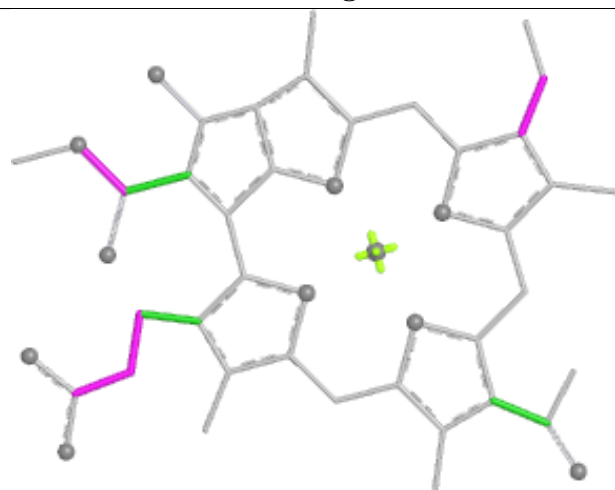
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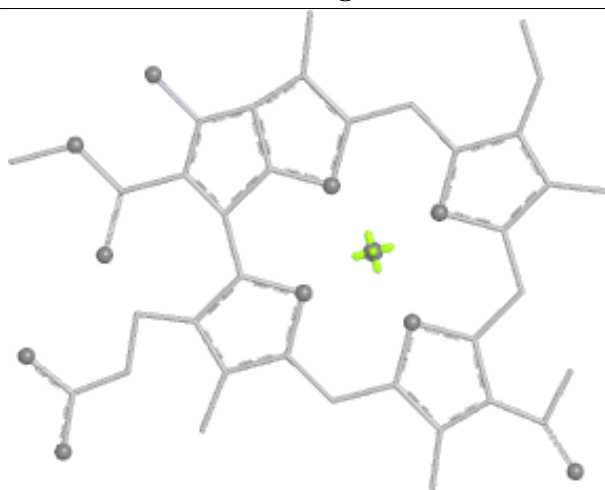
Bond lengths



Bond angles

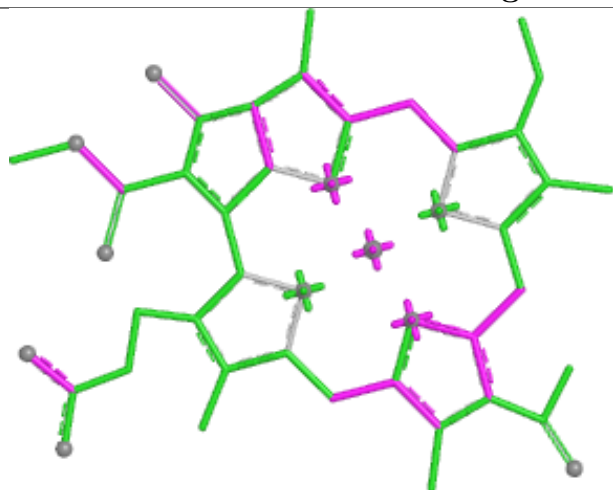


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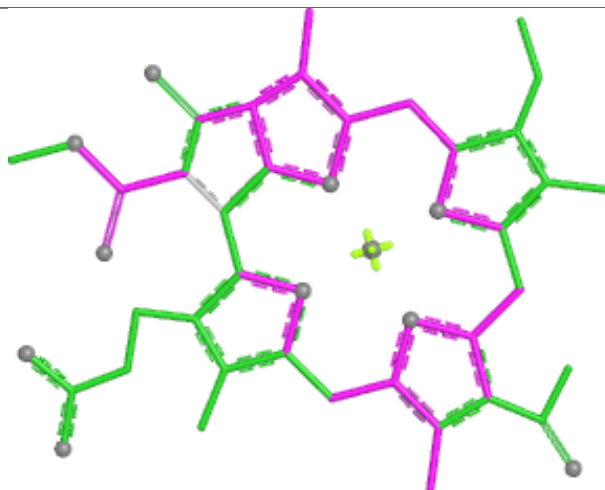


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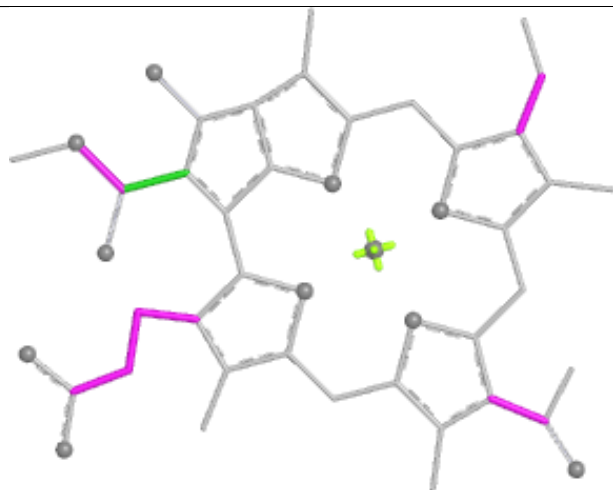
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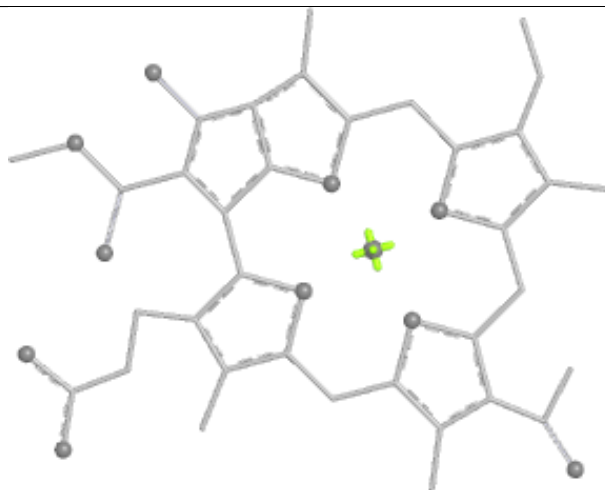
Bond lengths



Bond angles

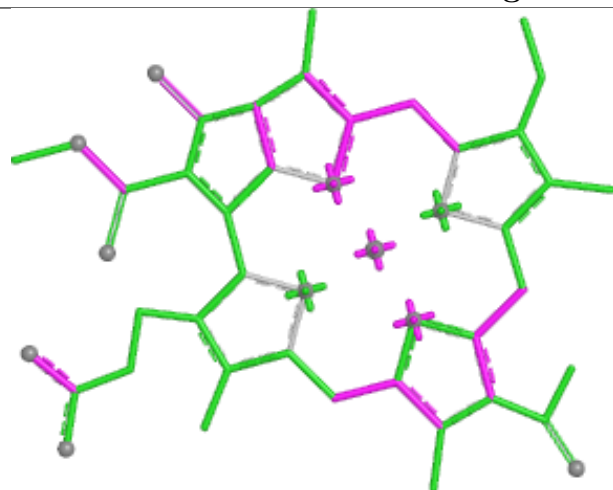


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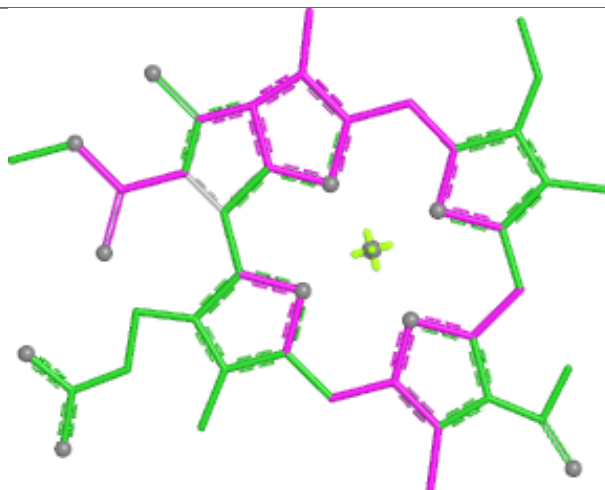


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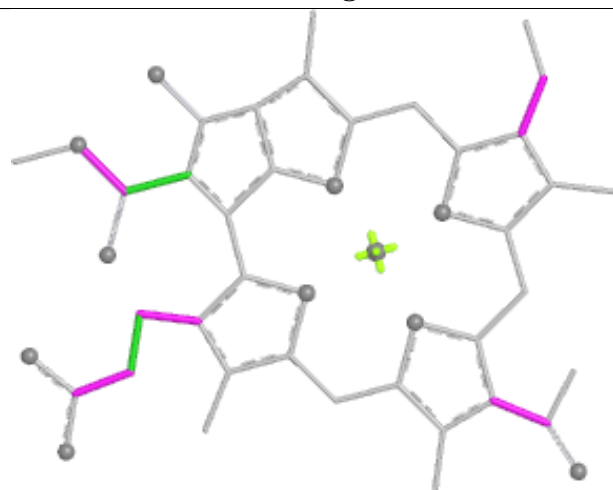
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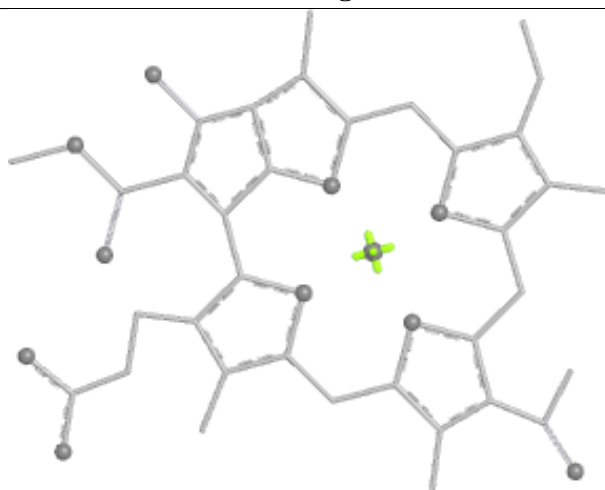
Bond lengths



Bond angles

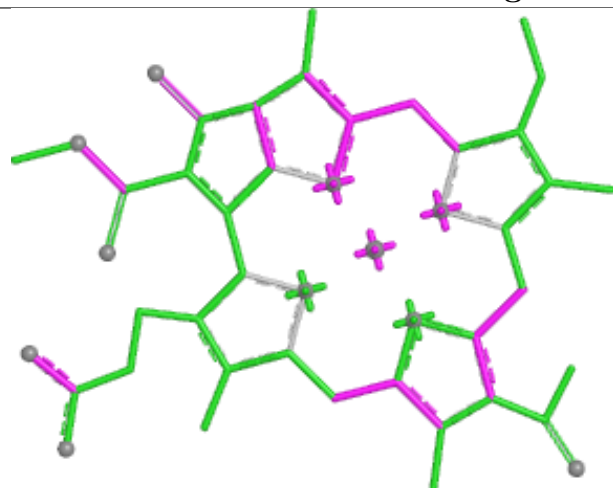


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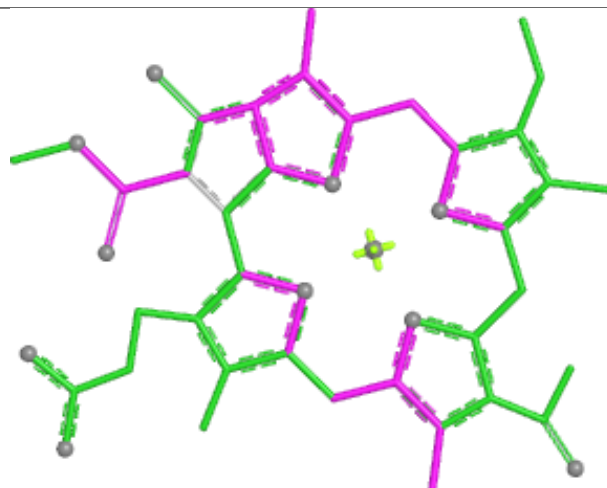


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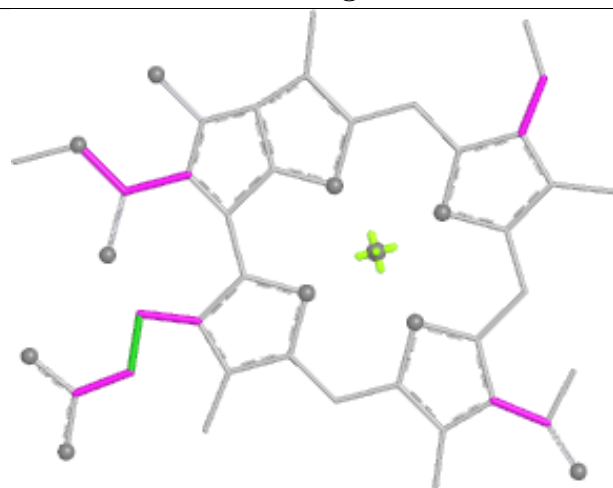
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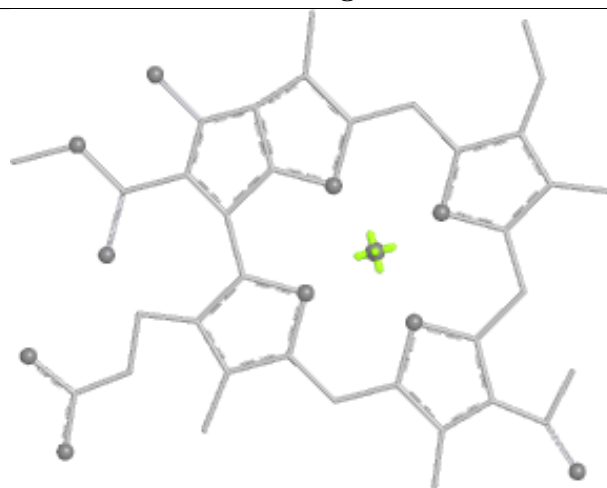
Bond lengths



Bond angles

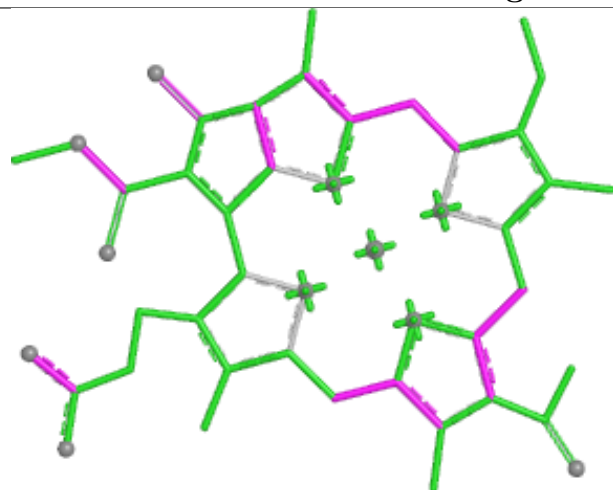


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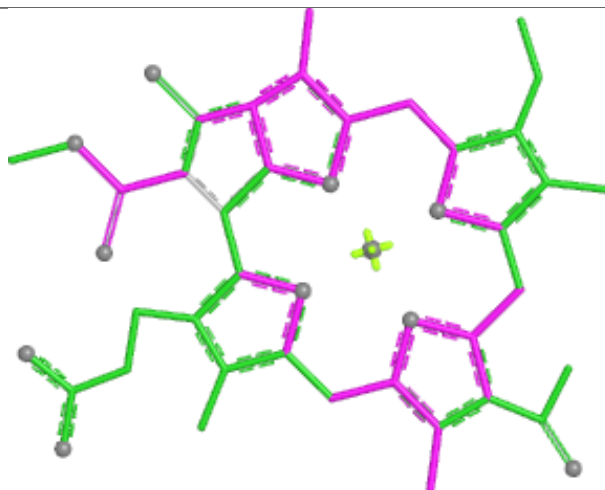


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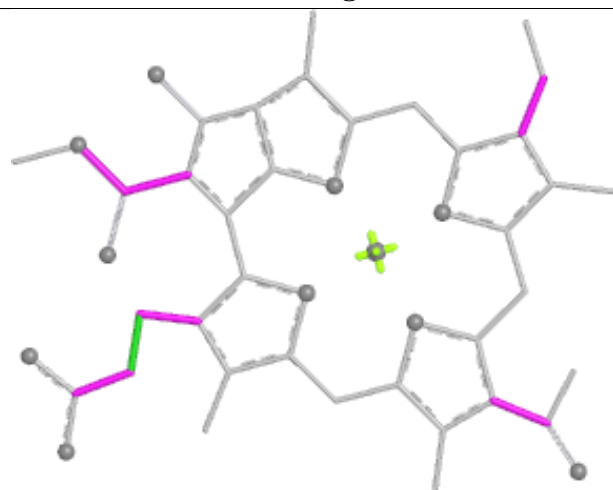
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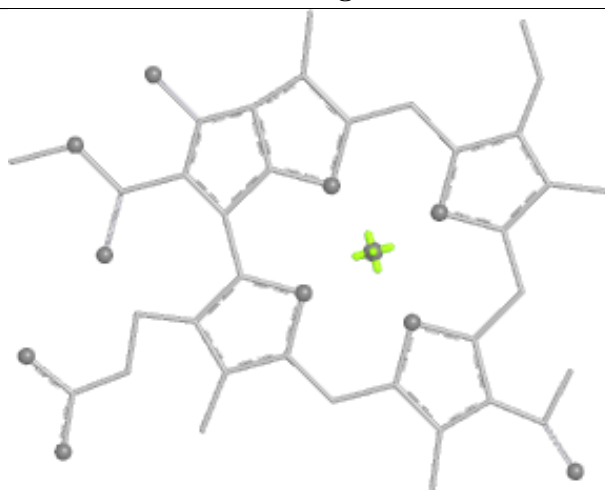
Bond lengths



Bond angles

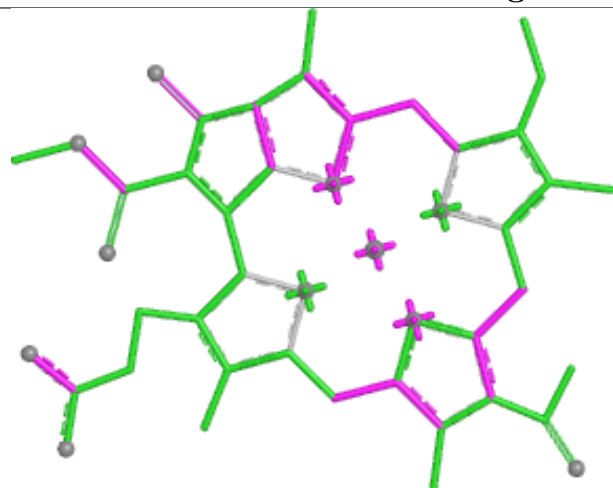


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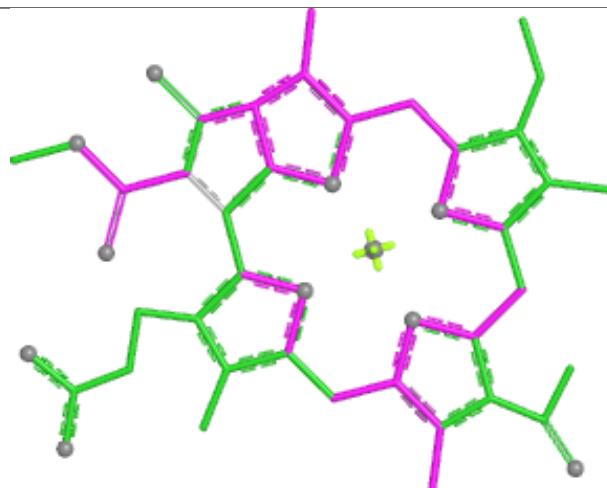


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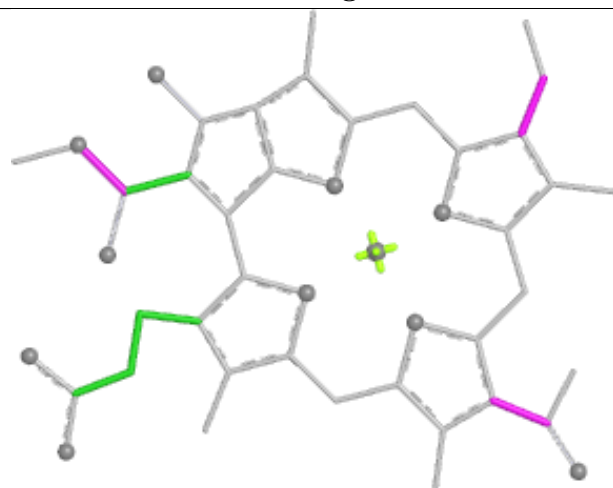
Ligand BCL A4 101



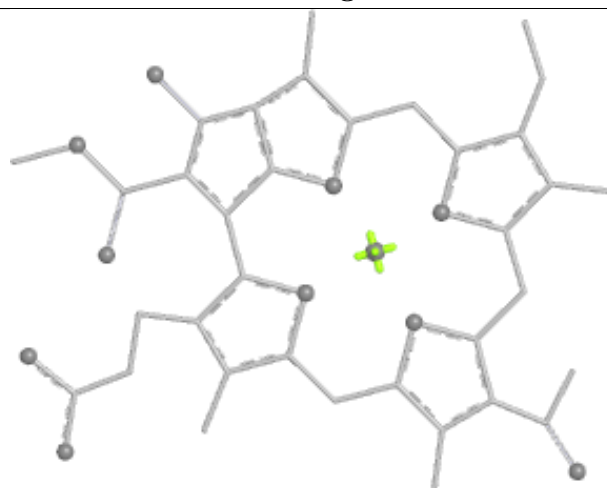
Bond lengths



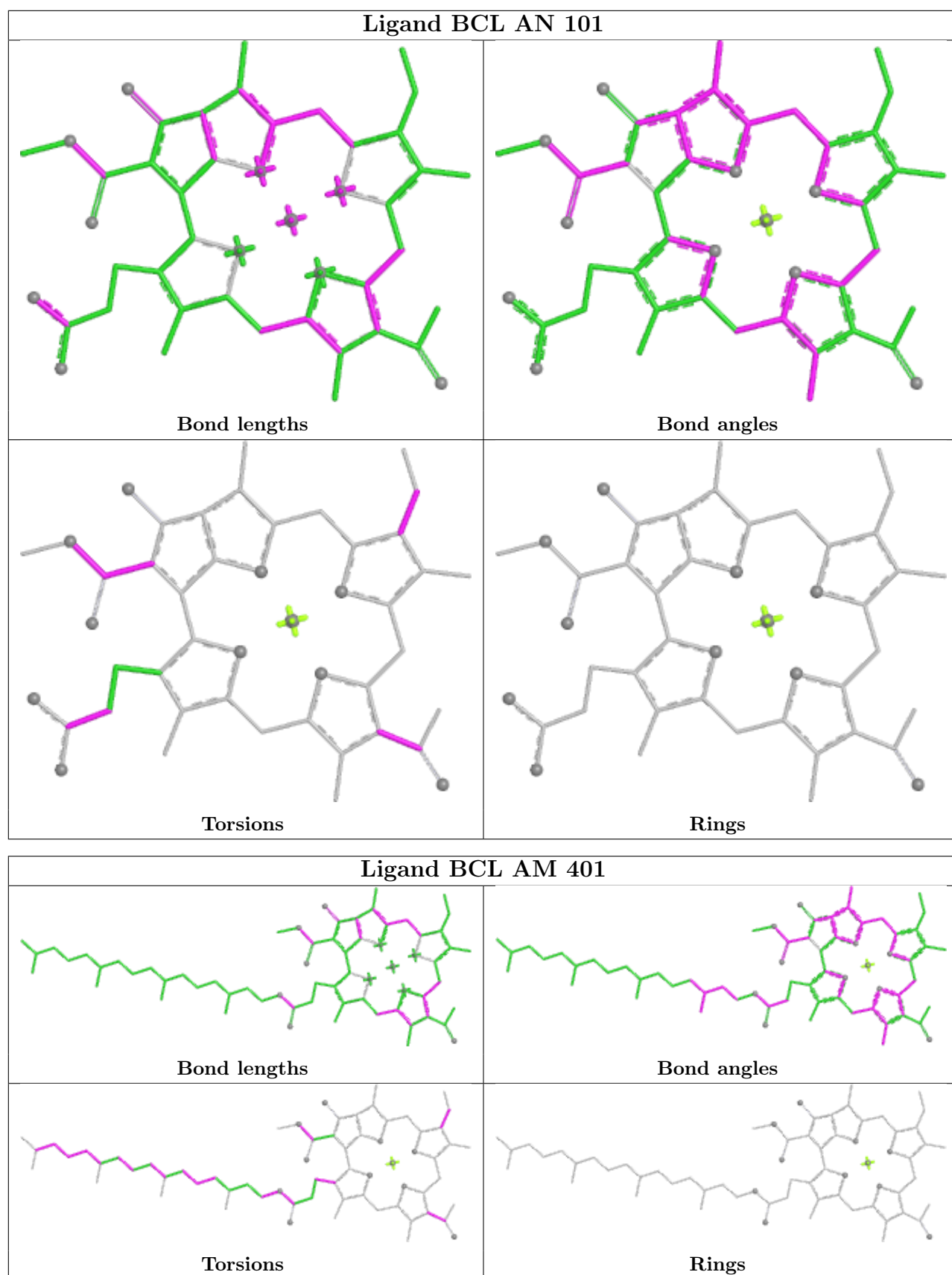
Bond angles



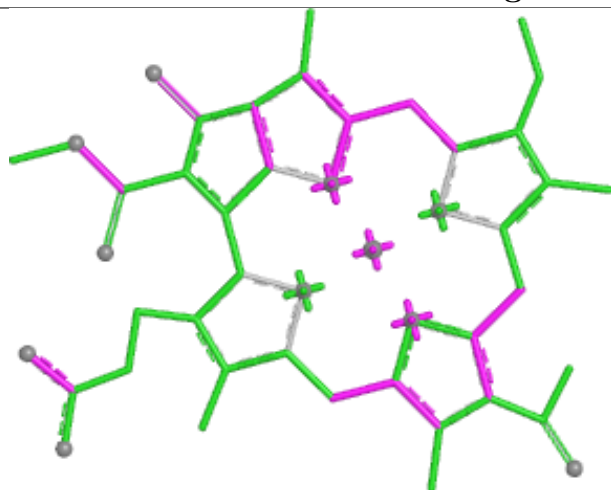
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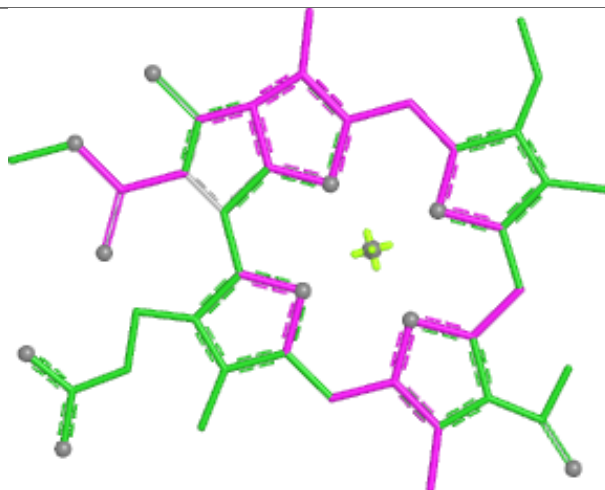
Rings



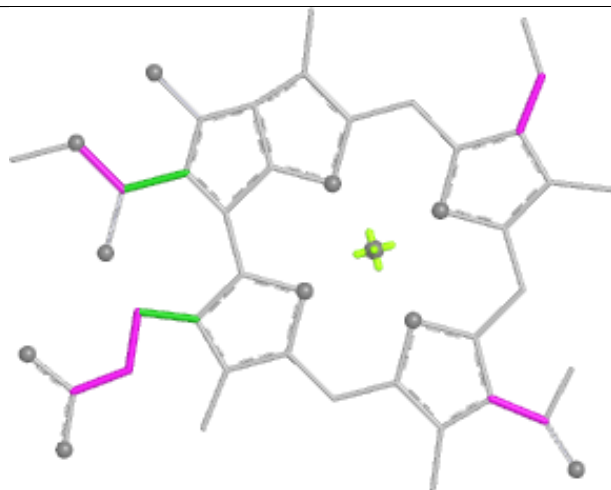
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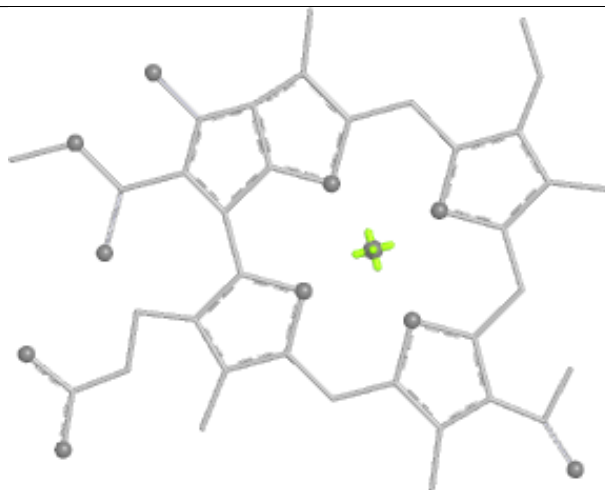
Bond lengths



Bond angles

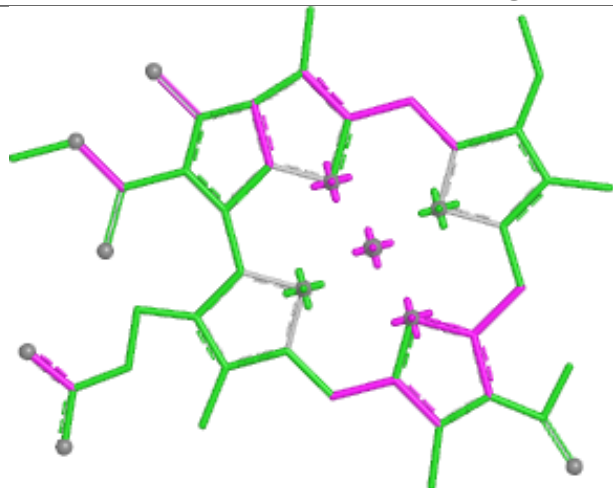


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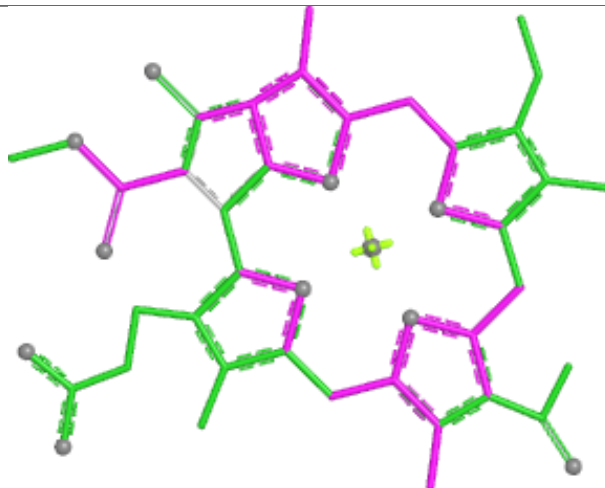


Rings

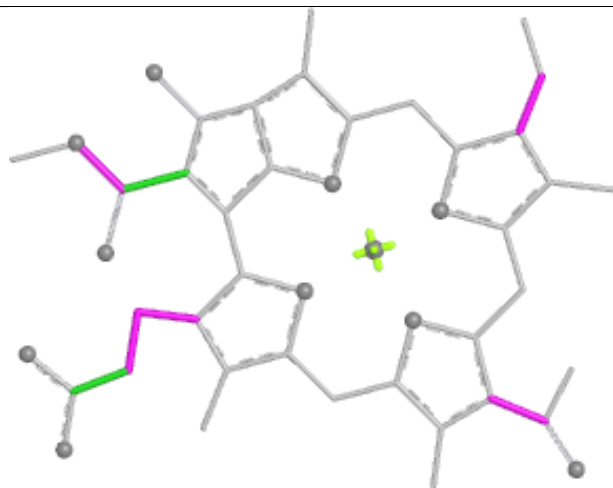
Ligand BCL A2 101



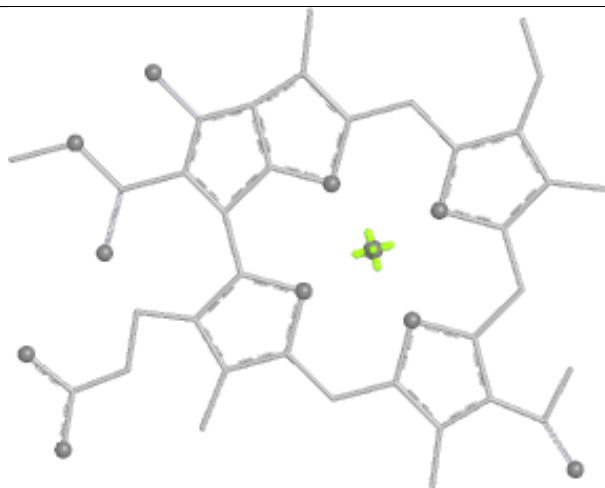
Bond lengths



Bond angles

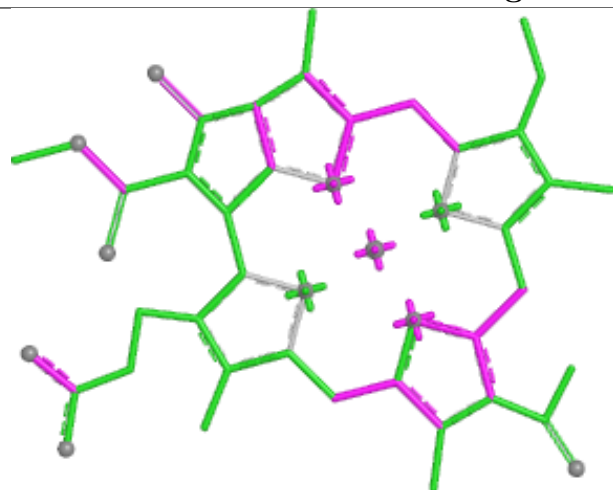


Torsions

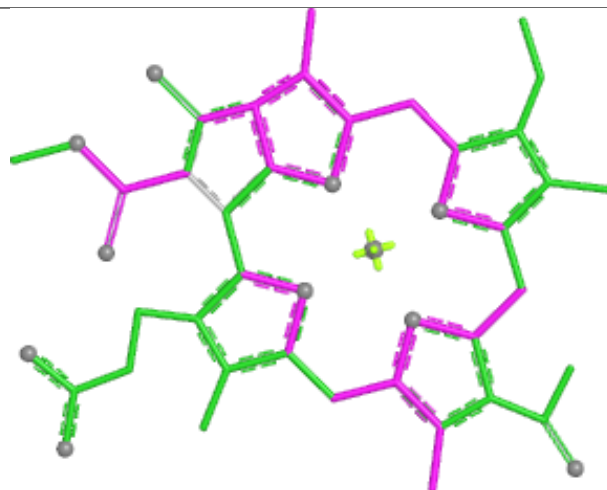


Rings

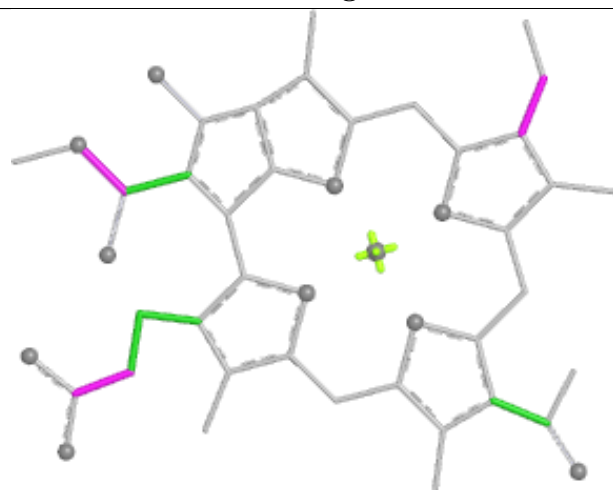
Ligand BCL BP 102



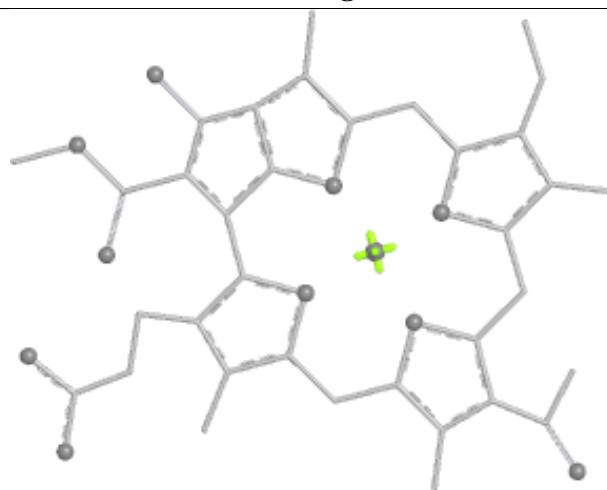
Bond lengths



Bond angles

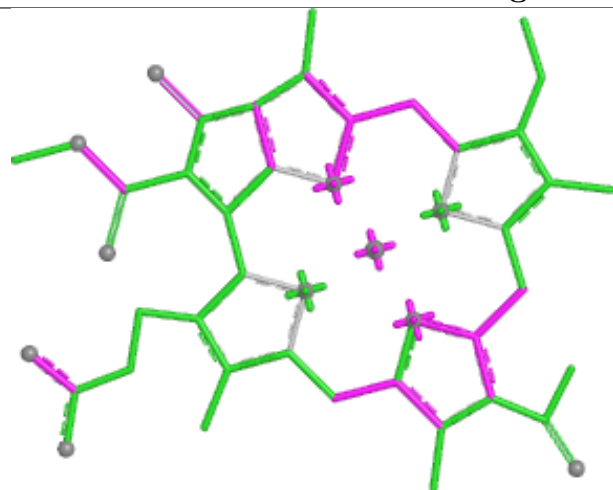


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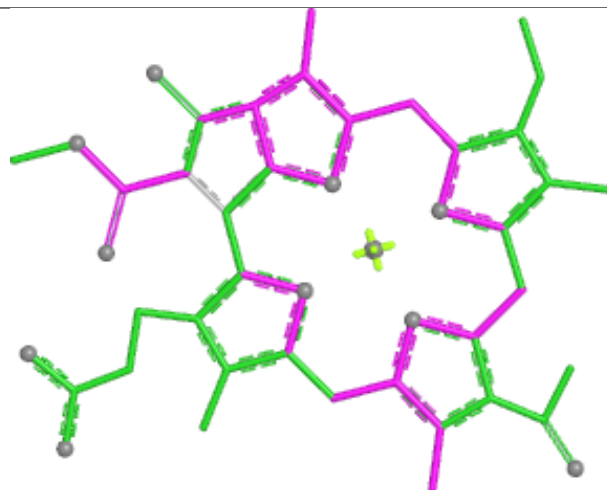


Rings

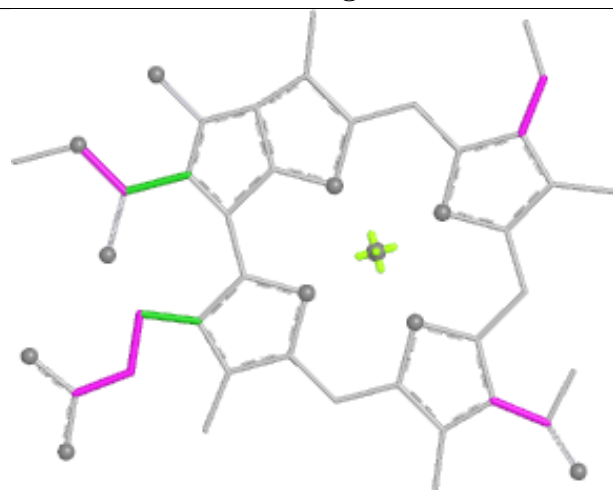
Ligand BCL AI 101



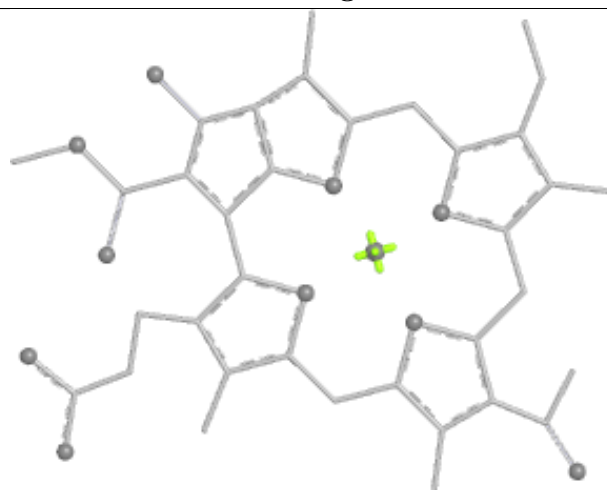
Bond lengths



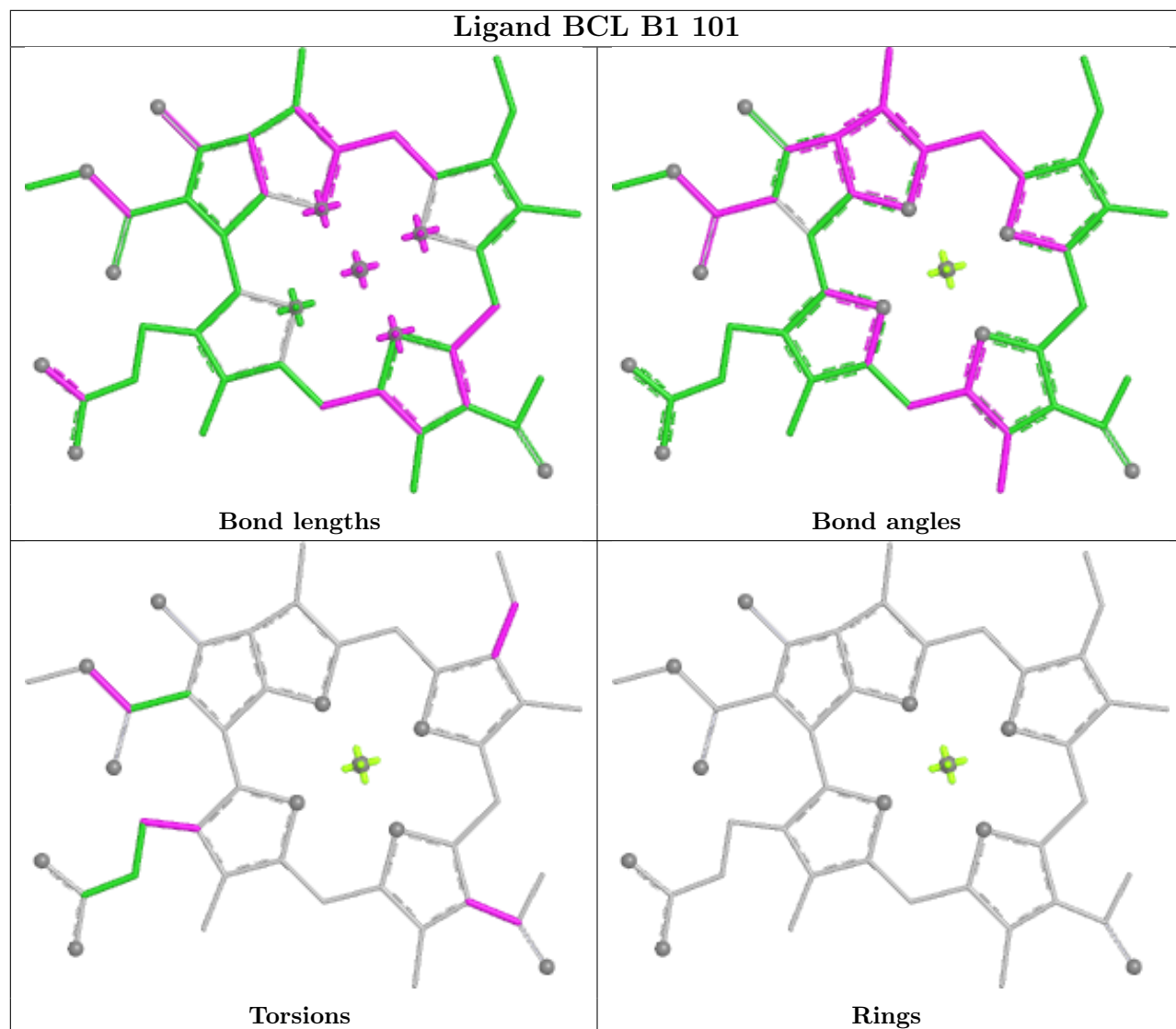
Bond angles



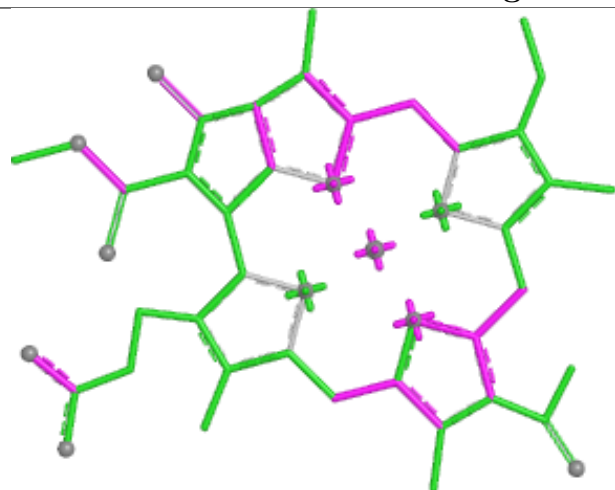
Torsions



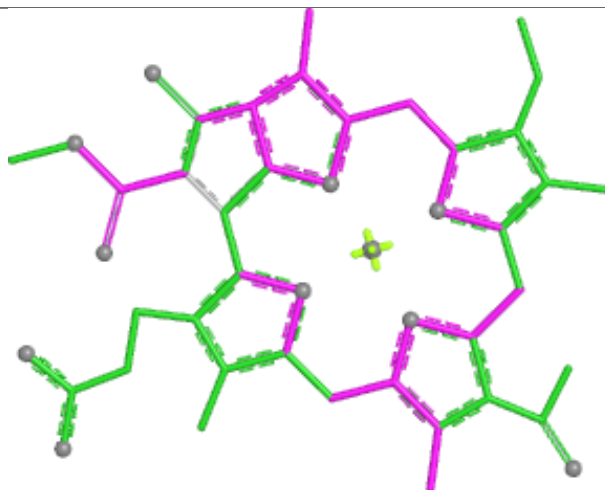
Rings



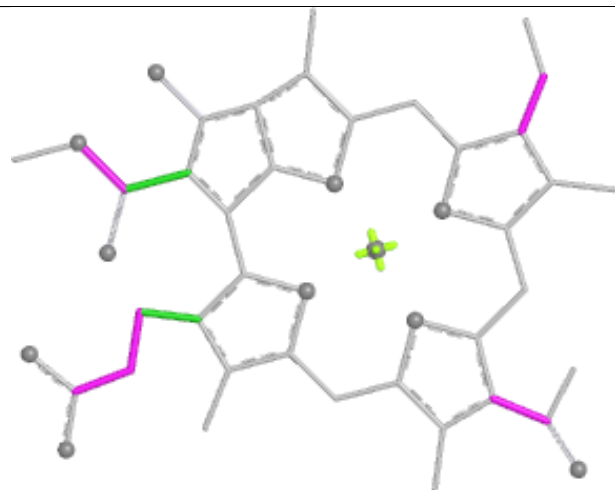
Ligand BCL AO 101



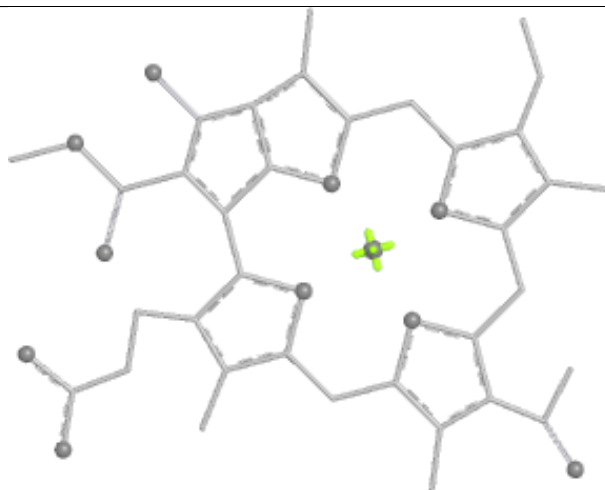
Bond lengths



Bond angles

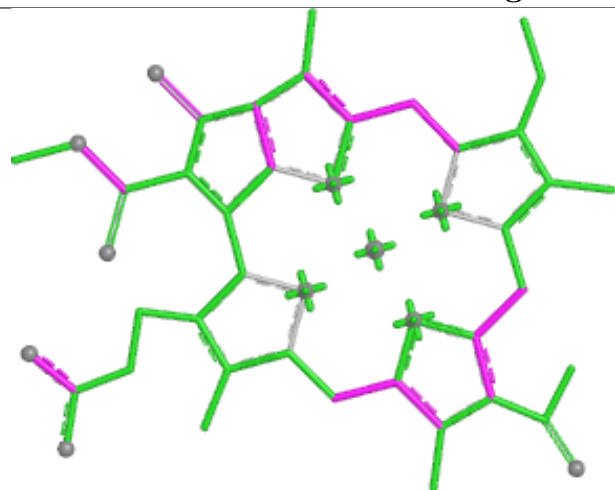


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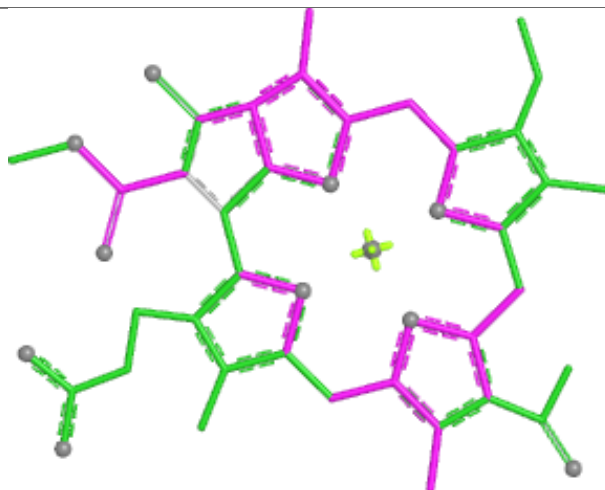


Rings

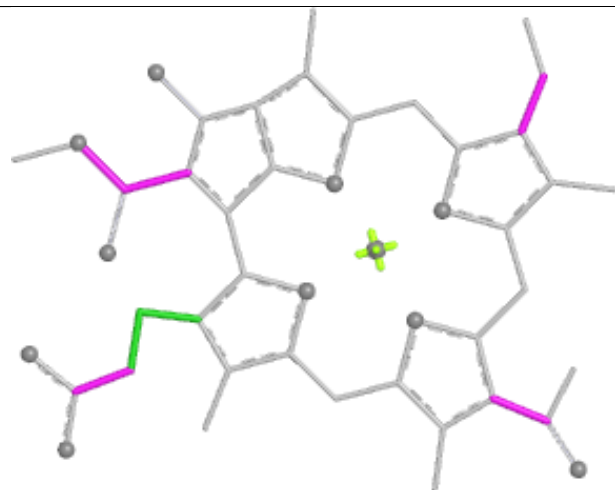
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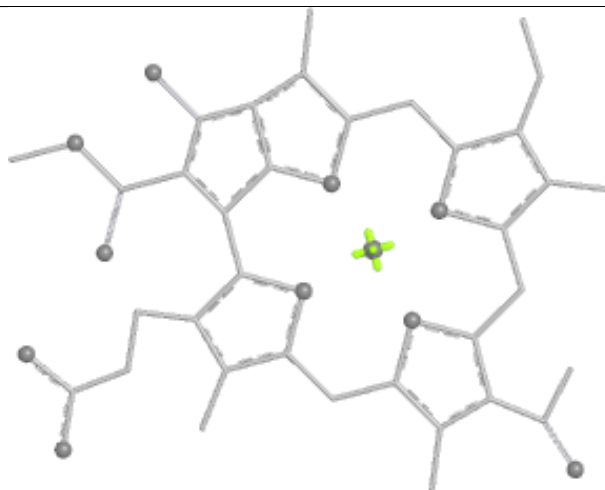
Bond lengths



Bond angles

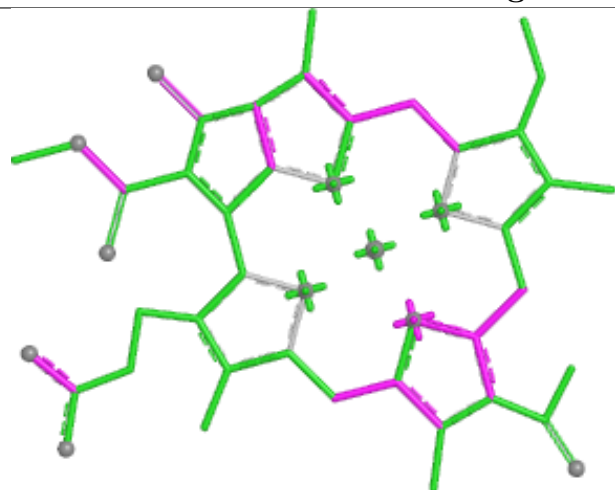


Torsions

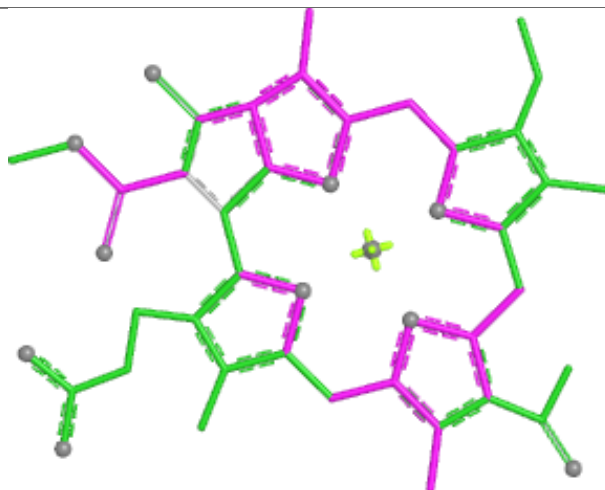


Rings

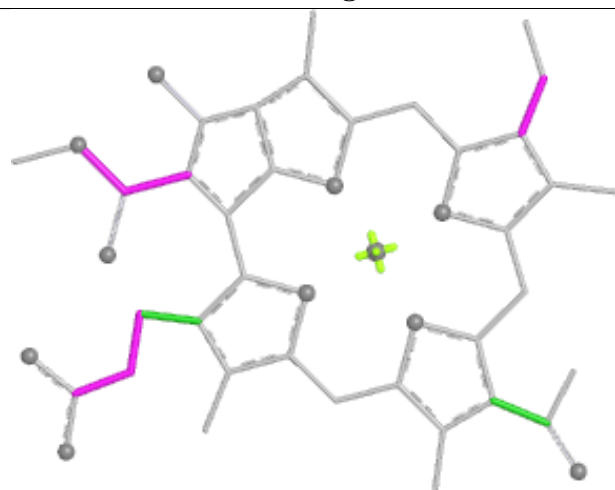
Ligand BCL A7 101



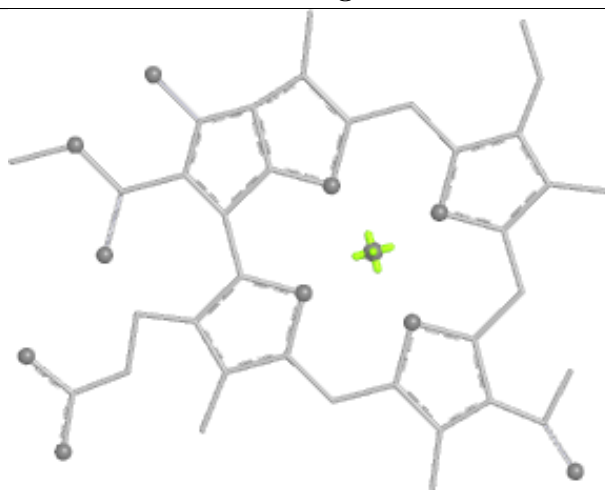
Bond lengths



Bond angles

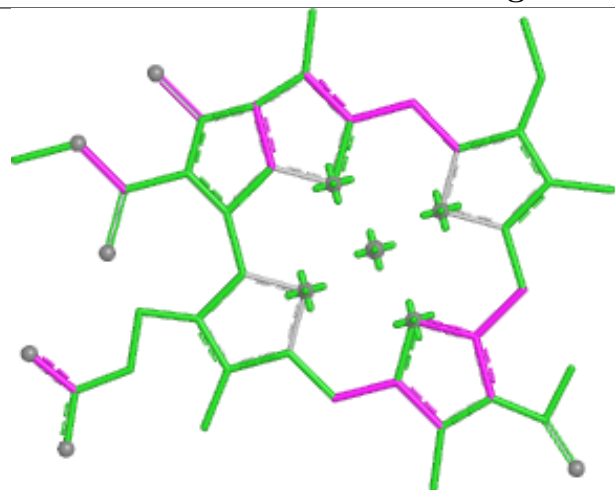


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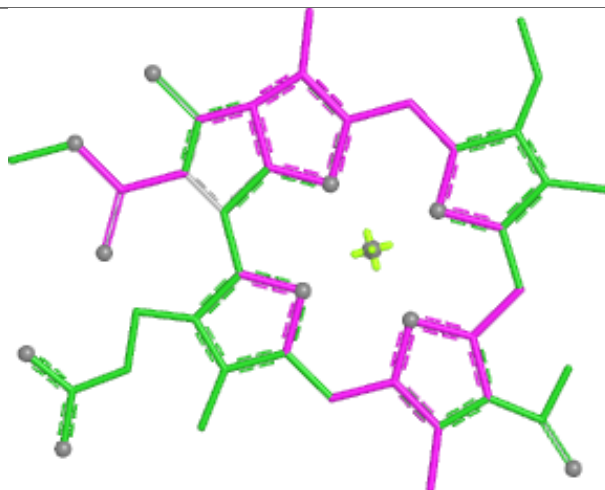


Rings

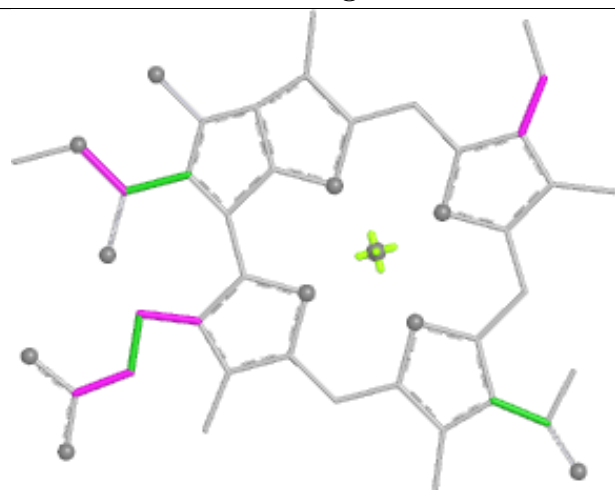
Ligand BCL A8 101



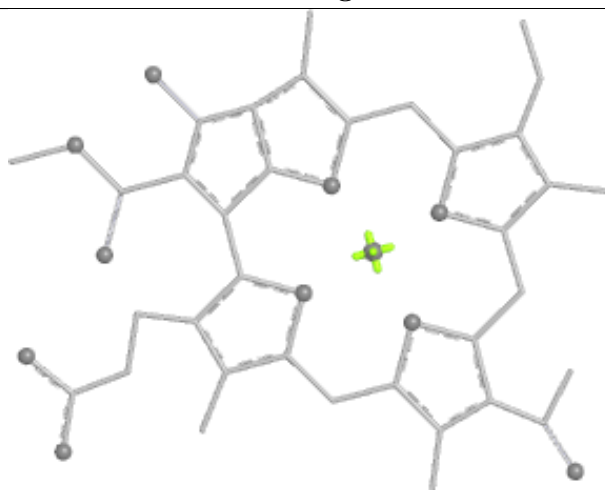
Bond lengths



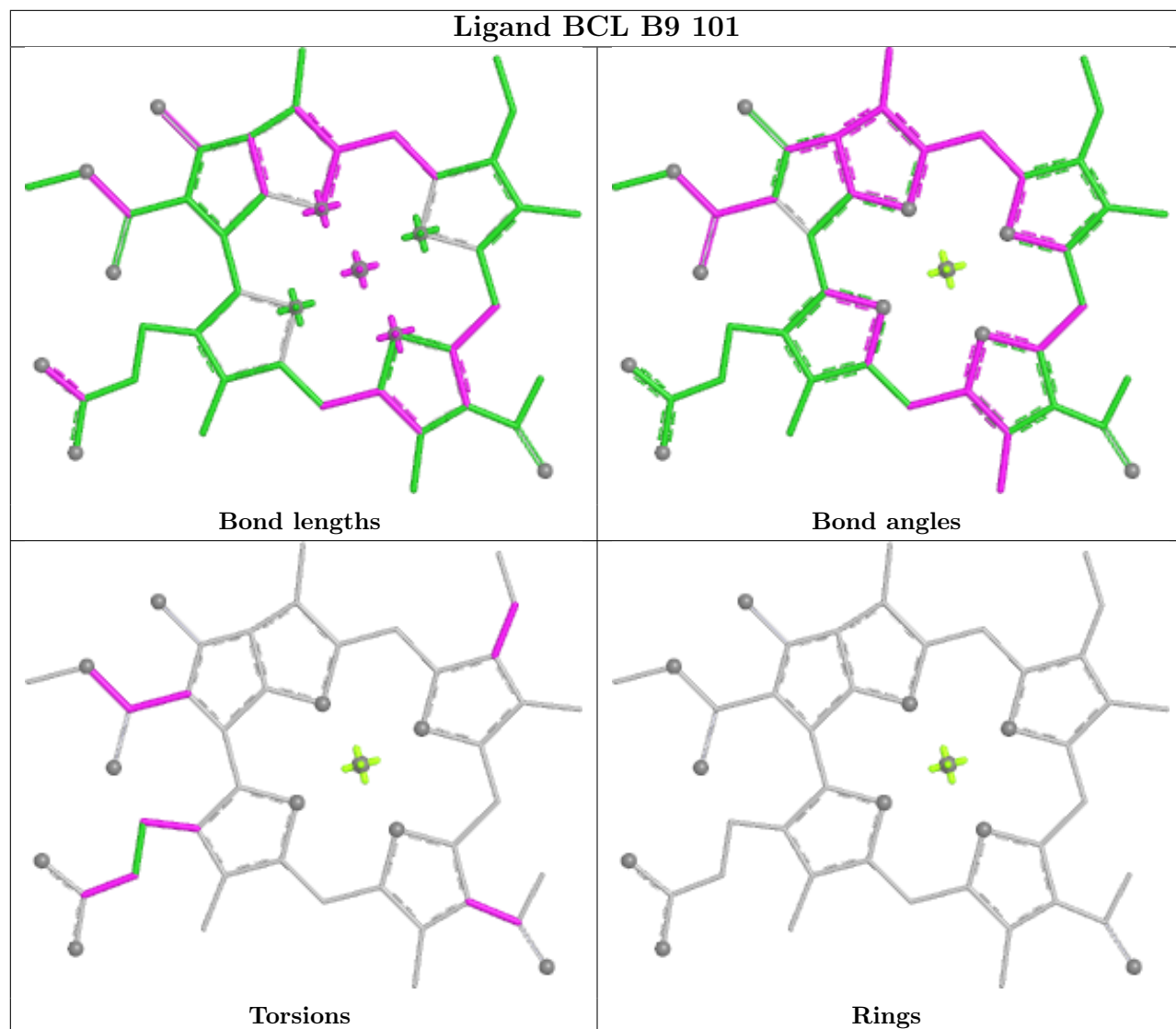
Bond angles

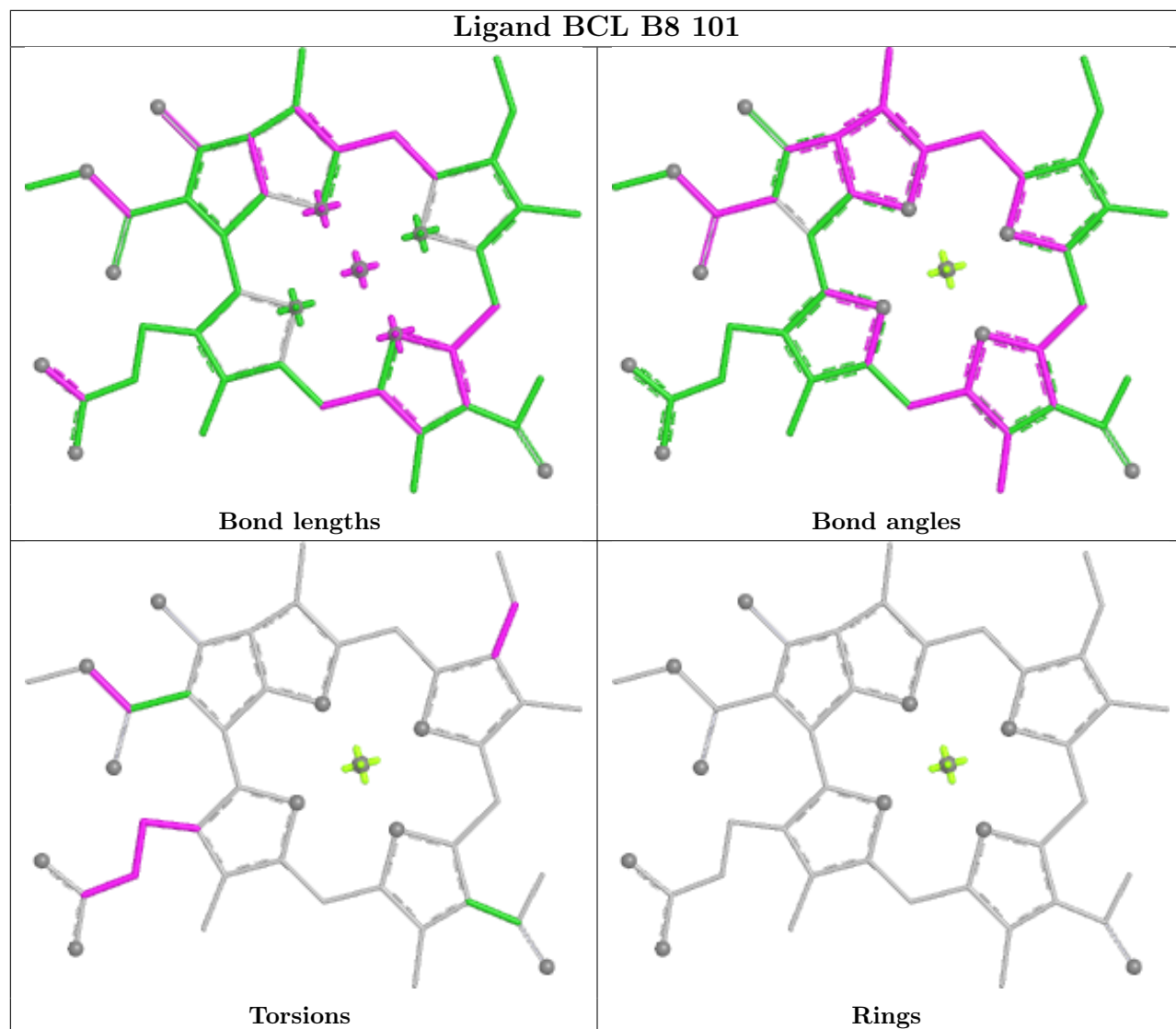


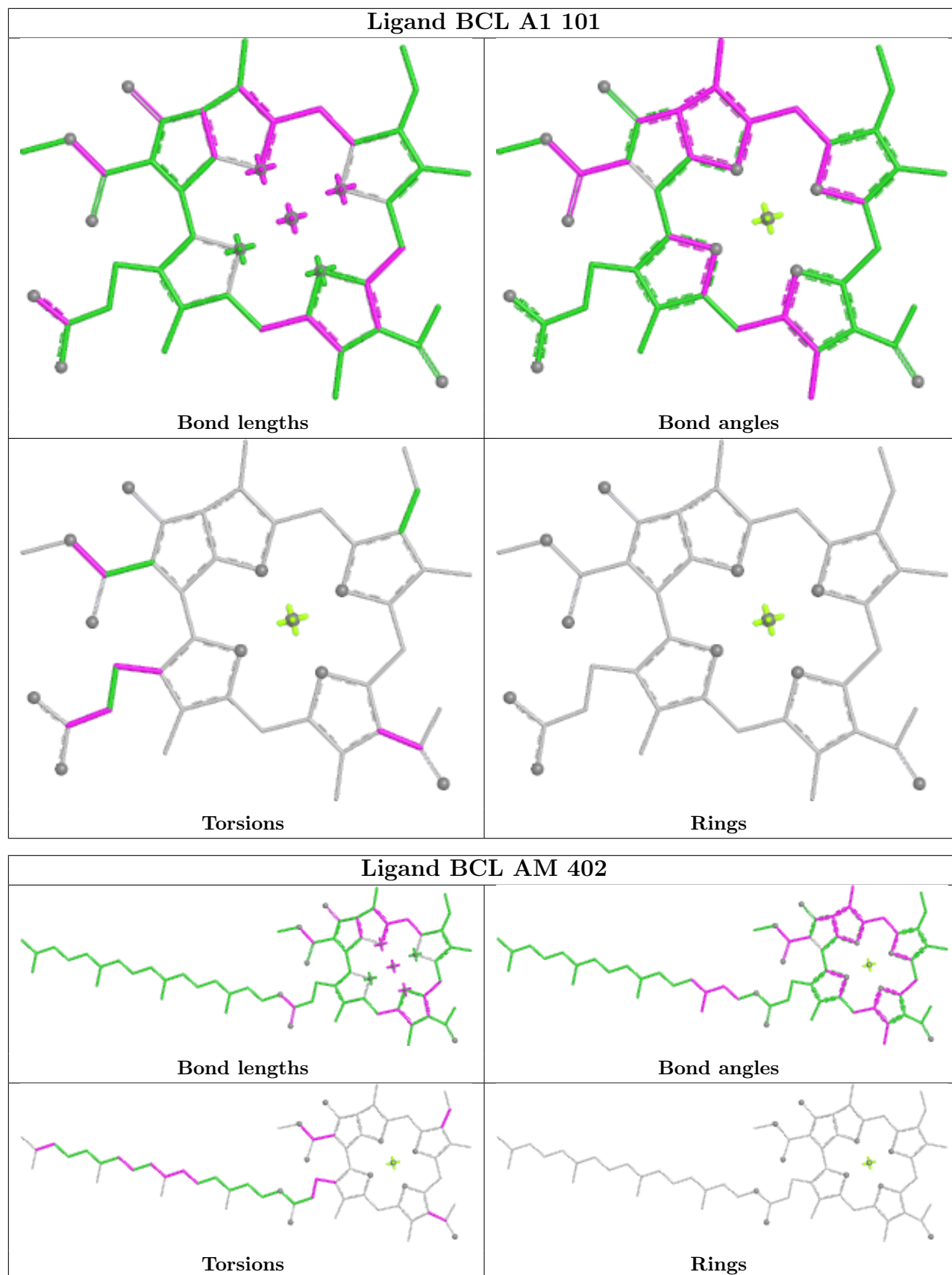
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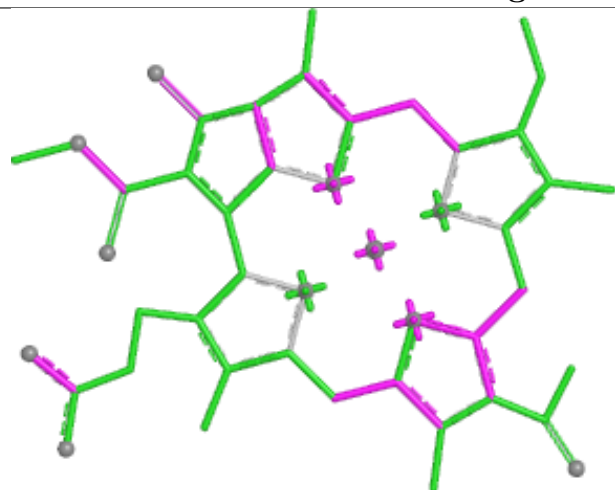
Rings



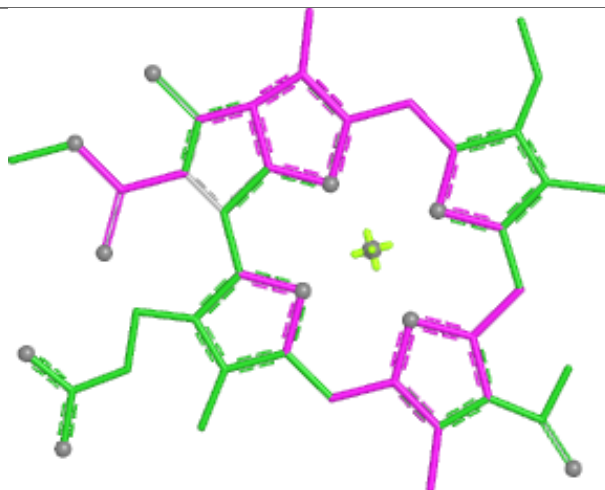




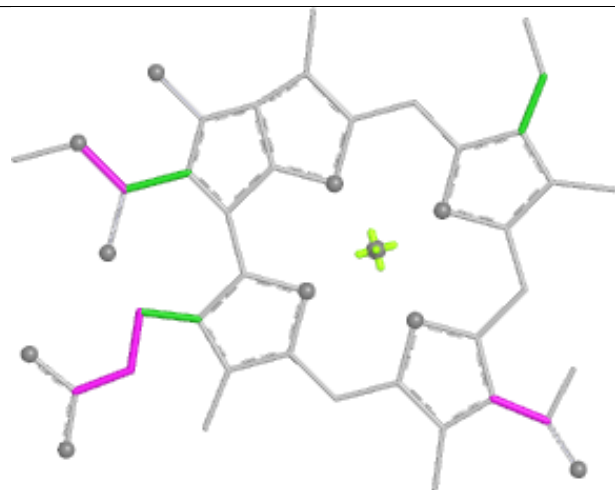
Ligand BCL B5 101



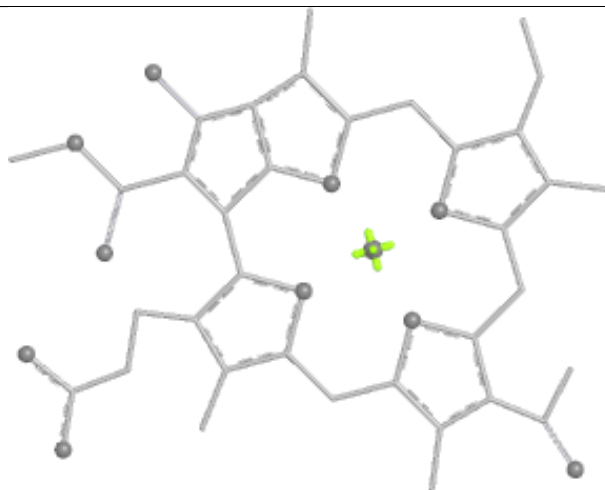
Bond lengths



Bond angles

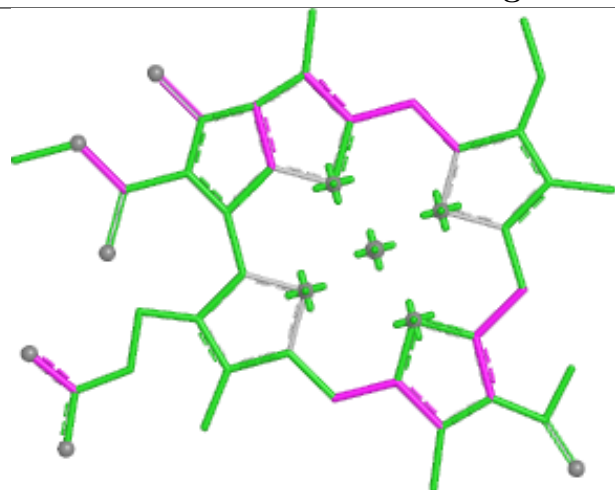


Torsions

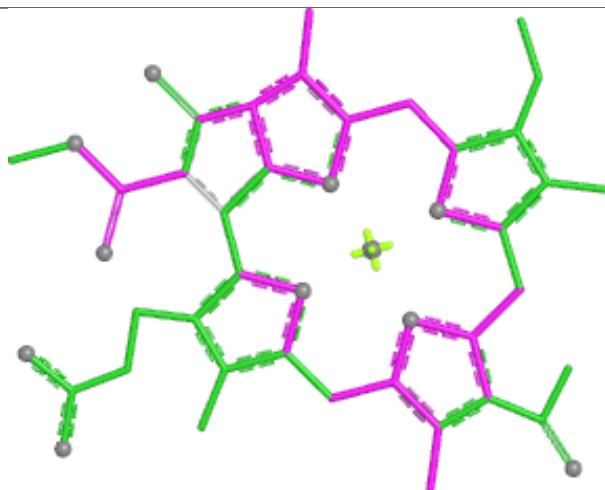


Rings

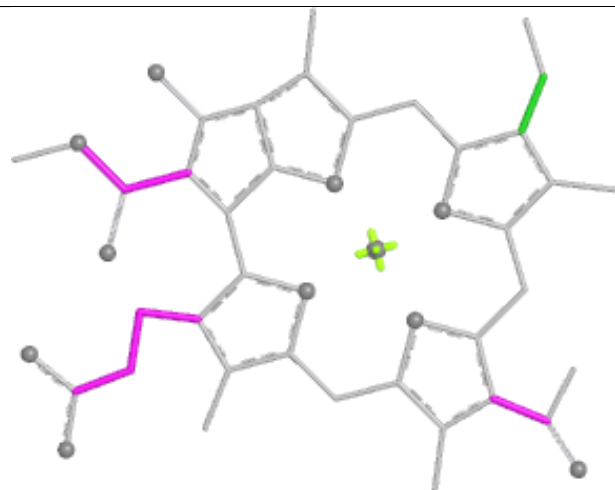
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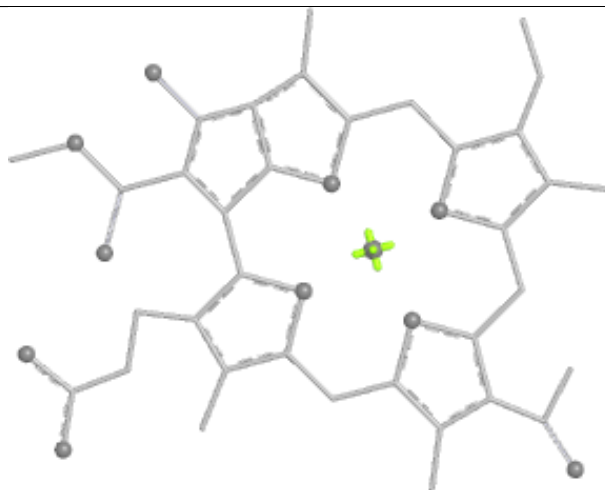
Bond lengths



Bond angles

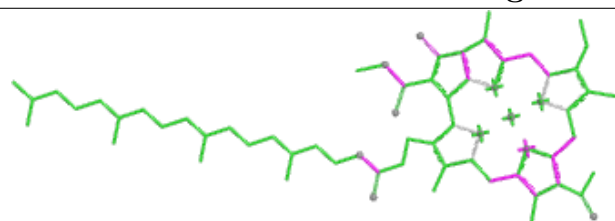


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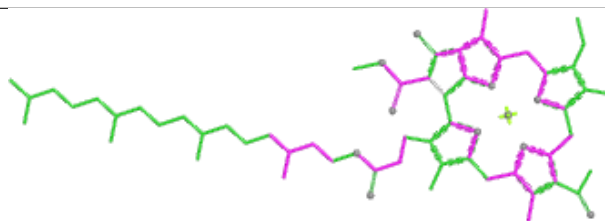


Rings

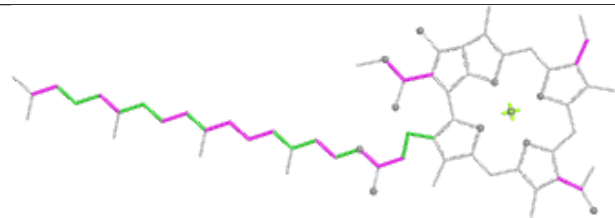
Ligand BCL BL 301



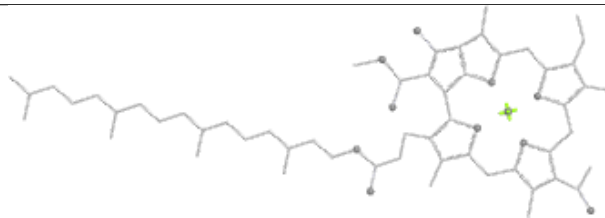
Bond lengths



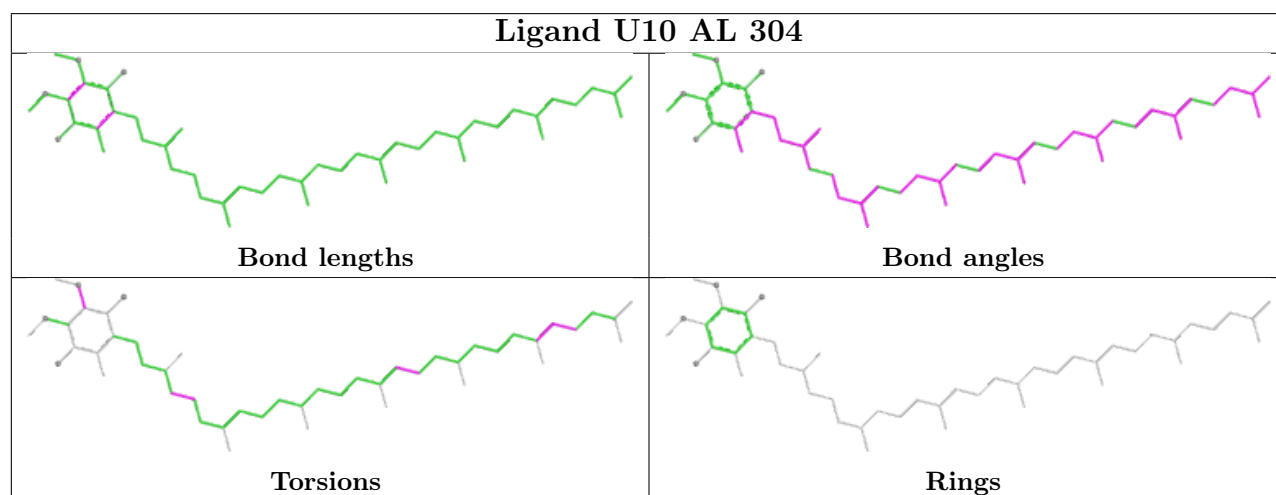
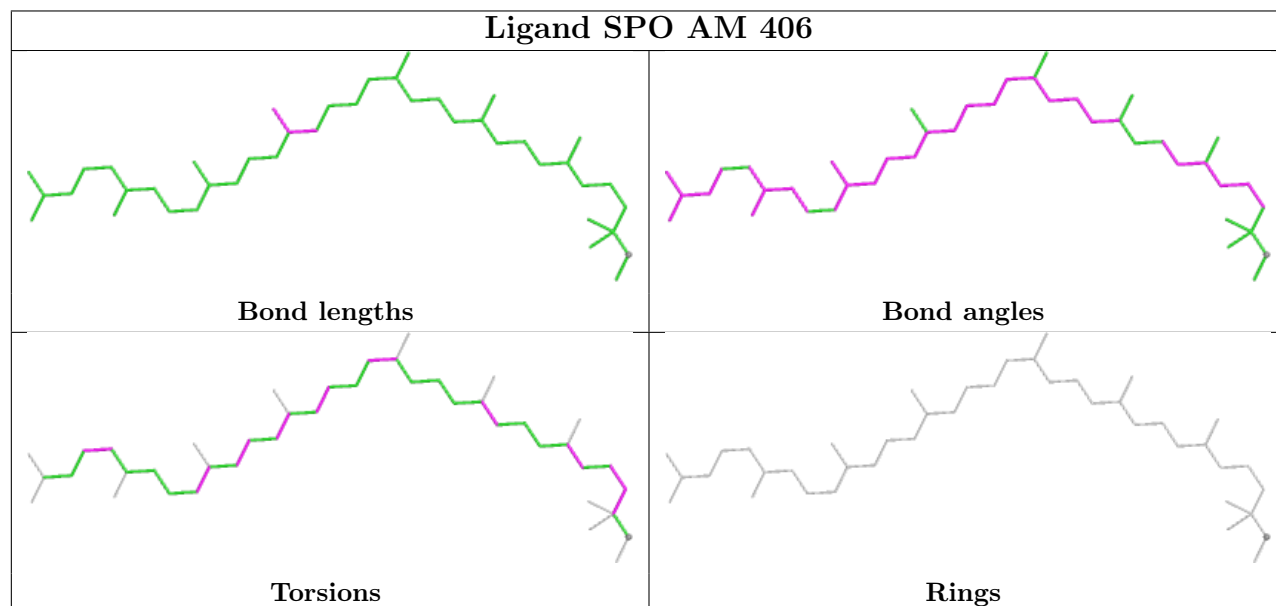
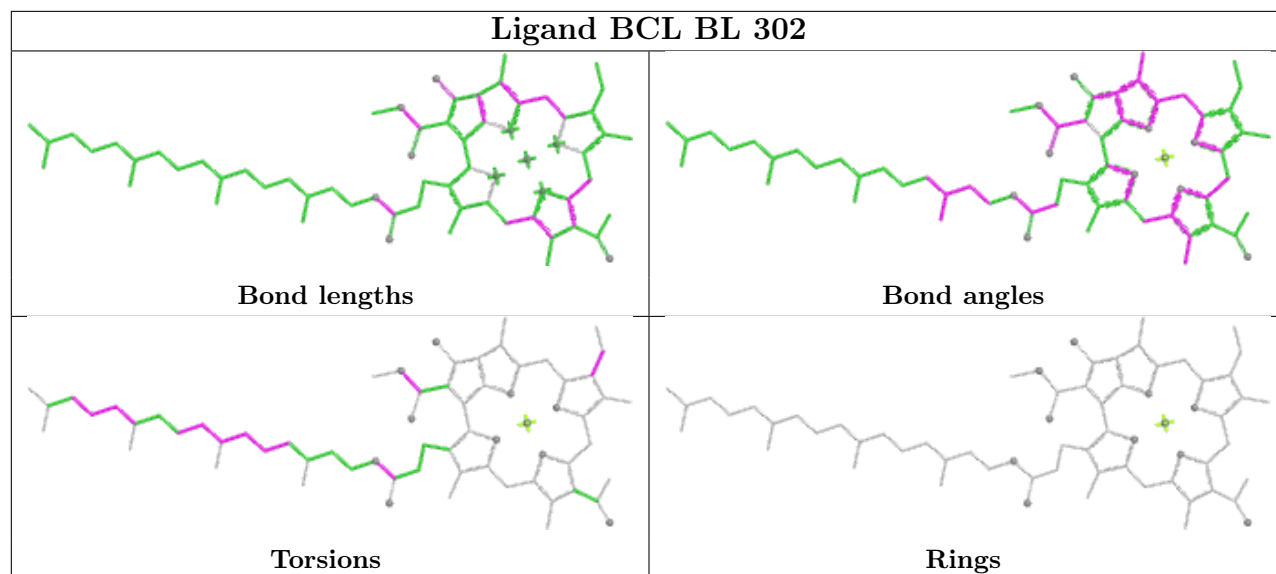
Bond angles



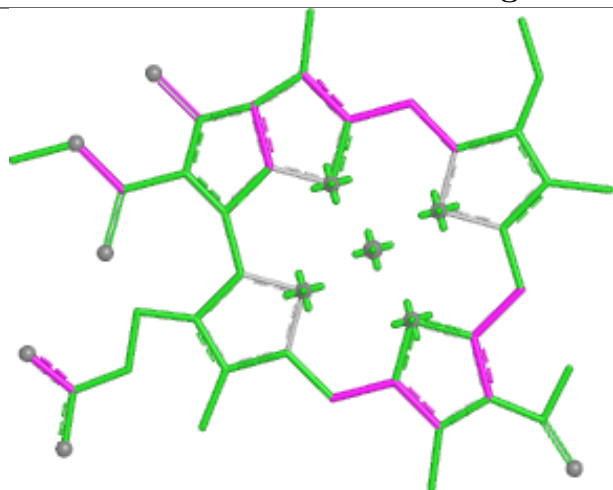
Torsions



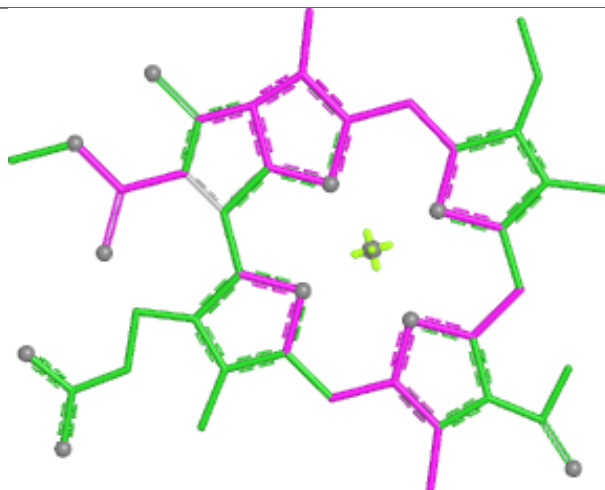
Rings



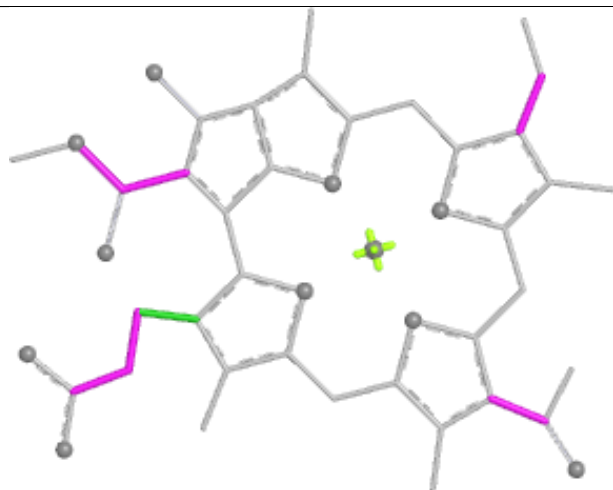
Ligand BCL AD 101



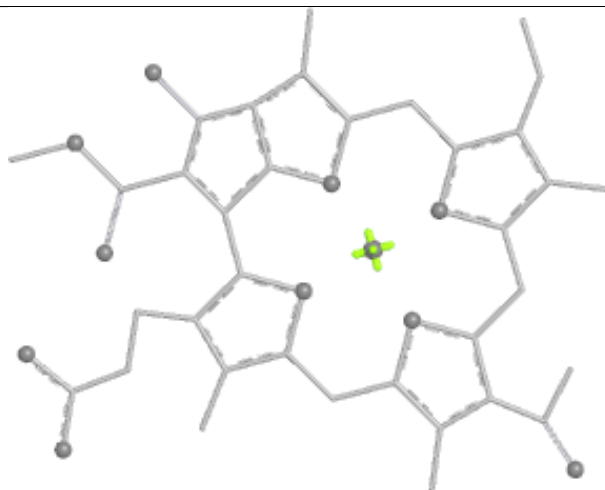
Bond lengths



Bond angles

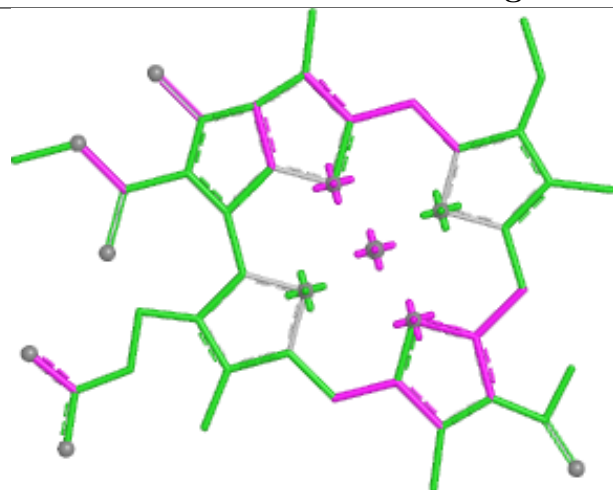


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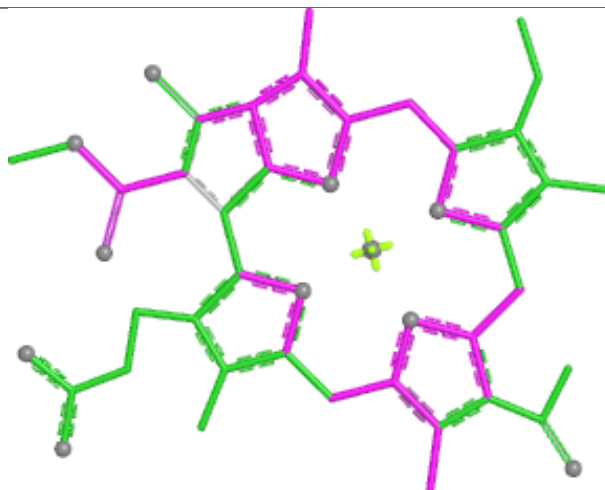


Rings

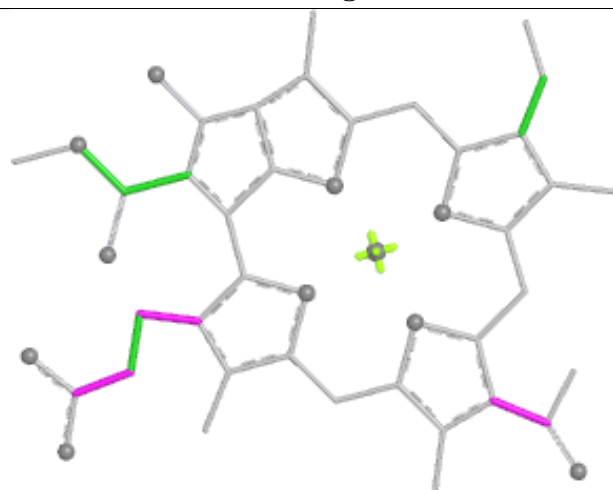
Ligand BCL BT 101



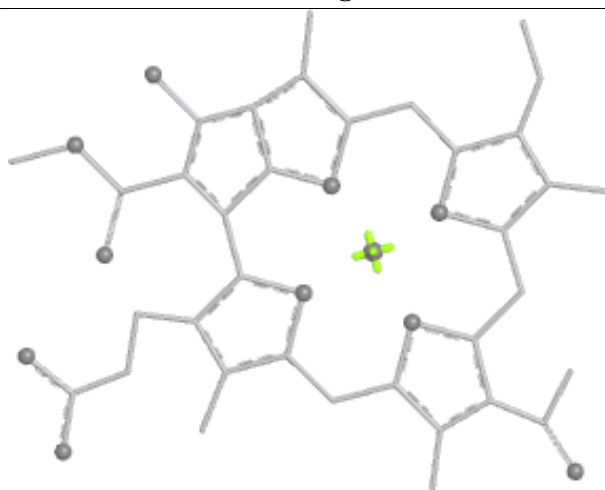
Bond lengths



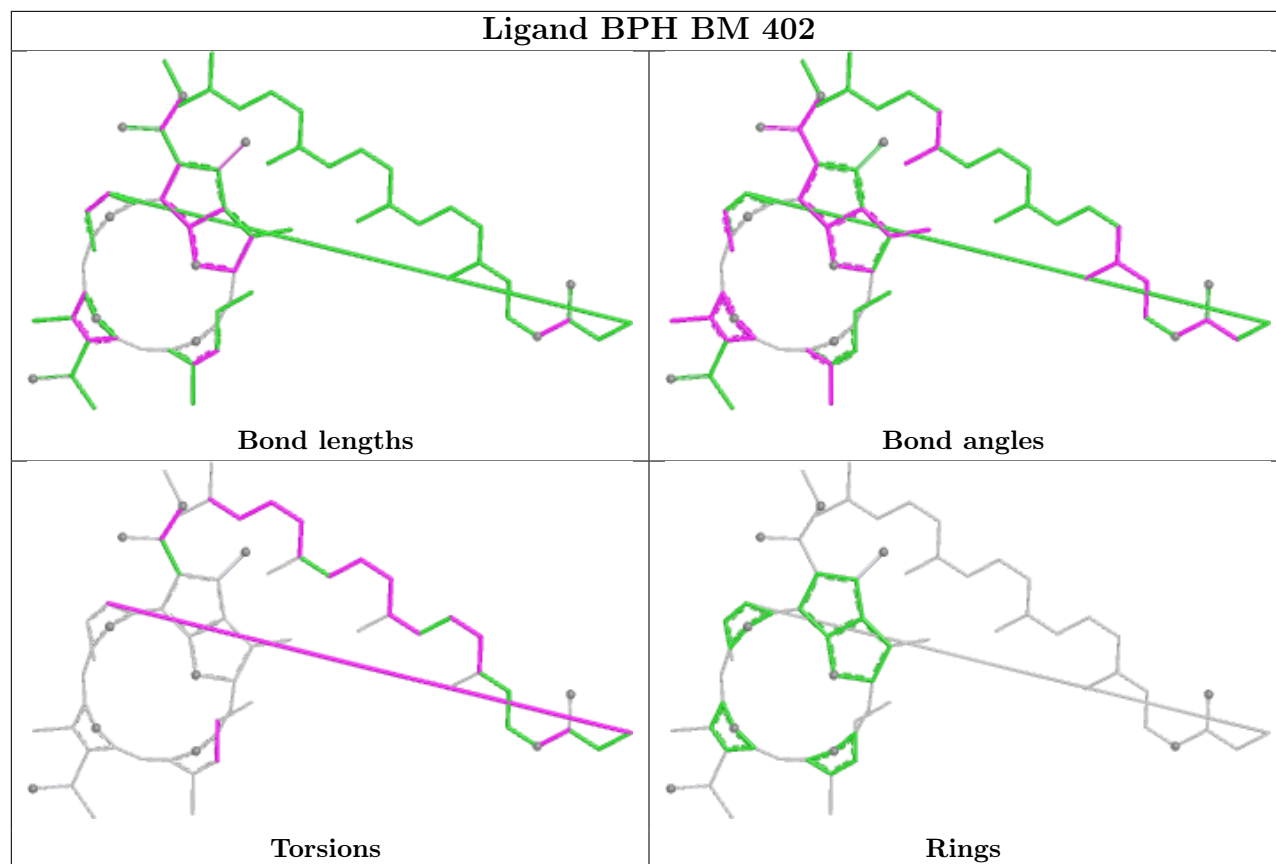
Bond angles



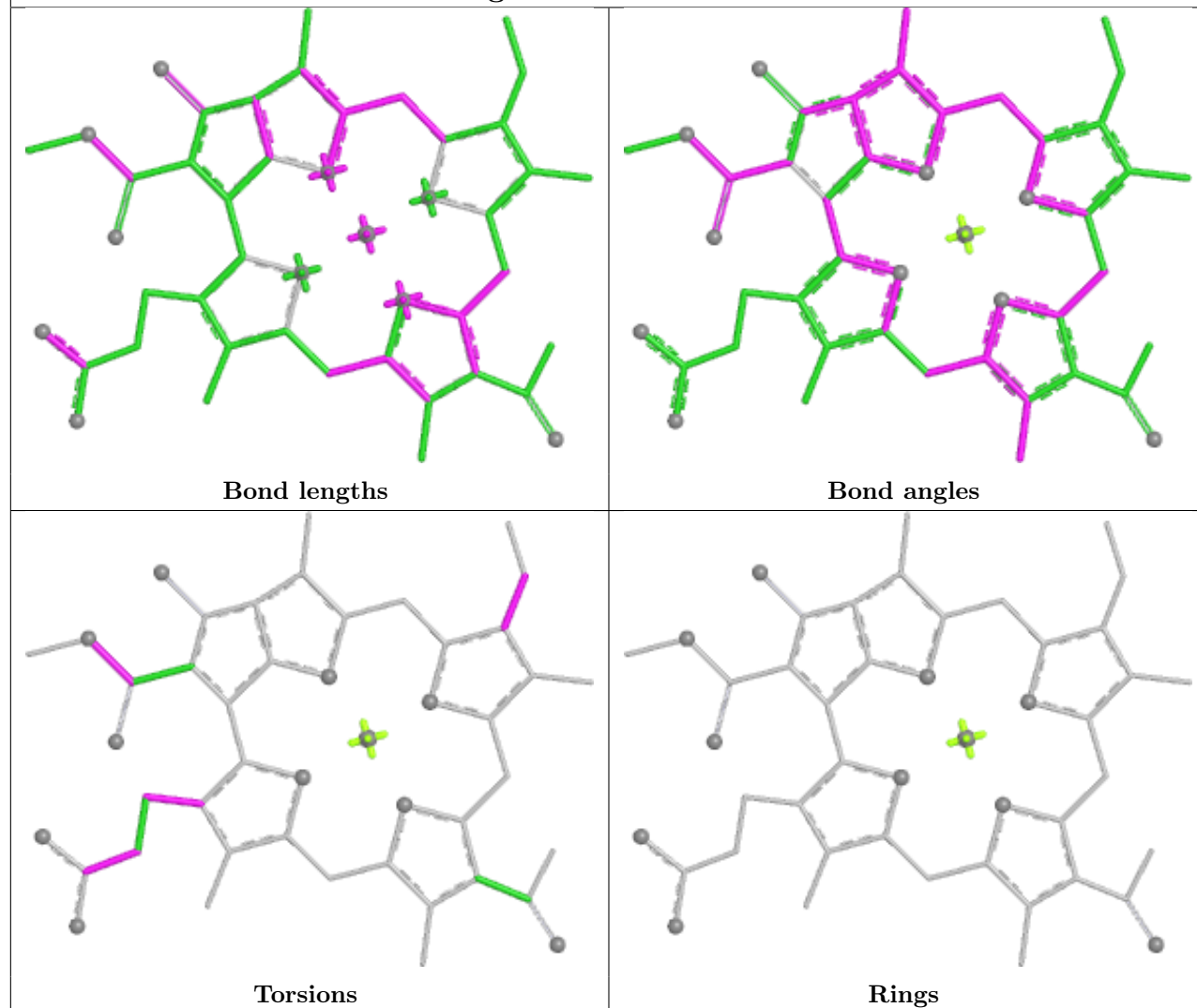
Torsions



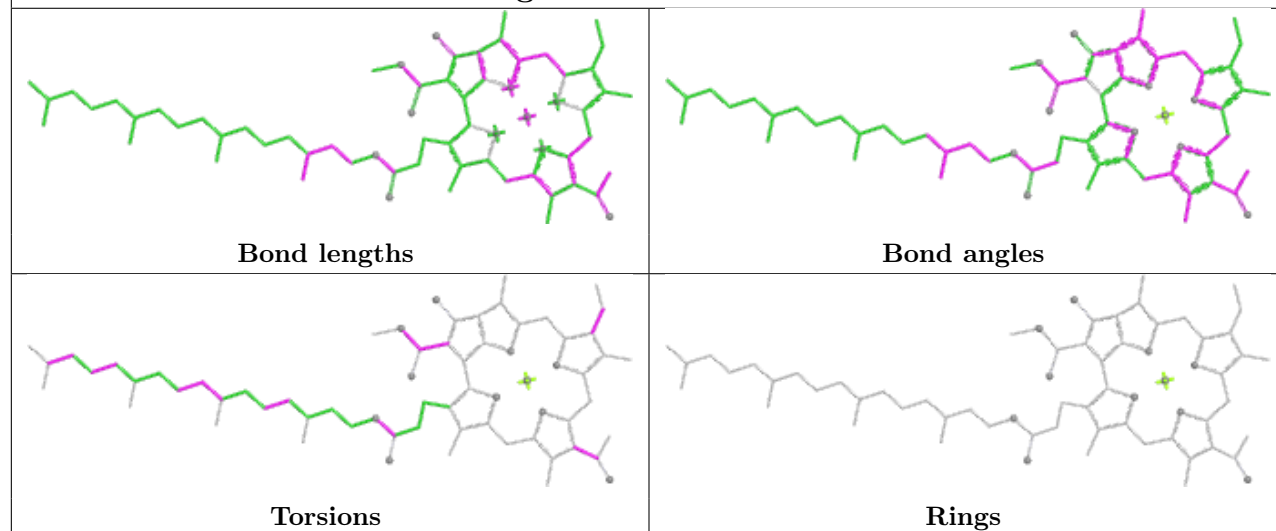
Rings



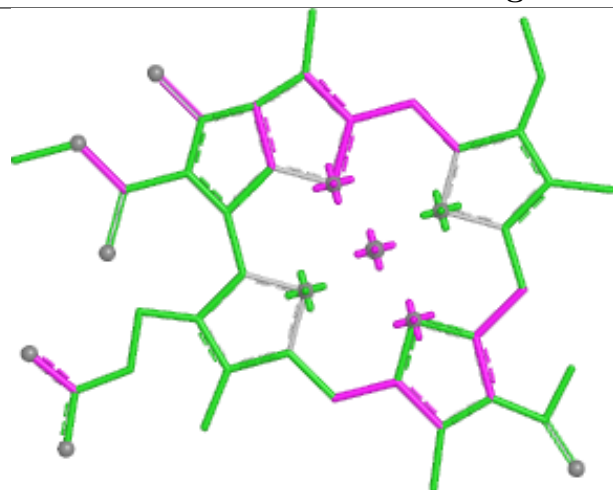
Ligand BCL AP 102



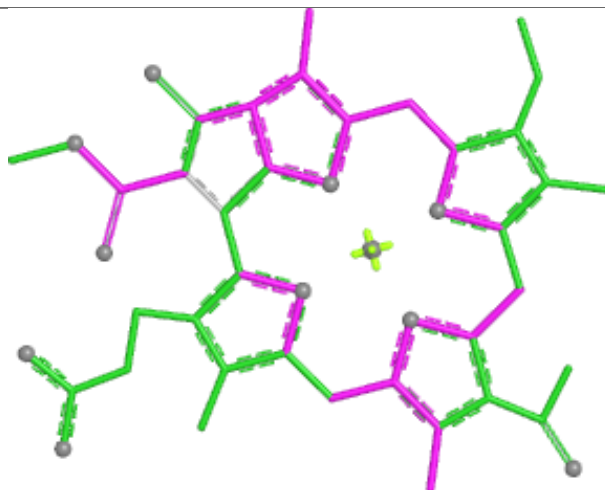
Ligand BCL BM 401



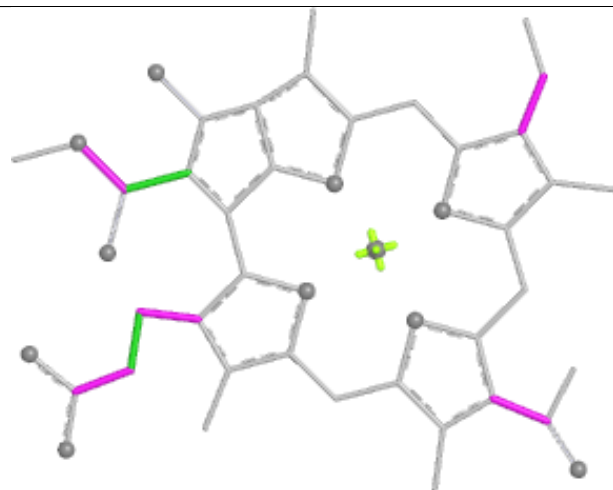
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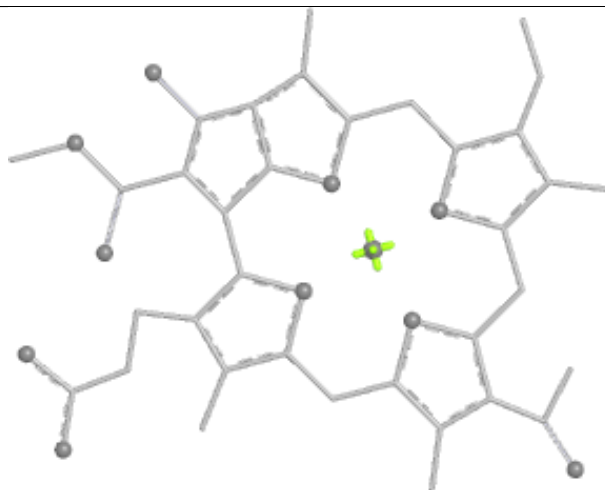
Bond lengths



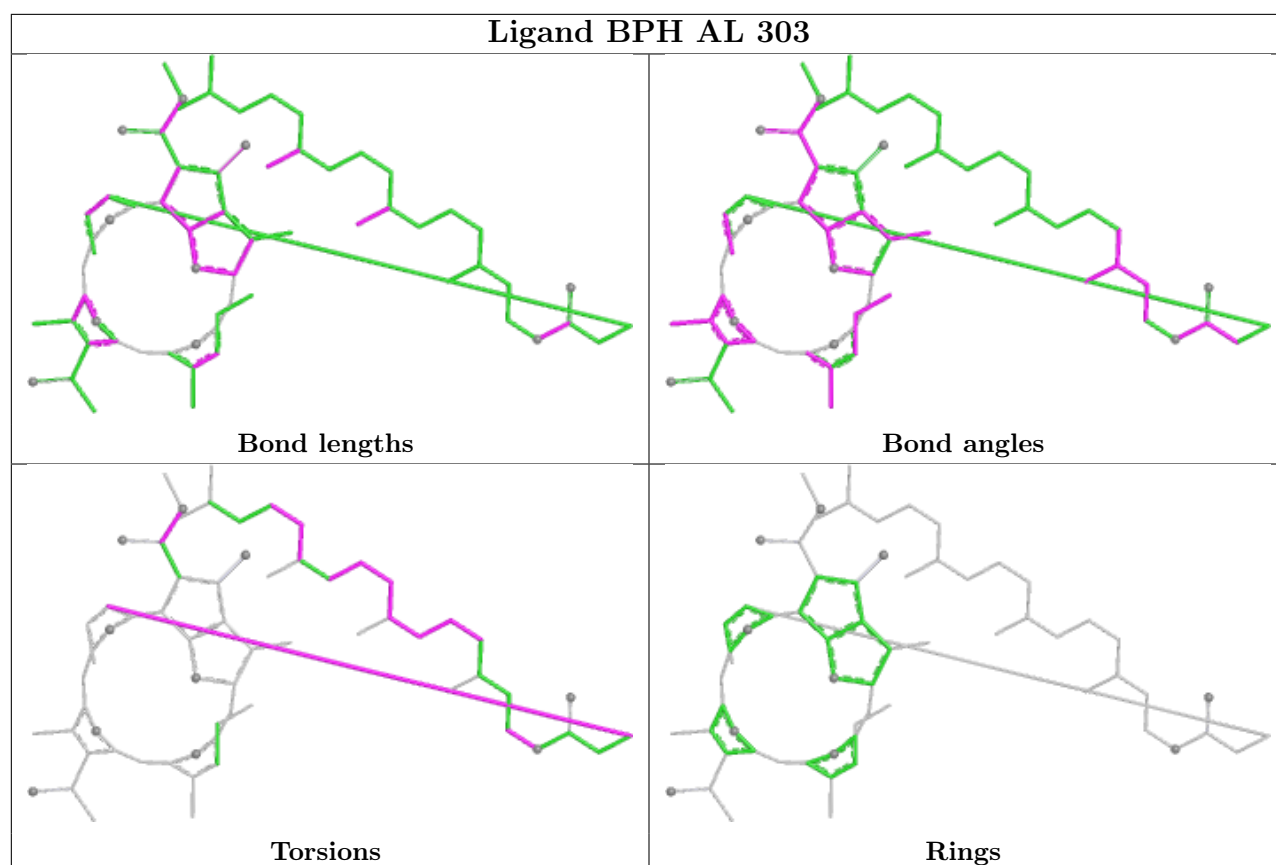
Bond angles



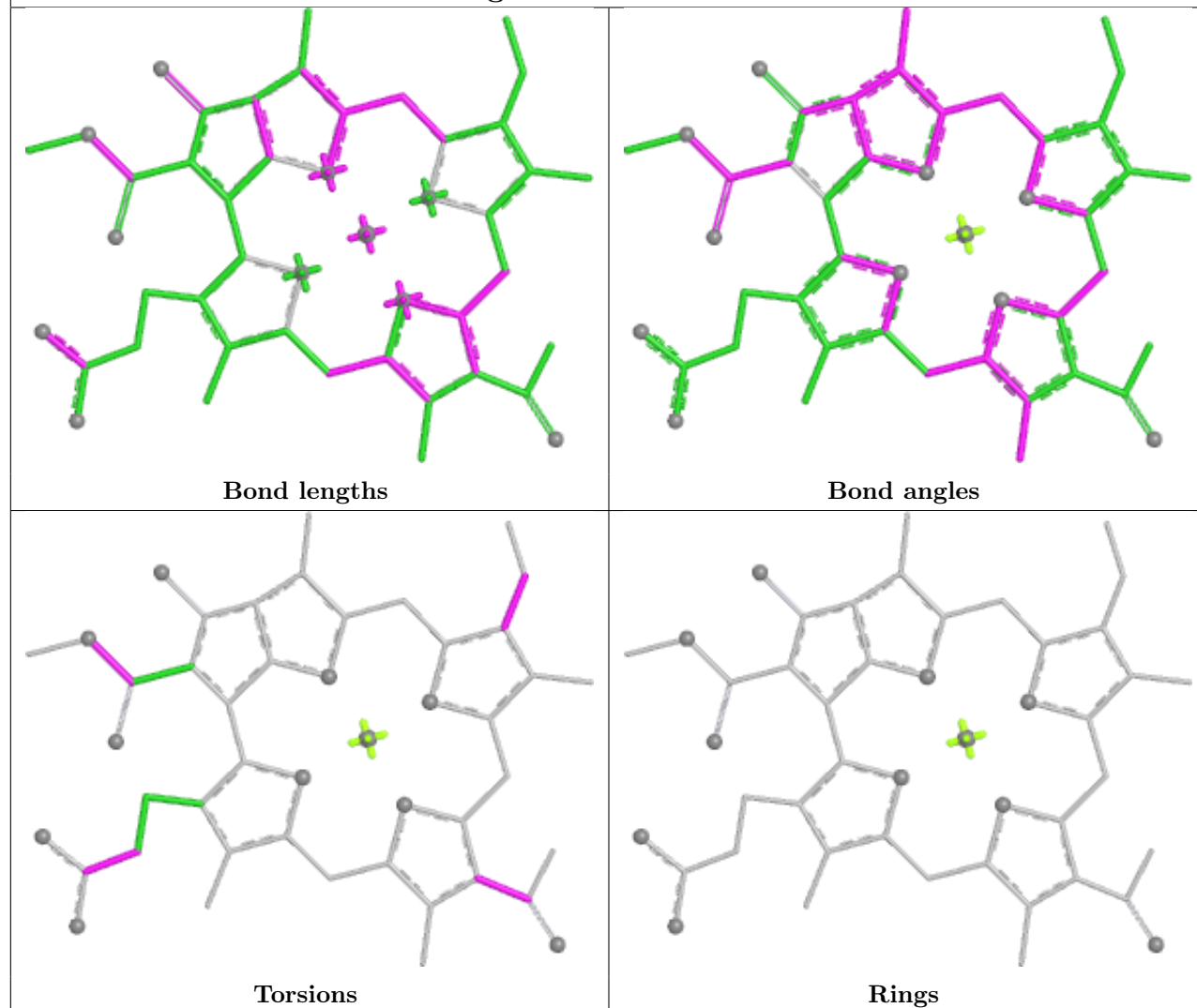
Torsions



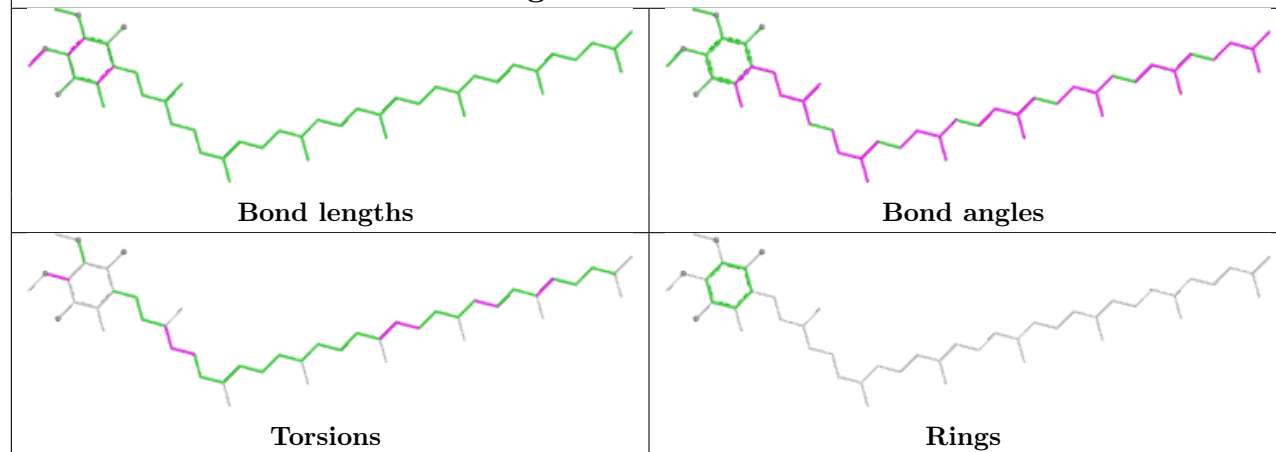
Rings



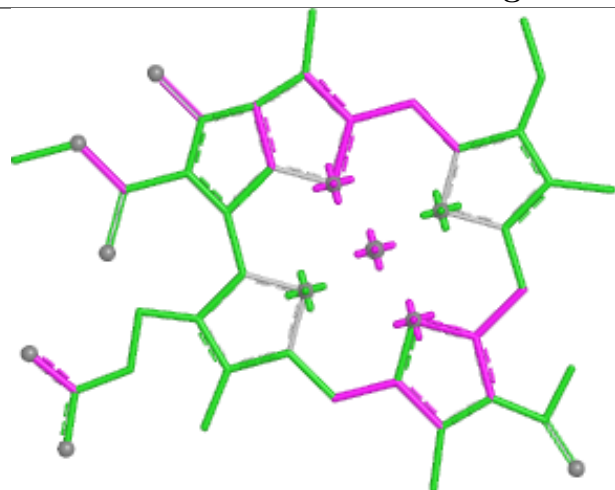
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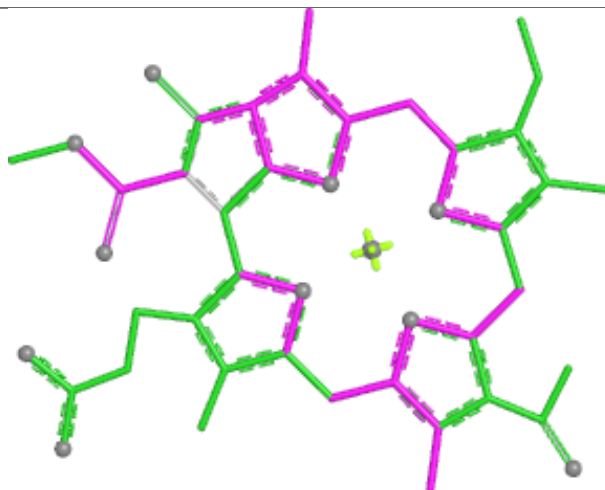
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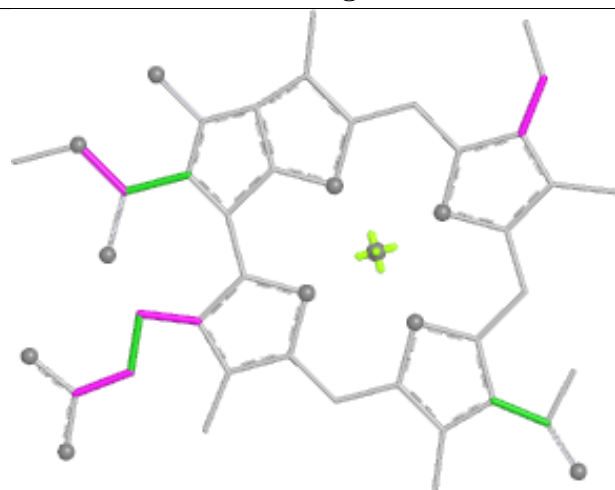
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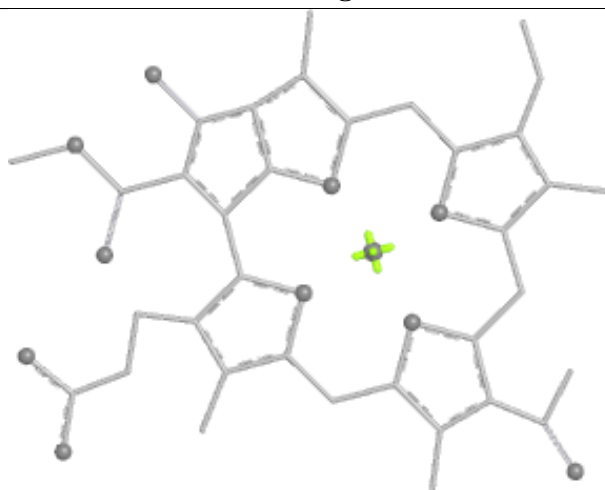
Bond lengths



Bond angles

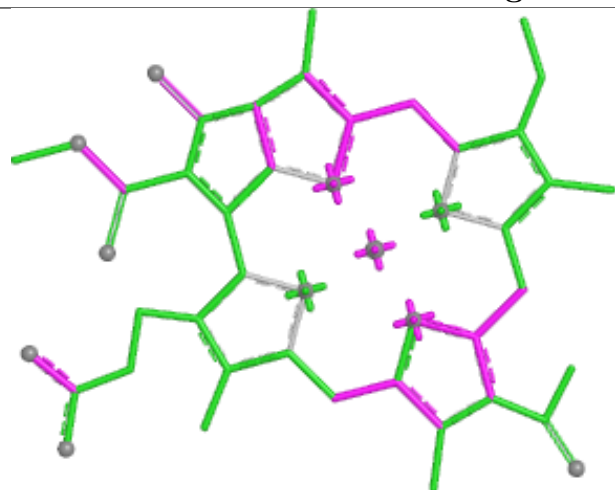


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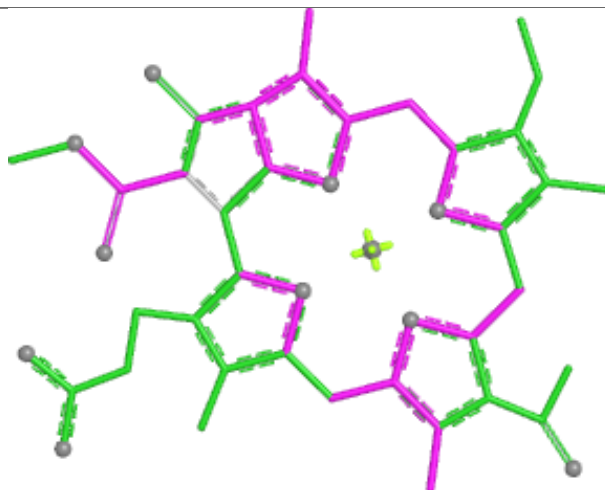


Rings

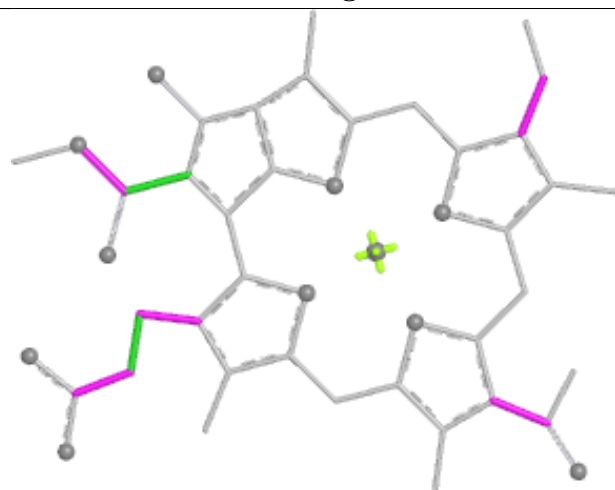
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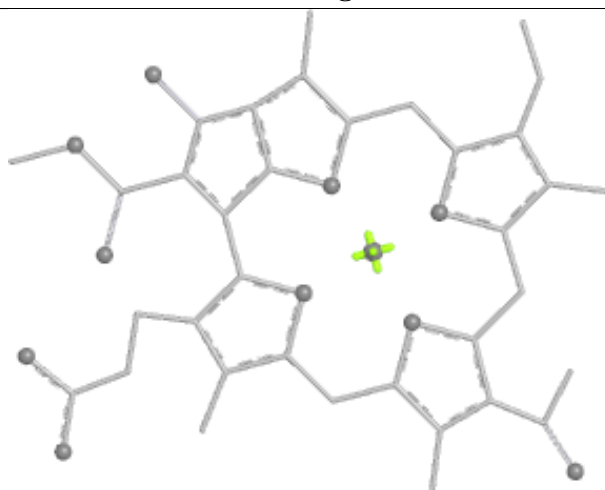
Bond lengths



Bond angles

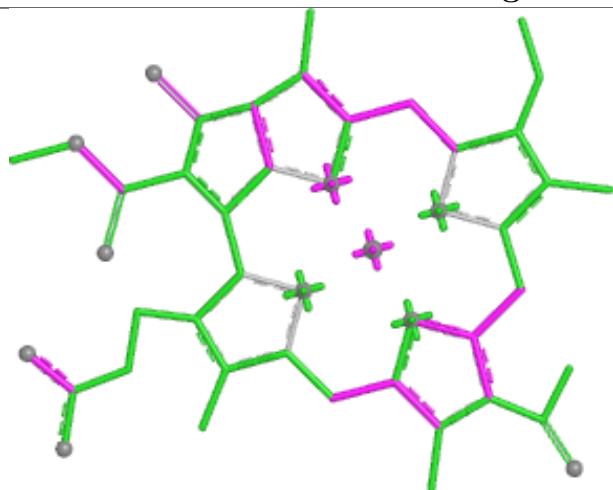


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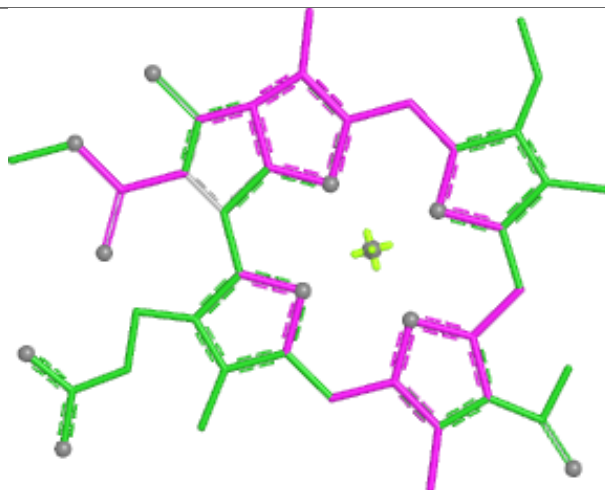


Rings

Ligand BCL AP 101



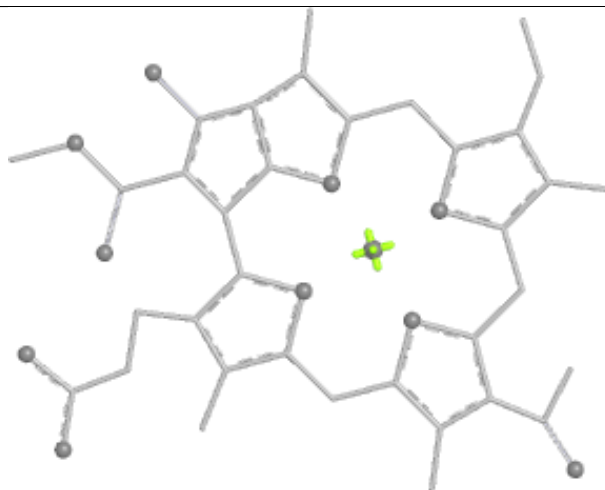
Bond lengths



Bond angles

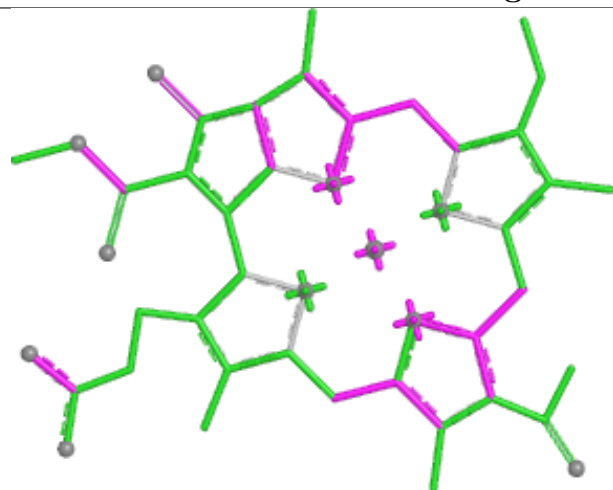


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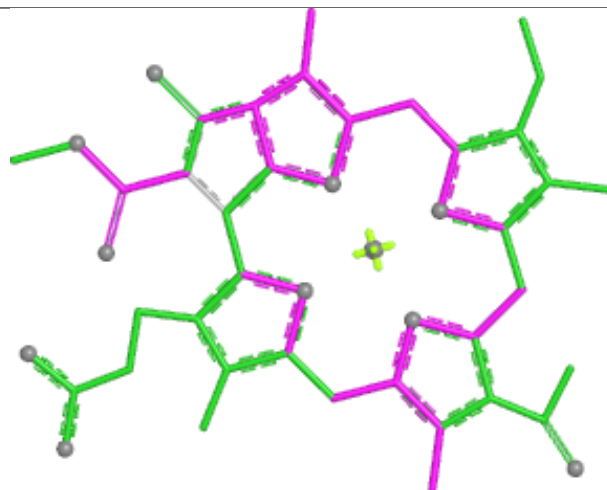


Rings

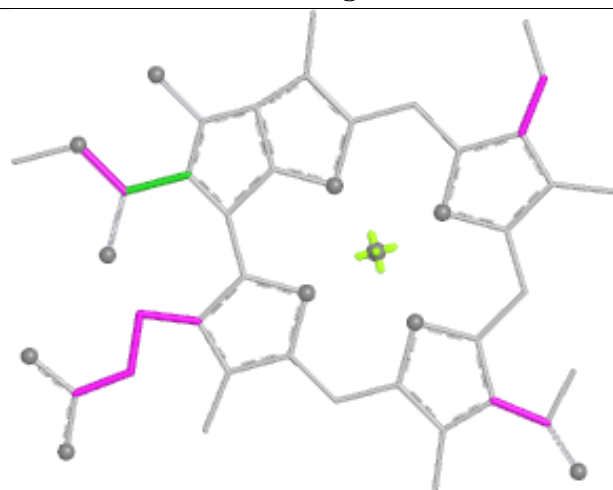
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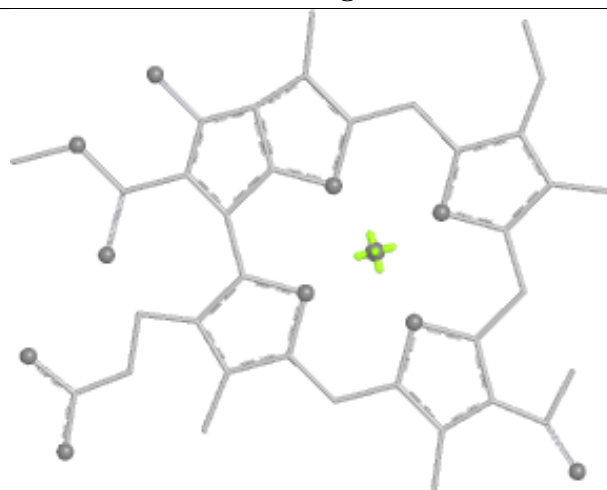
Bond lengths



Bond angles

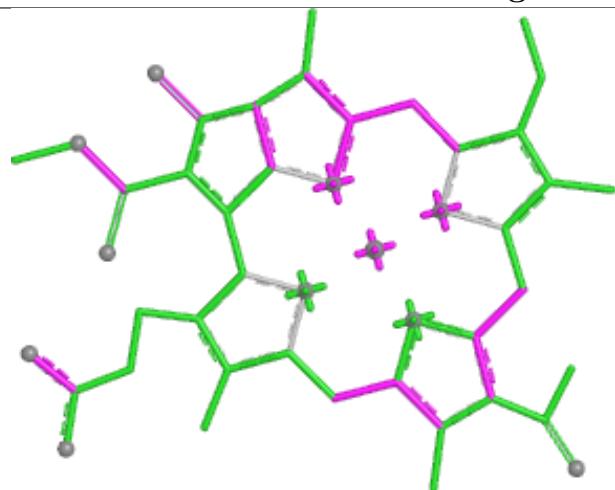


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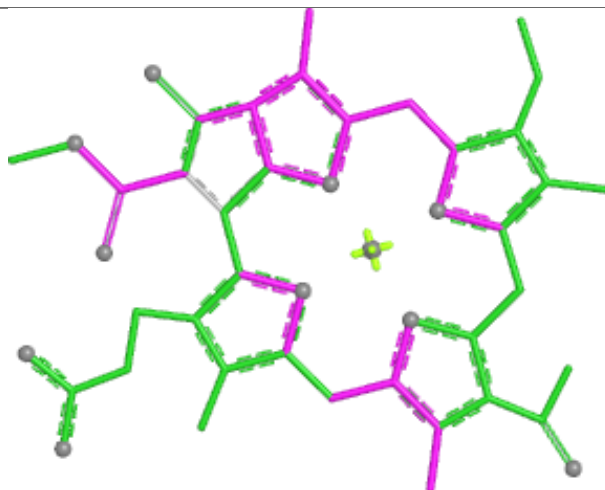


Rings

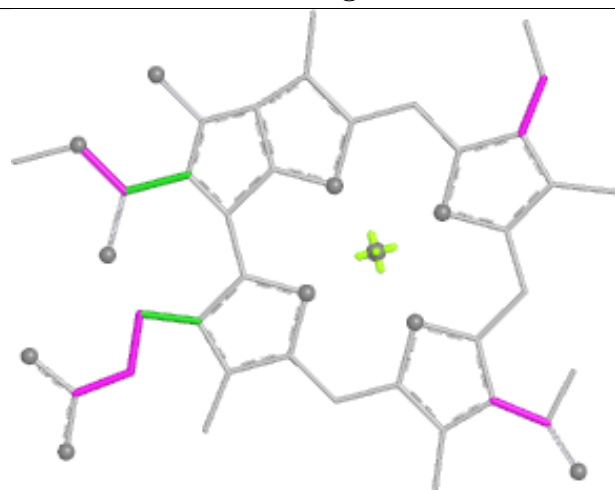
Ligand BCL B3 101



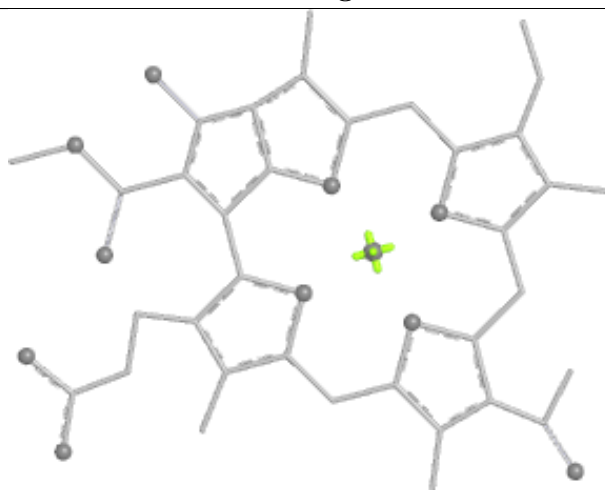
Bond lengths



Bond angles

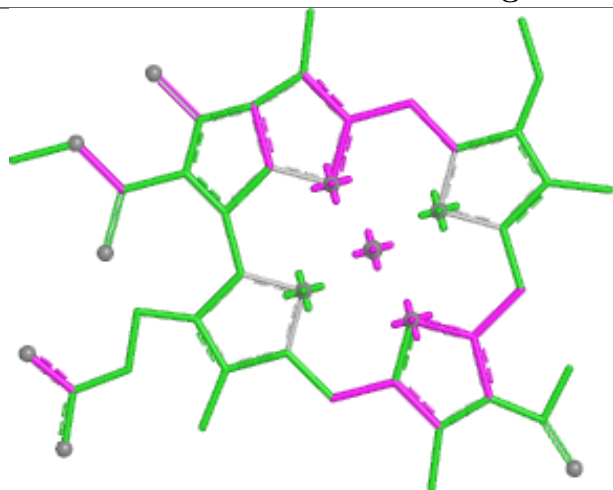


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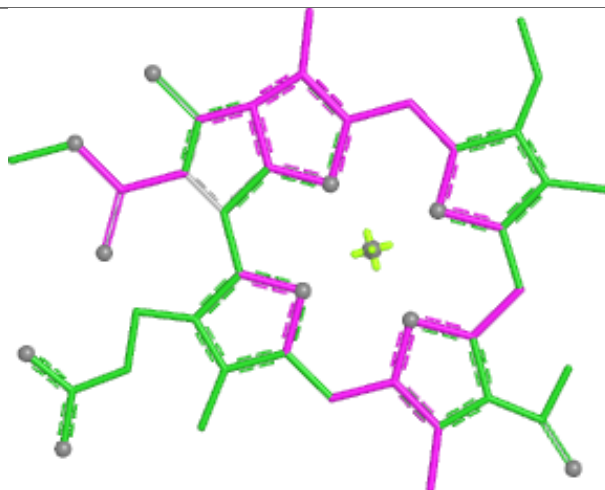


Rings

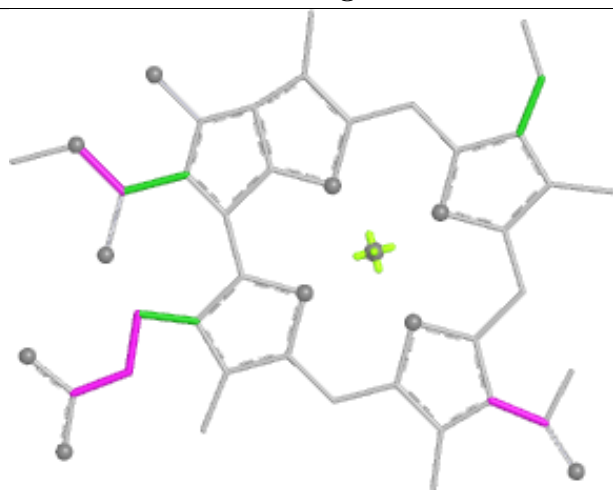
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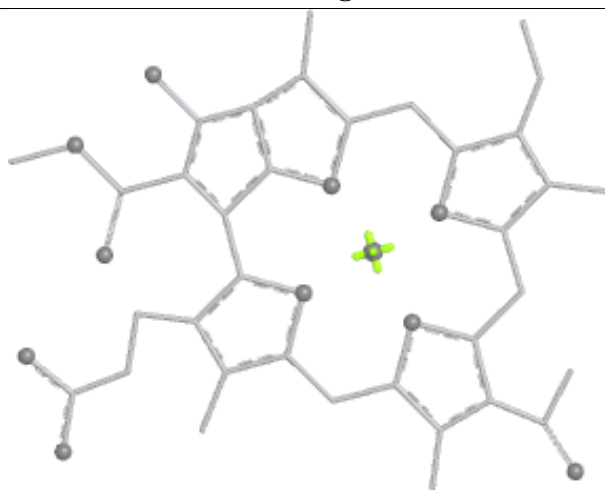
Bond lengths



Bond angles

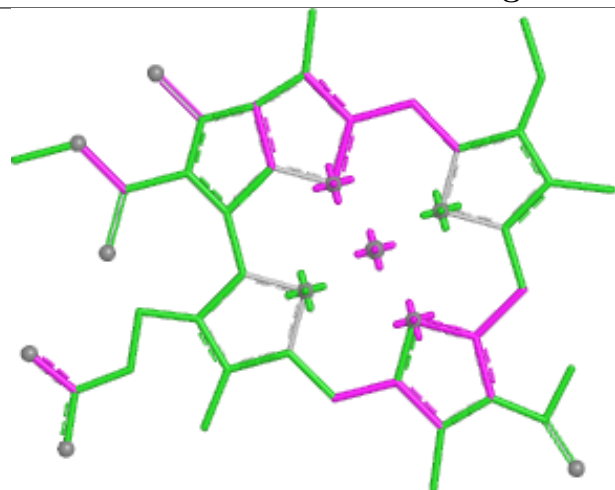


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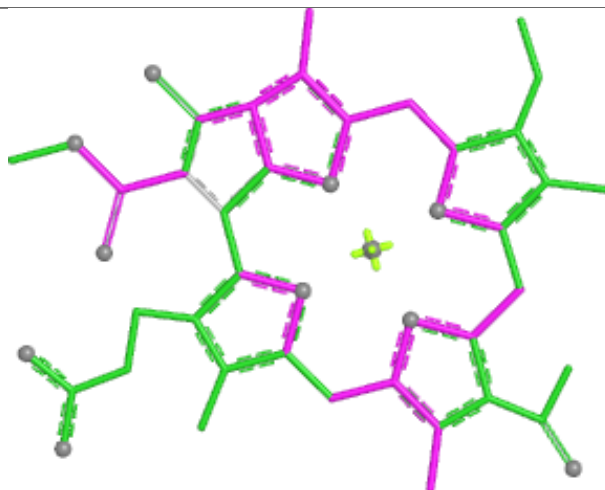


Rings

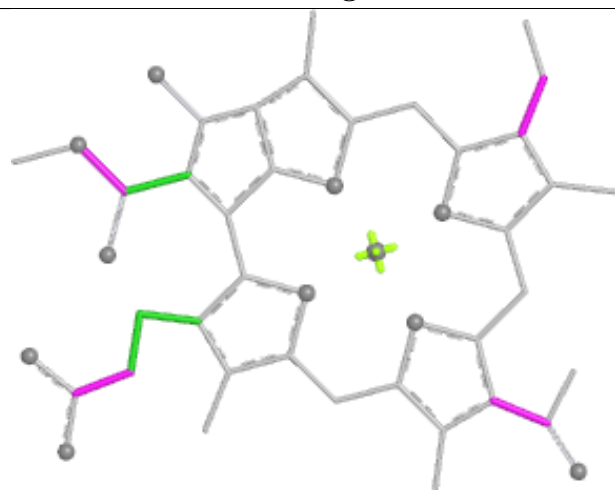
Ligand BCL AD 102



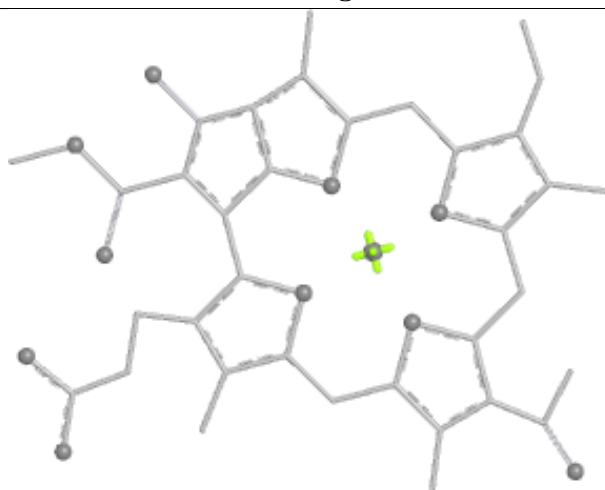
Bond lengths



Bond angles

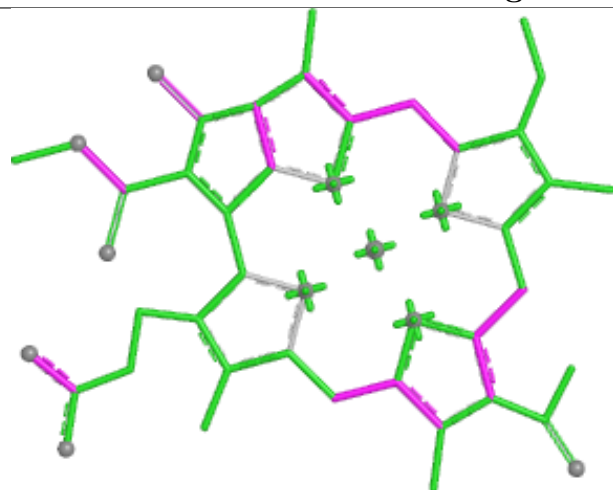


Torsions

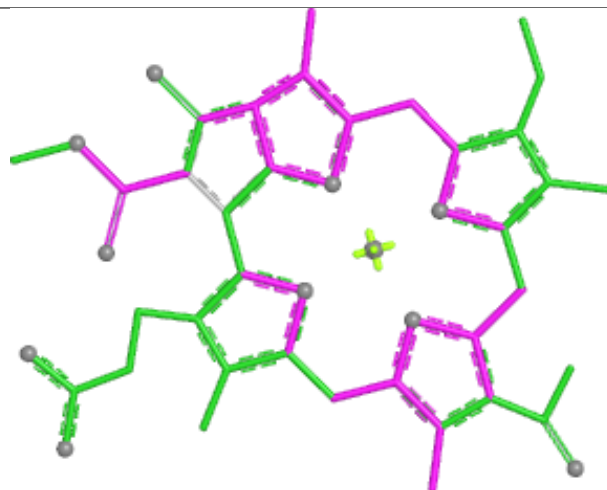


Rings

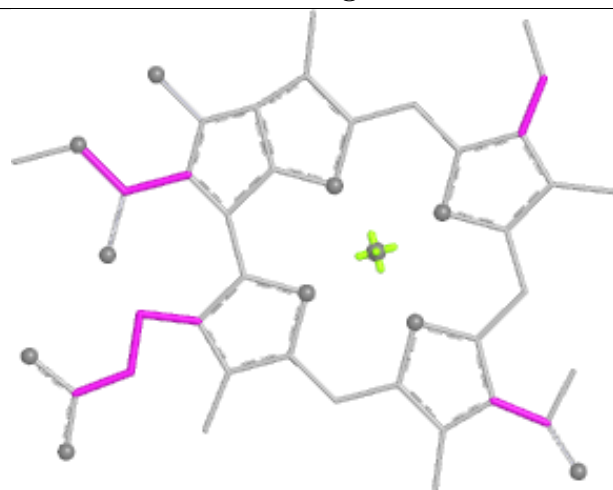
Ligand BCL AF 101



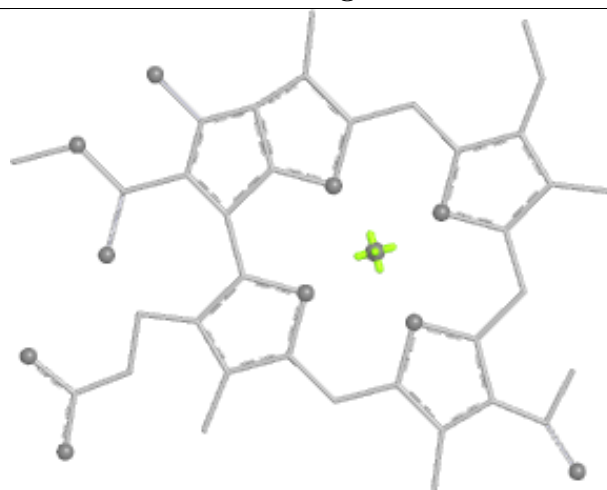
Bond lengths



Bond angles

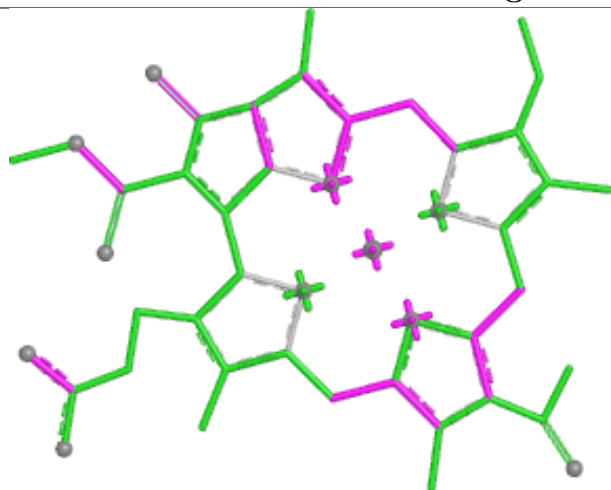


Torsions

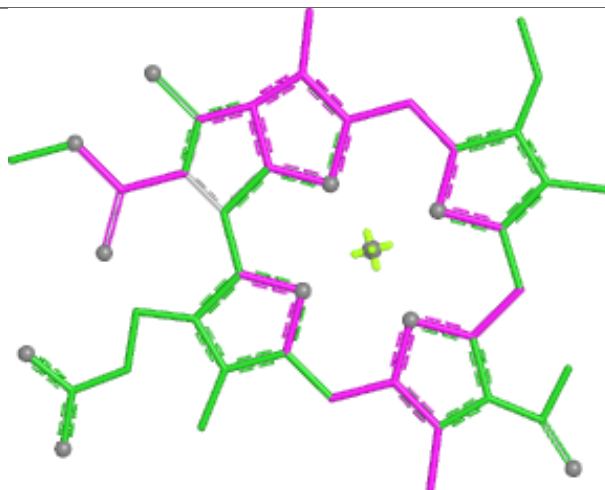


Rings

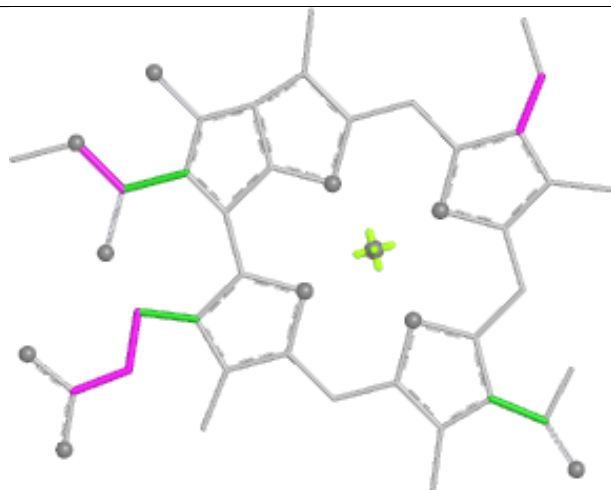
Ligand BCL AJ 101



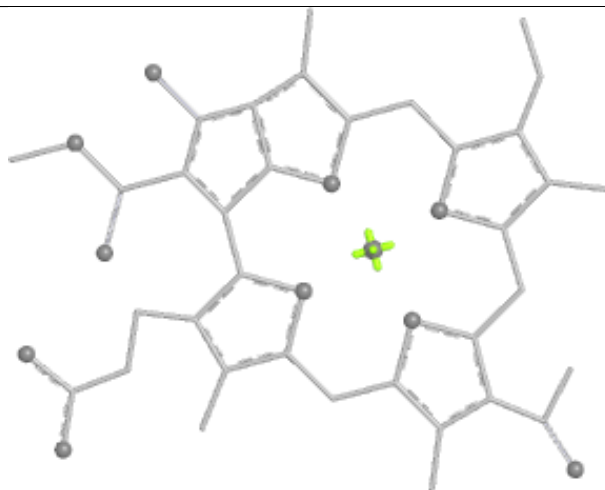
Bond lengths



Bond angles

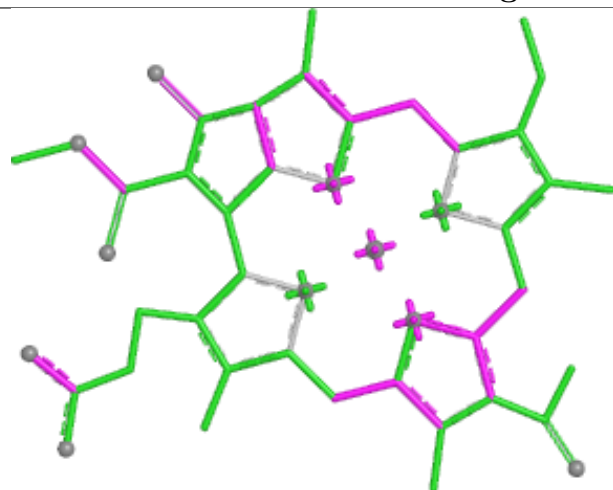


Torsions

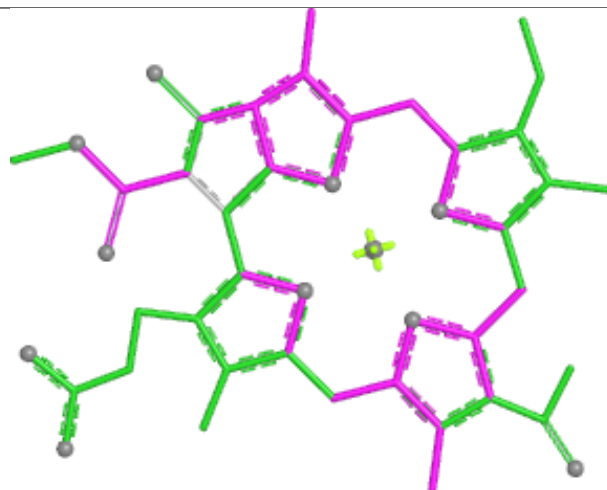


Rings

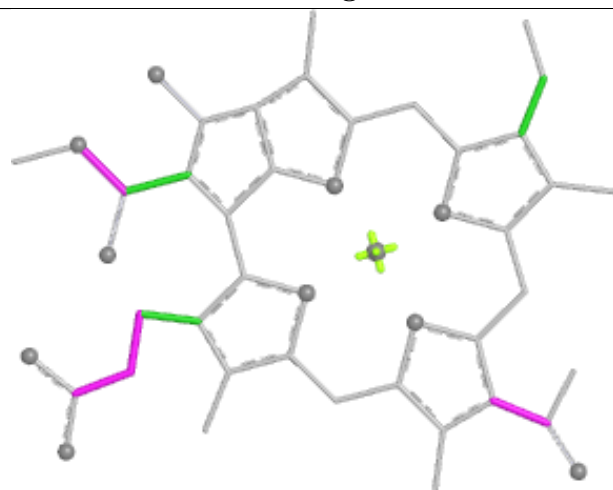
Ligand BCL AW 101



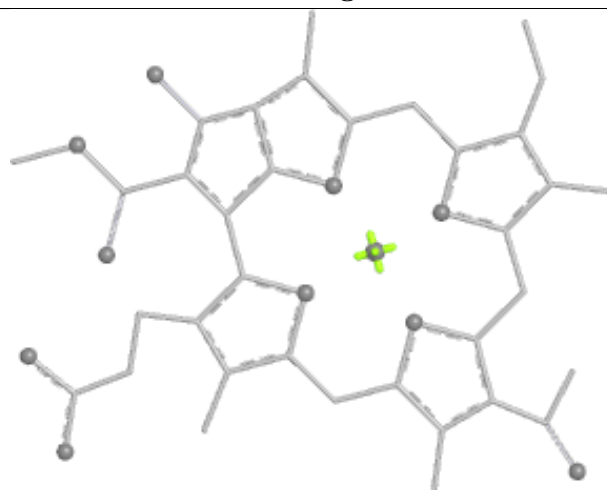
Bond lengths



Bond angles

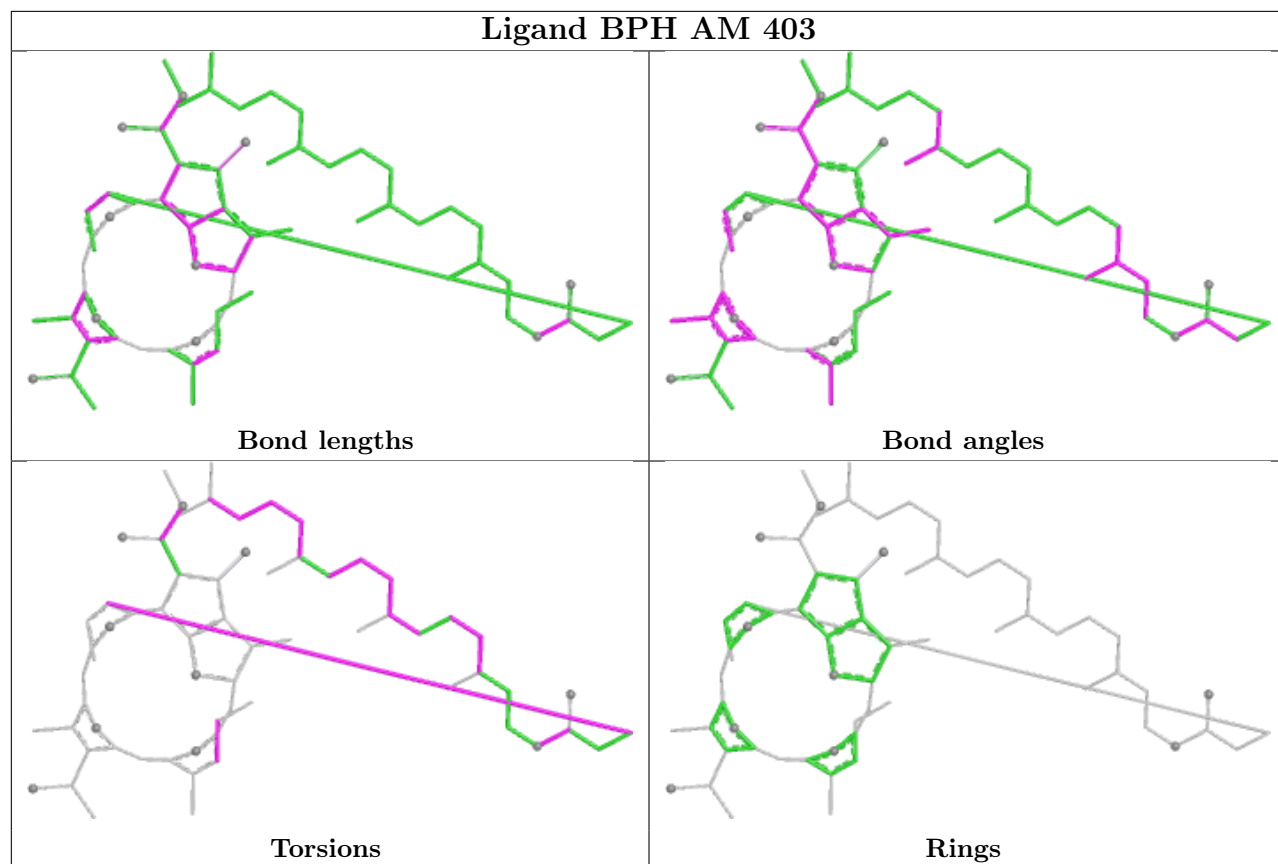


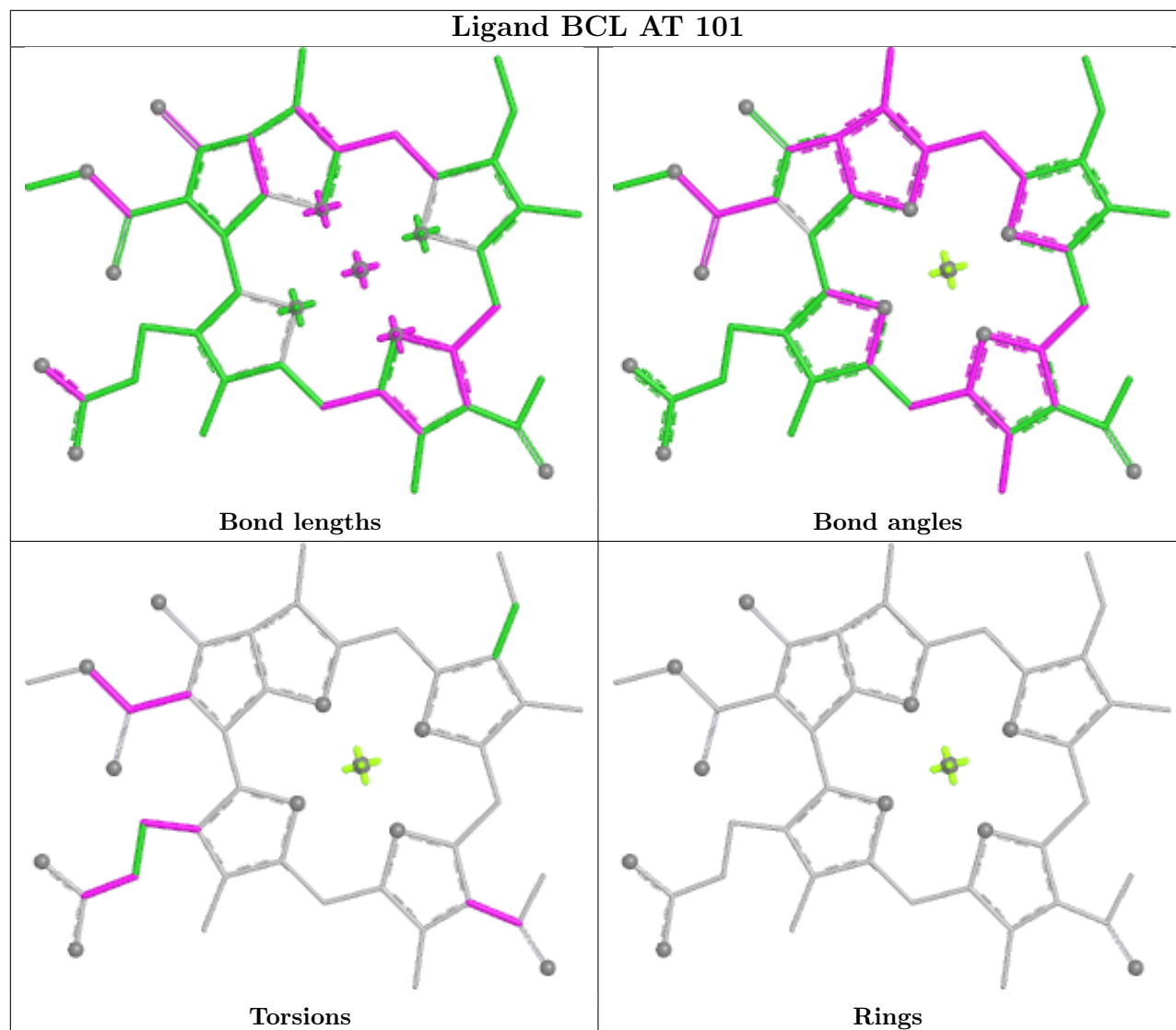
Torsions



Rings

Ligand BPH AM 403





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A1	42/58 (72%)	-1.31	0 100 100	135, 231, 388, 456	0
1	A2	42/58 (72%)	-1.02	0 100 100	182, 298, 500, 500	0
1	A3	42/58 (72%)	-0.92	0 100 100	162, 348, 498, 500	0
1	A5	42/58 (72%)	-1.20	0 100 100	87, 166, 318, 335	0
1	A7	42/58 (72%)	-1.01	0 100 100	217, 396, 500, 500	0
1	AD	42/58 (72%)	-1.04	1 (2%) 59 52	120, 190, 361, 392	0
1	AF	42/58 (72%)	-1.19	0 100 100	235, 399, 499, 500	0
1	AJ	42/58 (72%)	-1.29	0 100 100	42, 331, 460, 498	0
1	AN	42/58 (72%)	-1.18	0 100 100	149, 330, 490, 500	0
1	AP	42/58 (72%)	-1.21	0 100 100	163, 285, 365, 402	0
1	AT	42/58 (72%)	-1.15	0 100 100	171, 353, 500, 500	0
1	AV	42/58 (72%)	-1.06	0 100 100	310, 453, 500, 500	0
1	AX	42/58 (72%)	-0.89	0 100 100	270, 446, 500, 500	0
1	AZ	42/58 (72%)	-1.11	0 100 100	123, 321, 500, 500	0
1	B1	42/58 (72%)	-1.04	0 100 100	230, 429, 500, 500	0
1	B2	42/58 (72%)	-0.89	0 100 100	177, 354, 500, 500	0
1	B3	42/58 (72%)	-0.82	0 100 100	307, 434, 500, 500	0
1	B5	42/58 (72%)	-1.02	1 (2%) 59 52	146, 321, 429, 492	0
1	B7	42/58 (72%)	-1.25	0 100 100	162, 245, 500, 500	0
1	BD	42/58 (72%)	-0.80	1 (2%) 59 52	137, 211, 374, 482	0
1	BF	42/58 (72%)	-1.07	0 100 100	206, 417, 500, 500	0
1	BJ	42/58 (72%)	-1.10	0 100 100	204, 333, 500, 500	0
1	BN	42/58 (72%)	-1.17	0 100 100	113, 245, 500, 500	0
1	BP	42/58 (72%)	-1.00	0 100 100	182, 415, 500, 500	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	BT	42/58 (72%)	-1.10	0	100 100	214, 397, 484, 500	0
1	BV	42/58 (72%)	-0.98	0	100 100	295, 443, 500, 500	0
1	BX	42/58 (72%)	-0.86	0	100 100	285, 448, 500, 500	0
1	BZ	42/58 (72%)	-1.09	0	100 100	243, 355, 499, 500	0
2	AB	57/82 (69%)	-1.24	0	100 100	145, 257, 378, 461	0
2	BB	57/82 (69%)	-0.96	1 (1%)	67 58	306, 464, 500, 500	0
3	A4	48/49 (97%)	-1.01	1 (2%)	63 54	220, 382, 500, 500	0
3	A6	48/49 (97%)	-1.26	0	100 100	89, 180, 383, 405	0
3	A8	48/49 (97%)	-0.98	0	100 100	258, 408, 497, 500	0
3	A9	48/49 (97%)	-1.22	0	100 100	250, 475, 500, 500	0
3	AE	48/49 (97%)	-1.08	0	100 100	237, 329, 457, 500	0
3	AG	48/49 (97%)	-0.87	0	100 100	149, 384, 500, 500	0
3	AI	48/49 (97%)	-1.09	0	100 100	233, 385, 491, 500	0
3	AK	48/49 (97%)	-1.17	0	100 100	235, 383, 499, 500	0
3	AO	48/49 (97%)	-1.13	0	100 100	117, 342, 494, 500	0
3	AQ	48/49 (97%)	-1.12	0	100 100	94, 446, 500, 500	0
3	AS	48/49 (97%)	-1.21	0	100 100	170, 319, 496, 500	0
3	AU	48/49 (97%)	-1.15	0	100 100	331, 417, 500, 500	0
3	AW	48/49 (97%)	-0.97	0	100 100	232, 405, 500, 500	0
3	AY	48/49 (97%)	-1.10	0	100 100	262, 396, 500, 500	0
3	B4	48/49 (97%)	-0.99	0	100 100	202, 353, 488, 500	0
3	B6	48/49 (97%)	-1.15	0	100 100	116, 241, 375, 438	0
3	B8	48/49 (97%)	-0.87	0	100 100	225, 472, 500, 500	0
3	B9	48/49 (97%)	-1.09	0	100 100	187, 374, 462, 494	0
3	BE	48/49 (97%)	-1.02	0	100 100	177, 387, 500, 500	0
3	BG	48/49 (97%)	-0.95	0	100 100	274, 482, 500, 500	0
3	BI	48/49 (97%)	-1.03	0	100 100	242, 480, 500, 500	0
3	BK	48/49 (97%)	-0.93	0	100 100	356, 448, 500, 500	0
3	BO	48/49 (97%)	-1.10	0	100 100	206, 396, 500, 500	0
3	BQ	48/49 (97%)	-1.09	0	100 100	159, 401, 500, 500	0
3	BS	48/49 (97%)	-1.03	0	100 100	235, 426, 500, 500	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
3	BU	48/49 (97%)	-0.84	0	100 100	225, 487, 500, 500	0
3	BW	48/49 (97%)	-1.14	0	100 100	210, 382, 500, 500	0
3	BY	48/49 (97%)	-1.05	0	100 100	279, 460, 500, 500	0
4	AH	250/260 (96%)	-1.17	0	100 100	2, 101, 447, 500	0
4	BH	250/260 (96%)	-0.99	1 (0%)	88 79	16, 193, 470, 500	0
5	AL	281/282 (99%)	-1.11	0	100 100	2, 2, 194, 460	0
5	BL	281/282 (99%)	-1.04	0	100 100	2, 9, 249, 370	0
6	AM	304/308 (98%)	-1.06	0	100 100	1, 2, 215, 459	1 (0%)
6	BM	304/308 (98%)	-0.88	3 (0%)	79 68	2, 9, 269, 492	1 (0%)
All	All	4304/4860 (88%)	-1.05	9 (0%)	91 84	1, 273, 500, 500	2 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B5	40	SER	3.4
3	A4	36	VAL	3.4
1	AD	12	ASP	3.4
2	BB	31	ALA	2.9
6	BM	50	ILE	2.7

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BCL	AV	101	46/66	0.94	0.06	313,363,409,416	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	BCL	AP	102	46/66	0.94	0.06	212,236,270,272	0
7	BCL	A6	101	46/66	0.94	0.07	391,461,488,498	0
7	BCL	A4	101	46/66	0.94	0.07	289,335,362,369	0
7	BCL	B5	101	46/66	0.94	0.09	460,484,500,500	0
7	BCL	B3	101	46/66	0.94	0.07	442,492,500,500	0
7	BCL	B4	101	46/66	0.94	0.07	467,500,500,500	0
7	BCL	B9	101	46/66	0.95	0.11	500,500,500,500	0
8	BPH	BM	402	65/65	0.95	0.07	2,2,2,2	0
7	BCL	AY	102	46/66	0.96	0.05	360,384,441,448	0
7	BCL	B6	101	46/66	0.96	0.11	268,314,325,333	0
7	BCL	AY	101	46/66	0.96	0.07	438,471,494,500	0
7	BCL	BI	101	46/66	0.96	0.07	449,481,500,500	0
7	BCL	BL	301	66/66	0.96	0.07	2,2,2,2	0
7	BCL	BZ	102	46/66	0.96	0.07	340,425,460,469	0
7	BCL	BF	102	46/66	0.97	0.09	418,498,500,500	0
7	BCL	BY	102	46/66	0.97	0.04	192,221,234,245	0
7	BCL	B1	101	46/66	0.97	0.05	221,405,460,480	0
7	BCL	AP	101	46/66	0.97	0.07	196,268,280,290	0
7	BCL	BK	101	46/66	0.97	0.08	471,500,500,500	0
7	BCL	AI	101	46/66	0.97	0.04	277,287,302,304	0
7	BCL	BL	303	66/66	0.97	0.07	2,2,2,2	0
7	BCL	BO	101	46/66	0.97	0.09	500,500,500,500	0
9	U10	BL	306	48/63	0.97	0.05	2,2,2,2	0
7	BCL	BP	102	46/66	0.98	0.04	172,203,216,217	0
7	BCL	AD	102	46/66	0.98	0.07	145,169,200,210	0
7	BCL	A1	101	46/66	0.98	0.04	317,355,399,417	0
7	BCL	AT	102	46/66	0.98	0.11	368,404,465,495	0
7	BCL	A3	101	46/66	0.98	0.05	245,269,314,322	0
7	BCL	BU	101	46/66	0.98	0.07	292,480,500,500	0
7	BCL	AL	301	66/66	0.98	0.07	2,2,2,2	0
7	BCL	A9	101	46/66	0.98	0.05	318,386,396,414	0
7	BCL	BV	101	46/66	0.98	0.08	326,464,500,500	0
7	BCL	AO	101	46/66	0.98	0.06	247,260,266,272	0
7	BCL	BK	102	46/66	0.98	0.04	321,390,455,471	0
7	BCL	BD	102	46/66	0.98	0.06	313,347,446,472	0
7	BCL	BL	302	66/66	0.98	0.10	2,2,2,2	0
7	BCL	A7	101	46/66	0.98	0.04	180,198,207,213	0
7	BCL	BM	401	66/66	0.98	0.07	2,2,2,2	0
8	BPH	AM	403	65/65	0.98	0.05	2,2,2,2	0
8	BPH	BL	304	65/65	0.98	0.07	2,2,2,2	0
7	BCL	AW	101	46/66	0.98	0.06	388,435,462,478	0
9	U10	AL	304	48/63	0.98	0.06	2,2,2,2	0

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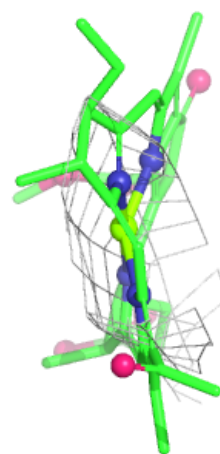
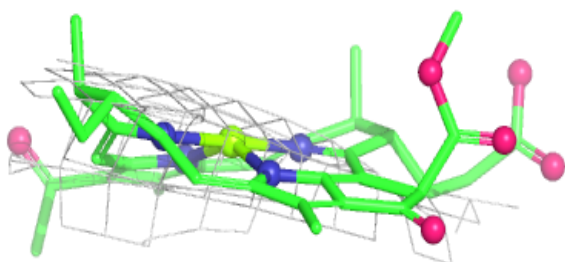
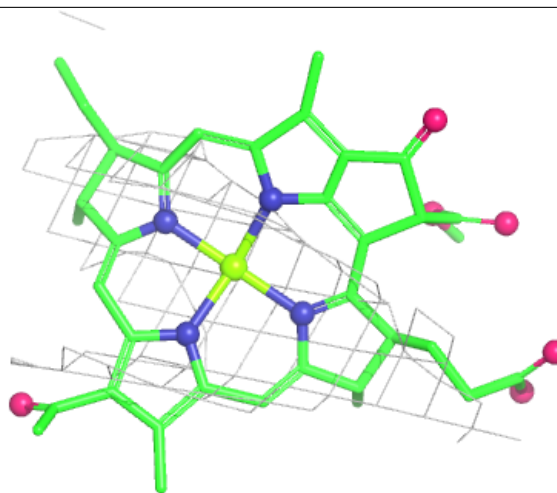
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	U10	AM	405	48/63	0.98	0.07	2,2,2,2	0
7	BCL	B2	101	46/66	0.98	0.07	171,220,230,232	0
7	BCL	BZ	101	46/66	0.99	0.06	411,455,500,500	0
7	BCL	AG	101	46/66	0.99	0.06	329,398,418,422	0
7	BCL	AS	101	46/66	0.99	0.04	275,321,356,360	0
7	BCL	AK	101	46/66	0.99	0.06	422,500,500,500	0
7	BCL	BO	102	46/66	0.99	0.04	152,179,187,204	0
7	BCL	AD	101	46/66	0.99	0.05	133,145,160,169	0
7	BCL	AL	302	66/66	0.99	0.04	2,2,2,2	0
7	BCL	BY	101	46/66	0.99	0.04	283,306,315,316	0
7	BCL	AM	401	66/66	0.99	0.04	2,2,2,2	0
7	BCL	AM	402	66/66	0.99	0.07	2,2,2,2	0
7	BCL	B8	101	46/66	0.99	0.05	233,268,304,309	0
7	BCL	AJ	101	46/66	0.99	0.04	241,343,392,401	0
7	BCL	BT	101	46/66	0.99	0.04	274,316,329,331	0
7	BCL	A2	101	46/66	0.99	0.07	451,500,500,500	0
7	BCL	BV	102	46/66	0.99	0.06	332,395,420,424	0
7	BCL	A6	102	46/66	0.99	0.07	205,301,379,402	0
7	BCL	B7	101	46/66	0.99	0.04	159,184,195,199	0
7	BCL	AN	101	46/66	0.99	0.05	263,334,370,376	0
8	BPH	AL	303	65/65	0.99	0.06	2,2,2,2	0
7	BCL	BF	101	46/66	0.99	0.07	374,453,480,499	0
7	BCL	AT	101	46/66	0.99	0.05	241,267,280,281	0
7	BCL	AF	101	46/66	0.99	0.04	204,214,229,239	0
7	BCL	AZ	101	46/66	0.99	0.07	500,500,500,500	0
7	BCL	BP	101	46/66	0.99	0.03	142,147,153,161	0
7	BCL	A8	101	46/66	0.99	0.07	301,369,400,413	0
10	PO4	AL	305	5/5	0.99	0.03	2,2,2,2	0
12	SPO	AM	406	42/42	0.99	0.07	2,2,2,2	0
10	PO4	BL	307	5/5	1.00	0.02	2,2,2,2	0
11	FE2	AM	404	1/1	1.00	0.03	2,2,2,2	0
11	FE2	BL	305	1/1	1.00	0.06	2,2,2,2	0
7	BCL	BD	101	46/66	1.00	0.06	233,299,305,307	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.

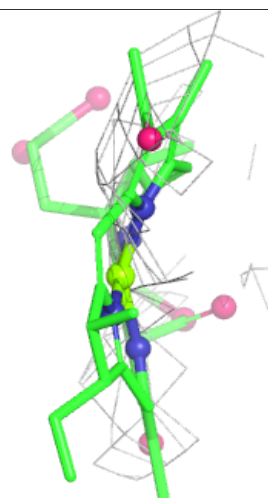
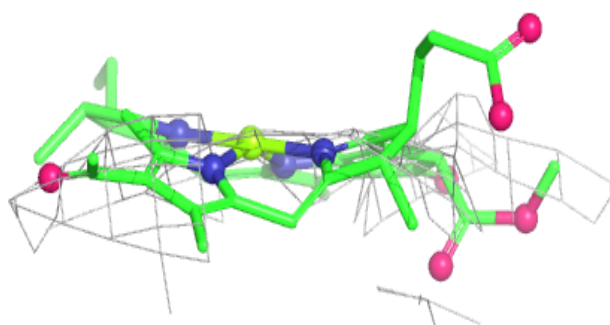
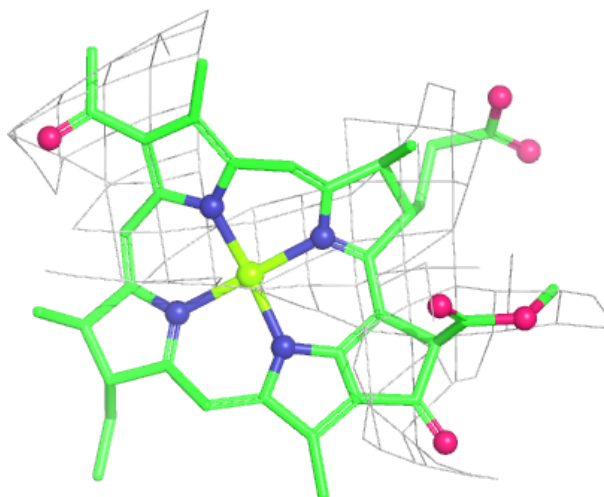
Electron density around BCL AV 101:

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



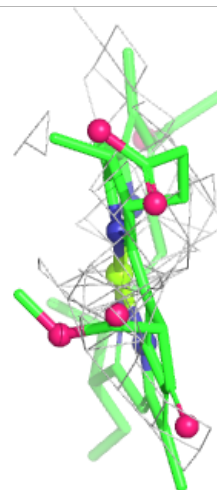
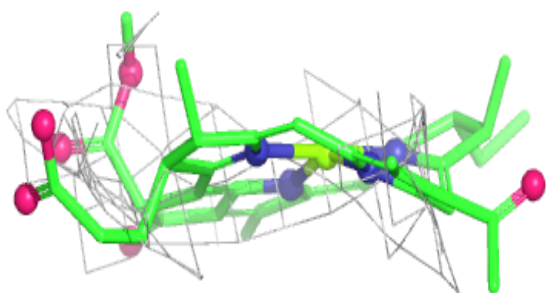
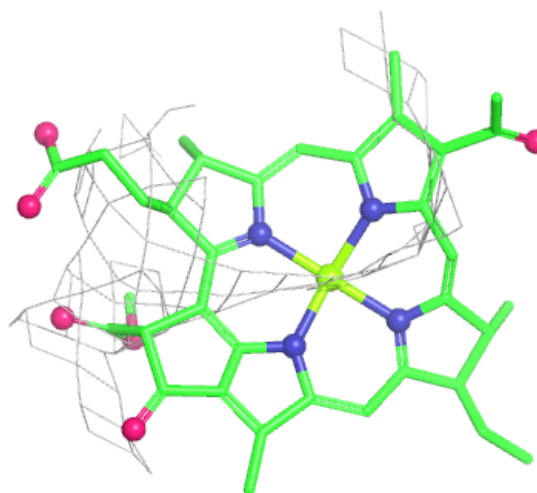
Electron density around BCL AP 102:

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



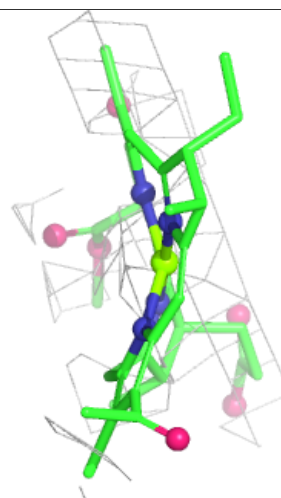
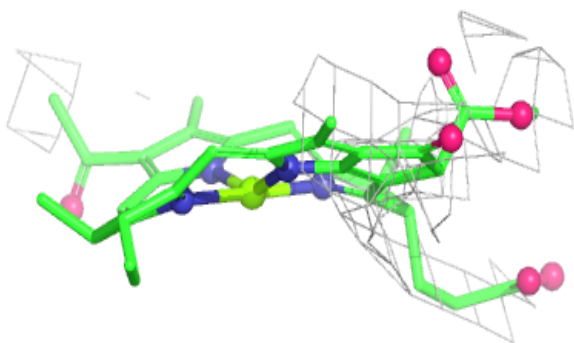
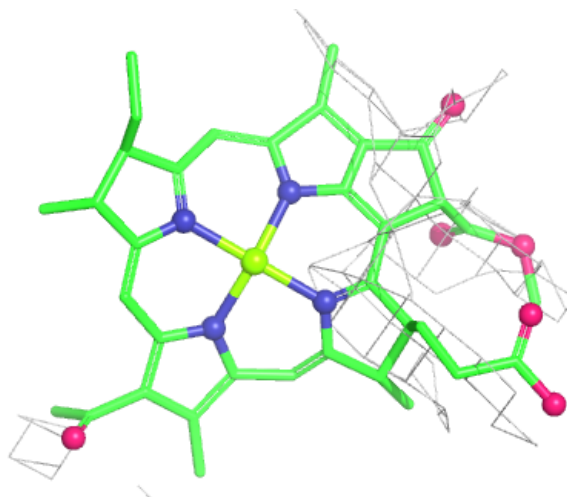
Electron density around BCL A6 101:

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



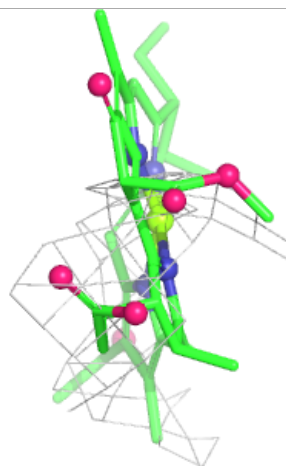
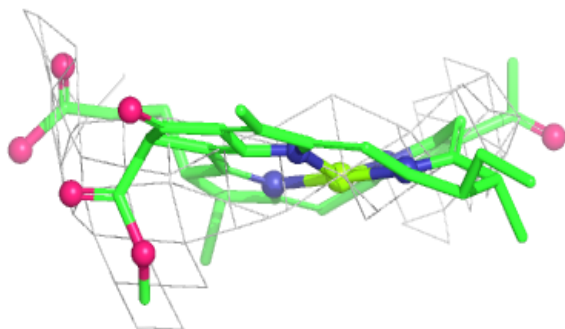
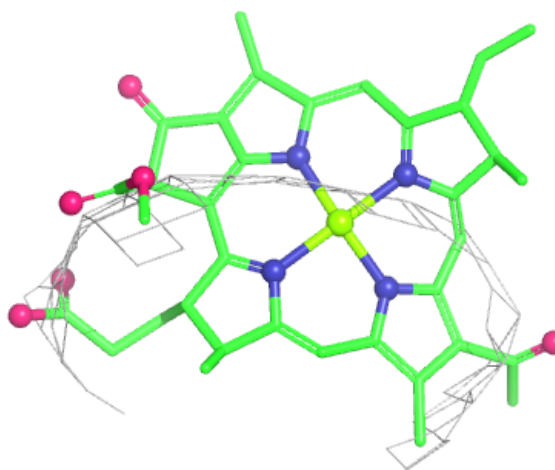
Electron density around BCL A4 101:

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



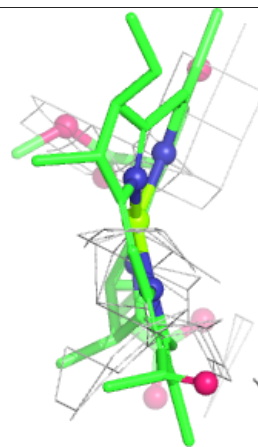
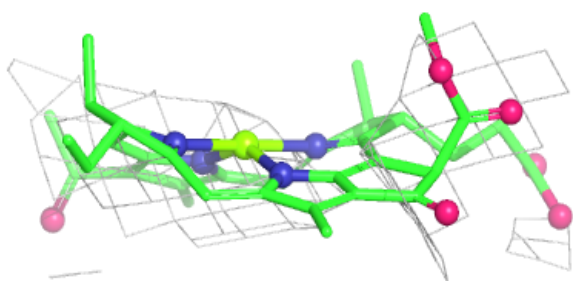
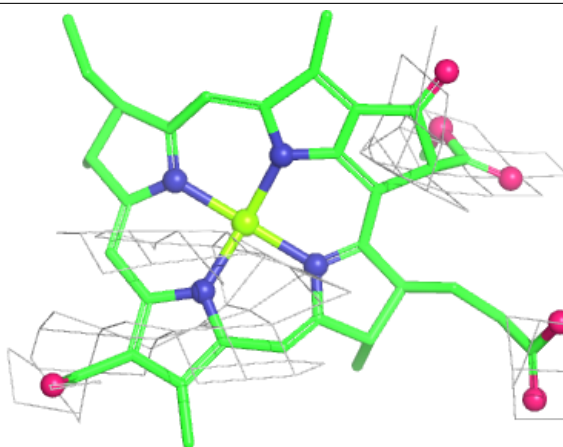
Electron density around BCL B5 101:

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



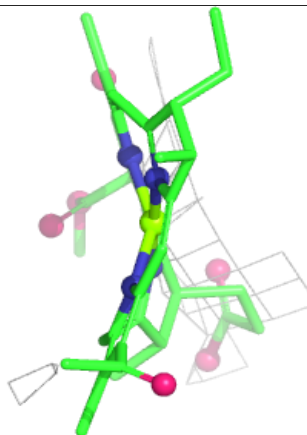
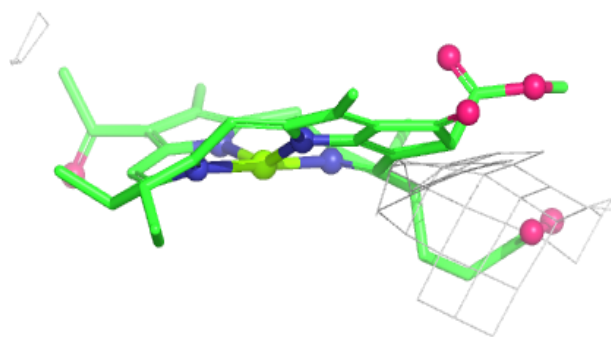
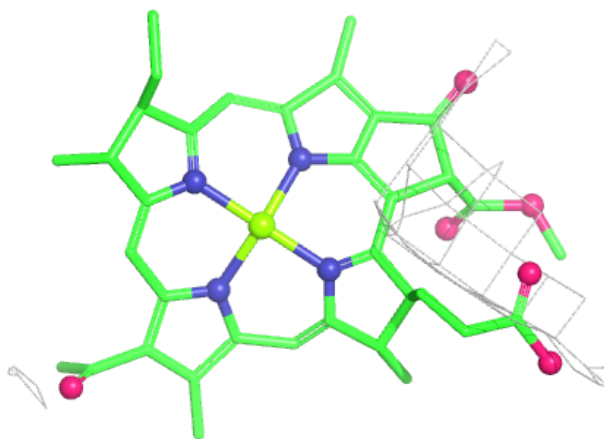
Electron density around BCL B3 101:

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



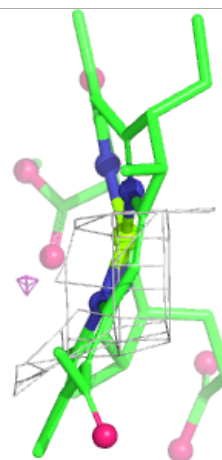
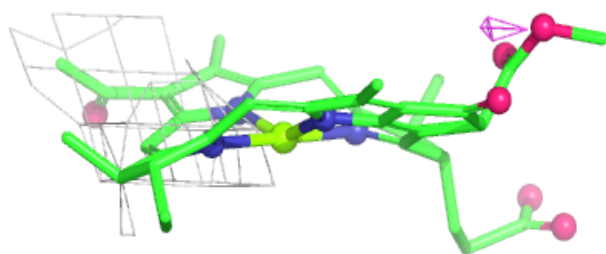
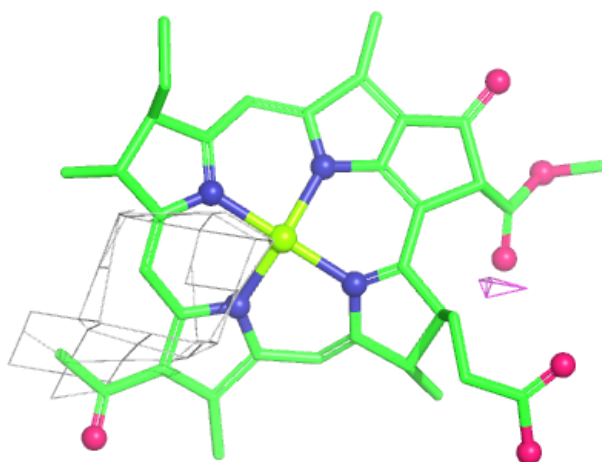
Electron density around BCL B4 101:

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



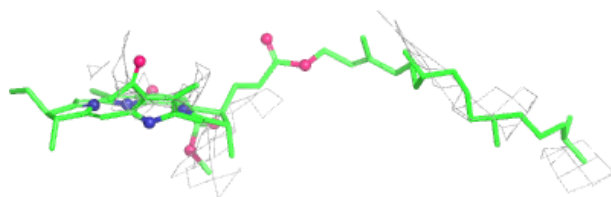
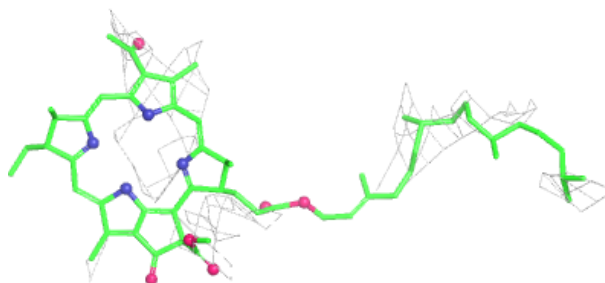
Electron density around BCL B9 101:

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



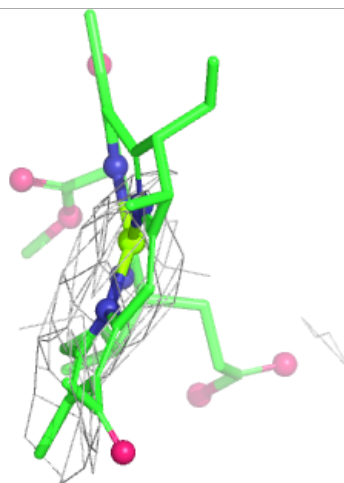
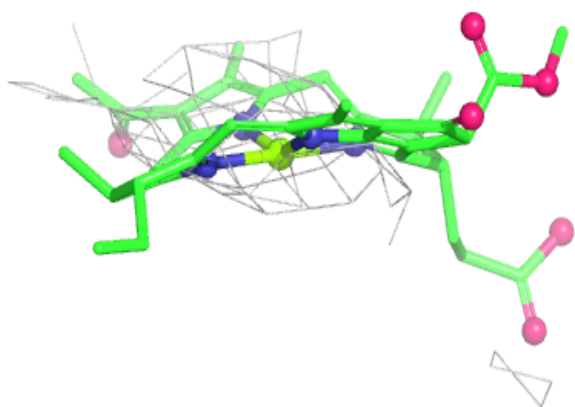
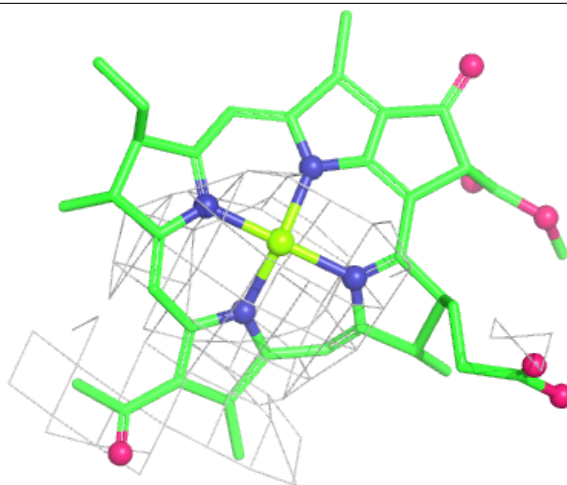
Electron density around BPH BM 402:

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



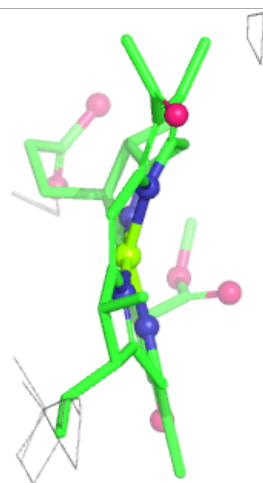
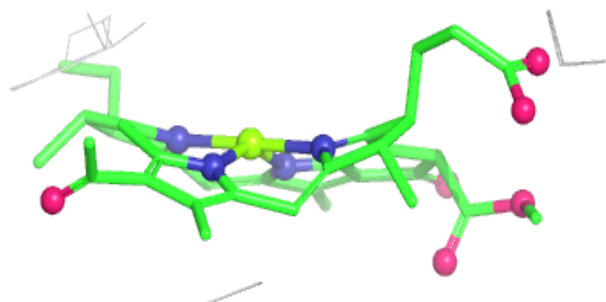
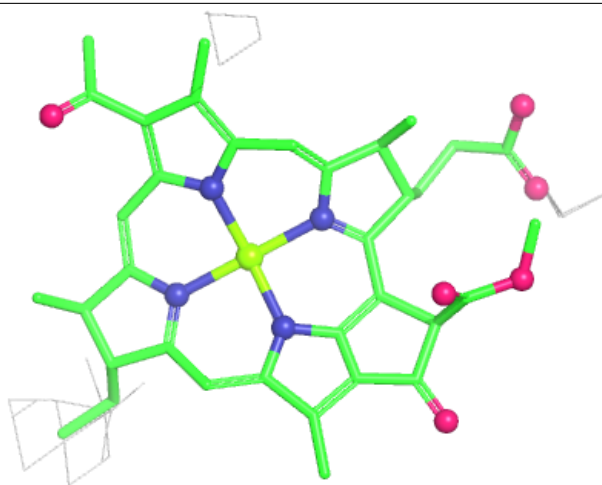
Electron density around BCL AY 102:

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



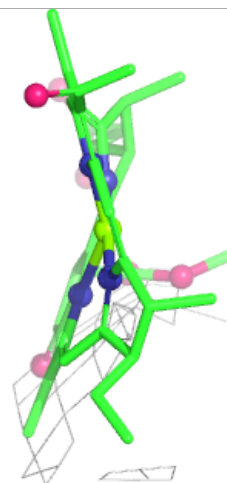
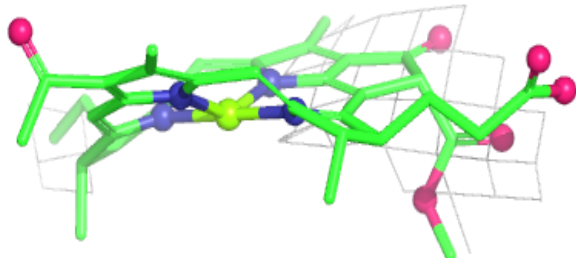
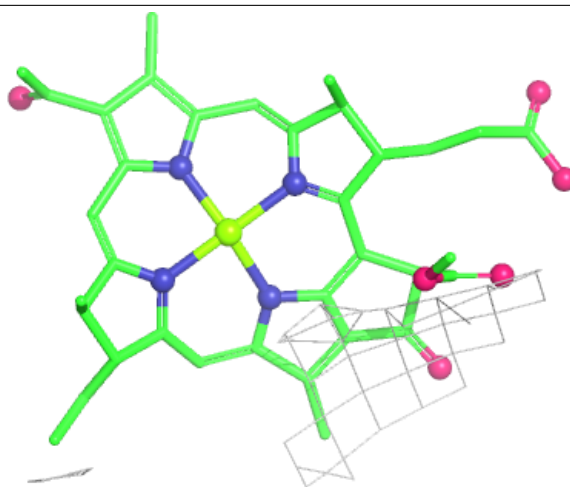
Electron density around BCL B6 101:

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



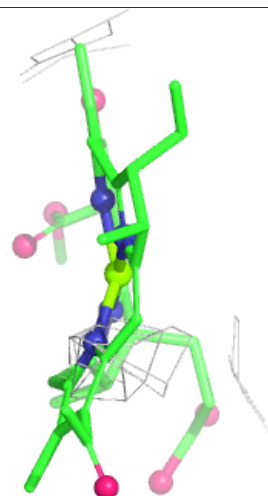
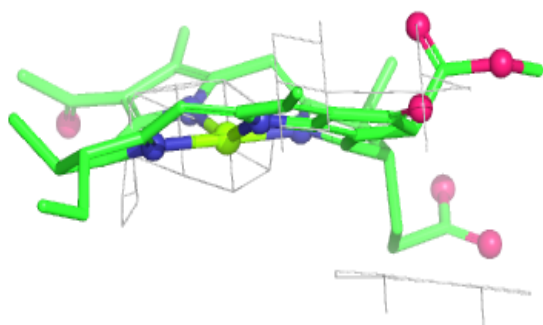
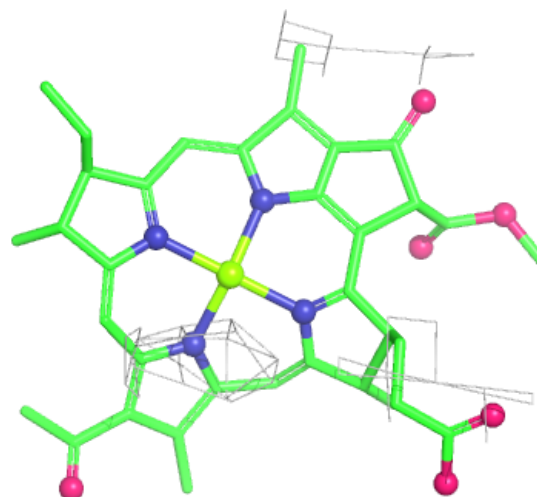
Electron density around BCL AY 101:

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



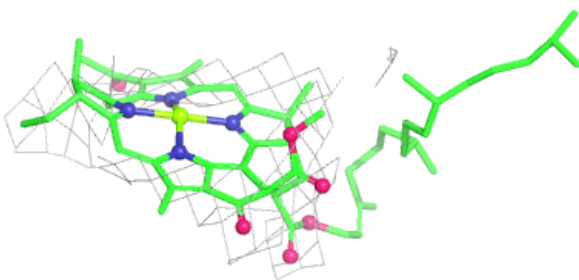
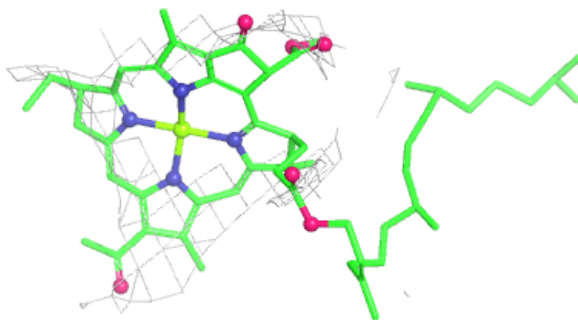
Electron density around BCL BI 101:

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



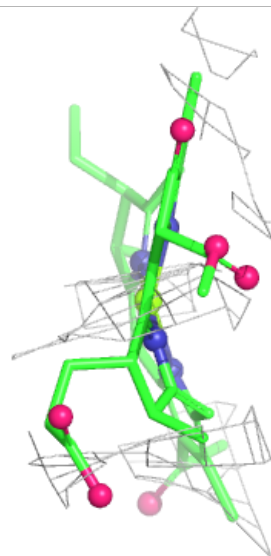
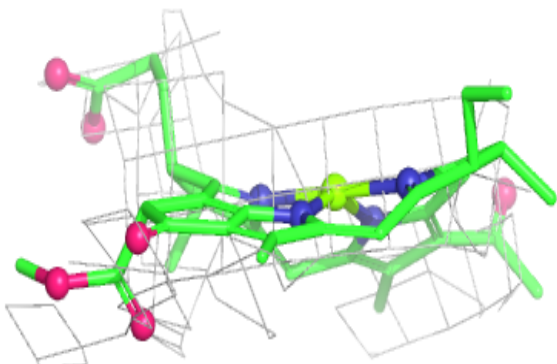
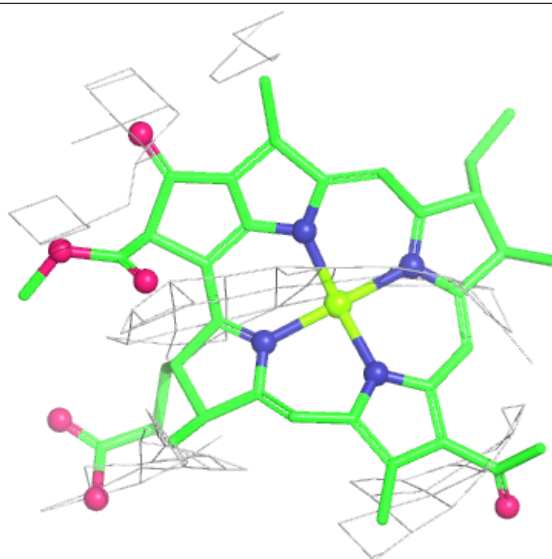
Electron density around BCL BL 301:

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



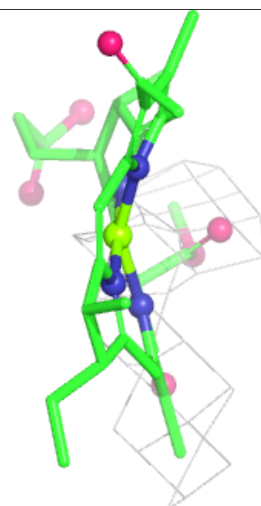
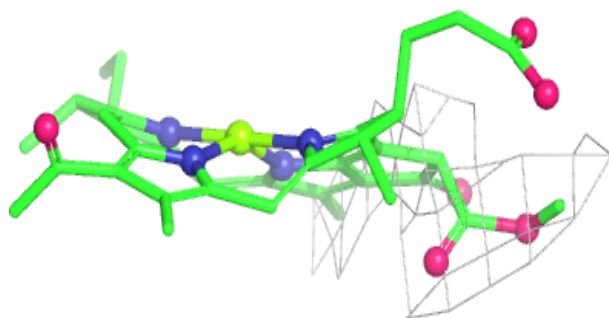
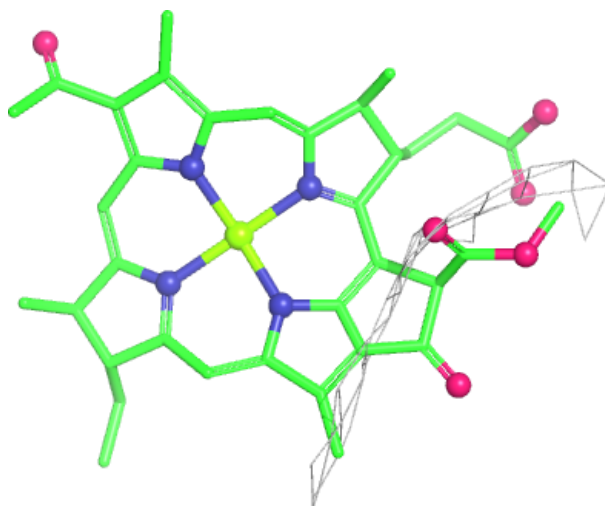
Electron density around BCL BZ 102:

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



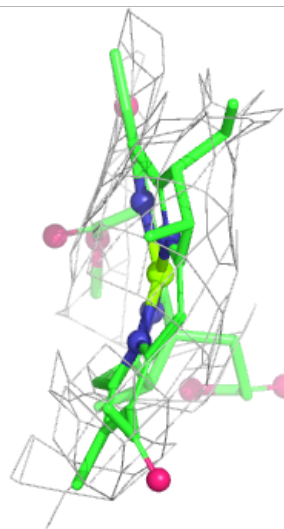
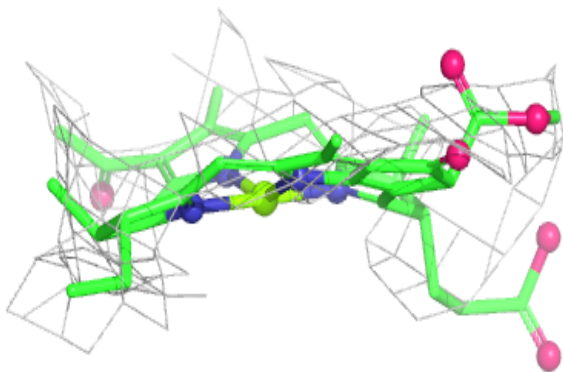
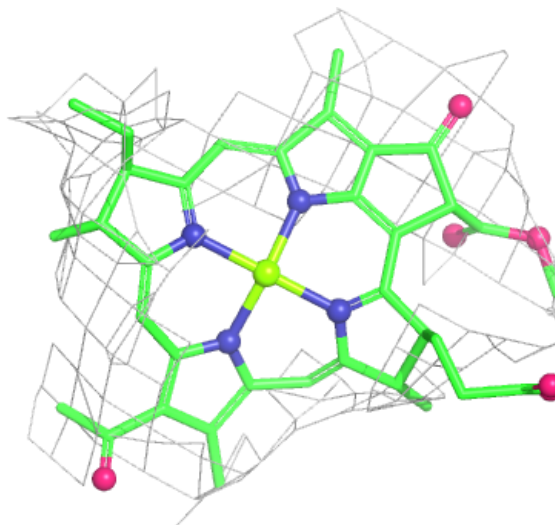
Electron density around BCL BF 102:

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



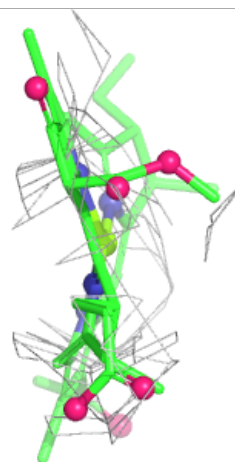
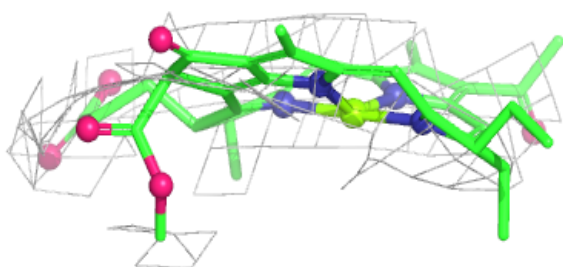
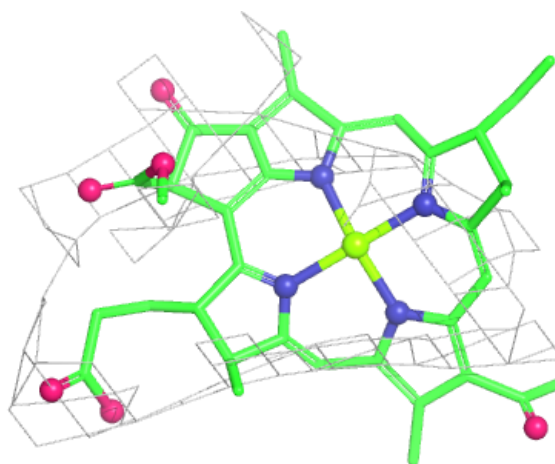
Electron density around BCL BY 102:

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



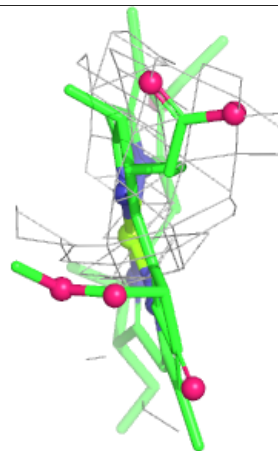
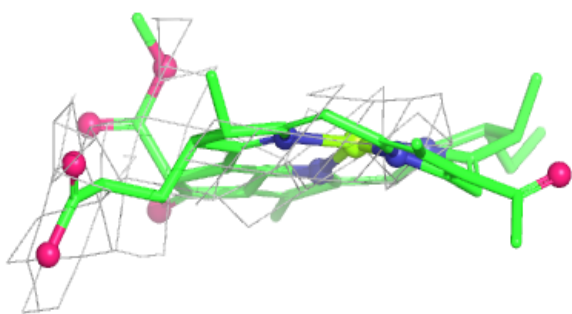
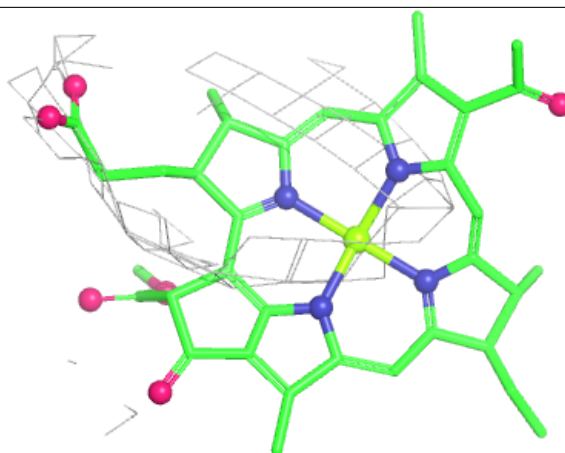
Electron density around BCL B1 101:

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



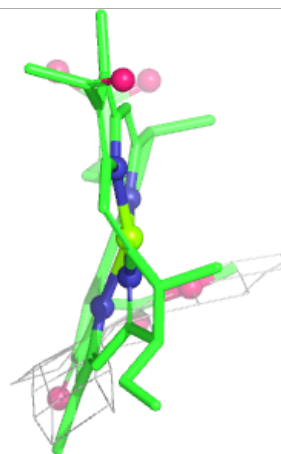
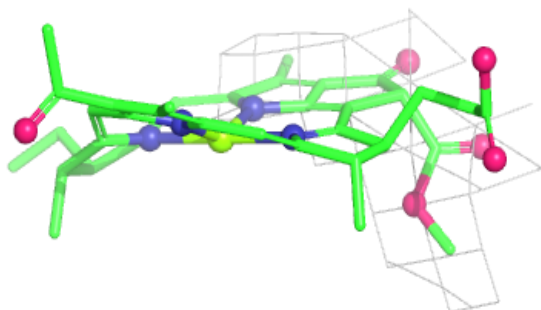
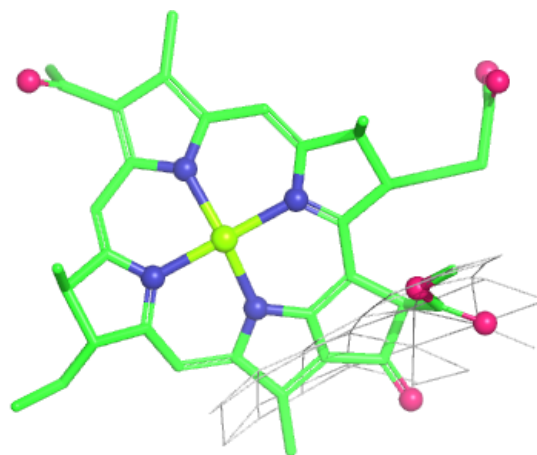
Electron density around BCL AP 101:

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



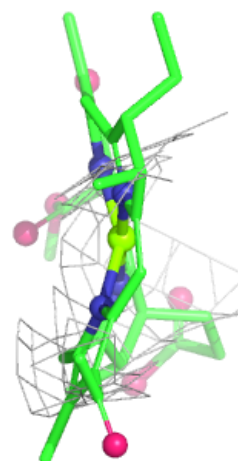
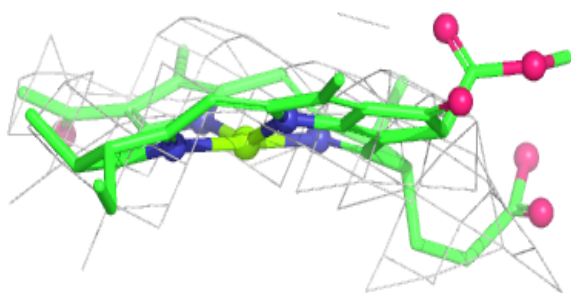
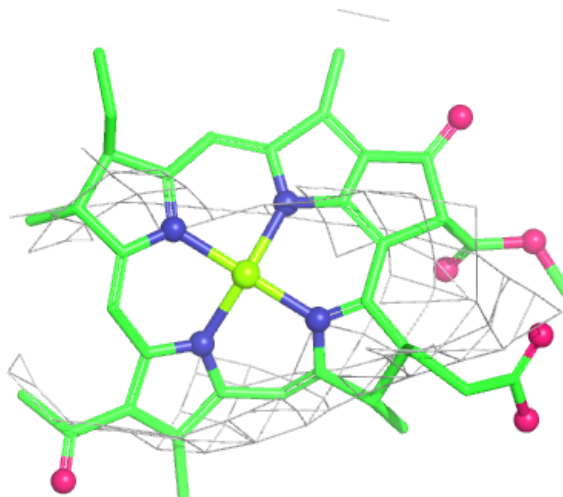
Electron density around BCL BK 101:

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



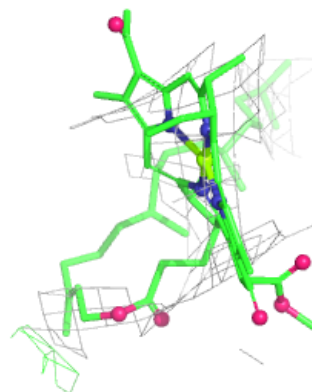
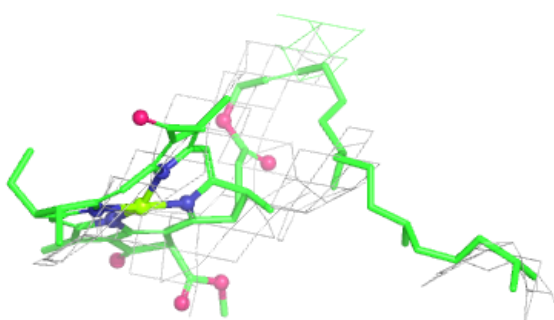
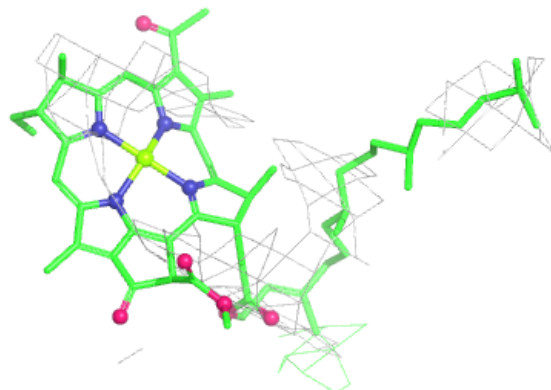
Electron density around BCL AI 101:

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



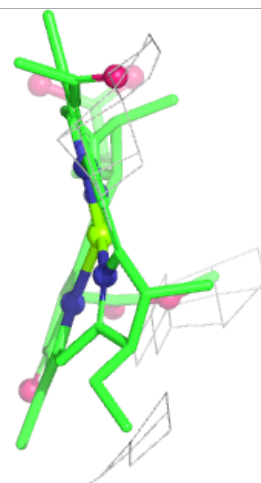
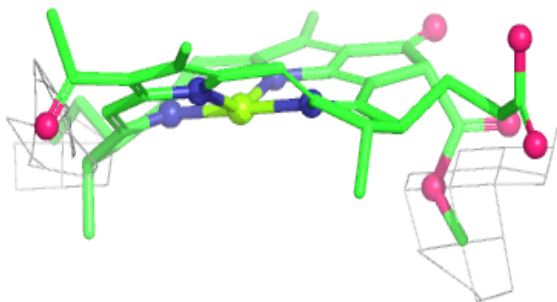
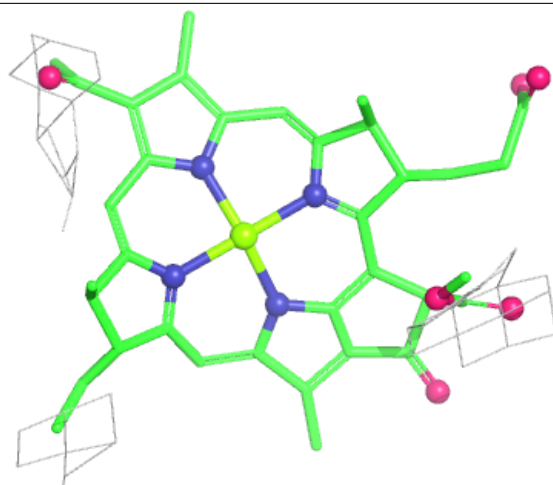
Electron density around BCL BL 303:

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



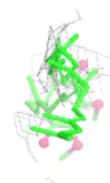
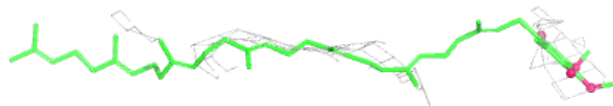
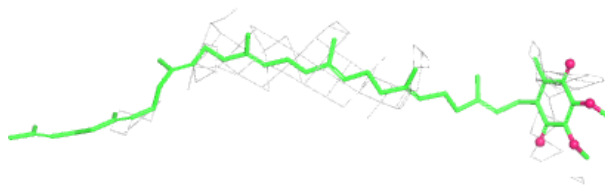
Electron density around BCL BO 101:

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



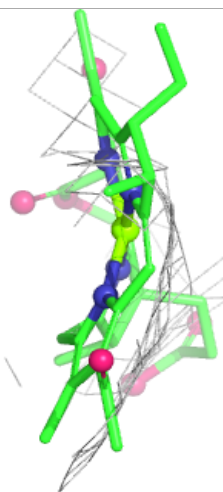
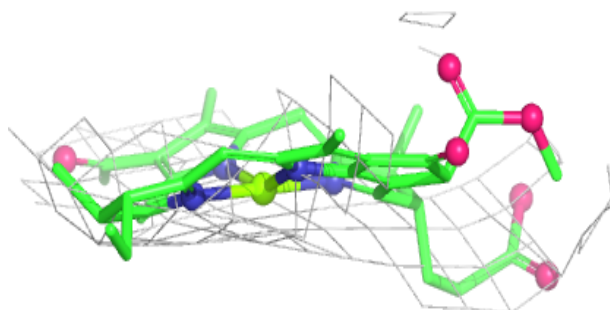
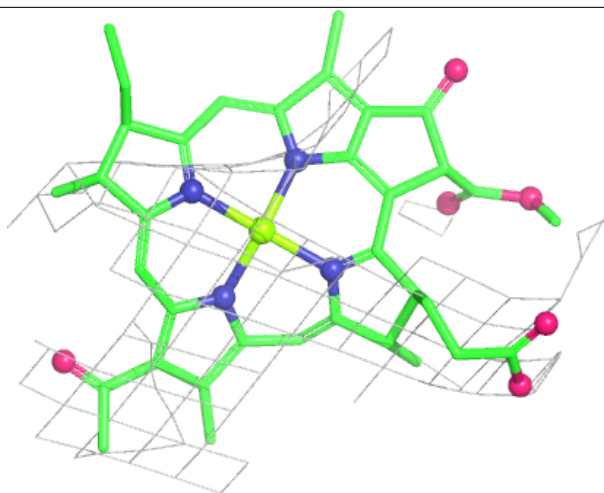
Electron density around U10 BL 306:

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



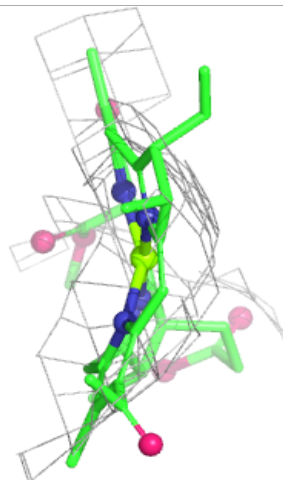
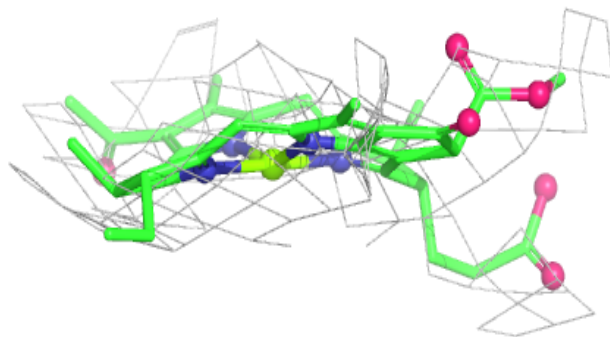
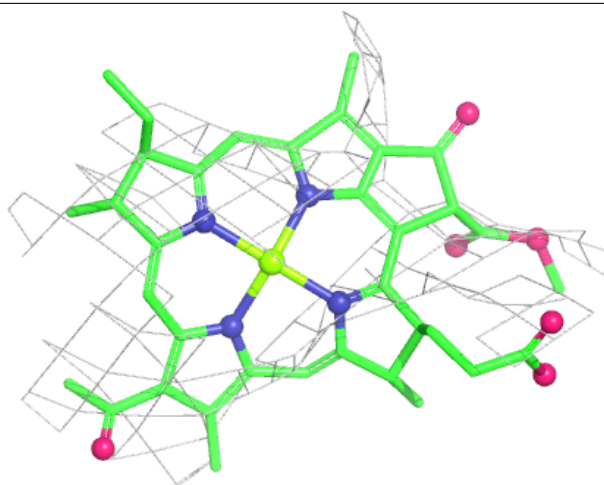
Electron density around BCL BP 102:

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



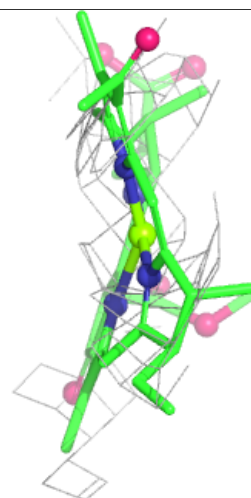
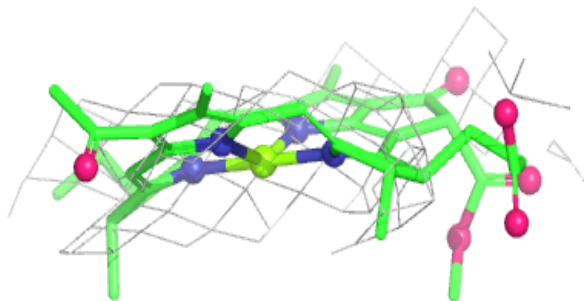
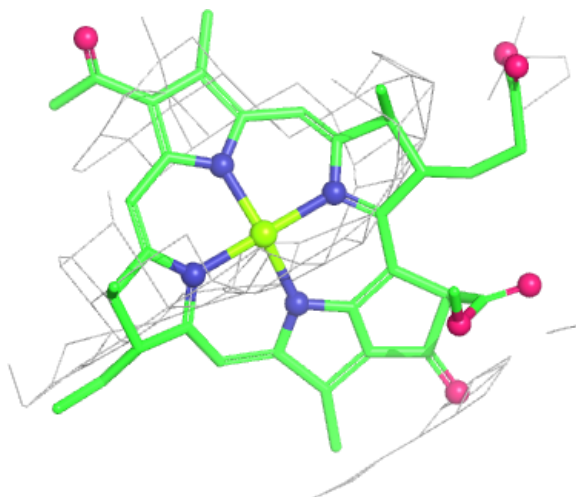
Electron density around BCL AD 102:

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



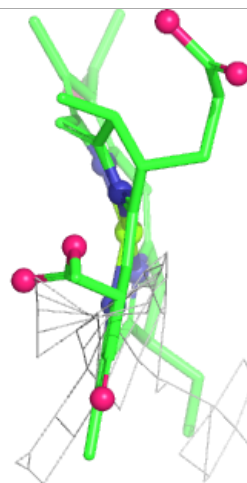
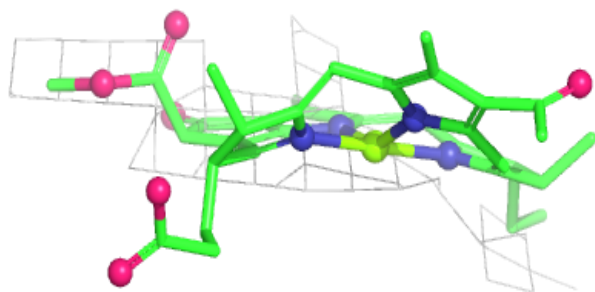
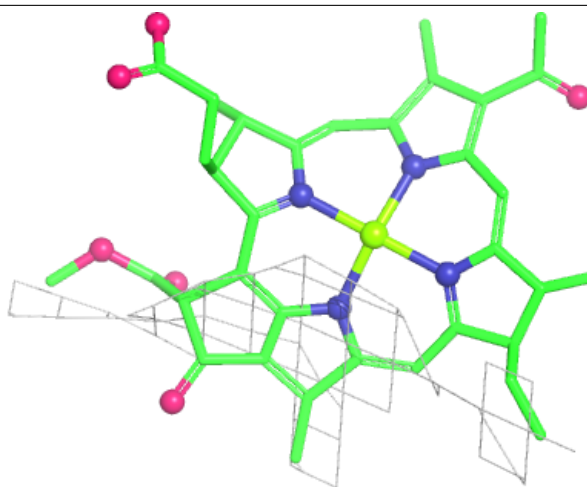
Electron density around BCL A1 101:

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



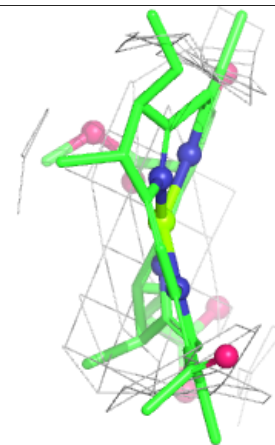
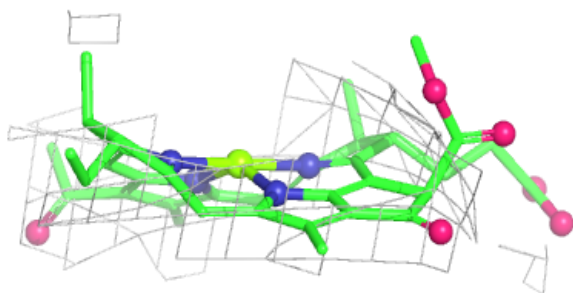
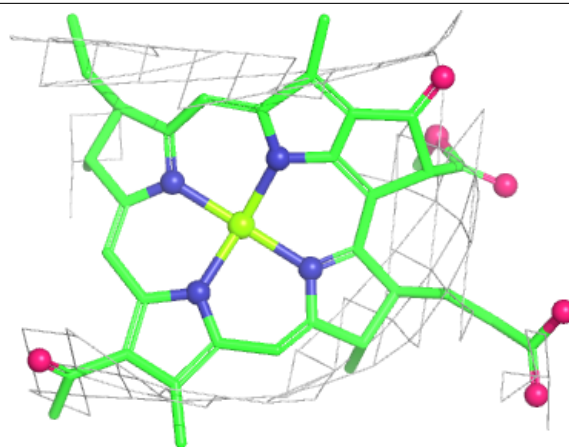
Electron density around BCL AT 102:

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



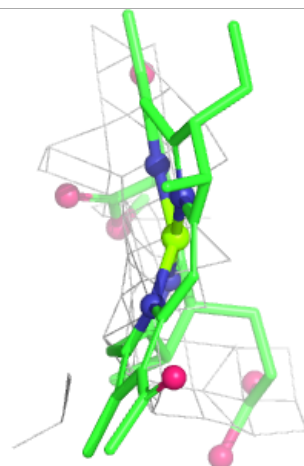
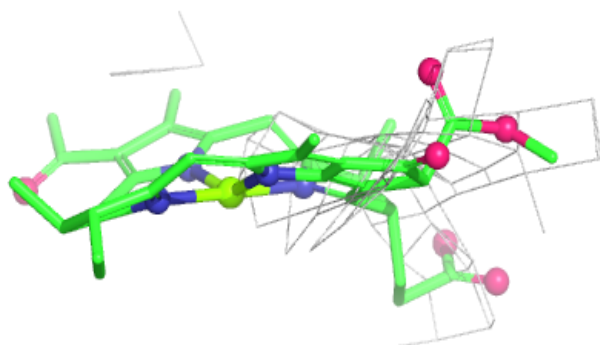
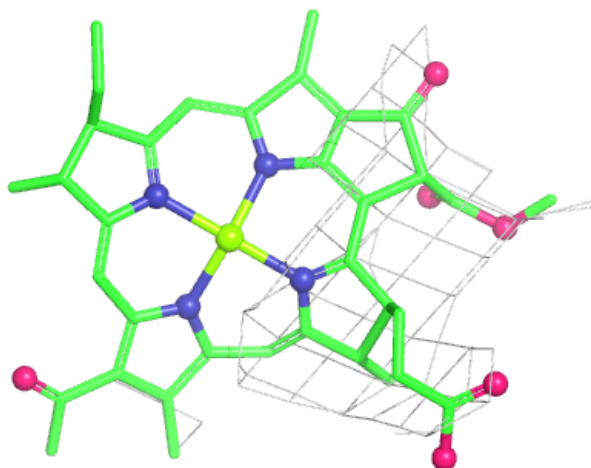
Electron density around BCL A3 101:

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



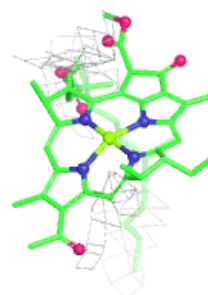
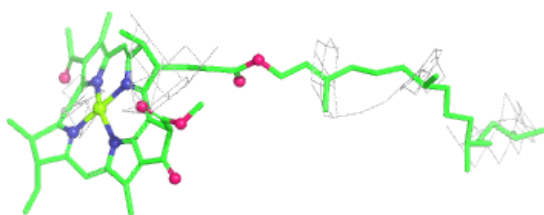
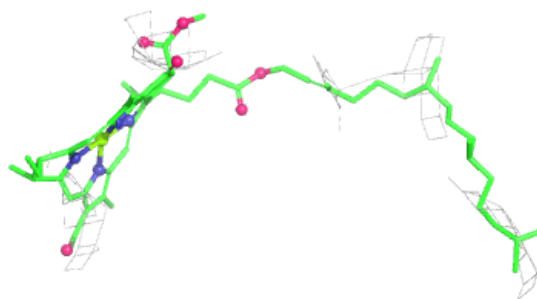
Electron density around BCL BU 101:

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



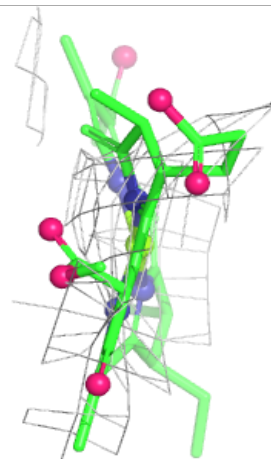
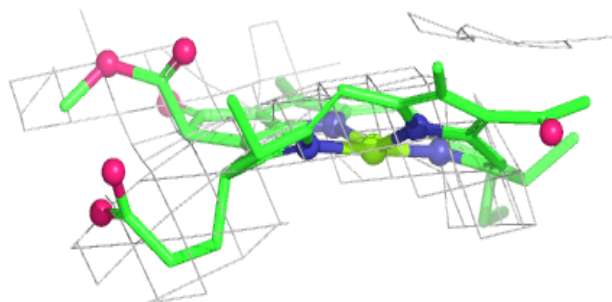
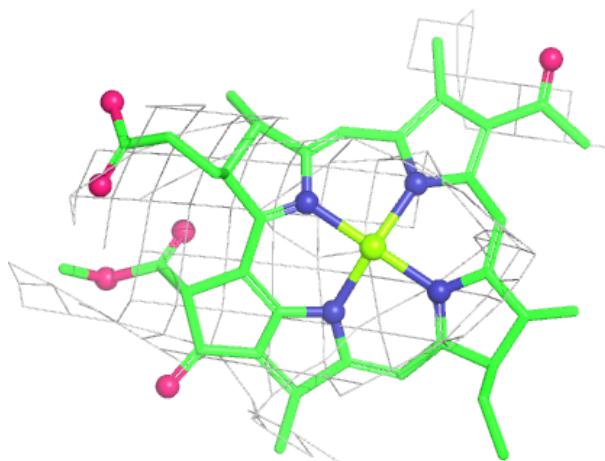
Electron density around BCL AL 301:

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



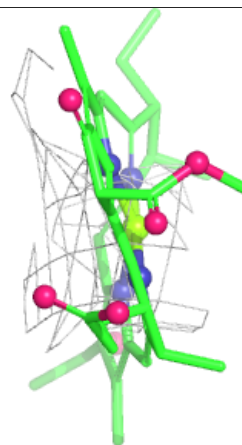
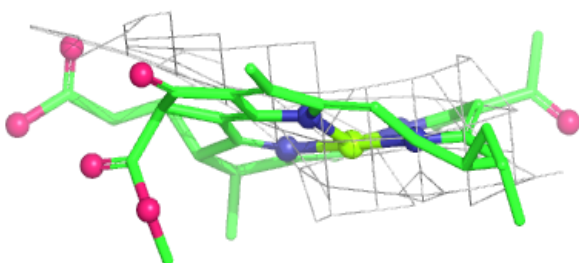
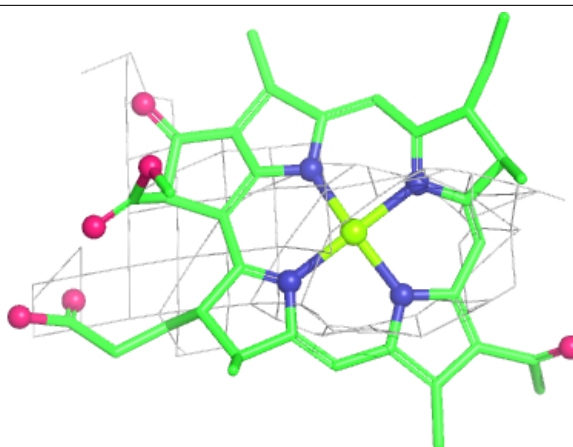
Electron density around BCL A9 101:

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



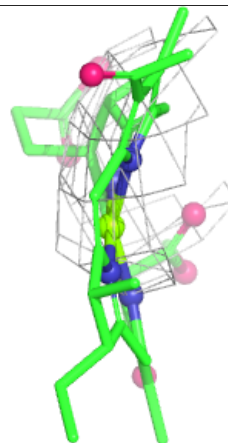
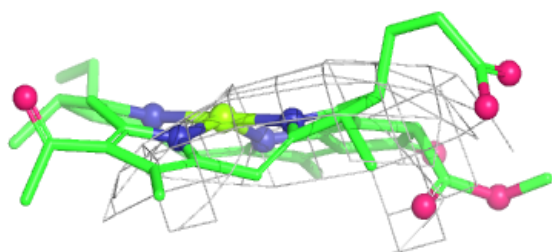
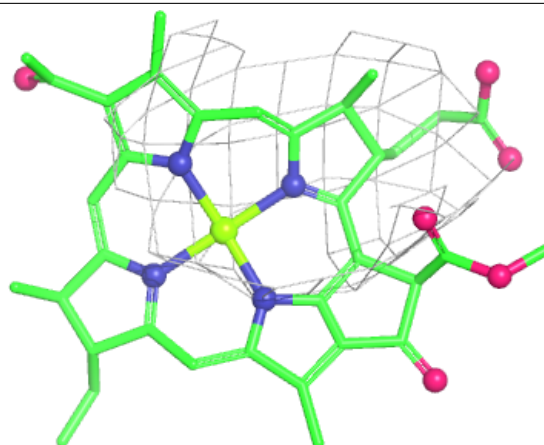
Electron density around BCL BV 101:

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



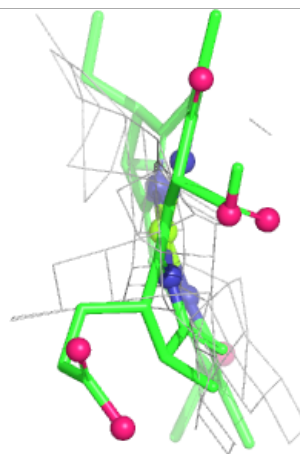
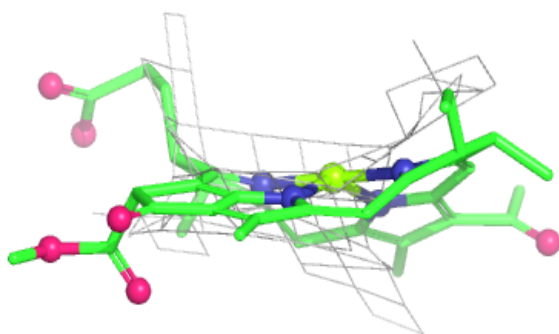
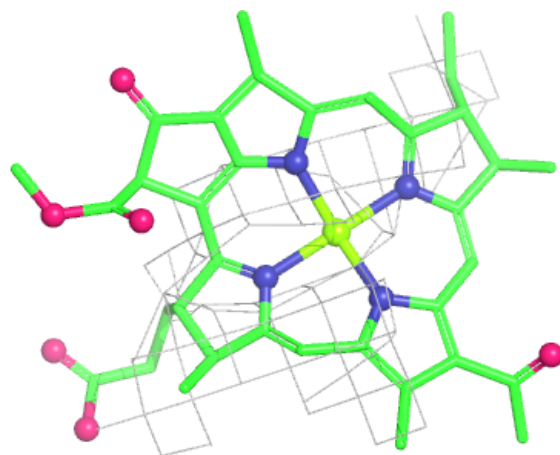
Electron density around BCL AO 101:

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



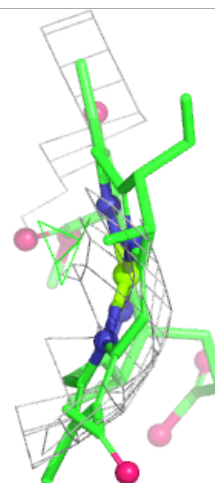
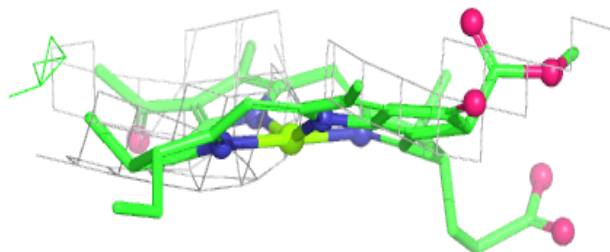
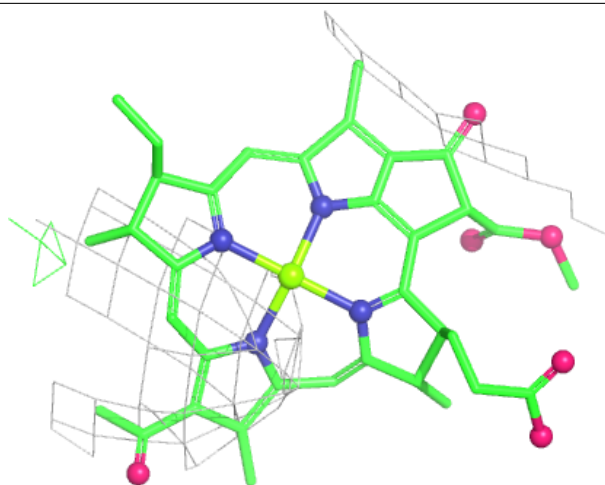
Electron density around BCL BK 102:

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



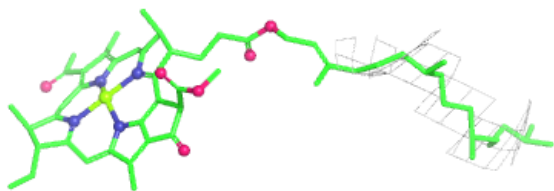
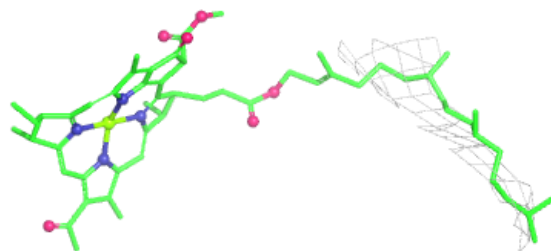
Electron density around BCL BD 102:

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



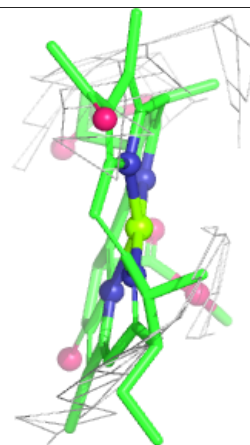
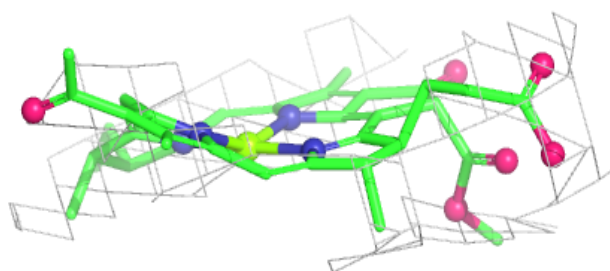
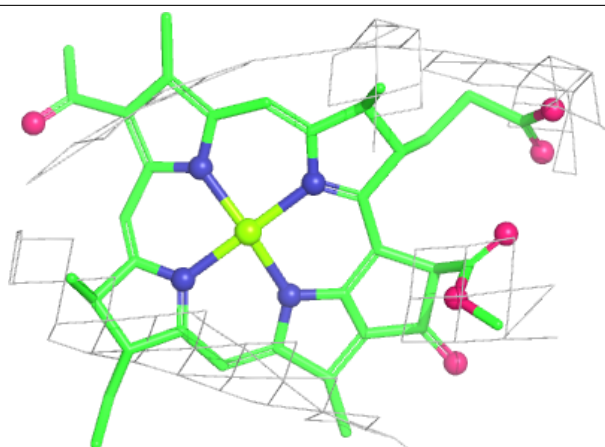
Electron density around BCL BL 302:

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



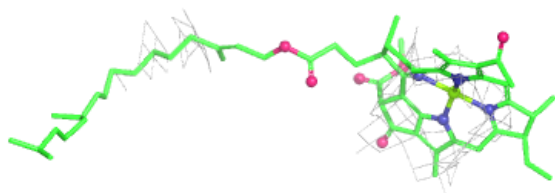
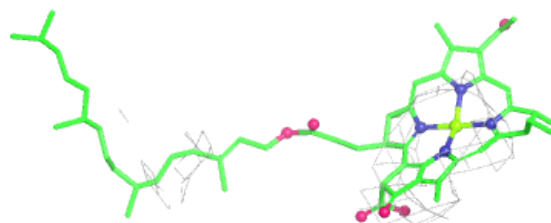
Electron density around BCL A7 101:

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

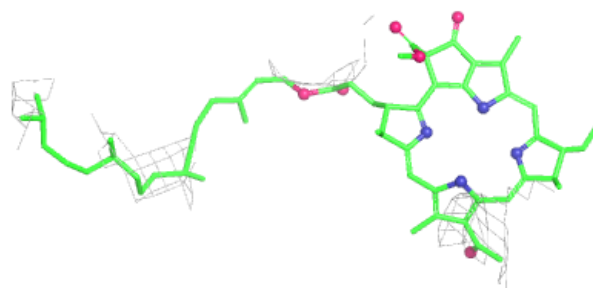


Electron density around BCL BM 401:

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

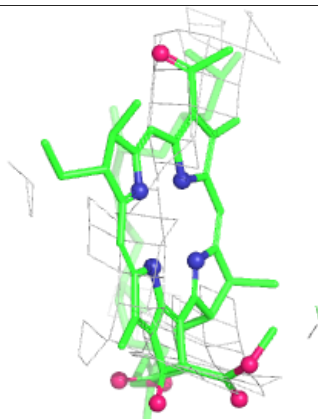
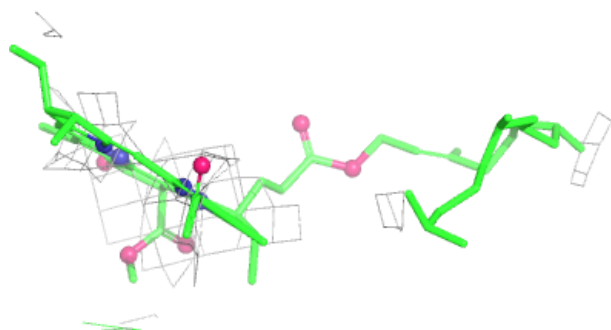
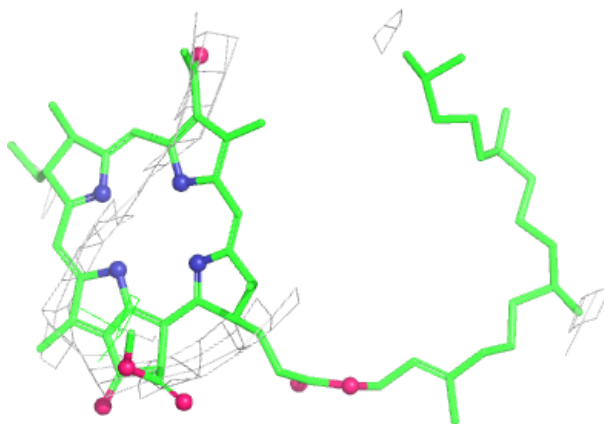
**Electron density around BPH AM 403:**

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



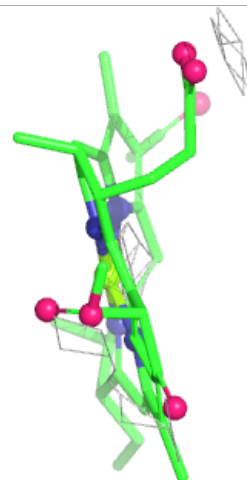
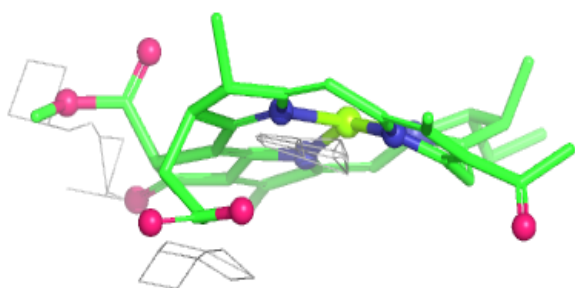
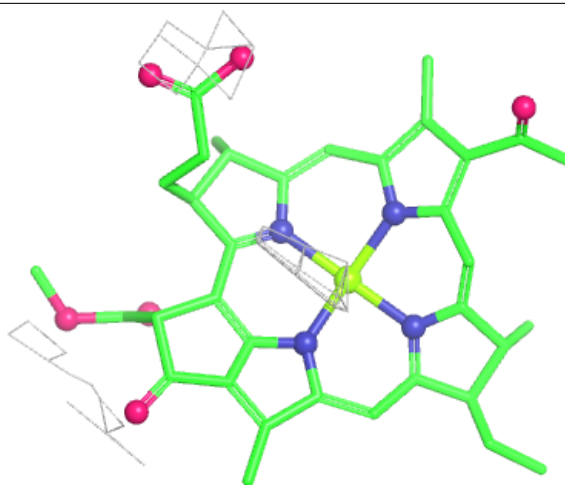
Electron density around BPH BL 304:

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



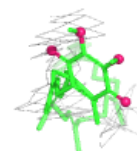
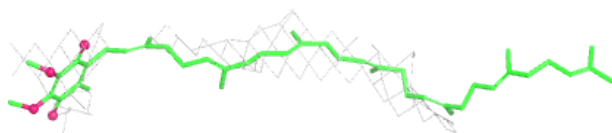
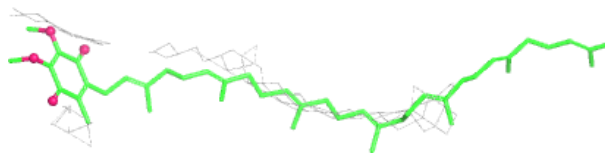
Electron density around BCL AW 101:

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

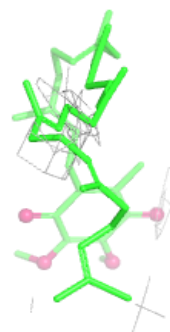
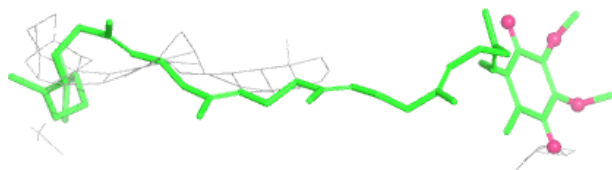
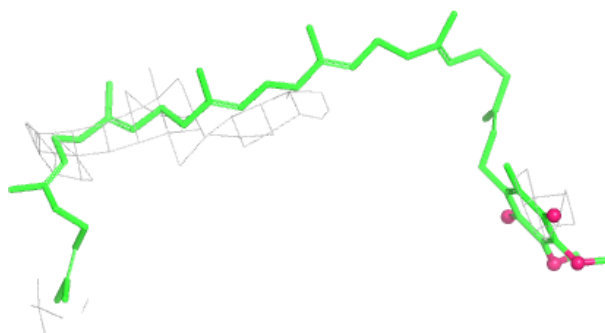


Electron density around U10 AL 304:

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

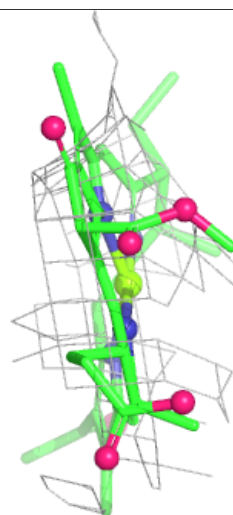
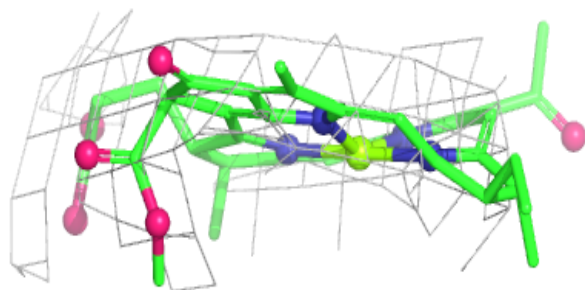
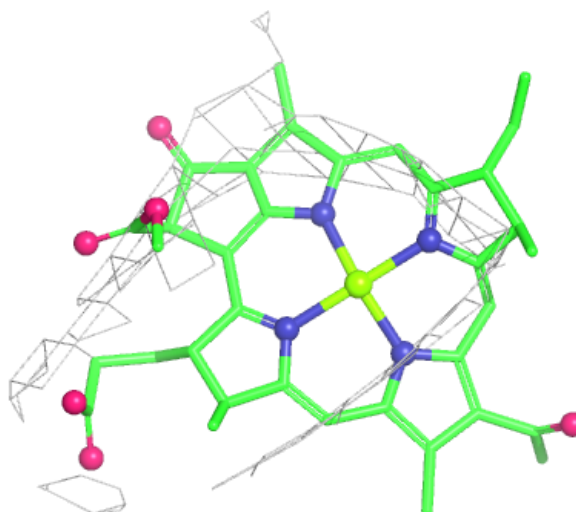
**Electron density around U10 AM 405:**

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



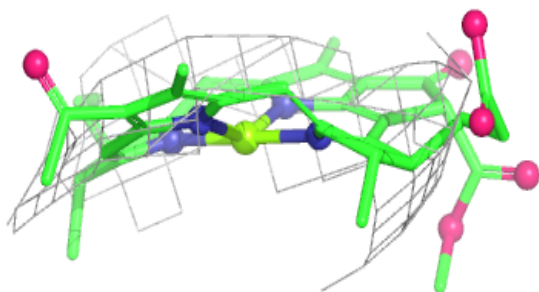
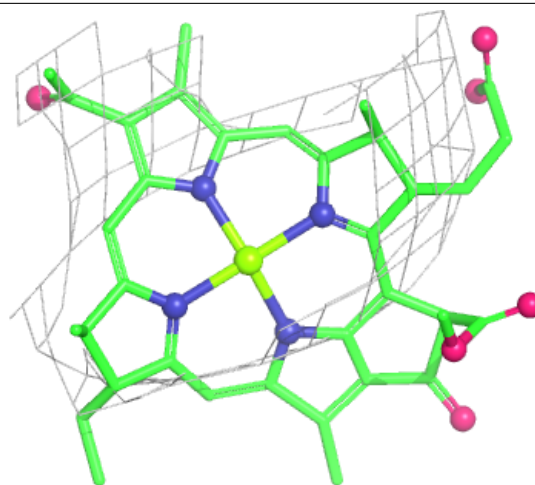
Electron density around BCL B2 101:

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



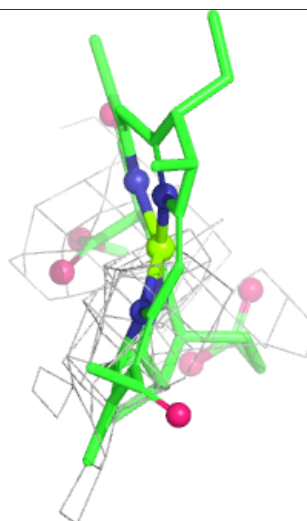
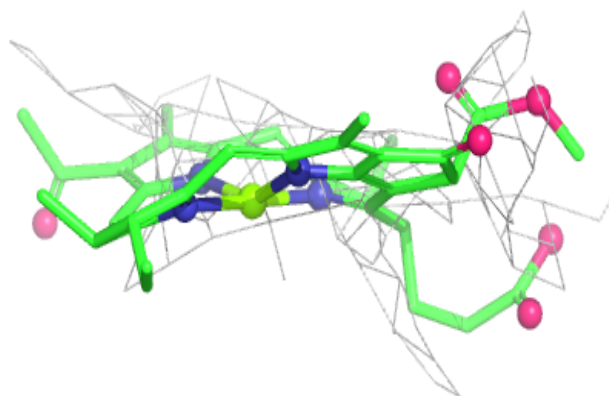
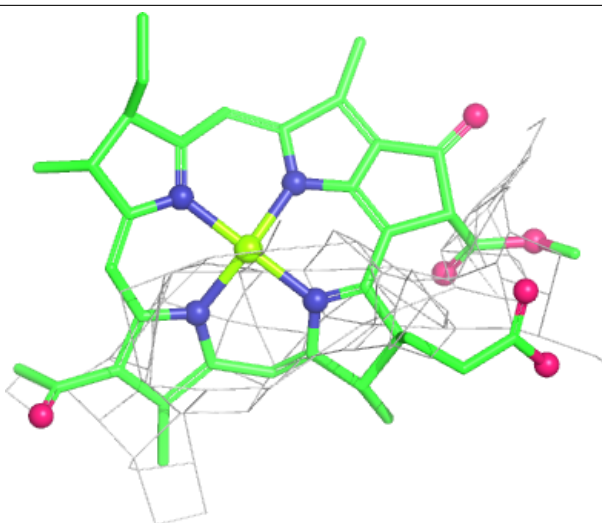
Electron density around BCL BZ 101:

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



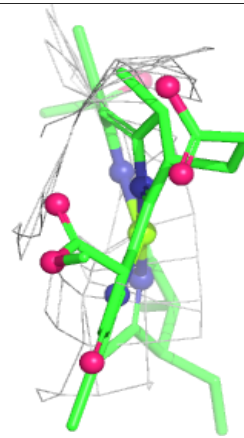
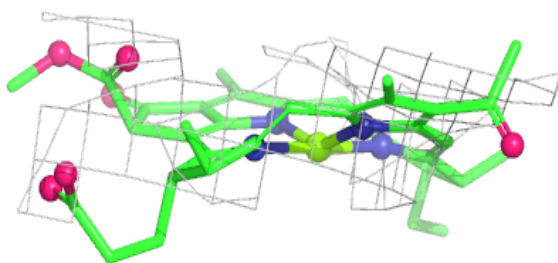
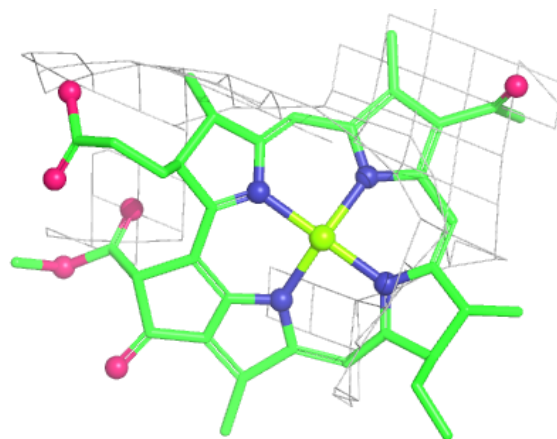
Electron density around BCL AG 101:

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



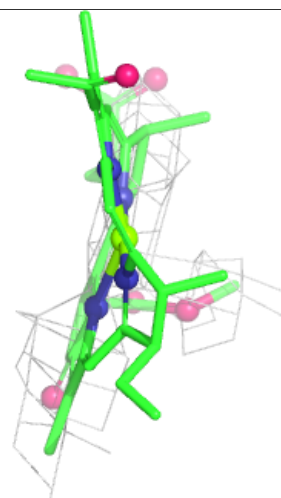
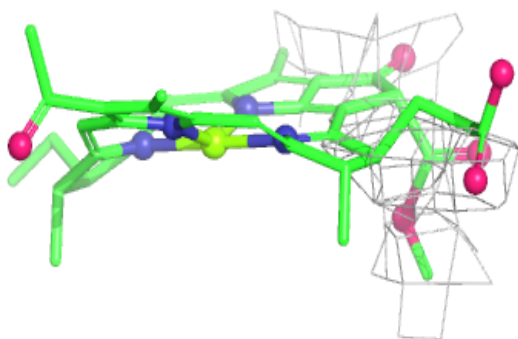
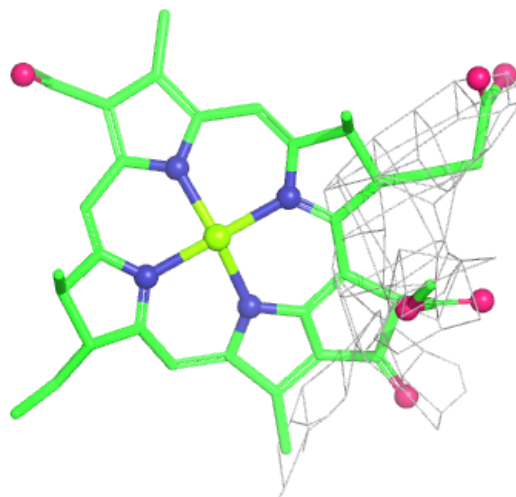
Electron density around BCL AS 101:

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



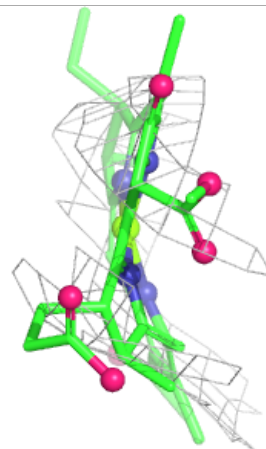
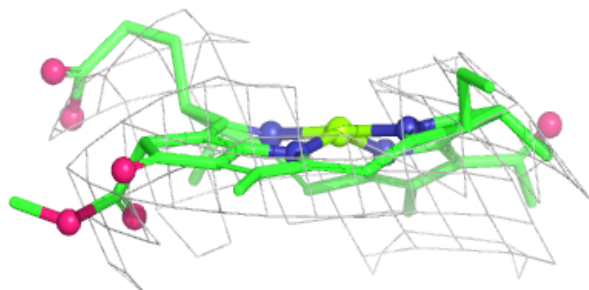
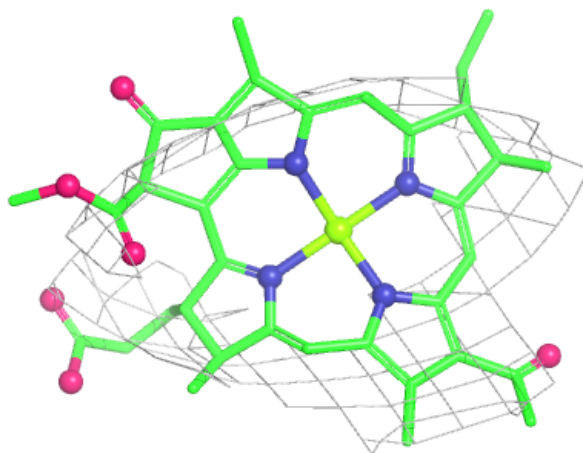
Electron density around BCL AK 101:

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



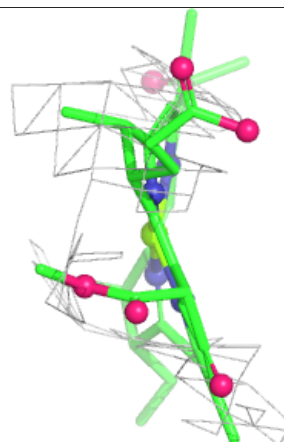
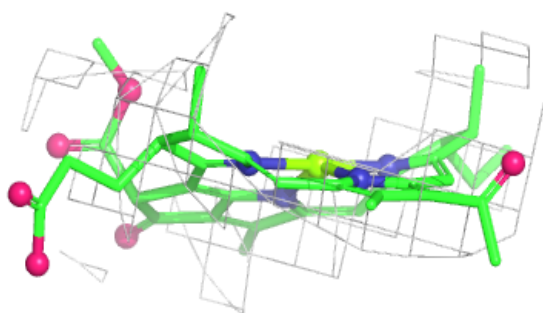
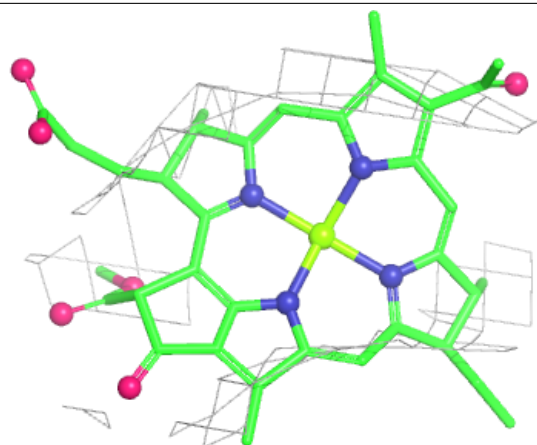
Electron density around BCL BO 102:

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



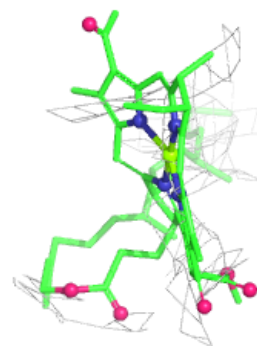
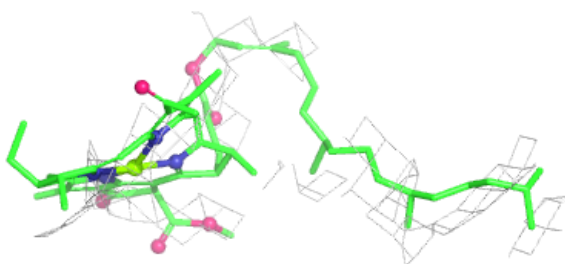
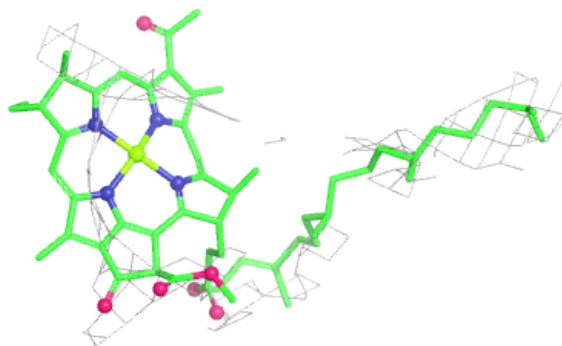
Electron density around BCL AD 101:

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



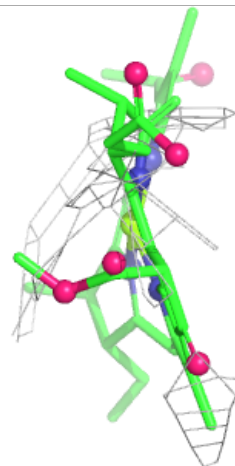
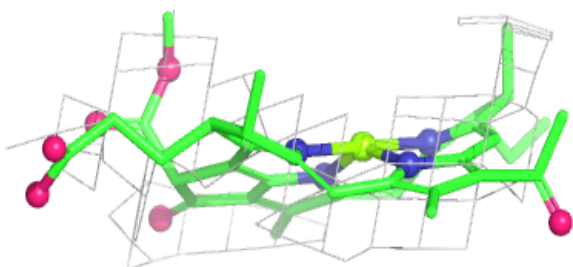
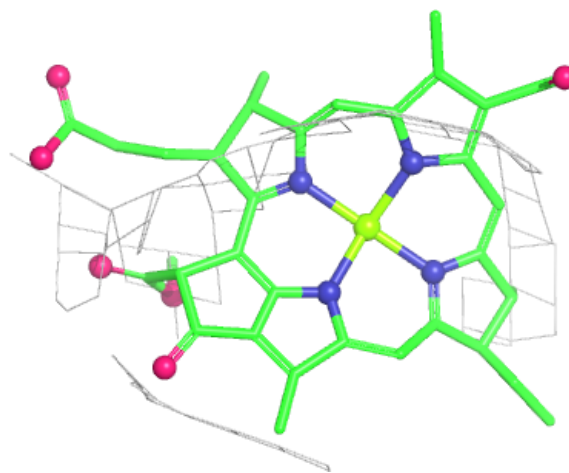
Electron density around BCL AL 302:

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



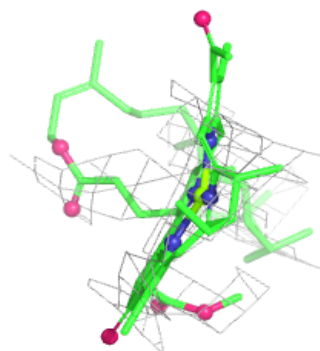
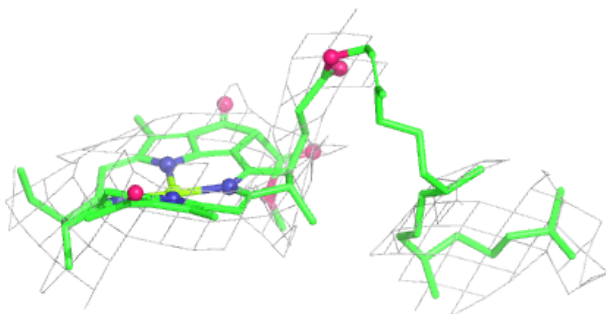
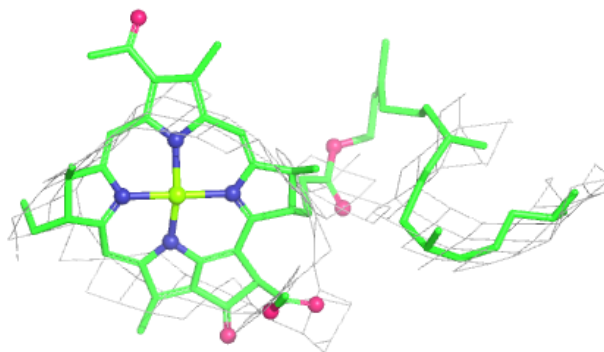
Electron density around BCL BY 101:

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

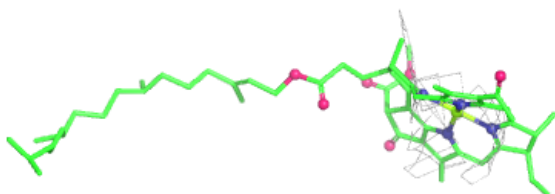
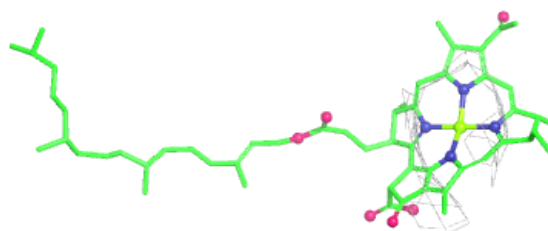


Electron density around BCL AM 401:

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

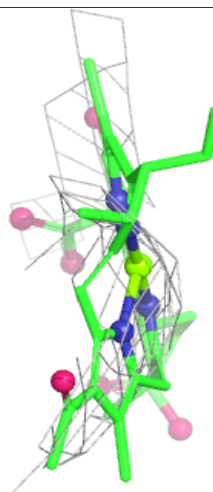
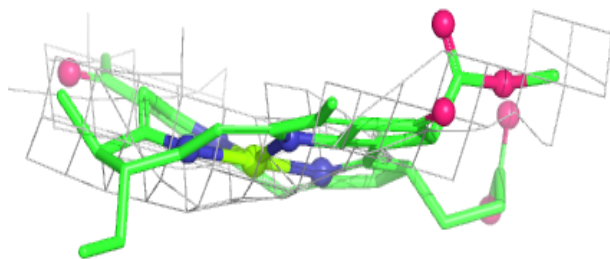
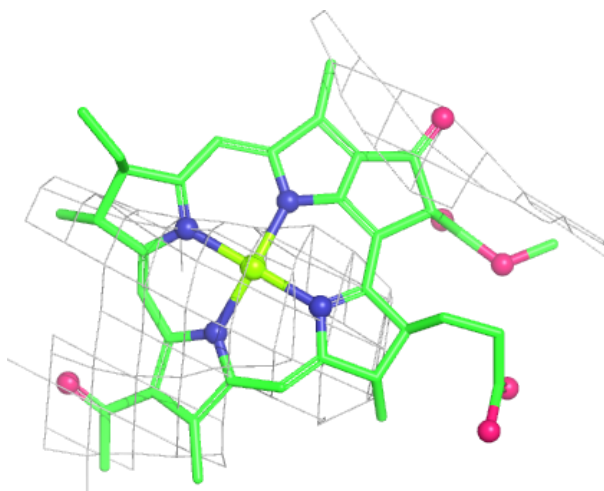
**Electron density around BCL AM 402:**

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



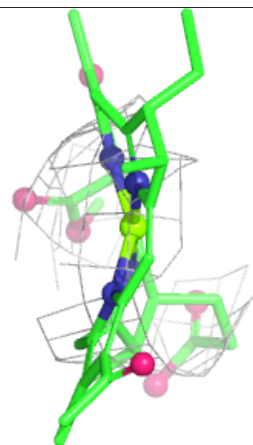
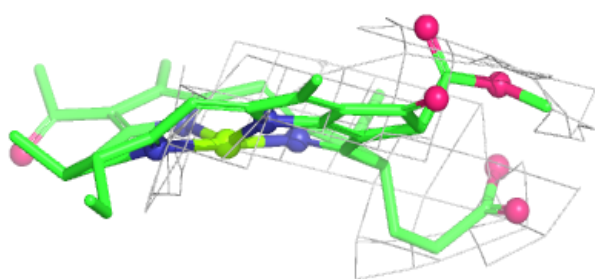
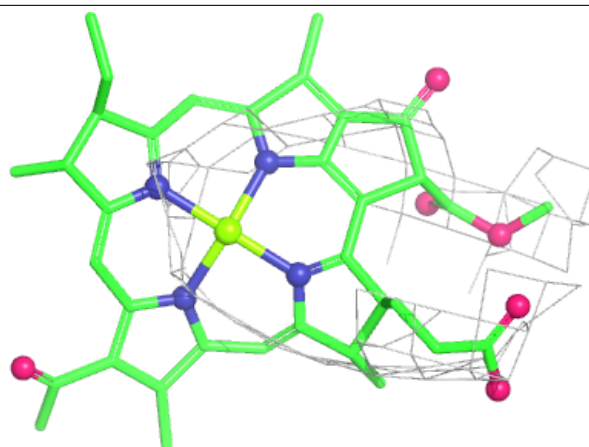
Electron density around BCL B8 101:

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



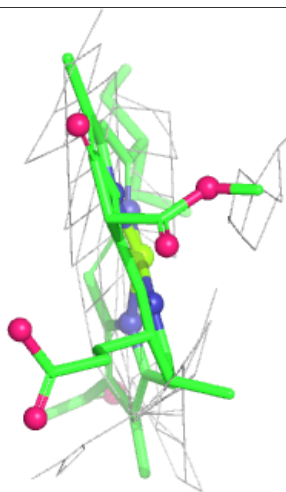
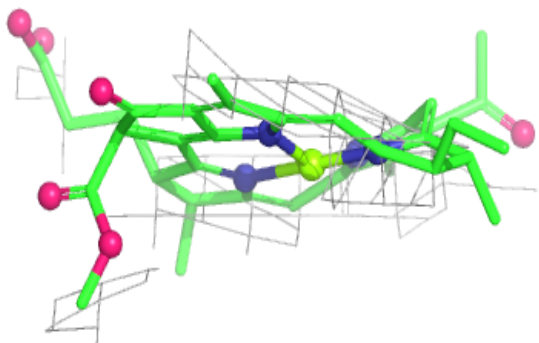
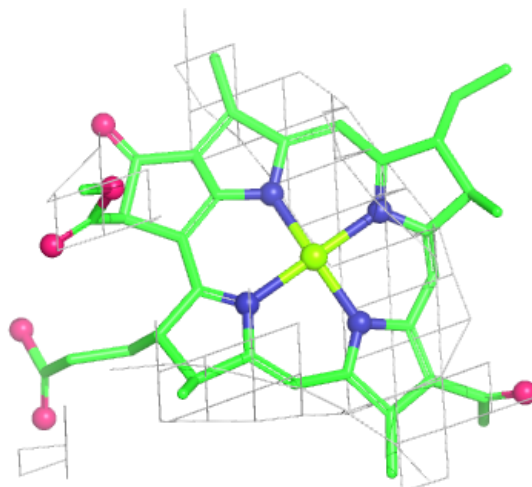
Electron density around BCL AJ 101:

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



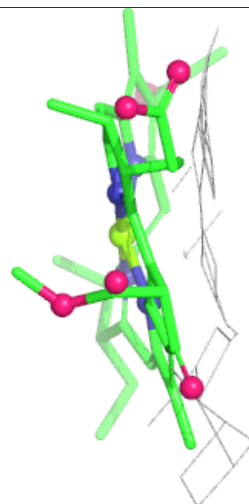
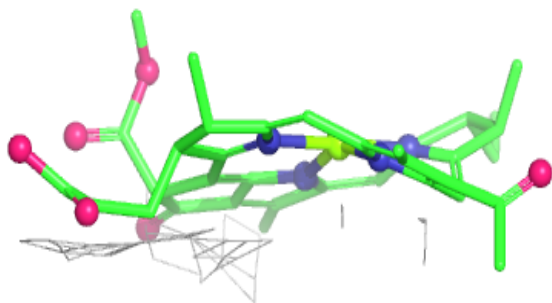
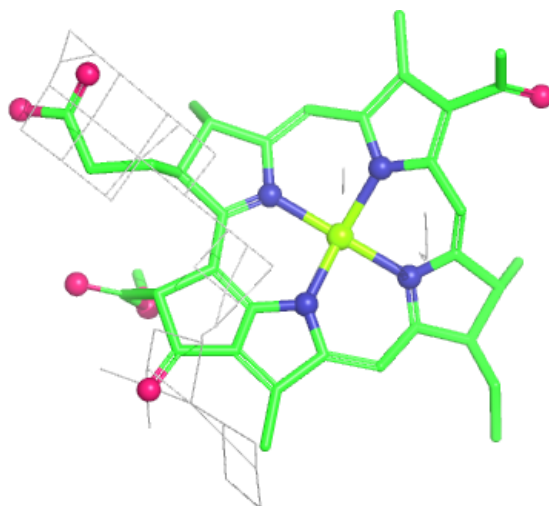
Electron density around BCL BT 101:

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



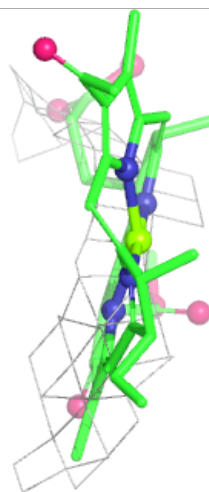
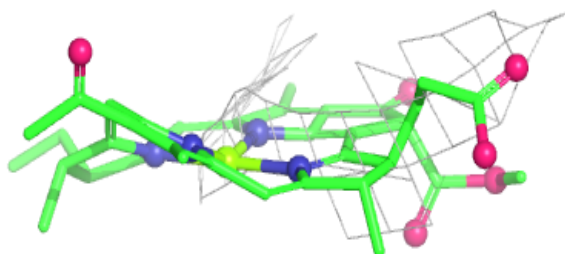
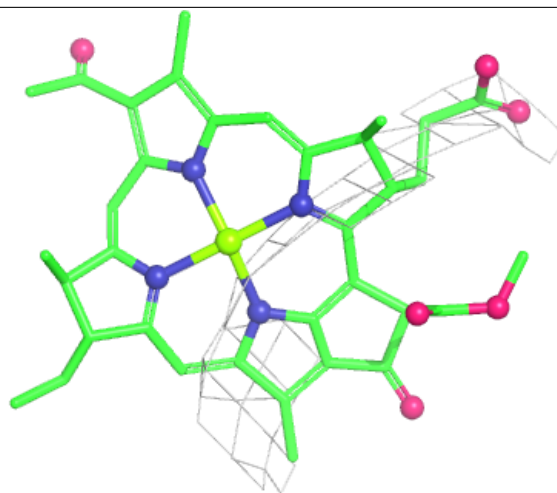
Electron density around BCL A2 101:

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



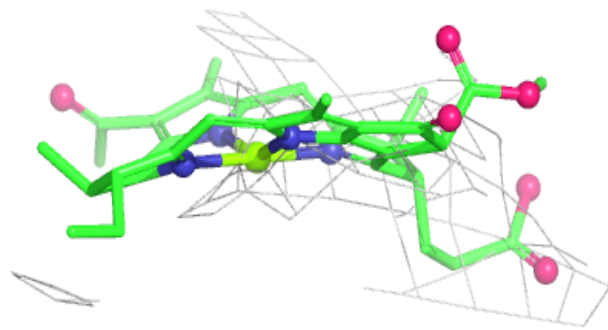
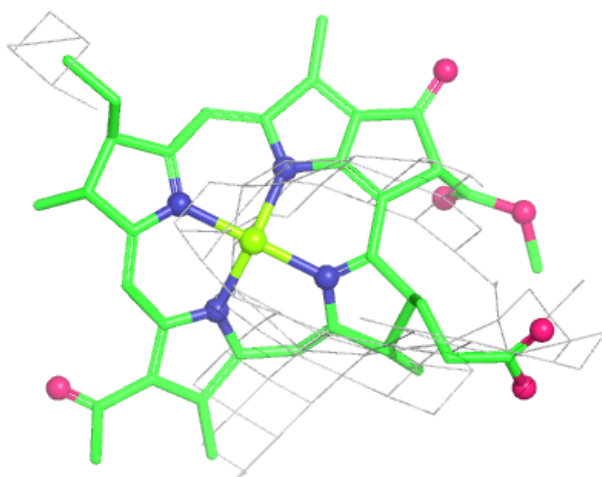
Electron density around BCL BV 102:

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



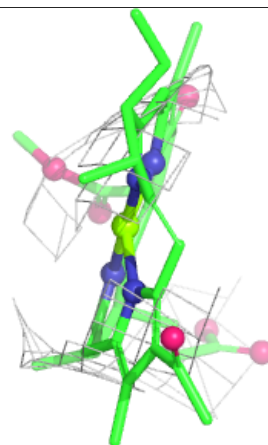
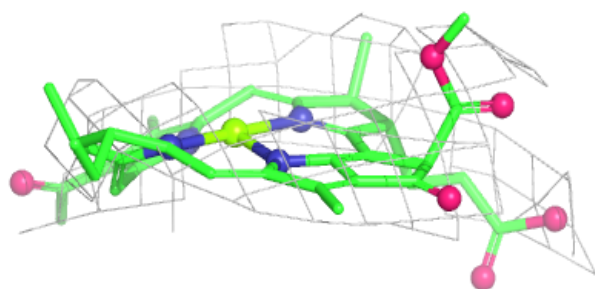
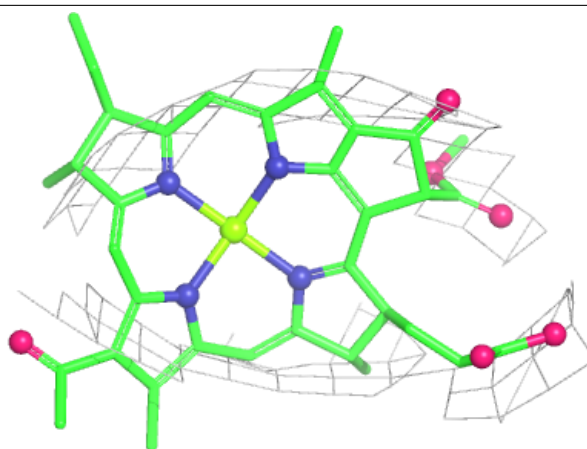
Electron density around BCL A6 102:

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



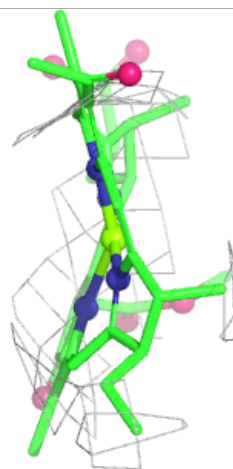
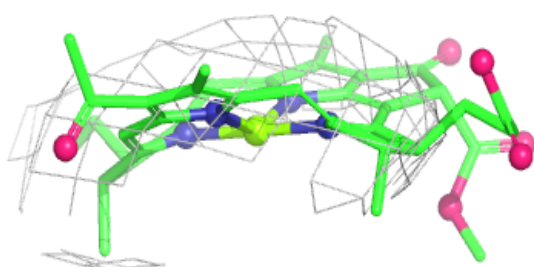
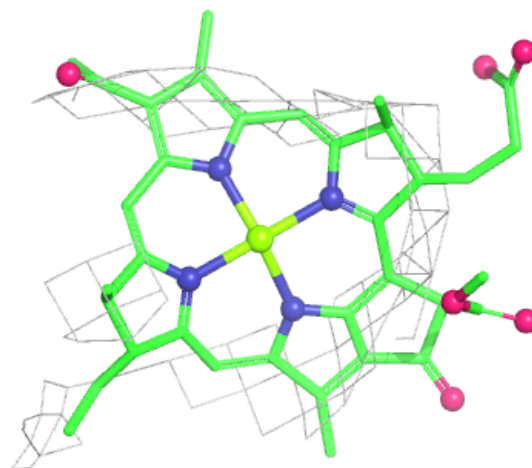
Electron density around BCL B7 101:

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



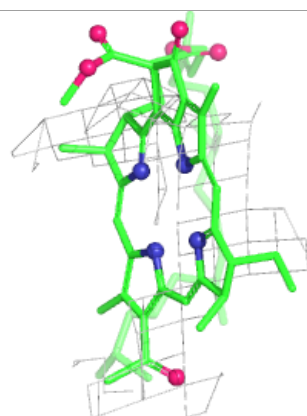
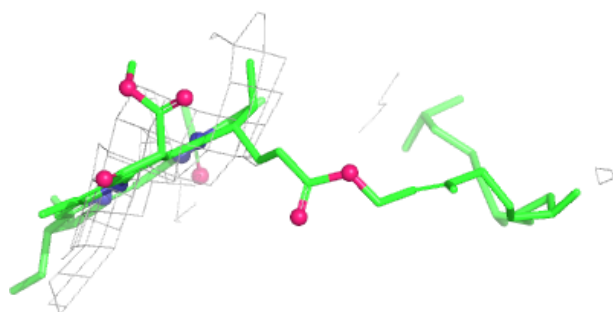
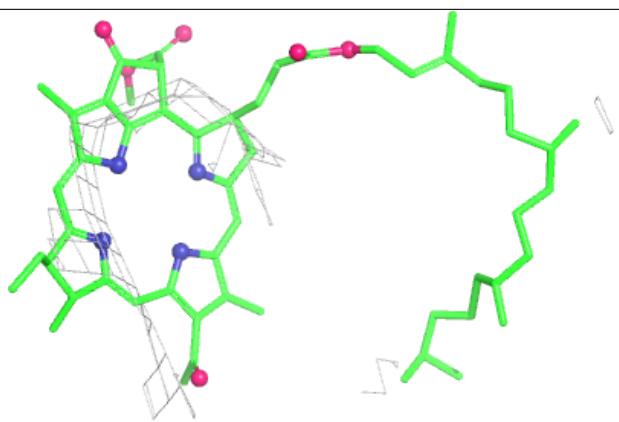
Electron density around BCL AN 101:

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

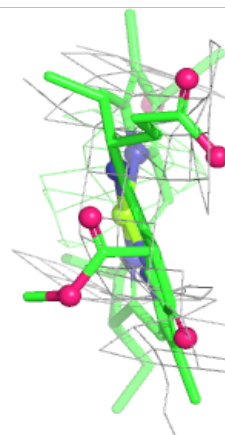
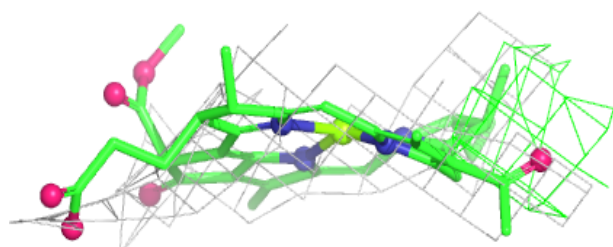
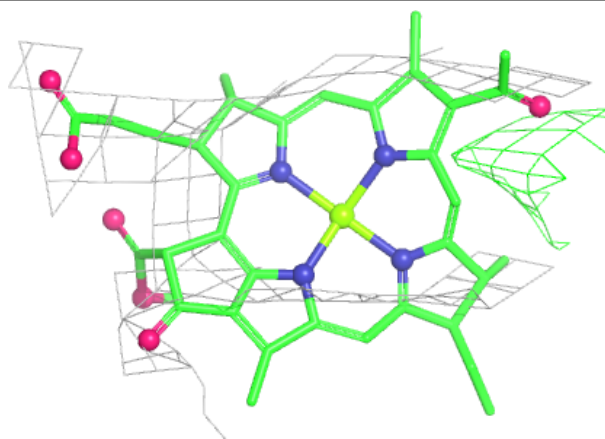


Electron density around BPH AL 303:

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

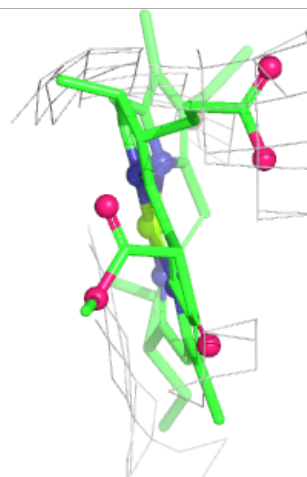
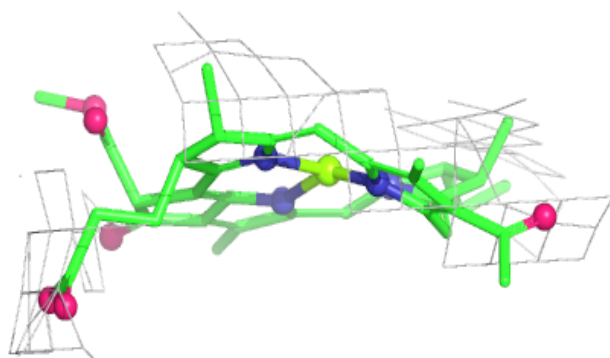
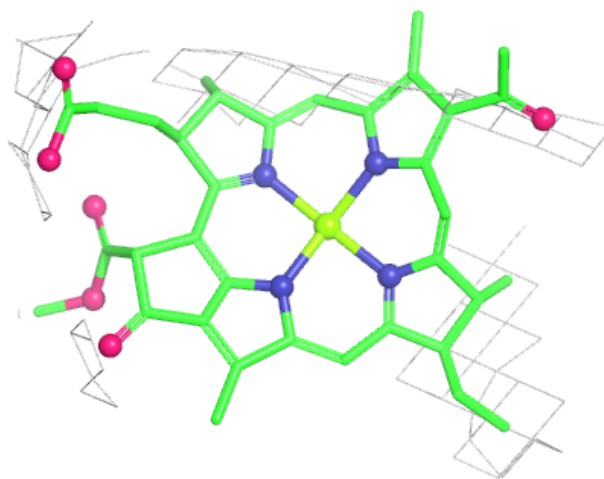
**Electron density around BCL BF 101:**

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



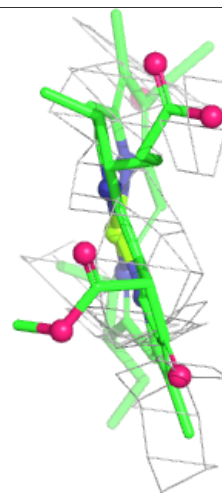
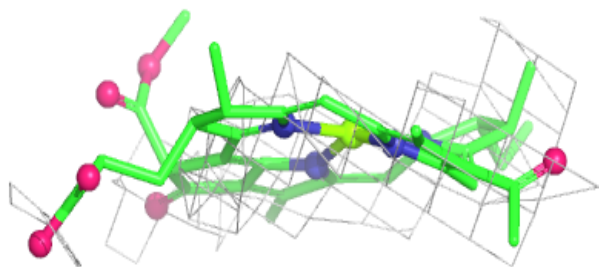
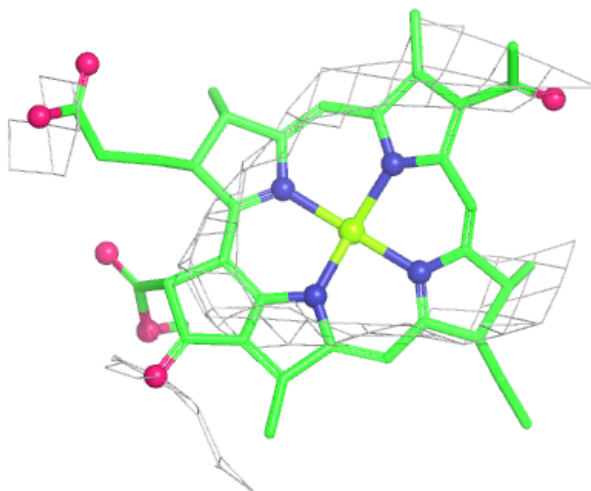
Electron density around BCL AT 101:

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



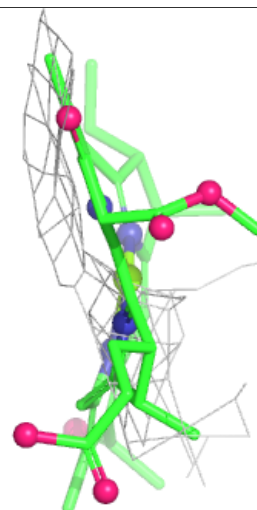
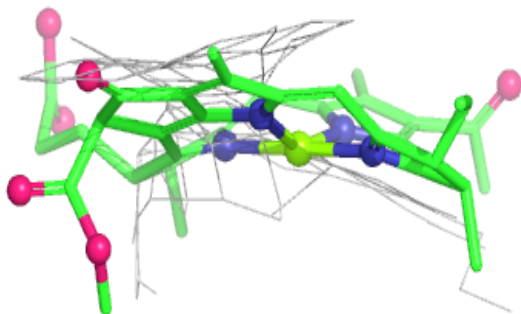
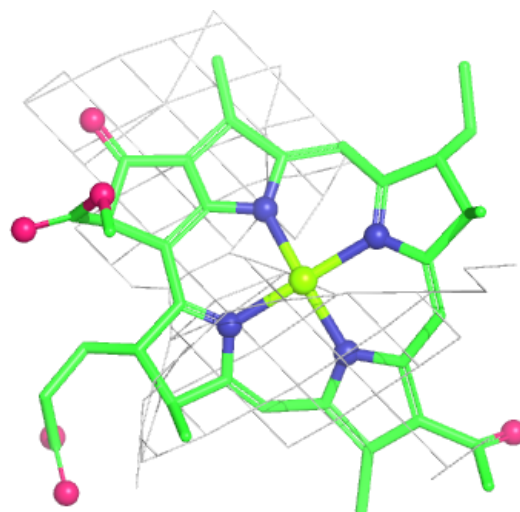
Electron density around BCL AF 101:

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



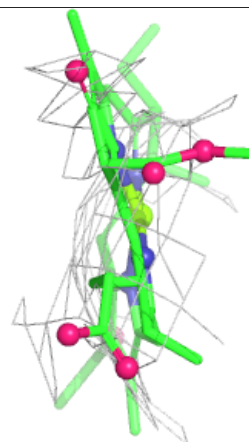
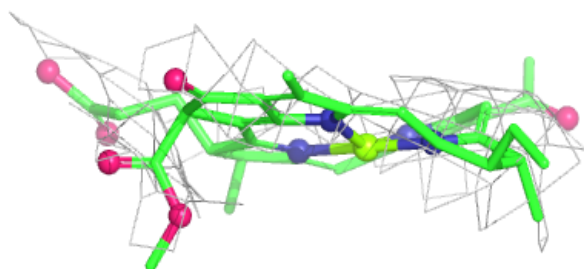
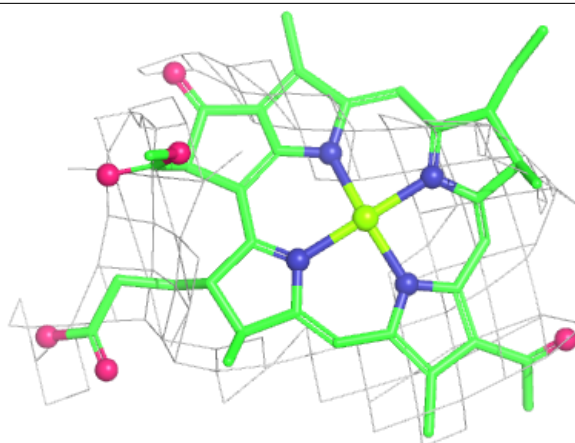
Electron density around BCL AZ 101:

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



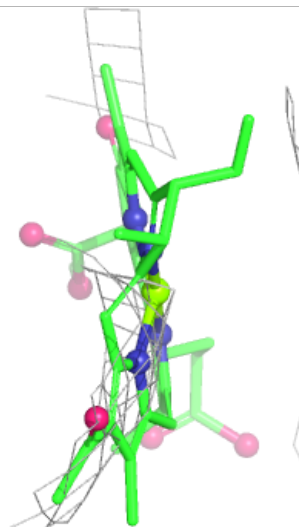
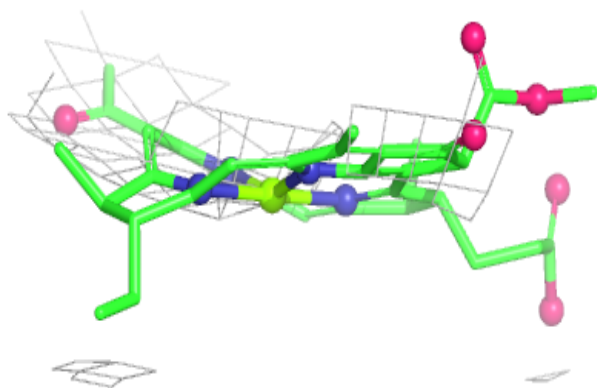
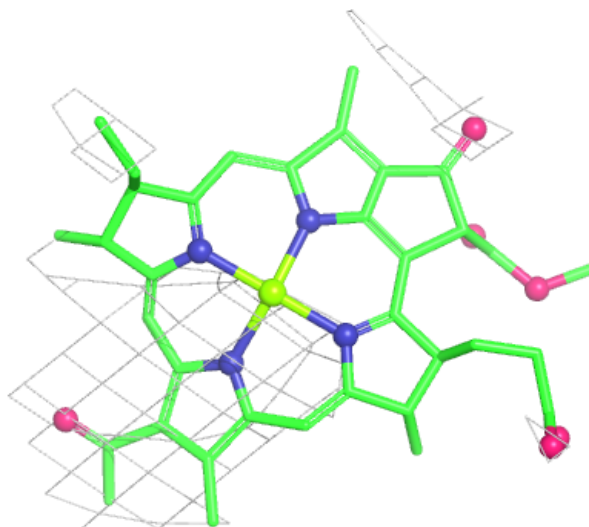
Electron density around BCL BP 101:

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



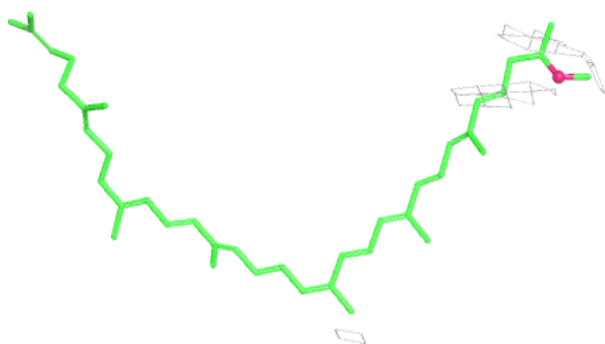
Electron density around BCL A8 101:

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

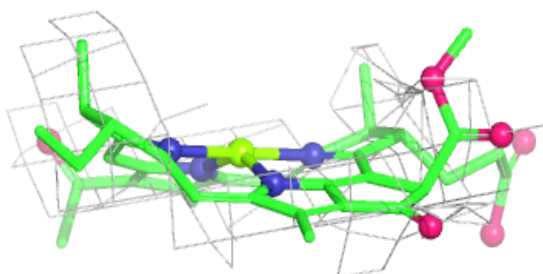
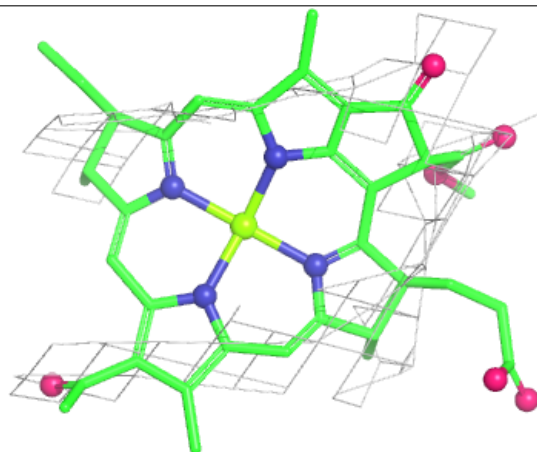


Electron density around SPO AM 406:

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

**Electron density around BCL BD 101:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.