wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 07:28 pm BST

PDB ID	:	1PYH
Title	:	Crystal structure of RC-LH1 core complex from Rhodopseudomonas palustris
Authors	:	Roszak, A.W.; Howard, T.D.; Southall, J.; Gardiner, A.T.; Law, C.J.; Isaacs, N.W.; Cogdell, R.J.
Deposited on	:	2003-07-08
Resolution	:	4.80 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

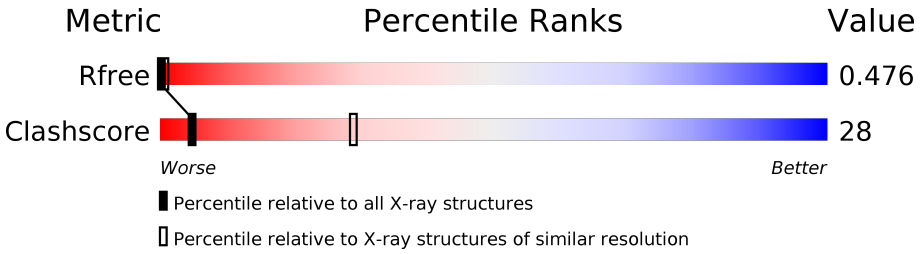
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1096 (5.80-3.80)
Clashscore	141614	1170 (5.80-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	281	99% .
2	B	302	99% .
3	C	241	96% .
4	1	26	96% .
4	3	26	96% .
4	5	26	96% .
4	7	26	96% .
4	D	26	100%
4	F	26	92% 8%

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Mol	Chain	Length	Quality of chain
4	H	26	100%
4	J	26	88% 12%
4	L	26	92% 8%
4	N	26	100%
4	P	26	100%
4	R	26	96%
4	T	26	96%
4	V	26	85% 15%
4	X	26	100%
4	Z	26	92% 8%
5	2	30	100%
5	4	30	100%
5	6	30	100%
5	8	30	100%
5	E	30	87% 13%
5	G	30	97%
5	I	30	100%
5	K	30	97%
5	M	30	97%
5	O	30	100%
5	Q	30	97%
5	S	30	97%
5	U	30	100%
5	W	30	97%
5	Y	30	93% 7%

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
6	BCL	1	38	-	-	-	X
6	BCL	5	38	-	-	-	X
6	BCL	6	36	-	-	-	X
6	BCL	7	38	-	-	-	X
6	BCL	8	36	-	-	-	X
6	BCL	A	301	-	-	-	X
6	BCL	A	302	-	-	-	X
6	BCL	B	303	-	-	-	X
6	BCL	B	304	-	-	-	X
6	BCL	D	2	-	-	-	X
6	BCL	E	1	-	-	-	X
6	BCL	F	4	-	-	-	X
6	BCL	I	5	-	-	-	X
6	BCL	J	8	-	-	X	-
6	BCL	L	10	-	-	X	-
6	BCL	N	38	-	-	X	-
6	BCL	P	38	-	-	X	-
6	BCL	P	39	-	-	X	-
6	BCL	S	36	-	-	-	X
6	BCL	U	36	-	-	-	X
6	BCL	V	38	-	-	-	X
6	BCL	W	36	-	-	-	X
6	BCL	Y	37	-	-	-	X
7	BPH	A	401	-	-	-	X
7	BPH	B	402	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10100 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	0	0	0
			1373	811	281	281			

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	0	0	0
			1474	870	302	302			

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	0	0	0
			1182	700	241	241			

- Molecule 4 is a protein called Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	F	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	H	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	J	26	Total	C	N	O	0	0	0
			127	75	26	26			
4	L	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	N	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	P	26	Total	C	N	O	0	0	0
			128	76	26	26			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	R	26	Total C N O 128 76 26 26	0	0	0
4	T	26	Total C N O 128 76 26 26	0	0	0
4	V	26	Total C N O 128 76 26 26	0	0	0
4	X	26	Total C N O 127 75 26 26	0	0	0
4	Z	26	Total C N O 128 76 26 26	0	0	0
4	1	26	Total C N O 128 76 26 26	0	0	0
4	3	26	Total C N O 128 76 26 26	0	0	0
4	5	26	Total C N O 128 76 26 26	0	0	0
4	7	26	Total C N O 128 76 26 26	0	0	0

- Molecule 5 is a protein called Light-harvesting protein B-800/850, beta chain.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	30	Total C N O 148 88 30 30	0	0	0
5	G	30	Total C N O 148 88 30 30	0	0	0
5	I	30	Total C N O 148 88 30 30	0	0	0
5	K	30	Total C N O 148 88 30 30	0	0	0
5	M	30	Total C N O 148 88 30 30	0	0	0
5	O	30	Total C N O 148 88 30 30	0	0	0
5	Q	30	Total C N O 148 88 30 30	0	0	0
5	S	30	Total C N O 148 88 30 30	0	0	0
5	U	30	Total C N O 148 88 30 30	0	0	0
5	W	30	Total C N O 148 88 30 30	0	0	0

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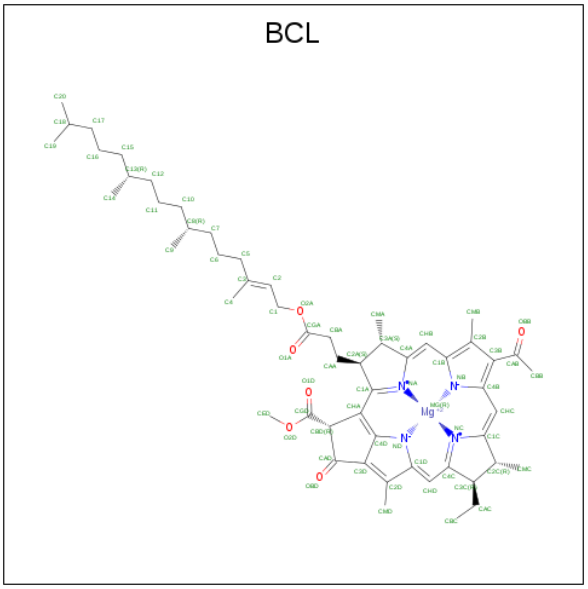
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	Y	30	Total C N O 148 88 30 30	0	0	0
5	2	30	Total C N O 148 88 30 30	0	0	0
5	4	30	Total C N O 148 88 30 30	0	0	0
5	6	30	Total C N O 148 88 30 30	0	0	0
5	8	30	Total C N O 148 88 30 30	0	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C Mg N O 66 55 1 4 6	0	0
6	A	1	Total C Mg N O 66 55 1 4 6	0	0
6	B	1	Total C Mg N O 66 55 1 4 6	0	0
6	B	1	Total C Mg N O 66 55 1 4 6	0	0
6	D	1	Total C Mg N O 47 36 1 4 6	0	0
6	E	1	Total C Mg N O 47 36 1 4 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	G	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	H	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	I	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	J	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	K	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	N	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	N	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	P	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	P	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	R	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	S	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	T	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	U	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	V	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	W	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

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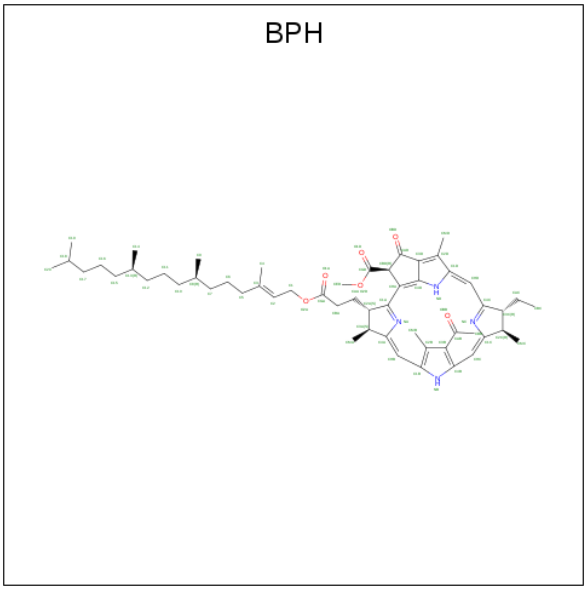
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	5	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	6	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	7	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			65	55	4	6		
7	B	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

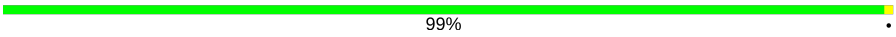
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe 1 1	0	0

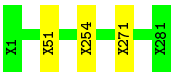
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Reaction center protein L chain

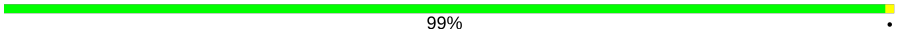
Chain A:





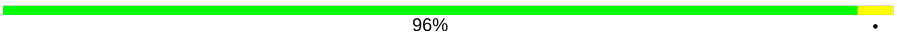
- Molecule 2: Reaction center protein M chain

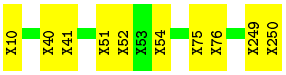
Chain B:



- Molecule 3: Reaction center protein H chain

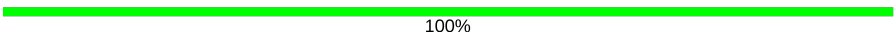
Chain C:





- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain D:



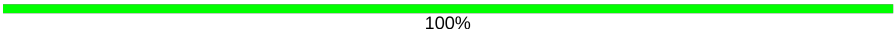
There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain F:

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

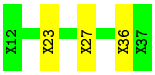
Chain H:



There are no outlier residues recorded for this chain.

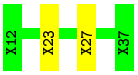
• Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain J:



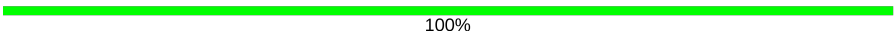
• Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain L:



• Molecule 4: Light-harvesting protein B-800/850, alpha chain

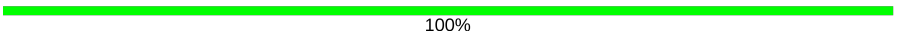
Chain N:



There are no outlier residues recorded for this chain.

• Molecule 4: Light-harvesting protein B-800/850, alpha chain

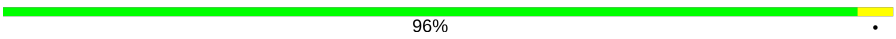
Chain P:



There are no outlier residues recorded for this chain.

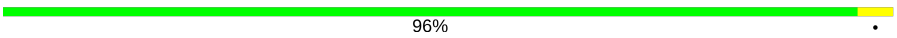
• Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain R:



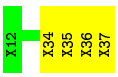
• Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain T:



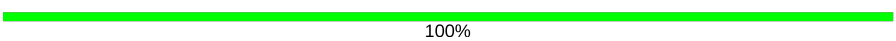
• Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain V:



• Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain X:

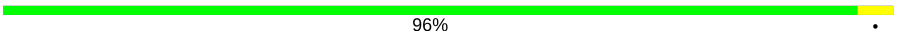


There are no outlier residues recorded for this chain.

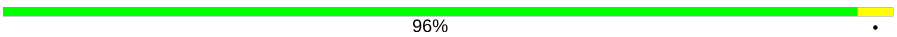
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain Z: 

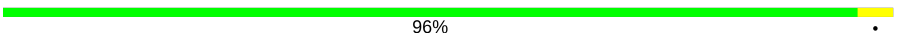
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 1: 

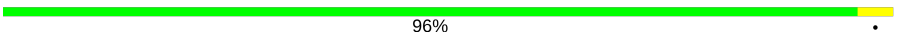
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 3: 

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

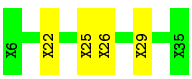
Chain 5: 

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

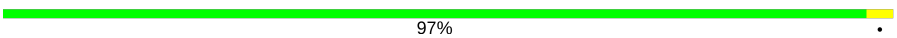
Chain 7: 

- Molecule 5: Light-harvesting protein B-800/850, beta chain

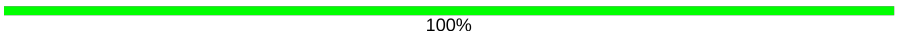
Chain E: 



- Molecule 5: Light-harvesting protein B-800/850, beta chain

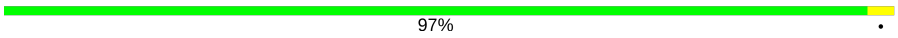
Chain G: 

• Molecule 5: Light-harvesting protein B-800/850, beta chain

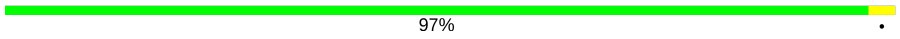
Chain I: 

There are no outlier residues recorded for this chain.

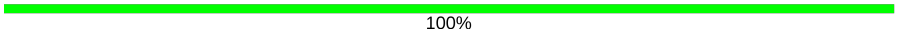
• Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain K: 

• Molecule 5: Light-harvesting protein B-800/850, beta chain

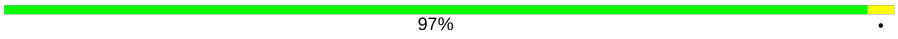
Chain M: 

• Molecule 5: Light-harvesting protein B-800/850, beta chain

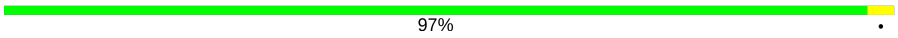
Chain O: 

There are no outlier residues recorded for this chain.

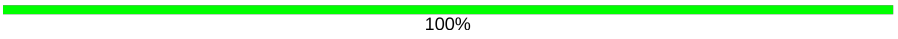
• Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain Q: 

• Molecule 5: Light-harvesting protein B-800/850, beta chain

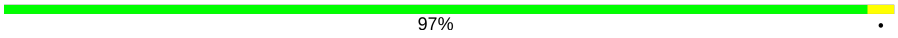
Chain S: 

• Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain U: 

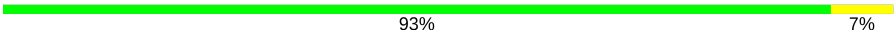
There are no outlier residues recorded for this chain.

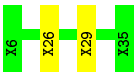
• Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain W: 

• Molecule 5: Light-harvesting protein B-800/850, beta chain

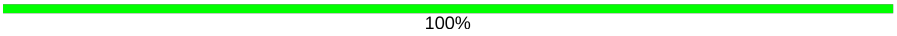
Chain Y:





• Molecule 5: Light-harvesting protein B-800/850, beta chain

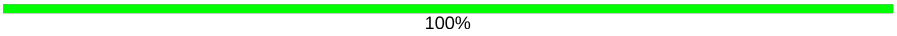
Chain 2:



There are no outlier residues recorded for this chain.

• Molecule 5: Light-harvesting protein B-800/850, beta chain

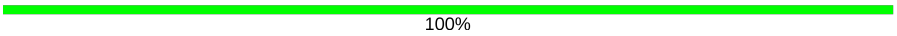
Chain 4:



There are no outlier residues recorded for this chain.

• Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 6:



There are no outlier residues recorded for this chain.

• Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 8:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.04Å 119.02Å 130.43Å 69.32° 72.69° 66.52°	Depositor
Resolution (Å)	60.00 – 4.80 59.99 – 4.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (60.00-4.80) 97.3 (59.99-4.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 4.86Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.467 , 0.491 0.454 , 0.476	Depositor DCC
R_{free} test set	944 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	202.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.03 , 999.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.76	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å^2)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, FE

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

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1373	0	257	10	0
2	B	1474	0	274	2	0
3	C	1182	0	230	13	0
4	1	128	0	26	2	0
4	3	128	0	26	1	0
4	5	128	0	26	1	0
4	7	128	0	26	2	0
4	D	128	0	26	0	0
4	F	128	0	26	7	0
4	H	128	0	26	0	0
4	J	127	0	25	7	0
4	L	128	0	26	3	0
4	N	128	0	26	0	0
4	P	128	0	26	0	0
4	R	128	0	26	1	0
4	T	128	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	128	0	26	5	0
4	X	127	0	25	0	0
4	Z	128	0	26	4	0
5	2	148	0	30	0	0
5	4	148	0	30	0	0
5	6	148	0	30	0	0
5	8	148	0	30	0	0
5	E	148	0	30	11	0
5	G	148	0	30	3	0
5	I	148	0	30	0	0
5	K	148	0	30	4	0
5	M	148	0	30	1	0
5	O	148	0	30	0	0
5	Q	148	0	30	5	0
5	S	148	0	30	1	0
5	U	148	0	30	0	0
5	W	148	0	30	2	0
5	Y	148	0	30	4	0
6	1	47	0	34	18	0
6	2	47	0	34	10	0
6	3	94	0	68	15	0
6	5	47	0	33	12	0
6	6	47	0	34	3	0
6	7	47	0	34	8	0
6	8	47	0	34	5	0
6	A	132	0	148	9	0
6	B	132	0	148	6	0
6	D	47	0	34	14	0
6	E	47	0	34	14	0
6	F	47	0	34	7	0
6	G	47	0	34	11	0
6	H	47	0	33	11	0
6	I	47	0	34	6	0
6	J	47	0	33	32	0
6	K	47	0	34	18	0
6	L	47	0	34	25	0
6	M	47	0	34	13	0
6	N	94	0	68	39	0
6	P	94	0	68	51	0
6	R	47	0	34	16	0
6	S	47	0	34	10	0
6	T	47	0	34	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	U	47	0	34	8	0
6	V	47	0	34	8	0
6	W	47	0	34	6	0
6	Y	94	0	68	23	0
7	A	65	0	76	5	0
7	B	65	0	76	0	0
8	B	1	0	0	0	0
All	All	10100	0	3090	367	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 28.

The worst 5 of 367 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)
6:N:38:BCL:HMC3	6:P:38:BCL:CBB	1.44	1.47
6:H:6:BCL:C1	6:H:6:BCL:O2A	1.63	1.46
6:R:38:BCL:O2A	6:R:38:BCL:C1	1.63	1.42
6:P:38:BCL:CBC	6:P:39:BCL:HMD2	1.56	1.33
6:L:10:BCL:CMB	6:N:11:BCL:HMA1	1.64	1.26

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 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	$\#\|Z\| > 2$
6	BCL	L	10	-	39,55,74	3.29	24 (61%)	46,92,115	5.22	19 (41%)
6	BCL	H	6	-	39,55,74	3.60	26 (66%)	46,92,115	5.14	19 (41%)
6	BCL	B	303	-	58,74,74	1.29	7 (12%)	69,115,115	1.57	13 (18%)
6	BCL	P	39	-	39,55,74	3.45	25 (64%)	46,92,115	5.24	20 (43%)
6	BCL	S	36	-	39,55,74	4.20	20 (51%)	46,92,115	4.19	22 (47%)
6	BCL	U	36	-	39,55,74	4.13	18 (46%)	46,92,115	4.12	20 (43%)
6	BCL	F	4	-	39,55,74	3.26	25 (64%)	46,92,115	5.15	20 (43%)
6	BCL	V	38	-	39,55,74	4.10	19 (48%)	46,92,115	4.30	24 (52%)
6	BCL	5	38	-	39,55,74	3.22	23 (58%)	46,92,115	5.34	20 (43%)
6	BCL	D	2	-	39,55,74	3.31	24 (61%)	46,92,115	5.16	20 (43%)
6	BCL	Y	37	-	39,55,74	3.22	25 (64%)	46,92,115	5.26	20 (43%)
6	BCL	A	301	-	58,74,74	1.16	5 (8%)	69,115,115	1.88	19 (27%)
6	BCL	N	11	-	39,55,74	3.99	17 (43%)	46,92,115	4.37	22 (47%)
7	BPH	B	402	-	64,70,70	0.84	1 (1%)	76,101,101	1.33	9 (11%)
6	BCL	A	302	-	58,74,74	1.16	3 (5%)	69,115,115	1.61	17 (24%)
6	BCL	N	38	-	39,55,74	3.26	24 (61%)	46,92,115	5.23	20 (43%)
6	BCL	3	39	-	39,55,74	3.20	24 (61%)	46,92,115	5.29	20 (43%)
6	BCL	7	38	-	39,55,74	3.24	22 (56%)	46,92,115	5.21	21 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BCL	3	38	-	39,55,74	3.92	18 (46%)	46,92,115	4.10	18 (39%)
6	BCL	R	38	-	39,55,74	3.45	24 (61%)	46,92,115	5.23	20 (43%)
6	BCL	E	1	-	39,55,74	4.21	18 (46%)	46,92,115	4.17	22 (47%)
6	BCL	2	36	-	39,55,74	4.03	18 (46%)	46,92,115	4.15	20 (43%)
6	BCL	Y	36	-	39,55,74	4.07	18 (46%)	46,92,115	4.08	19 (41%)
6	BCL	I	5	-	39,55,74	4.18	19 (48%)	46,92,115	4.27	22 (47%)
6	BCL	G	3	-	39,55,74	4.14	16 (41%)	46,92,115	4.18	21 (45%)
6	BCL	W	36	-	39,55,74	3.19	25 (64%)	46,92,115	5.22	20 (43%)
6	BCL	K	36	-	39,55,74	4.08	20 (51%)	46,92,115	4.21	18 (39%)
6	BCL	T	38	-	39,55,74	3.43	25 (64%)	46,92,115	5.19	20 (43%)
6	BCL	M	36	-	39,55,74	4.07	18 (46%)	46,92,115	4.26	21 (45%)
6	BCL	J	8	-	39,55,74	3.30	25 (64%)	46,92,115	5.11	19 (41%)
7	BPH	A	401	-	64,70,70	0.88	1 (1%)	76,101,101	1.43	12 (15%)
6	BCL	6	36	-	39,55,74	3.96	18 (46%)	46,92,115	4.11	20 (43%)
6	BCL	8	36	-	39,55,74	4.00	18 (46%)	46,92,115	4.17	23 (50%)
6	BCL	B	304	-	58,74,74	1.14	7 (12%)	69,115,115	1.52	15 (21%)
6	BCL	1	38	-	39,55,74	3.26	26 (66%)	46,92,115	5.37	20 (43%)
6	BCL	P	38	-	39,55,74	4.10	19 (48%)	46,92,115	4.27	20 (43%)

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
6	BCL	L	10	-	-	9/15/115/137	-
6	BCL	H	6	-	-	4/15/115/137	-
6	BCL	B	303	-	-	0/37/137/137	-
6	BCL	P	39	-	-	4/15/115/137	-
6	BCL	S	36	-	-	4/15/115/137	-
6	BCL	U	36	-	-	4/15/115/137	-
6	BCL	F	4	-	-	6/15/115/137	-
6	BCL	V	38	-	-	5/15/115/137	-
6	BCL	5	38	-	-	4/15/115/137	-
6	BCL	D	2	-	-	4/15/115/137	-
6	BCL	Y	37	-	-	4/15/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	A	301	-	-	10/37/137/137	-
6	BCL	N	11	-	-	2/15/115/137	-
7	BPH	B	402	-	-	7/54/105/105	0/5/6/6
6	BCL	A	302	-	-	7/37/137/137	-
6	BCL	N	38	-	-	3/15/115/137	-
6	BCL	3	39	-	-	5/15/115/137	-
6	BCL	7	38	-	-	2/15/115/137	-
6	BCL	3	38	-	-	0/15/115/137	-
6	BCL	R	38	-	-	5/15/115/137	-
6	BCL	E	1	-	-	3/15/115/137	-
6	BCL	2	36	-	-	1/15/115/137	-
6	BCL	Y	36	-	-	4/15/115/137	-
6	BCL	I	5	-	-	3/15/115/137	-
6	BCL	G	3	-	-	1/15/115/137	-
6	BCL	W	36	-	-	6/15/115/137	-
6	BCL	K	36	-	-	0/15/115/137	-
6	BCL	T	38	-	-	5/15/115/137	-
6	BCL	M	36	-	-	2/15/115/137	-
6	BCL	J	8	-	-	4/15/115/137	-
7	BPH	A	401	-	-	12/54/105/105	0/5/6/6
6	BCL	6	36	-	-	2/15/115/137	-
6	BCL	8	36	-	-	3/15/115/137	-
6	BCL	B	304	-	-	4/37/137/137	-
6	BCL	1	38	-	-	4/15/115/137	-
6	BCL	P	38	-	-	1/15/115/137	-

The worst 5 of 665 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	3	BCL	C1B-NB	17.27	1.50	1.35
6	I	5	BCL	C1B-NB	16.83	1.50	1.35
6	S	36	BCL	C1B-NB	16.76	1.50	1.35
6	E	1	BCL	C1B-NB	16.65	1.50	1.35
6	V	38	BCL	C1B-NB	16.61	1.50	1.35

The worst 5 of 695 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1	38	BCL	C4D-C3D-CAD	-28.61	92.52	108.47
6	5	38	BCL	C4D-C3D-CAD	-28.18	92.76	108.47
6	3	39	BCL	C4D-C3D-CAD	-28.04	92.83	108.47
6	Y	37	BCL	C4D-C3D-CAD	-28.04	92.83	108.47
6	W	36	BCL	C4D-C3D-CAD	-27.78	92.98	108.47

There are no chirality outliers.

5 of 144 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	10	BCL	C1A-C2A-CAA-CBA
6	L	10	BCL	C3A-C2A-CAA-CBA
6	L	10	BCL	C4C-C3C-CAC-CBC
6	L	10	BCL	CHA-CBD-CGD-O1D
6	L	10	BCL	CHA-CBD-CGD-O2D

There are no ring outliers.

35 monomers are involved in 341 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	10	BCL	25	0
6	H	6	BCL	11	0
6	B	303	BCL	4	0
6	P	39	BCL	27	0
6	S	36	BCL	10	0
6	U	36	BCL	8	0
6	F	4	BCL	7	0
6	V	38	BCL	8	0
6	5	38	BCL	12	0
6	D	2	BCL	14	0
6	Y	37	BCL	9	0
6	A	301	BCL	7	0
6	N	11	BCL	17	0
6	A	302	BCL	2	0
6	N	38	BCL	27	0
6	3	39	BCL	7	0
6	7	38	BCL	8	0
6	3	38	BCL	8	0
6	R	38	BCL	16	0
6	E	1	BCL	14	0
6	2	36	BCL	10	0
6	Y	36	BCL	17	0

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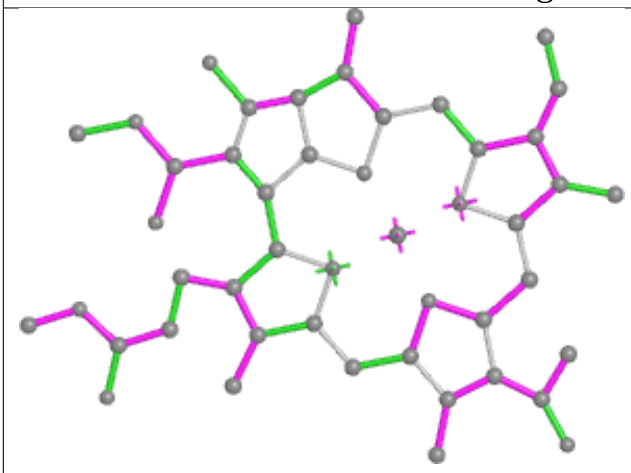
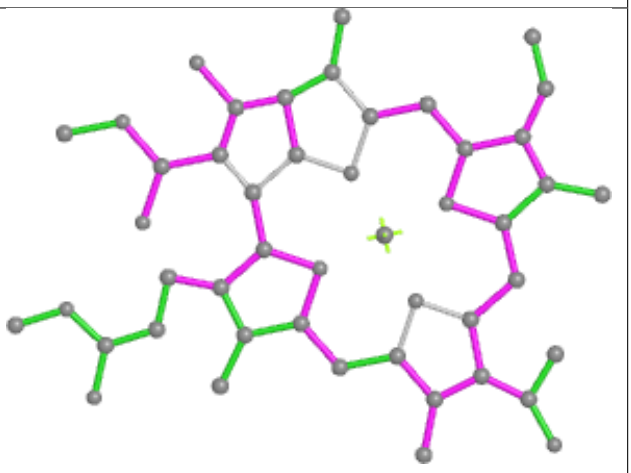
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	5	BCL	6	0
6	G	3	BCL	11	0
6	W	36	BCL	6	0
6	K	36	BCL	18	0
6	T	38	BCL	10	0
6	M	36	BCL	13	0
6	J	8	BCL	32	0
7	A	401	BPH	5	0
6	6	36	BCL	3	0
6	8	36	BCL	5	0
6	B	304	BCL	2	0
6	1	38	BCL	18	0
6	P	38	BCL	41	0

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

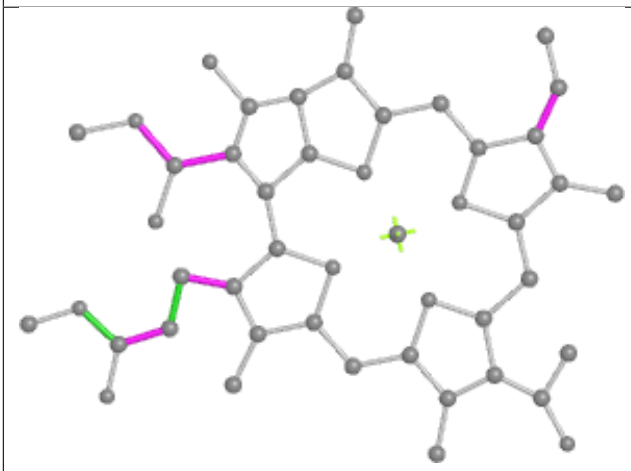
Ligand BCL L 10



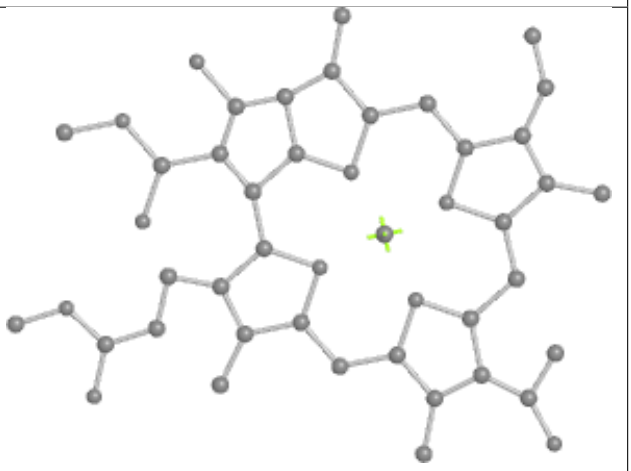
Bond lengths



Bond angles

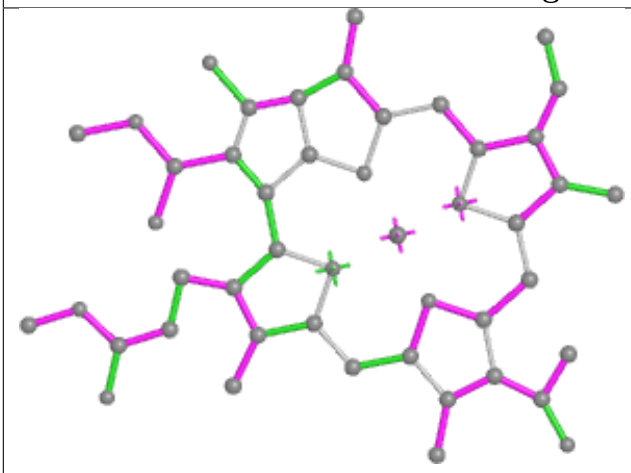


Torsions

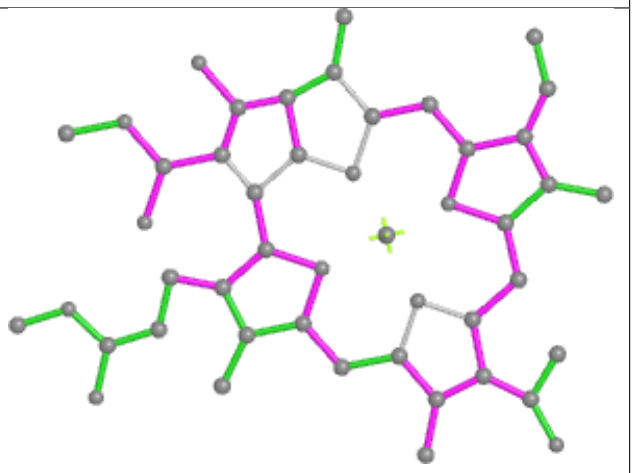


Rings

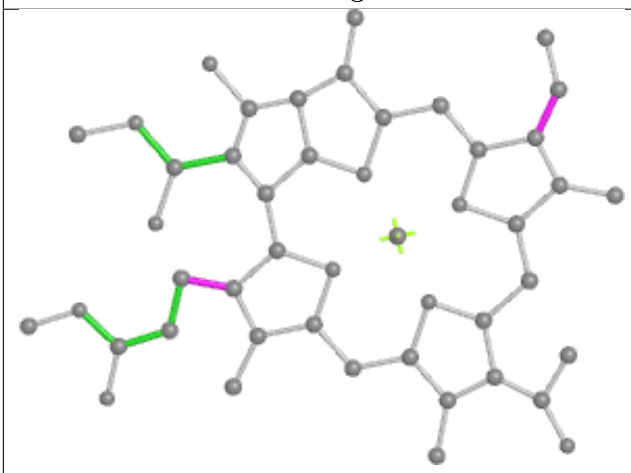
Ligand BCL H 6



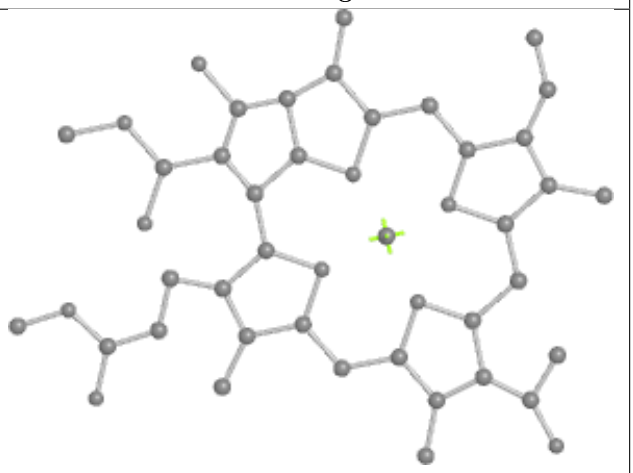
Bond lengths



Bond angles

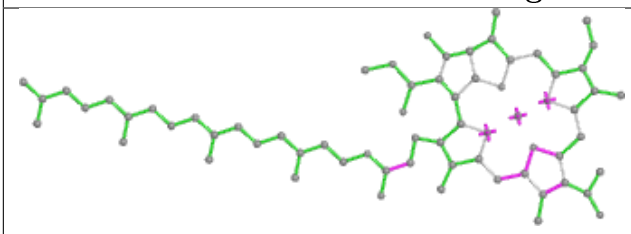


Torsions

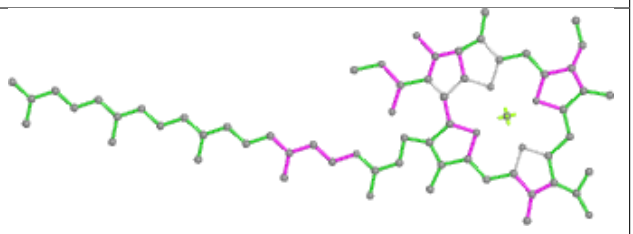


Rings

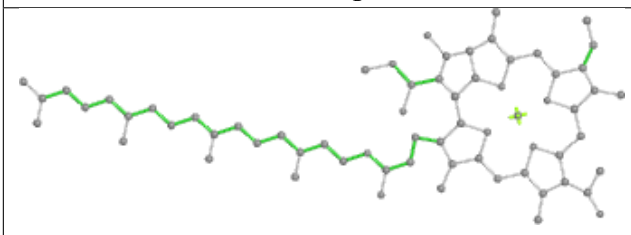
Ligand BCL B 303



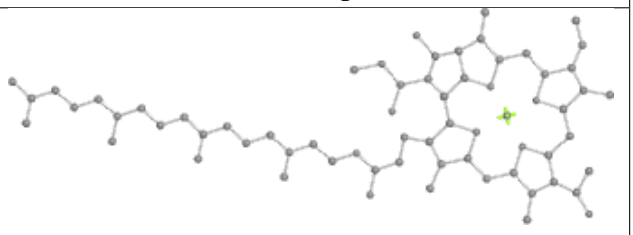
Bond lengths



Bond angles

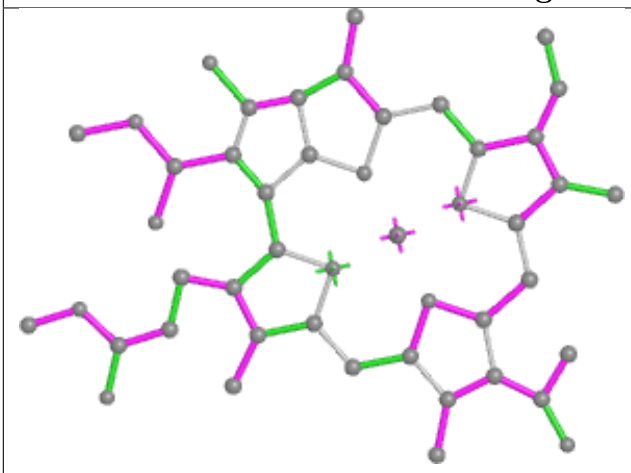


Torsions

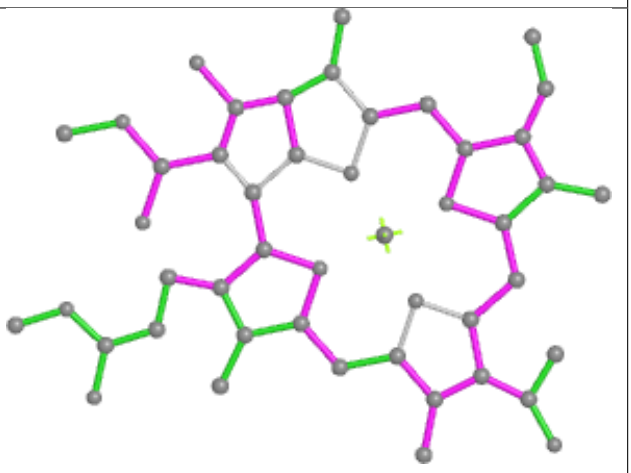


Rings

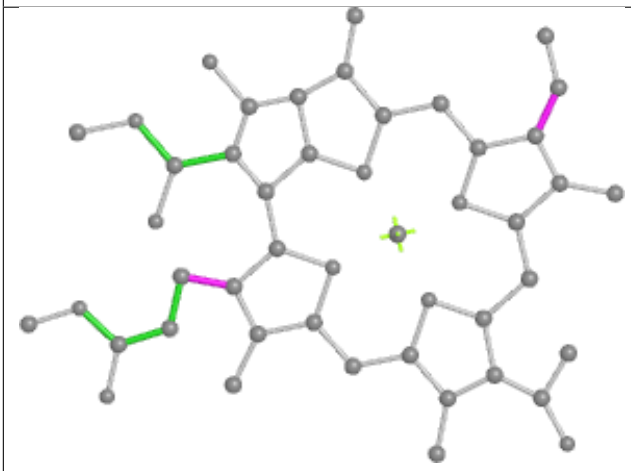
Ligand BCL P 39



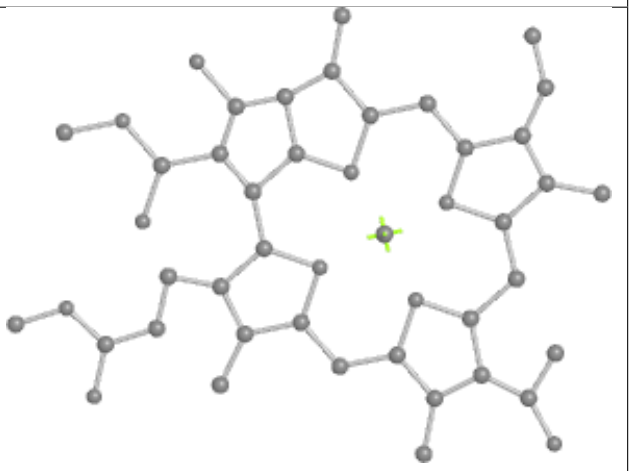
Bond lengths



Bond angles

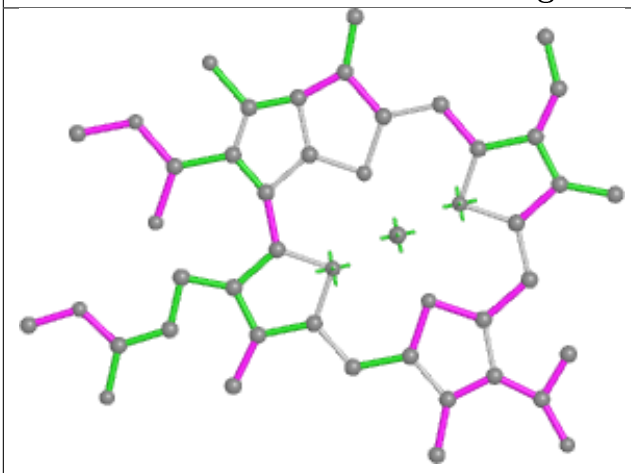


Torsions

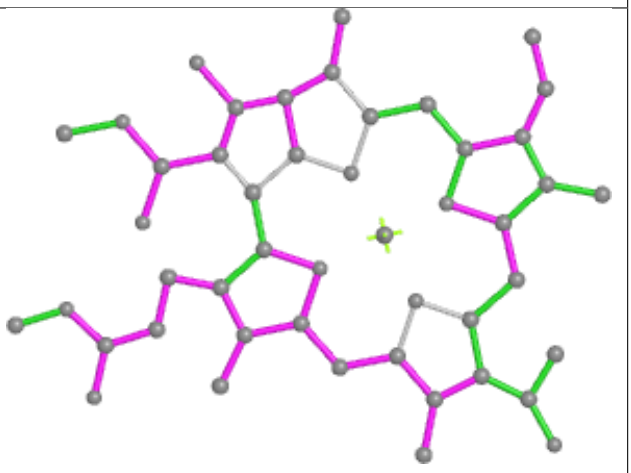


Rings

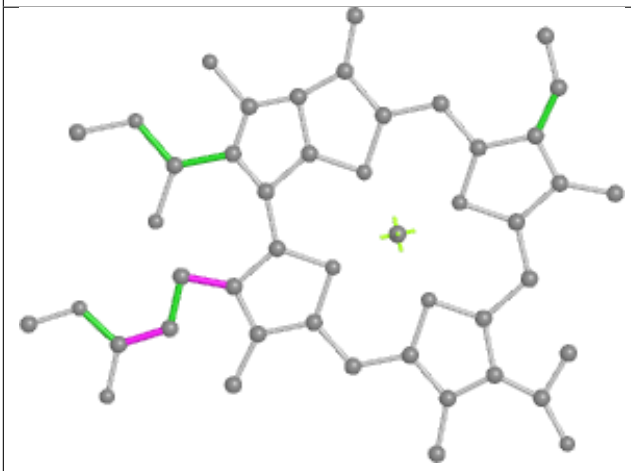
Ligand BCL S 36



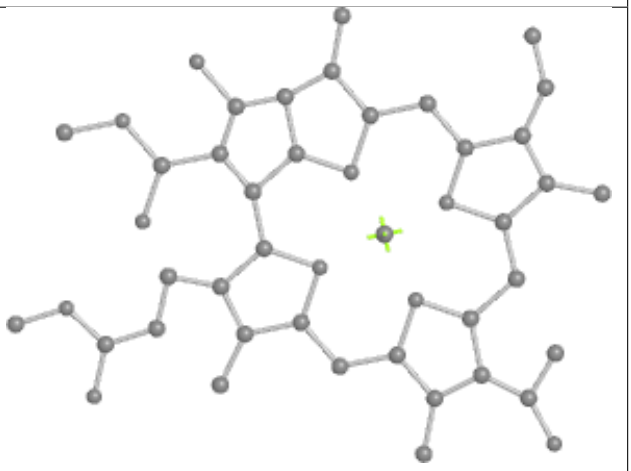
Bond lengths



Bond angles

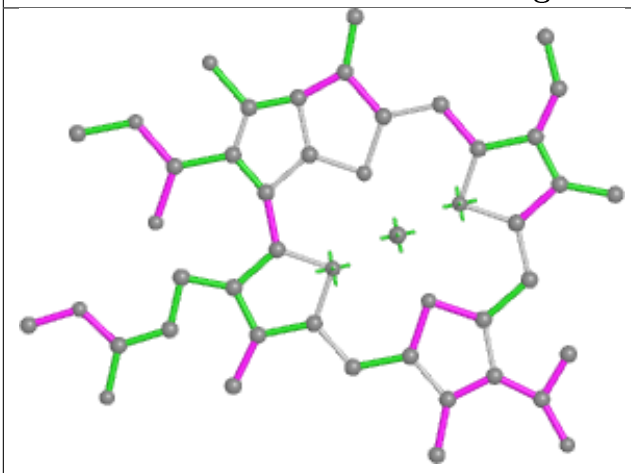


Torsions

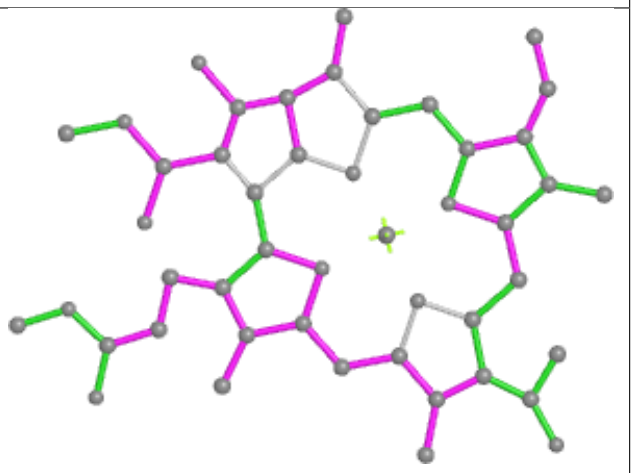


Rings

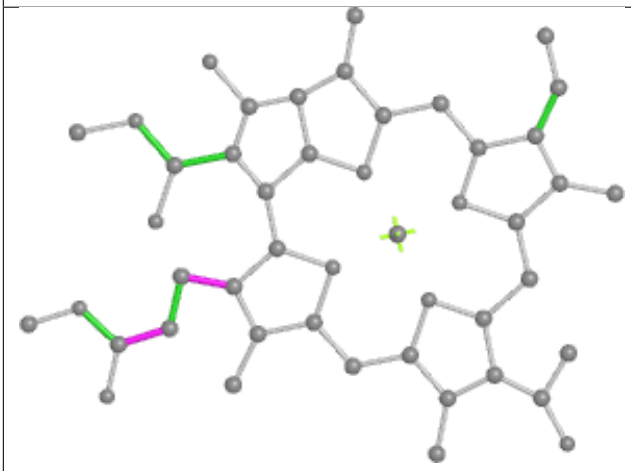
Ligand BCL U 36



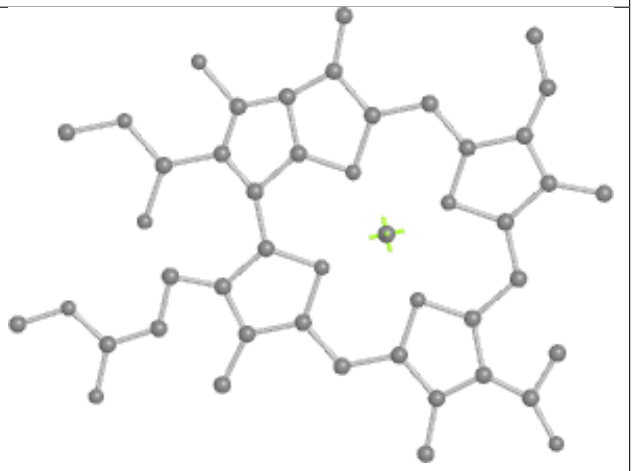
Bond lengths



Bond angles

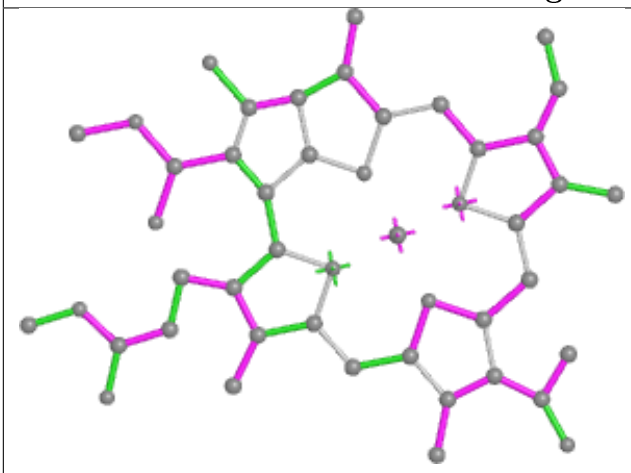


Torsions

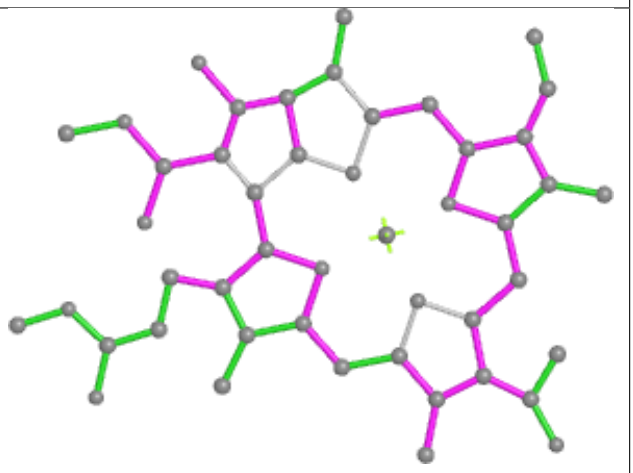


Rings

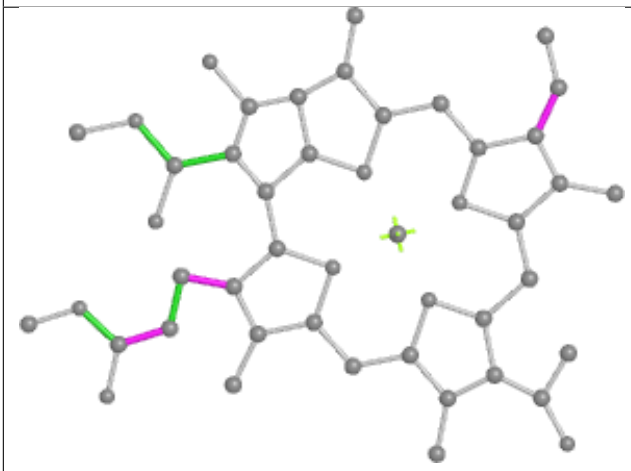
Ligand BCL F 4



Bond lengths



Bond angles



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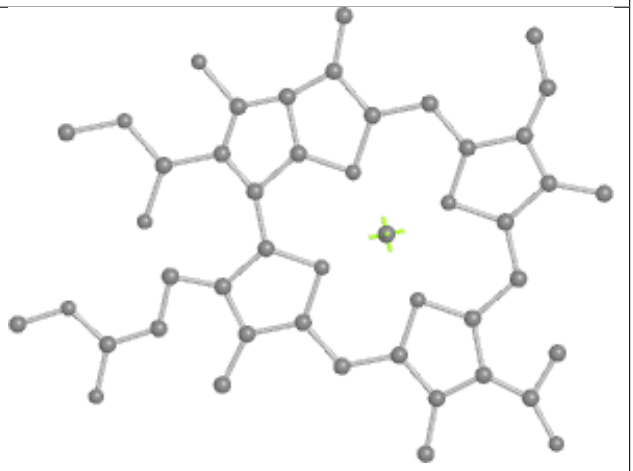
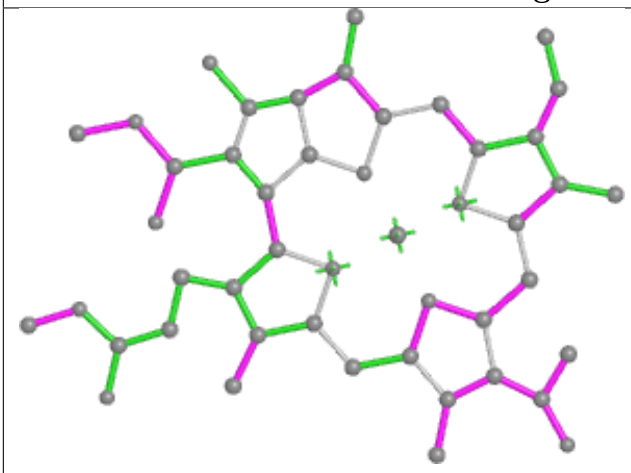


Rings

Ligand BCL V 38



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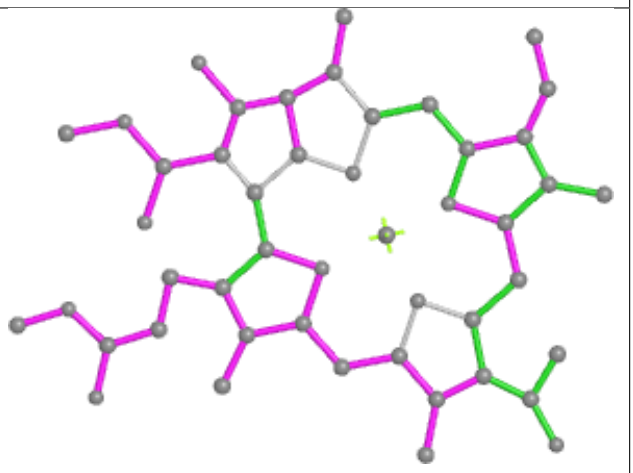
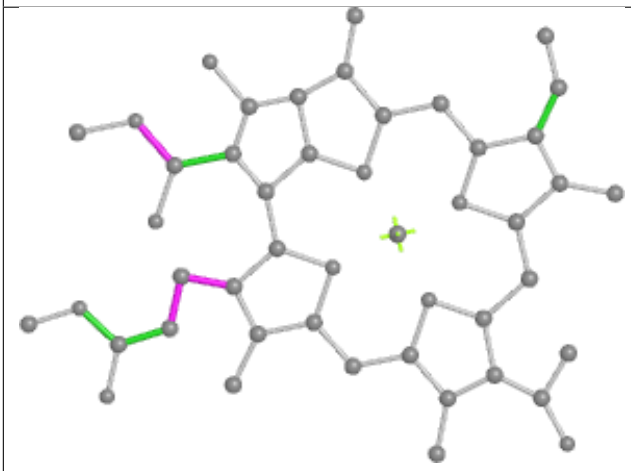


Bond angles



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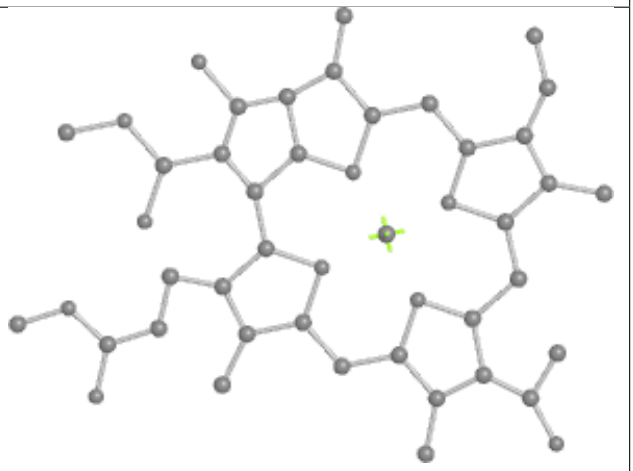
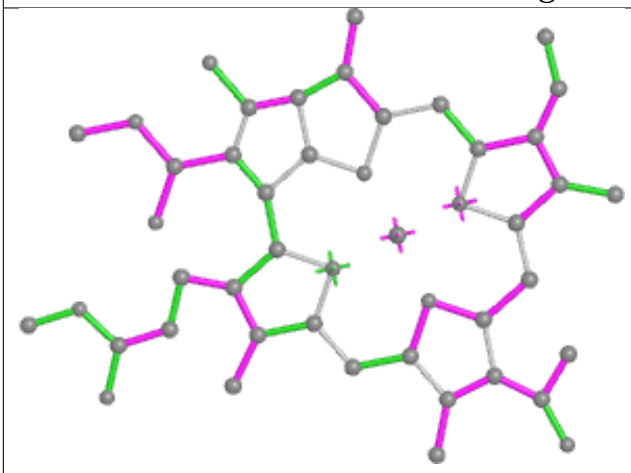
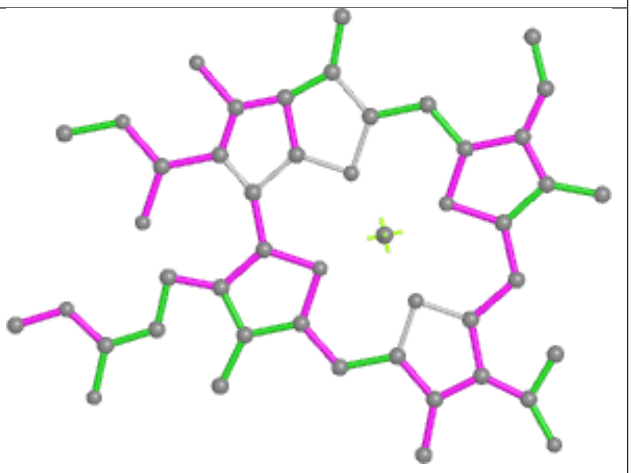


Rings

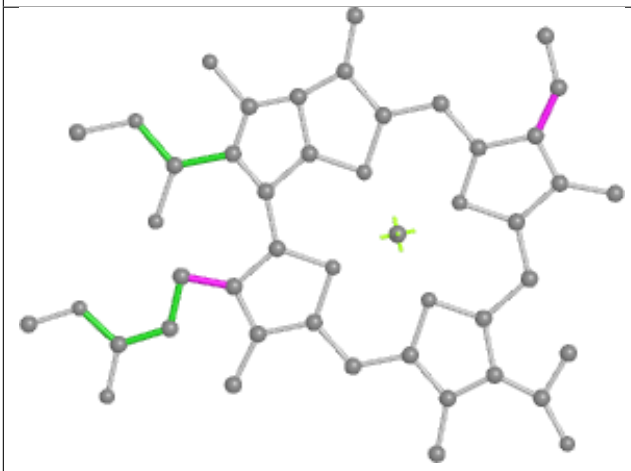
Ligand BCL 5 38



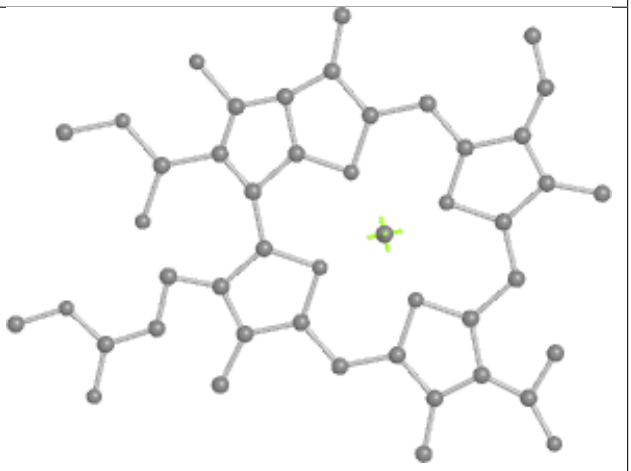
Bond lengths



Bond angles

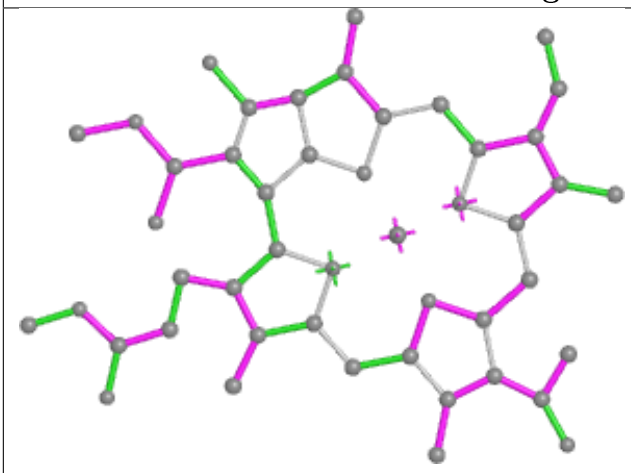


Torsions

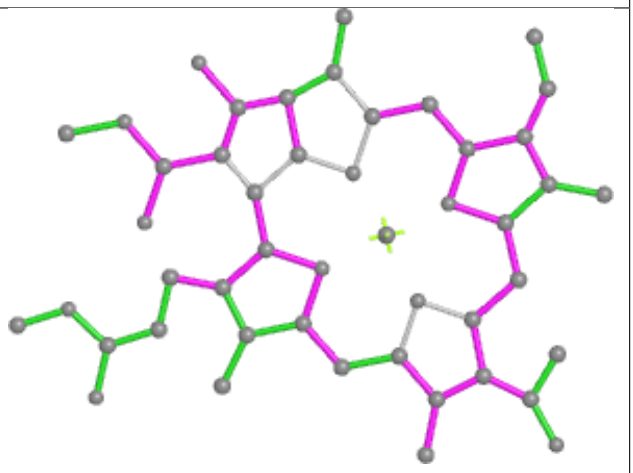


Rings

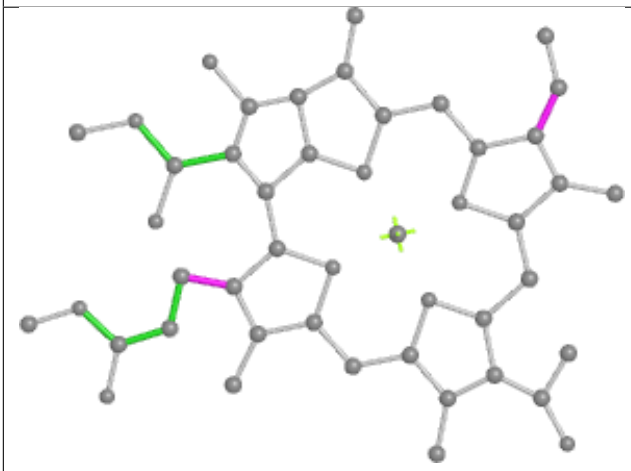
Ligand BCL D 2



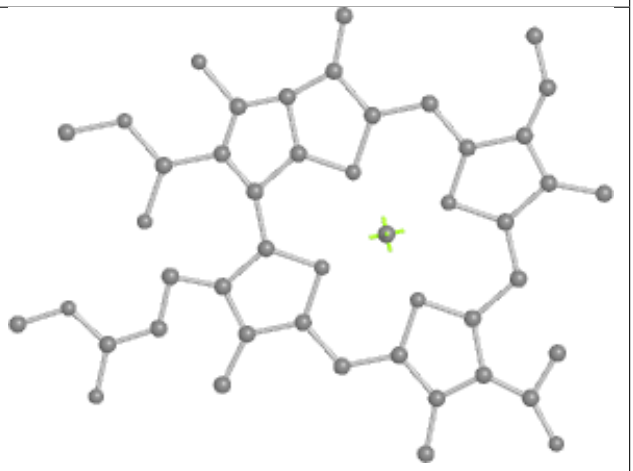
Bond lengths



Bond angles

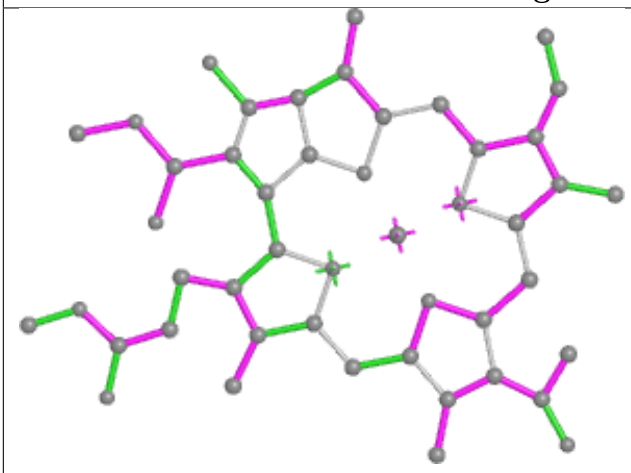


Torsions

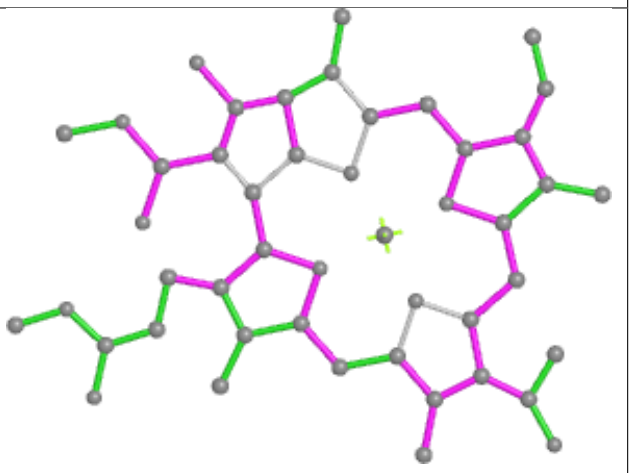


Rings

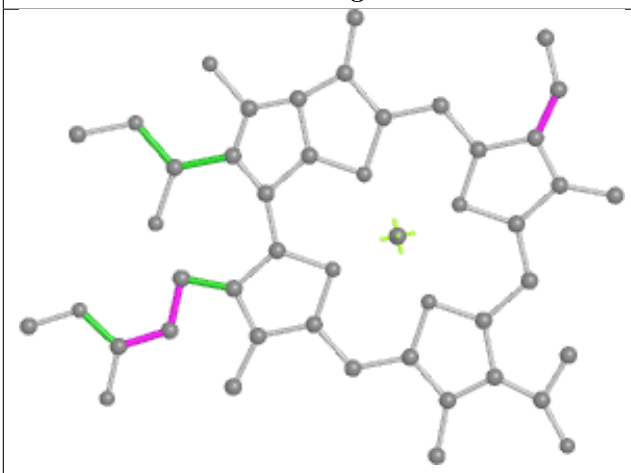
Ligand BCL Y 37



Bond lengths



Bond angles



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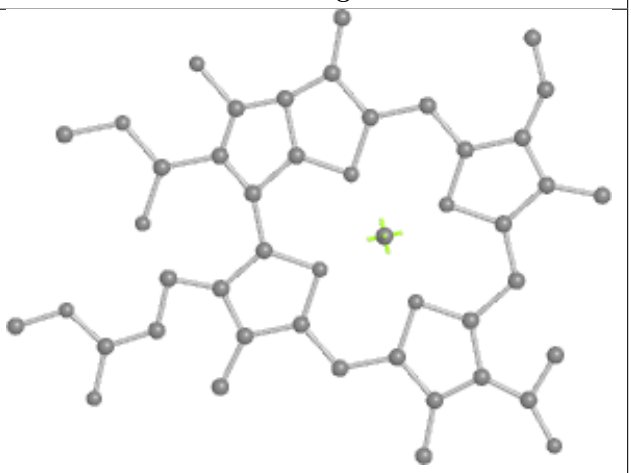
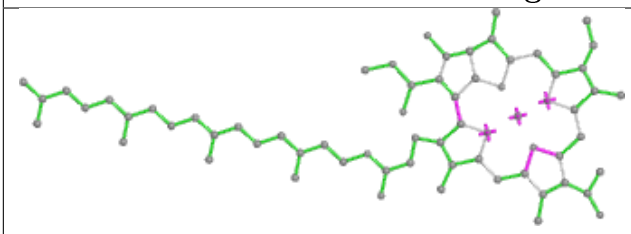
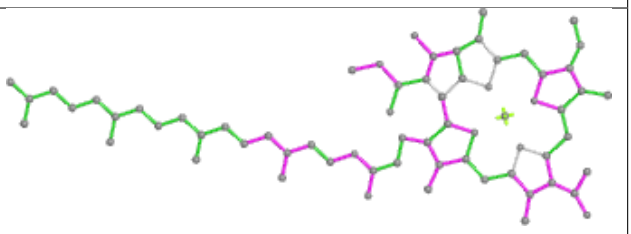


Rings

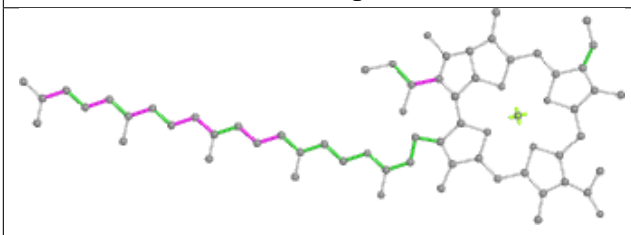
Ligand BCL A 301



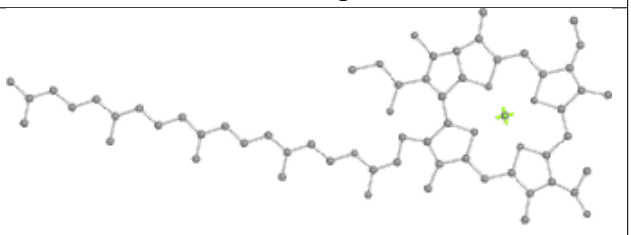
Bond lengths



Bond angles

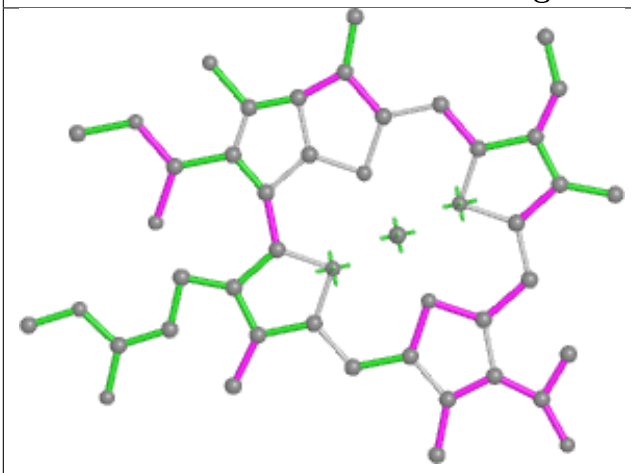


Torsions

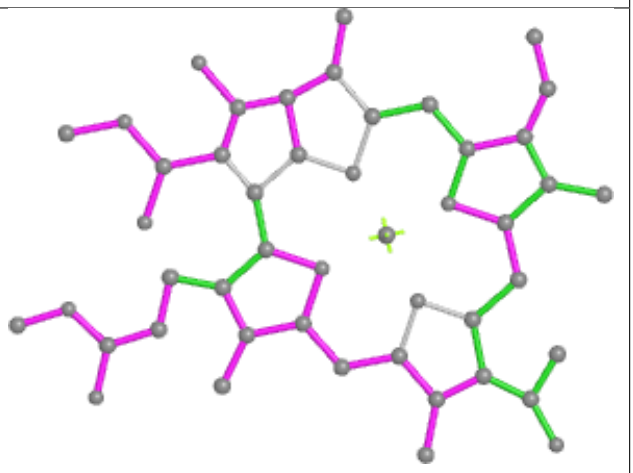


Rings

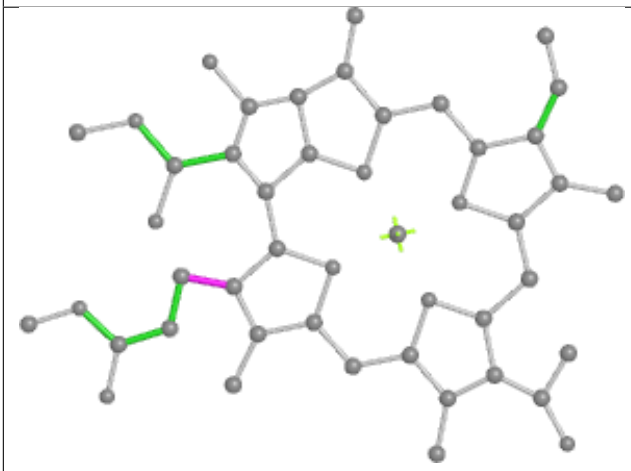
Ligand BCL N 11



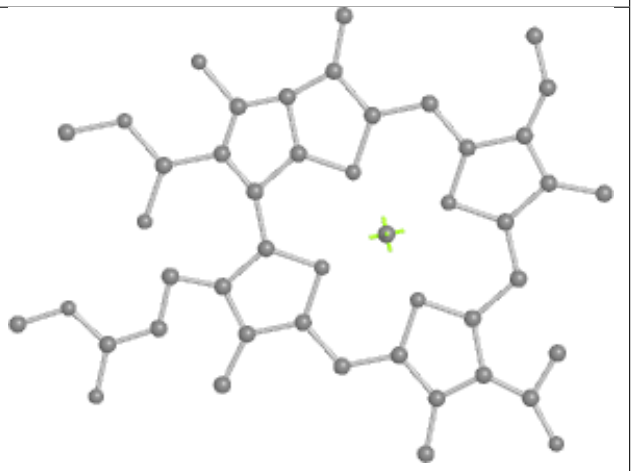
Bond lengths



Bond angles

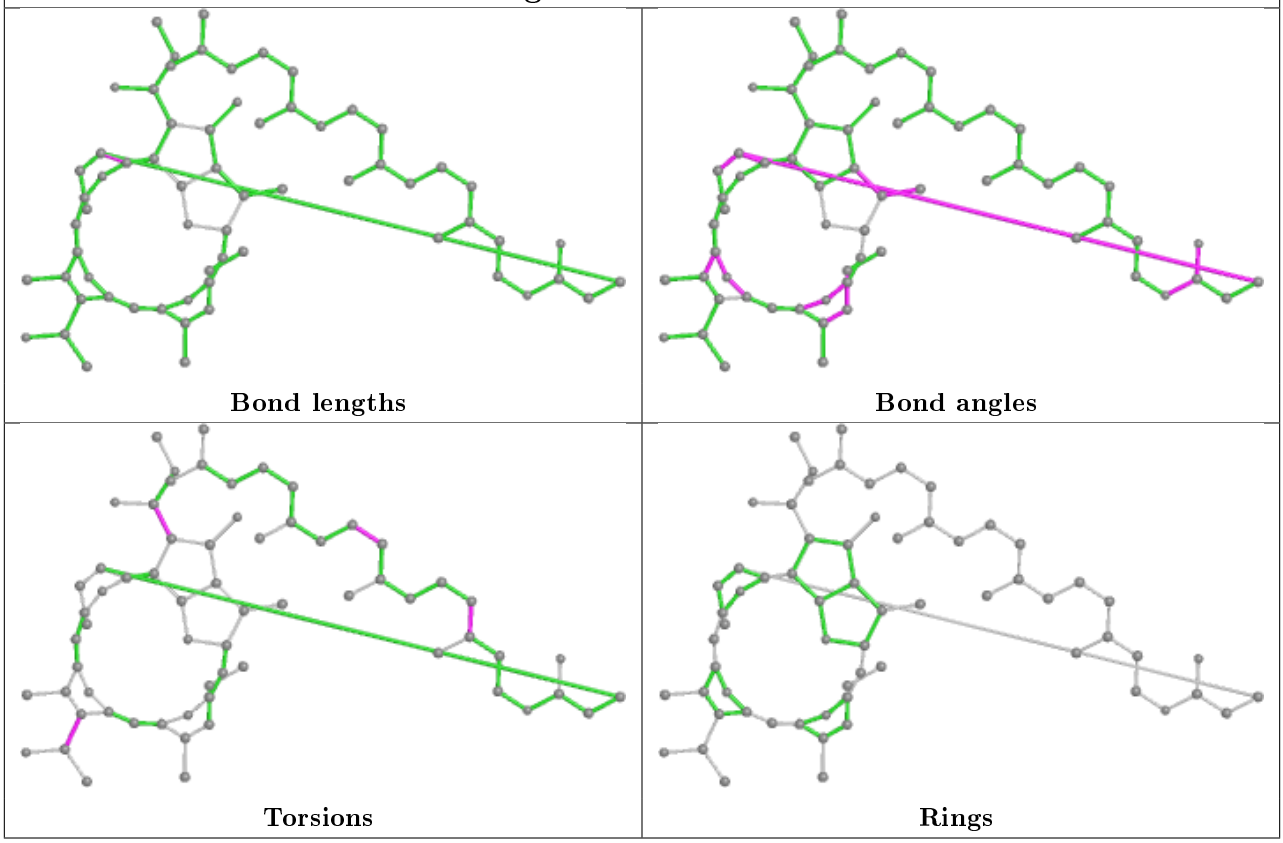


Torsions

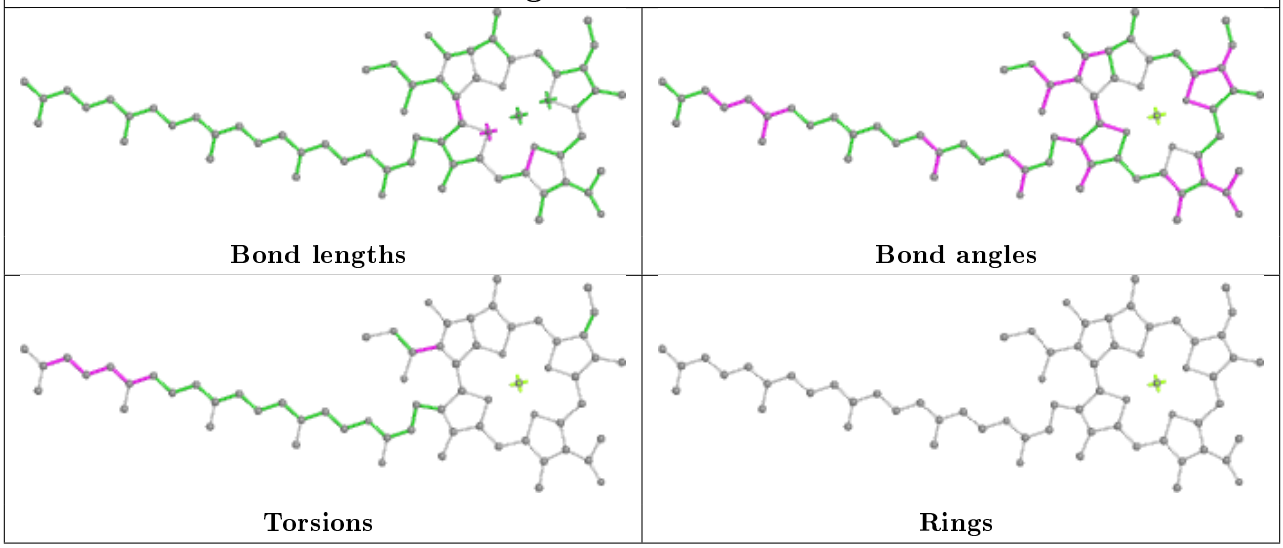


Rings

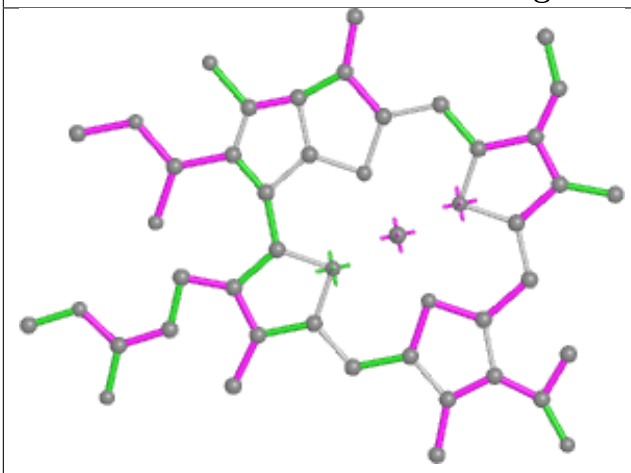
Ligand BPH B 402



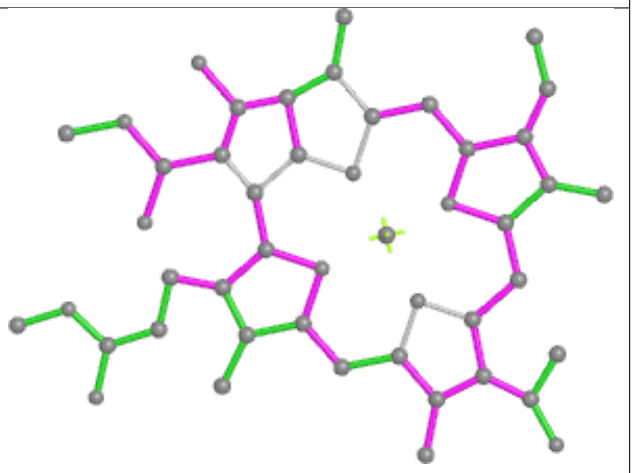
Ligand BCL A 302



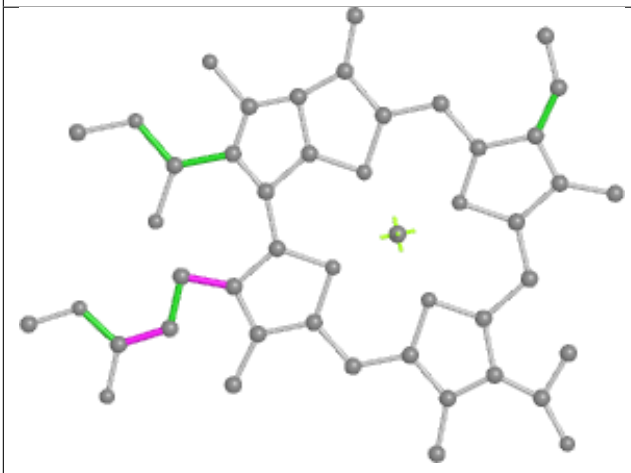
Ligand BCL N 38



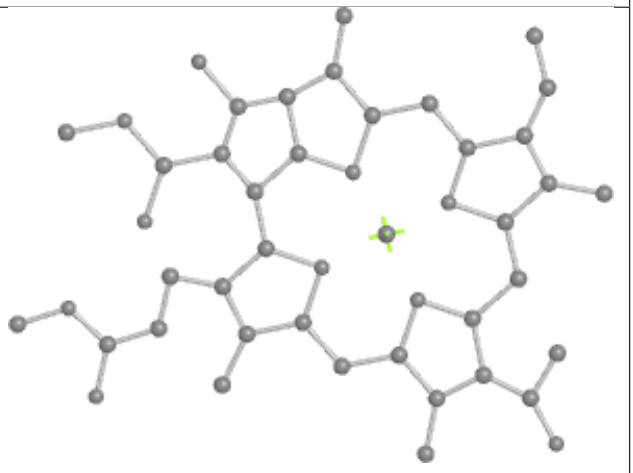
Bond lengths



Bond angles

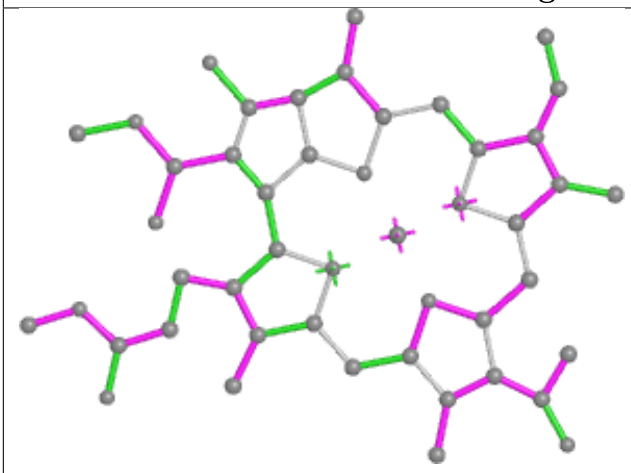


Torsions

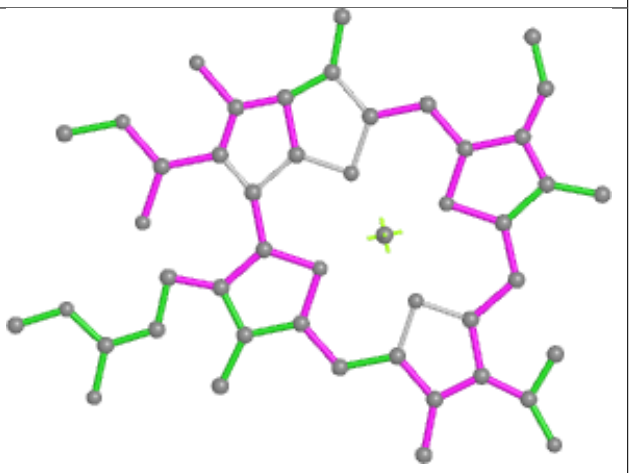


Rings

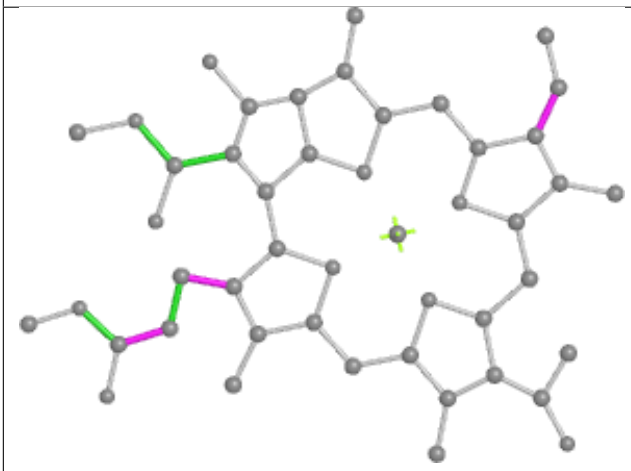
Ligand BCL 3 39



Bond lengths



Bond angles



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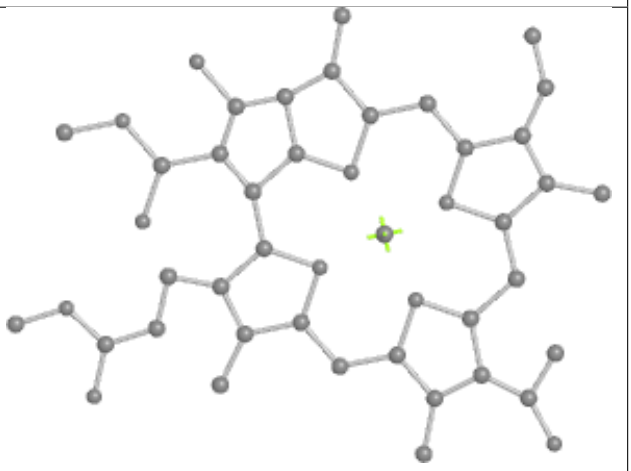
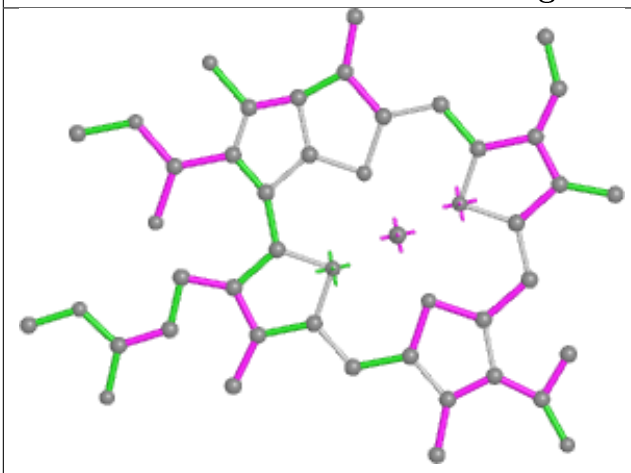
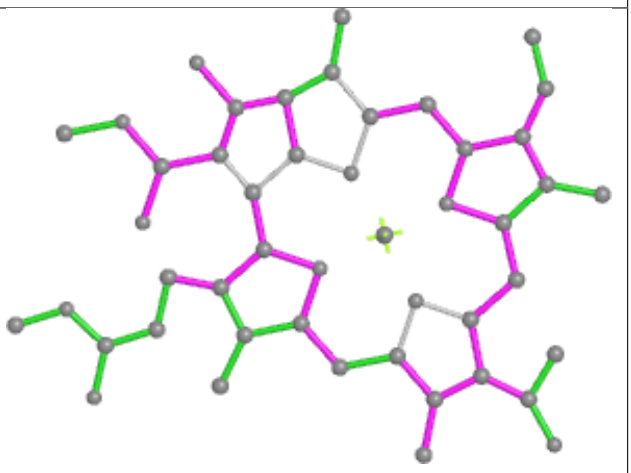


Rings

Ligand BCL 7 38



Bond lengths



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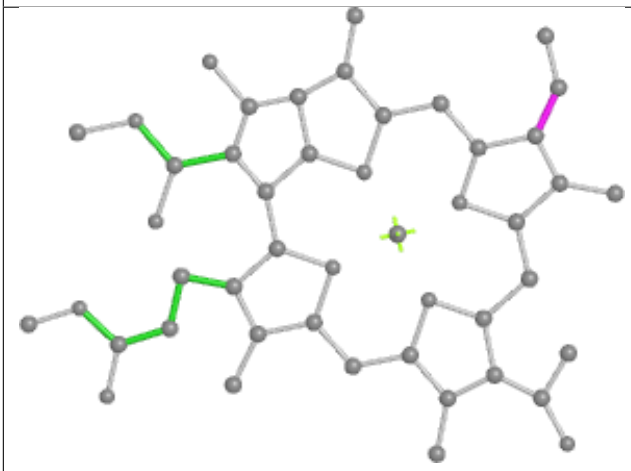

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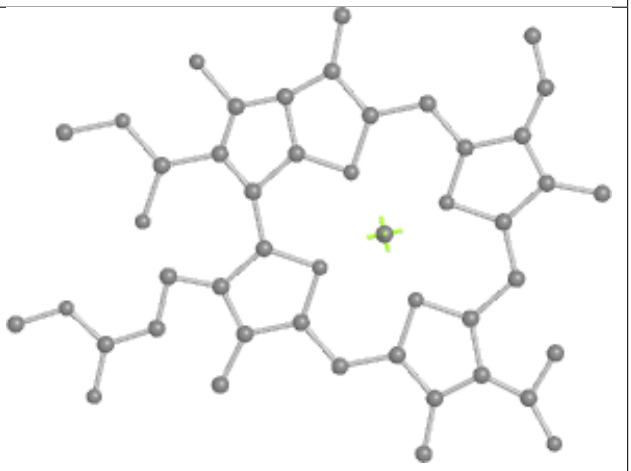
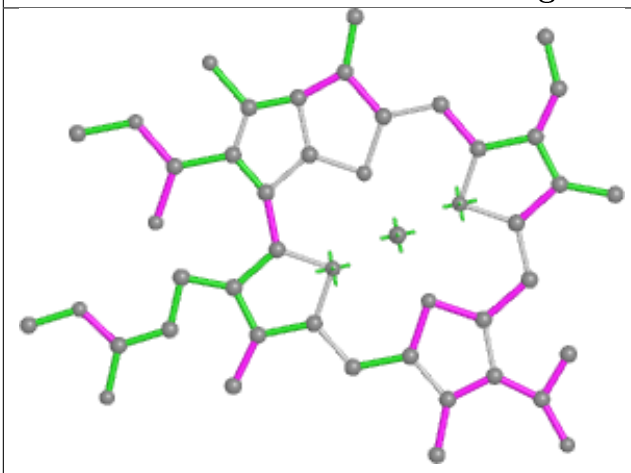


Rings

Ligand BCL 3 38



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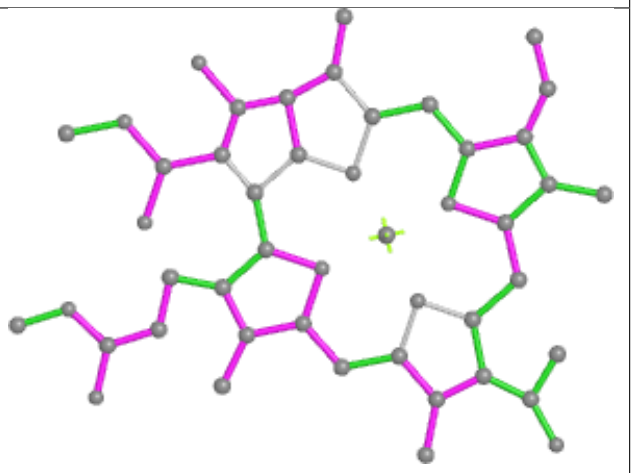

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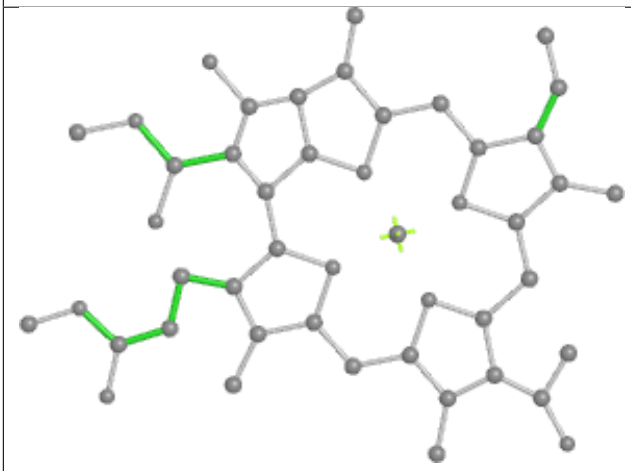

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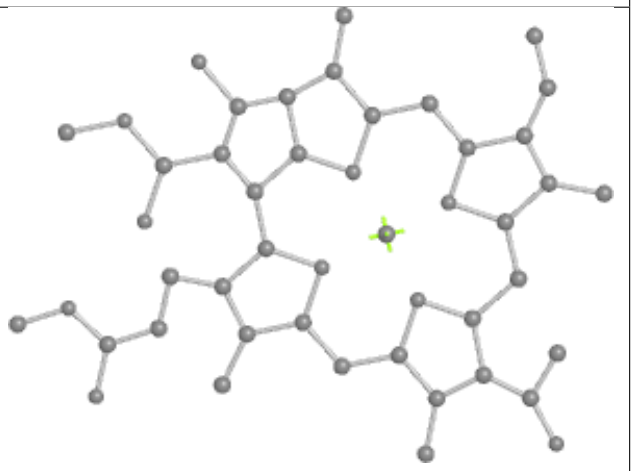
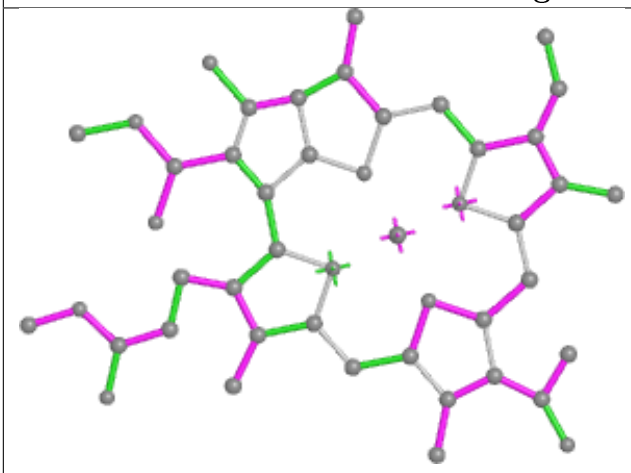


Rings

Ligand BCL R 38



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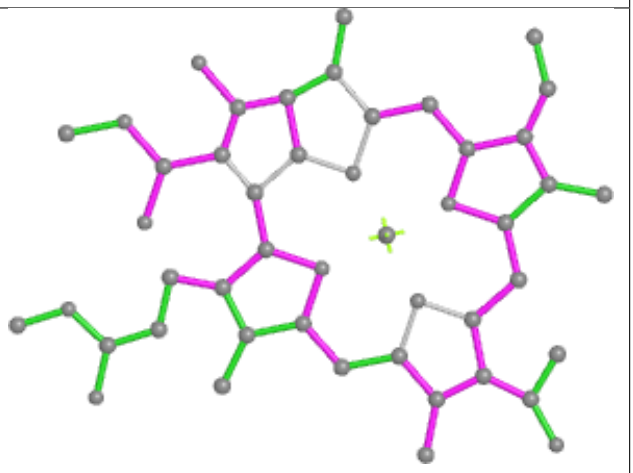
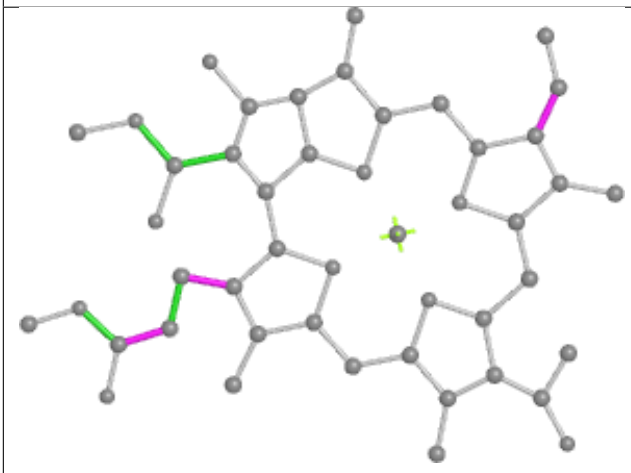


Bond angles



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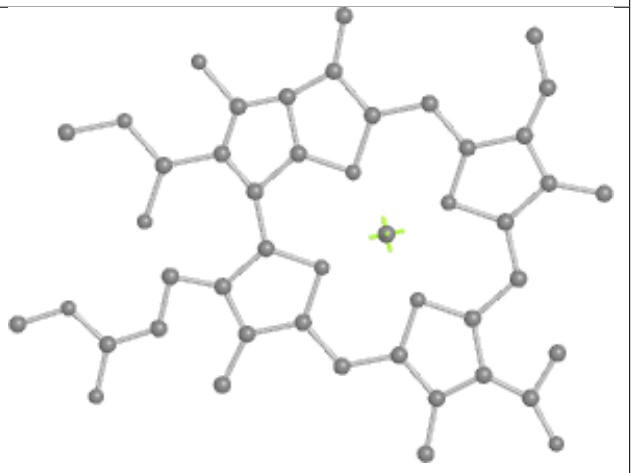
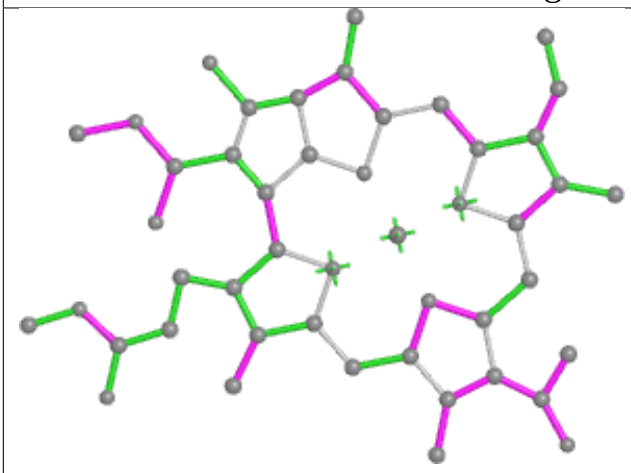


Rings

Ligand BCL E 1



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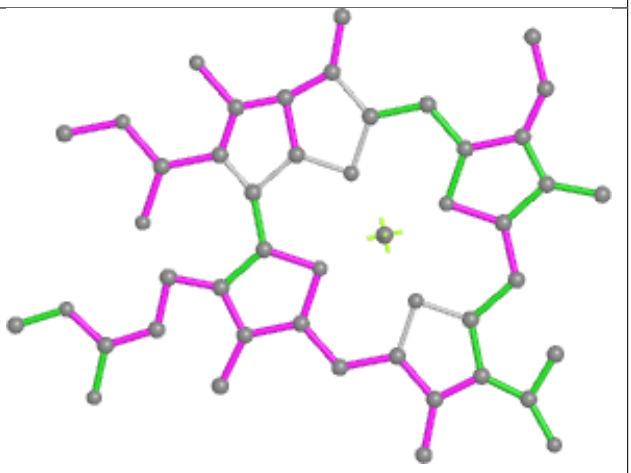

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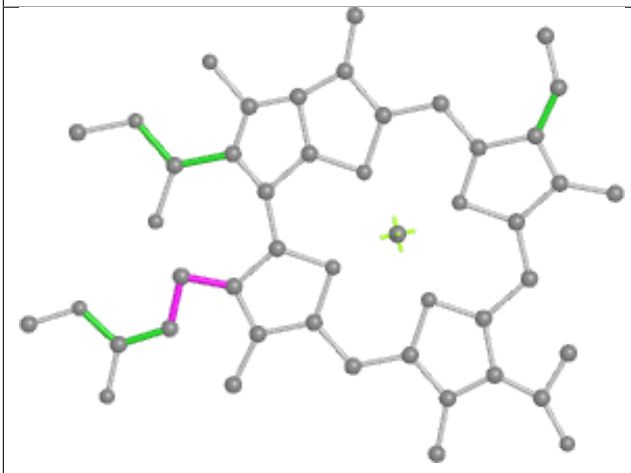

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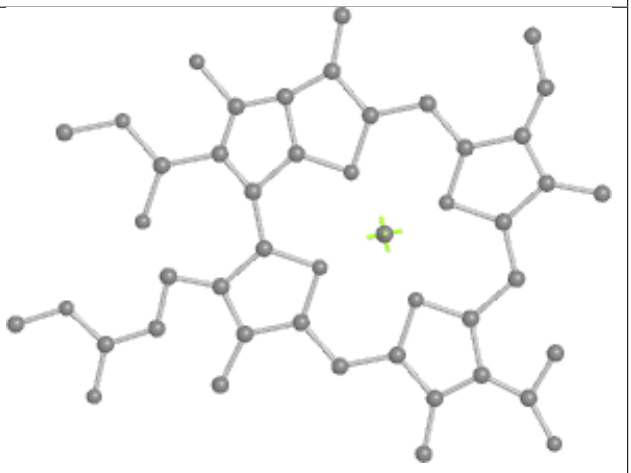
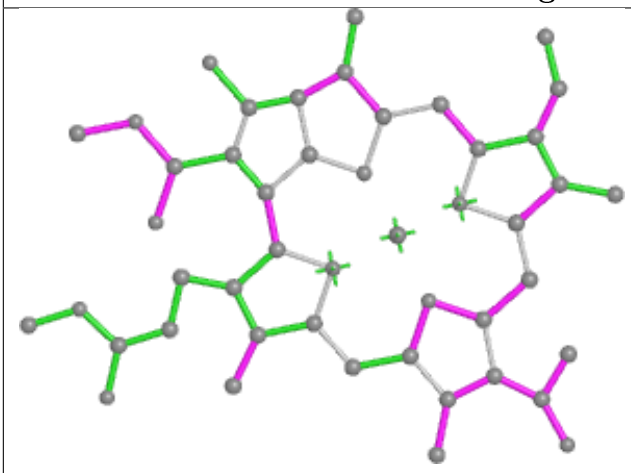


Rings

Ligand BCL 2 36



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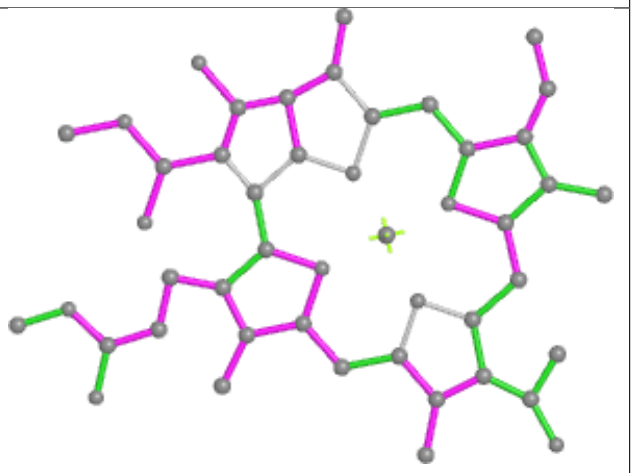
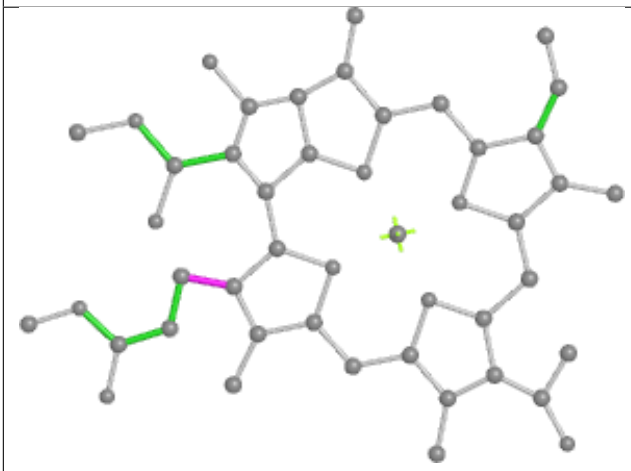
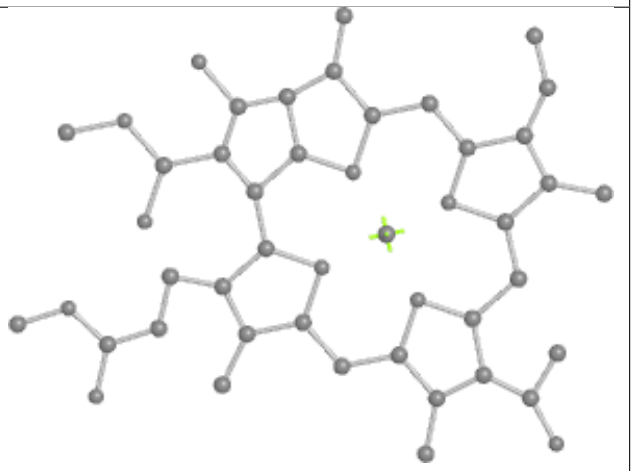


Bond angles

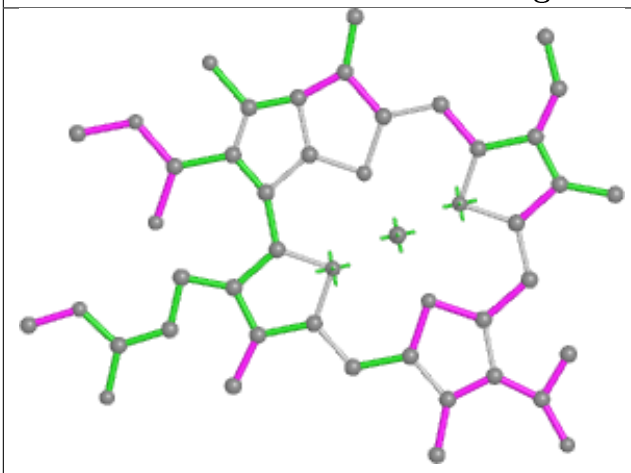


Torsions

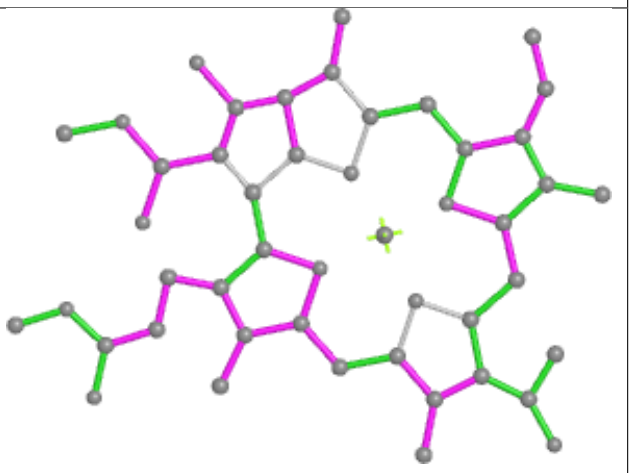


Rings

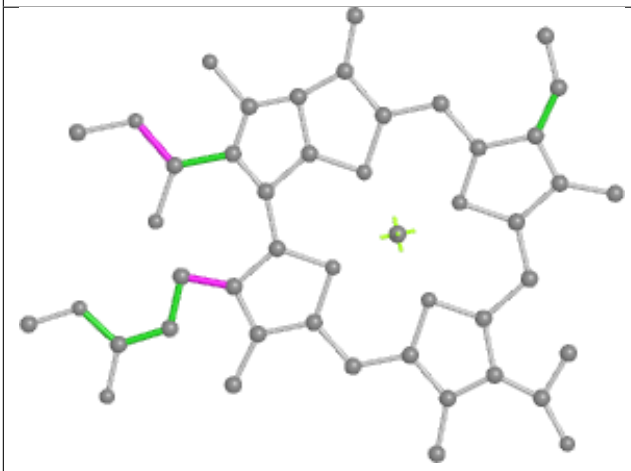
Ligand BCL Y 36



Bond lengths



Bond angles



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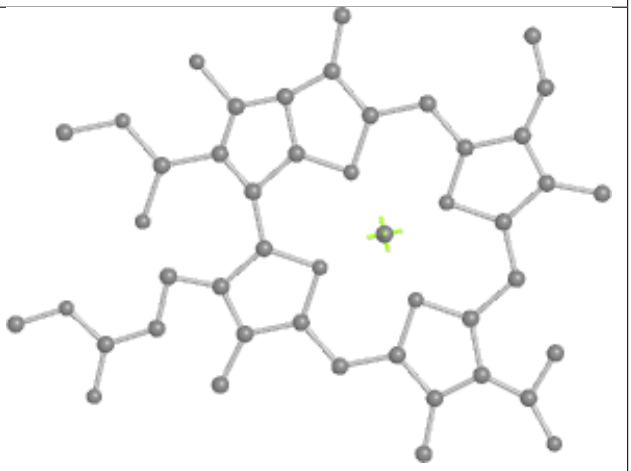
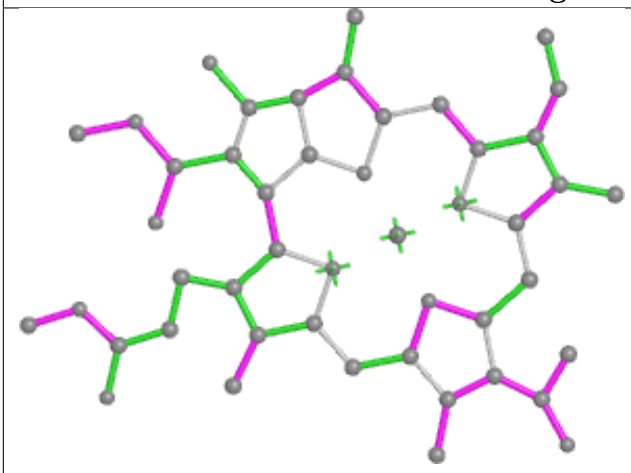


Rings

Ligand BCL I 5



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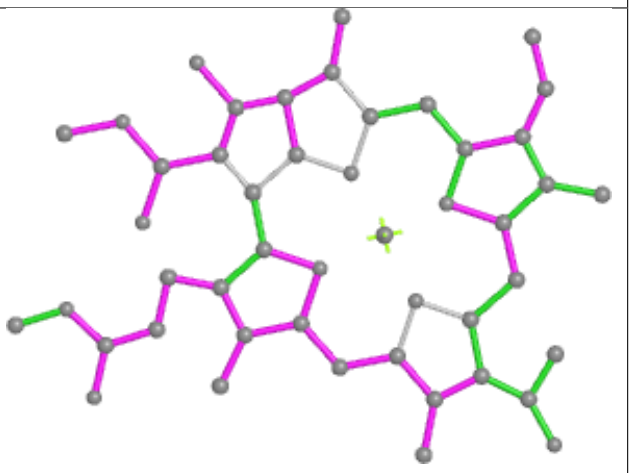
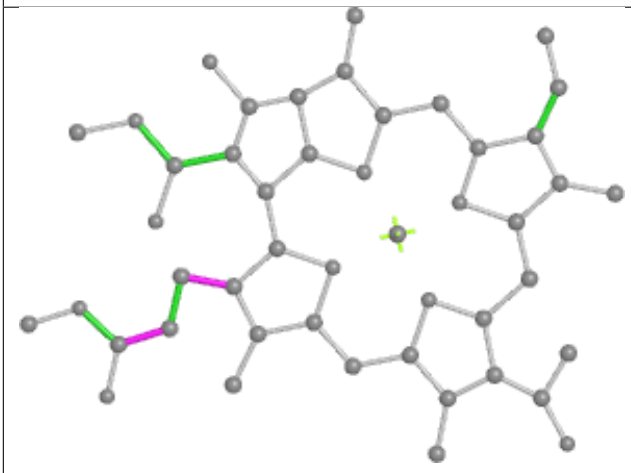


Bond angles



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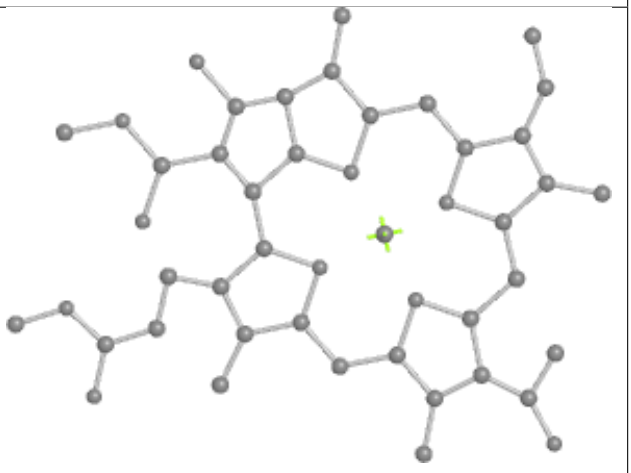
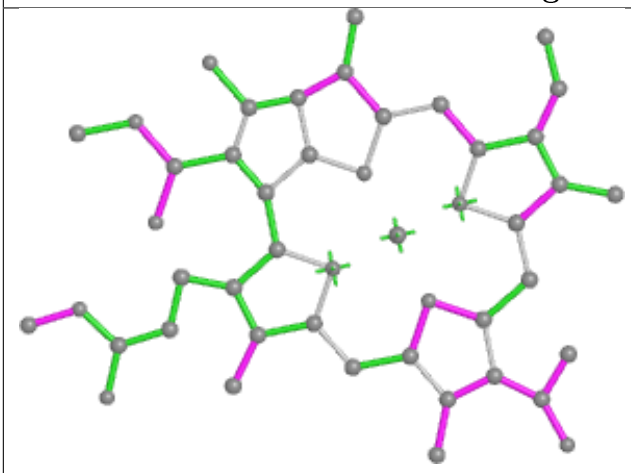
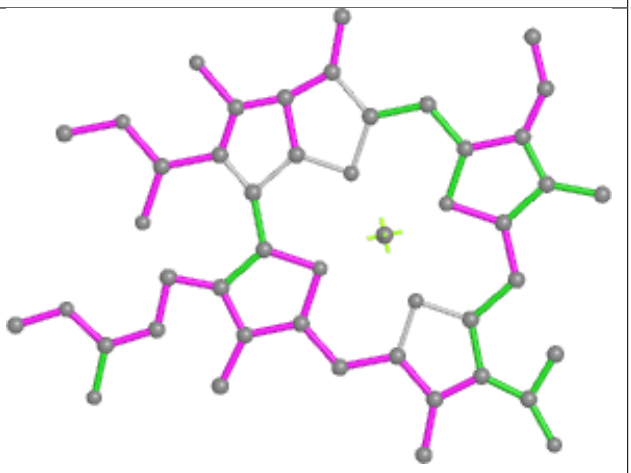


Rings

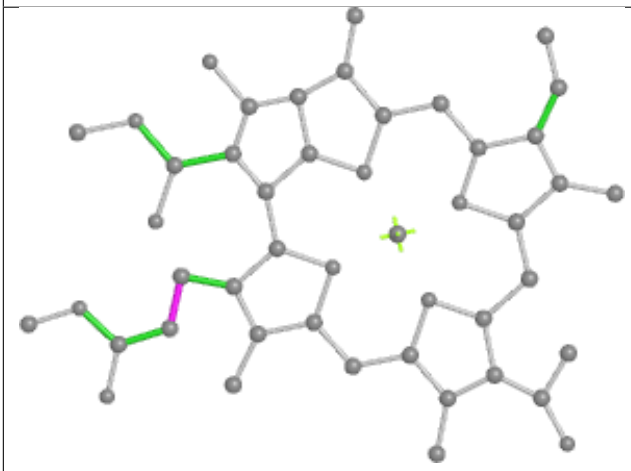
Ligand BCL G 3



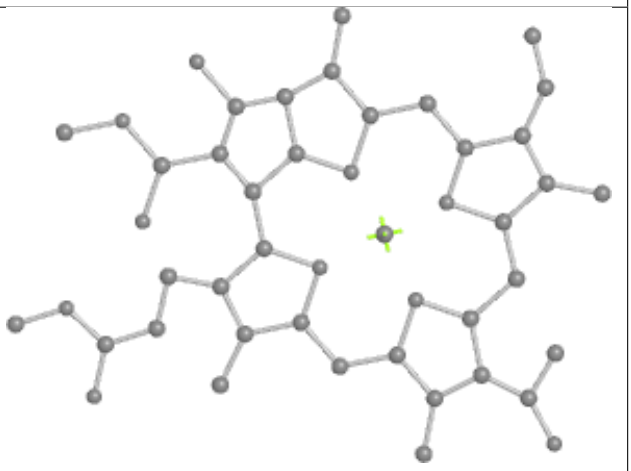
Bond lengths



Bond angles

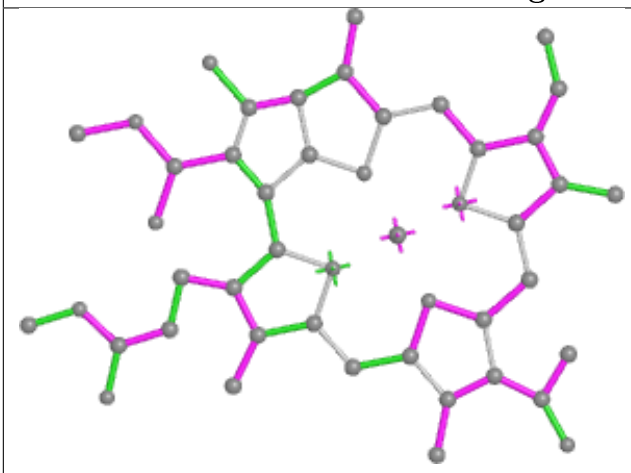


Torsions

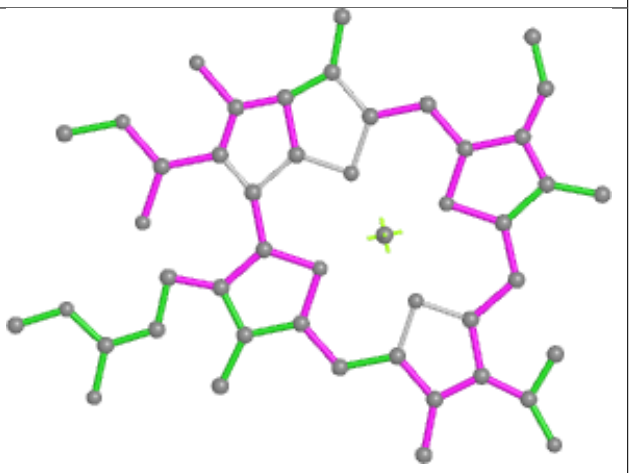


Rings

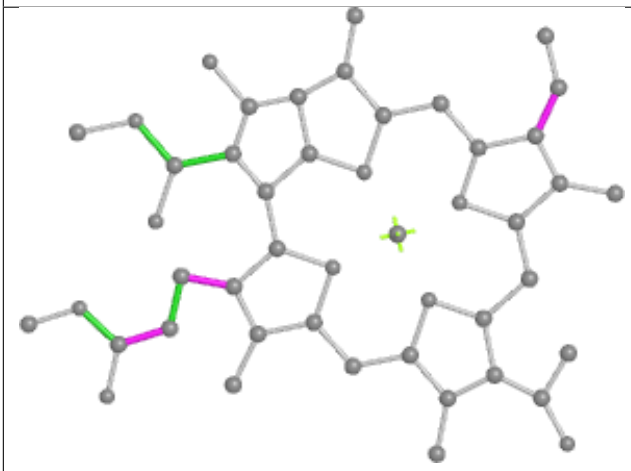
Ligand BCL W 36



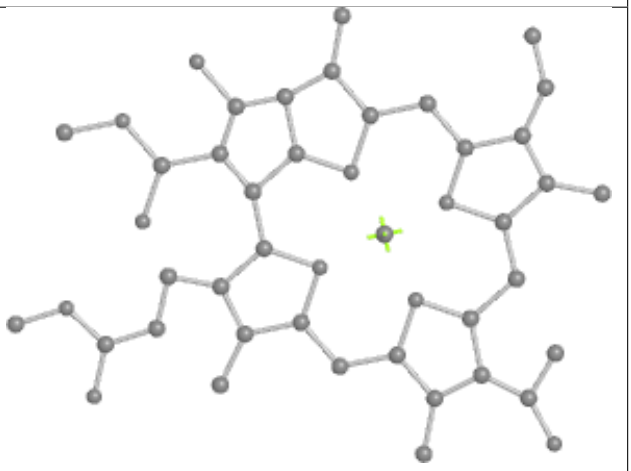
Bond lengths



Bond angles

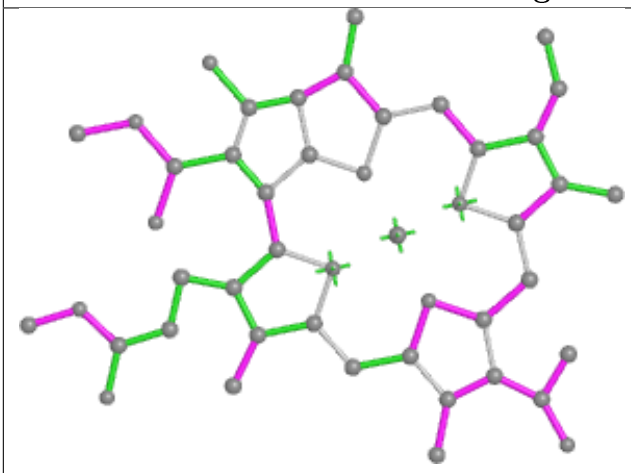


Torsions



Rings

Ligand BCL K 36



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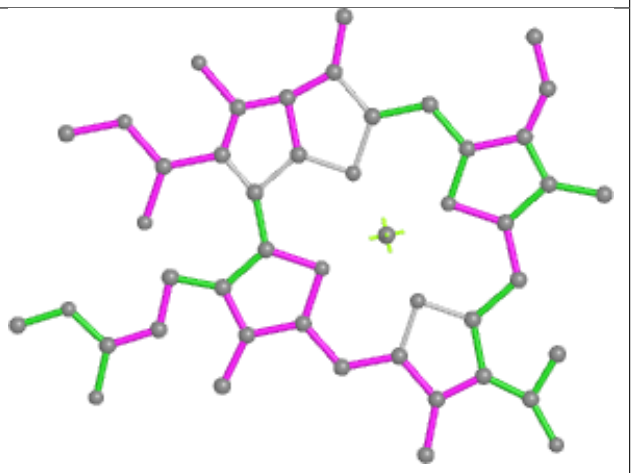
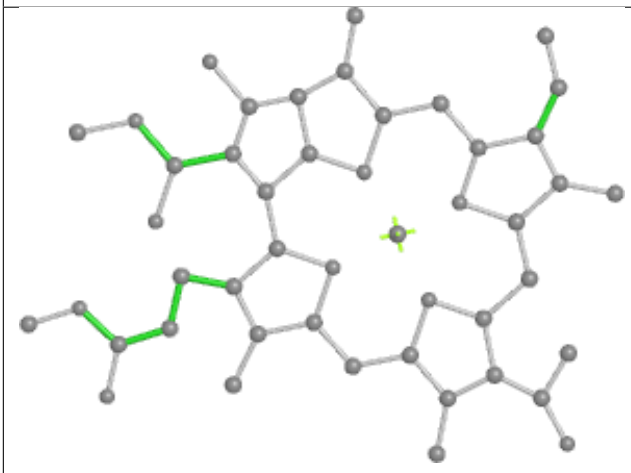


Bond angles



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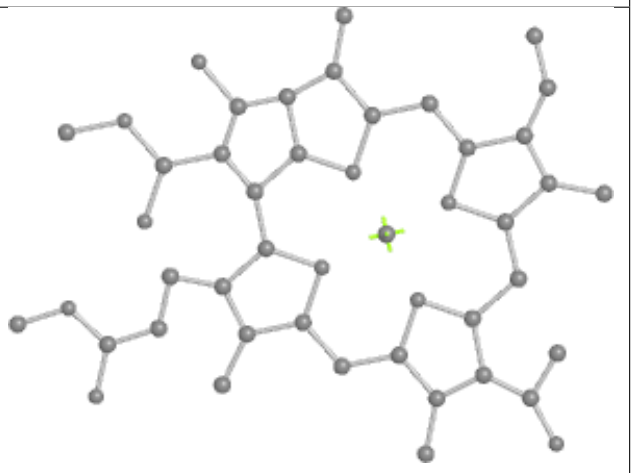
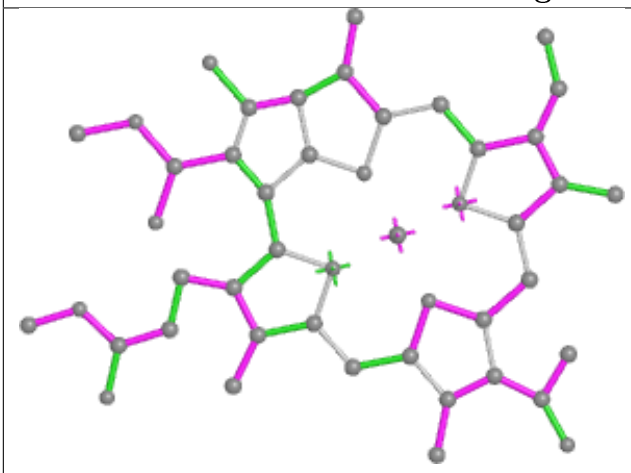
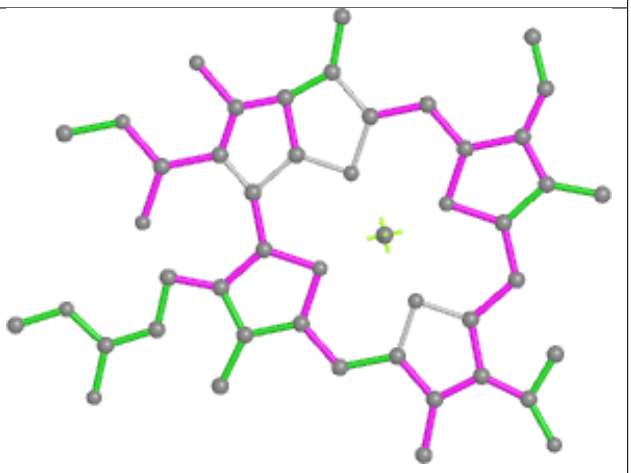


Rings

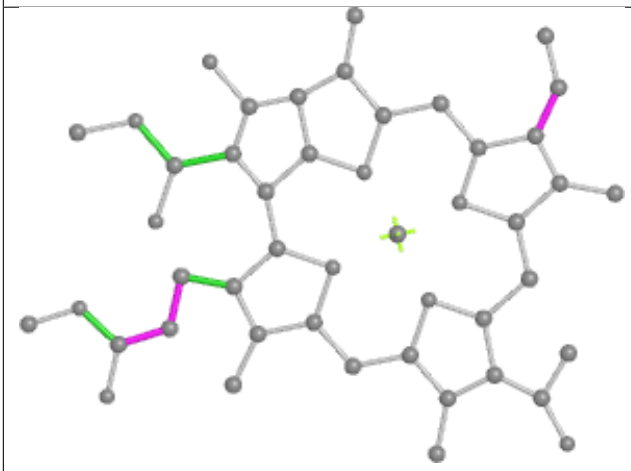
Ligand BCL T 38



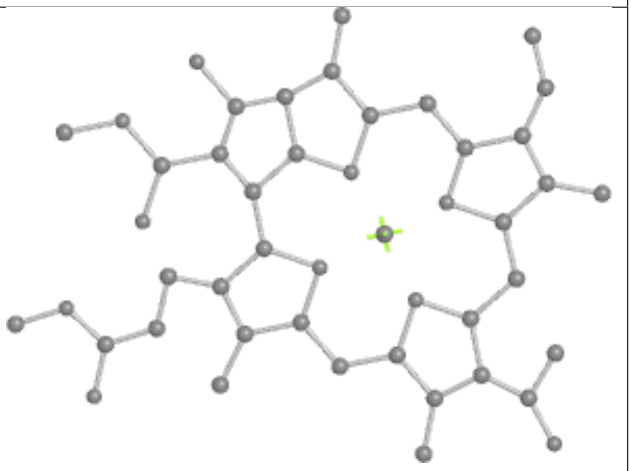
Bond lengths



Bond angles

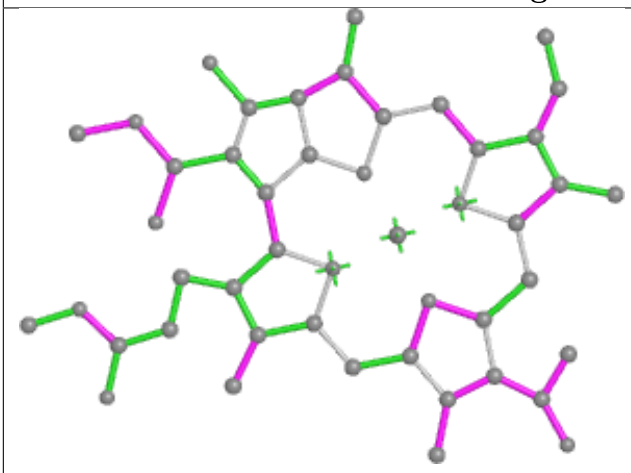


Torsions

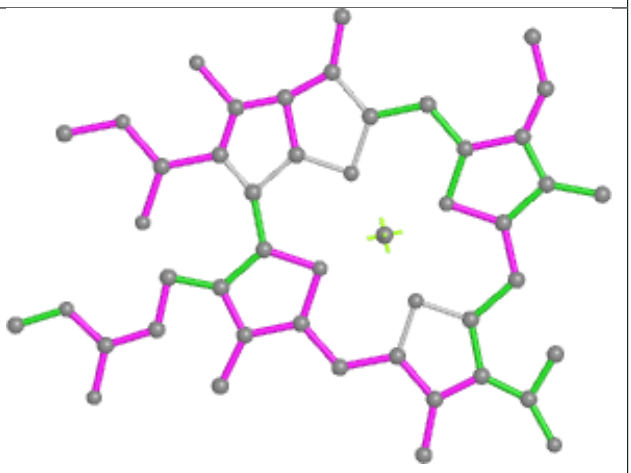


Rings

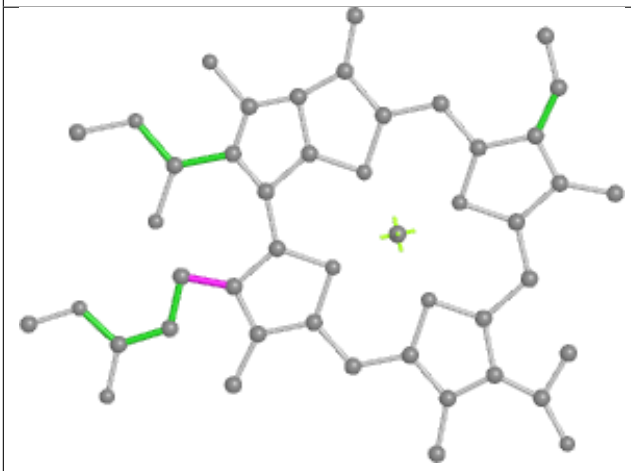
Ligand BCL M 36



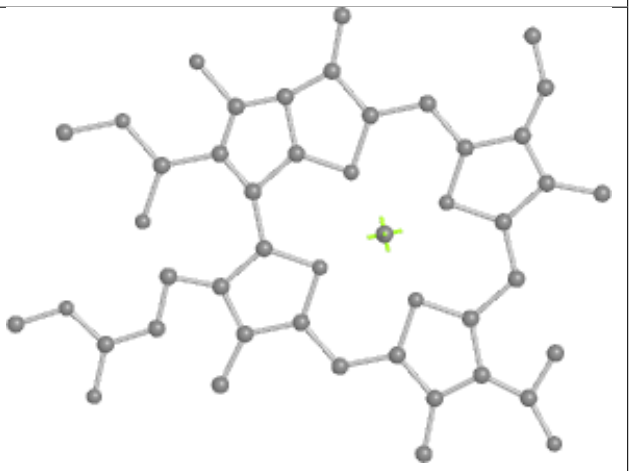
Bond lengths



Bond angles

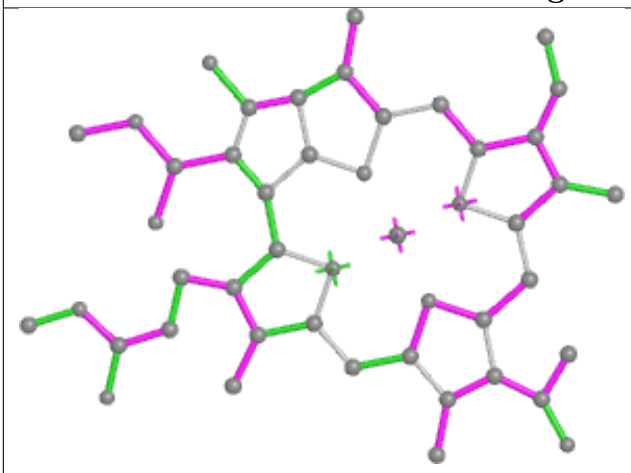


Torsions

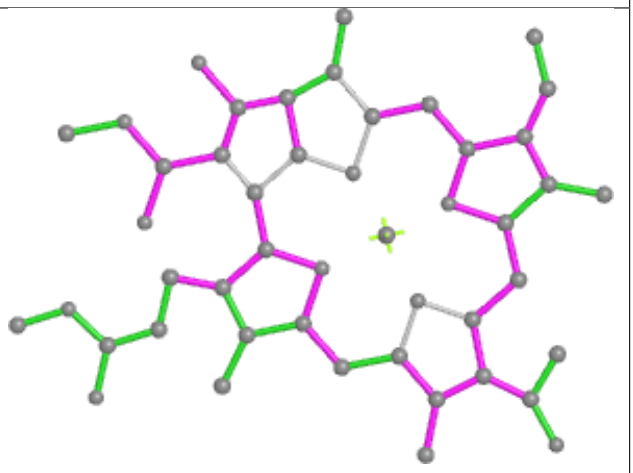


Rings

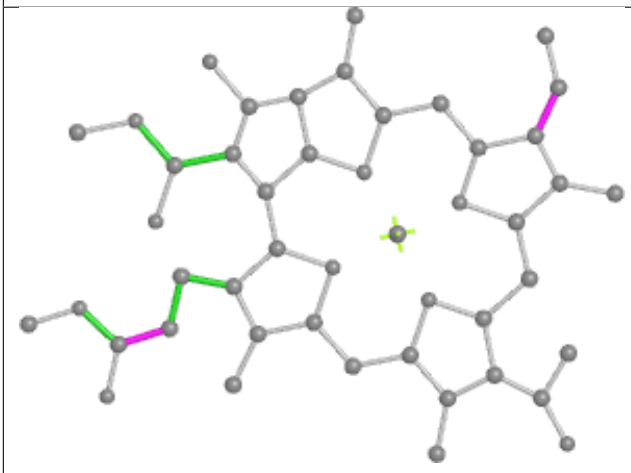
Ligand BCL J 8



Bond lengths



Bond angles



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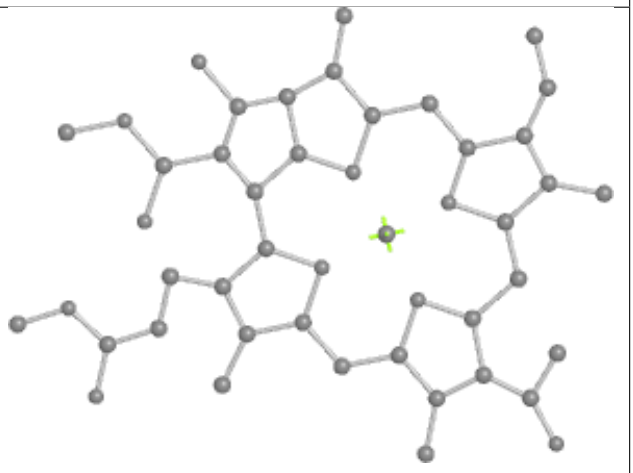
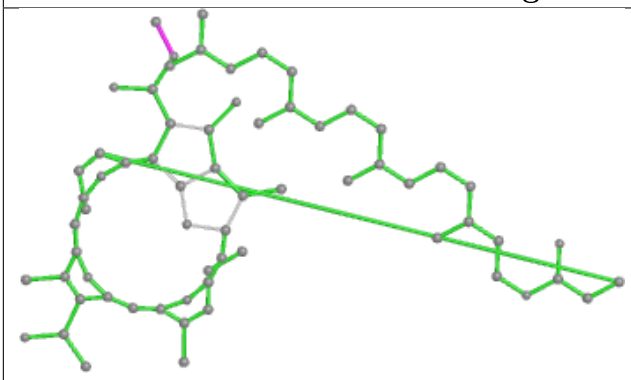
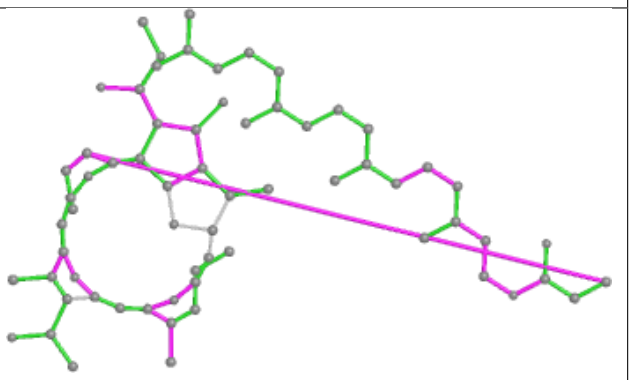


Rings

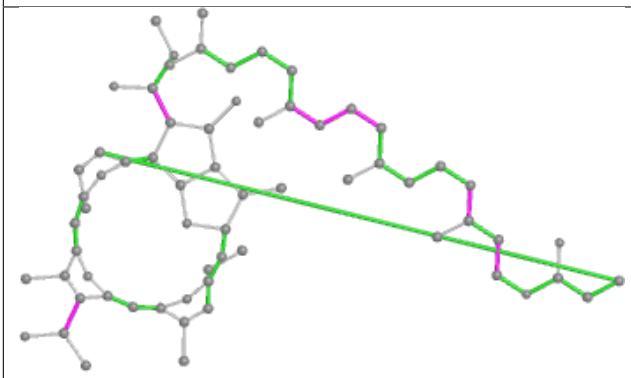
Ligand BPH A 401



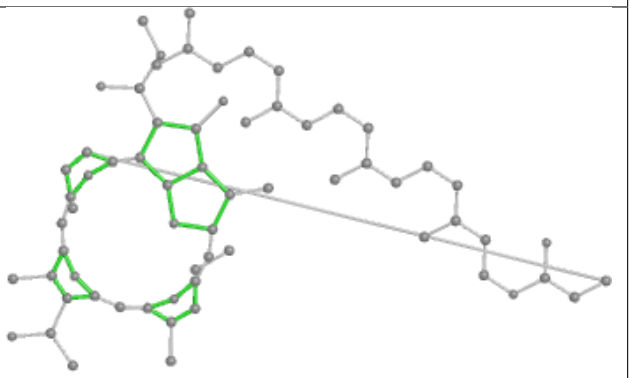
Bond lengths



Bond angles

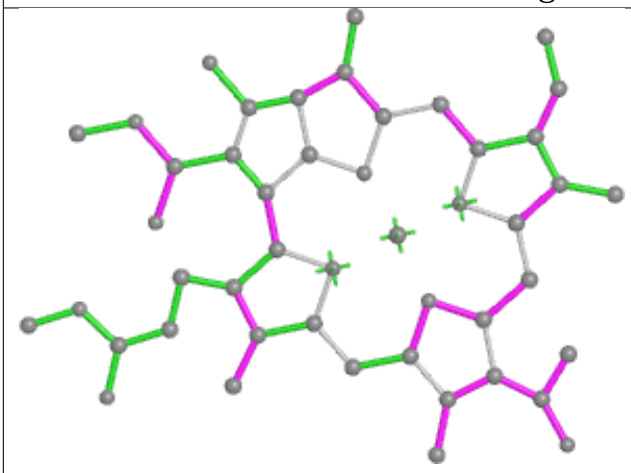


Torsions

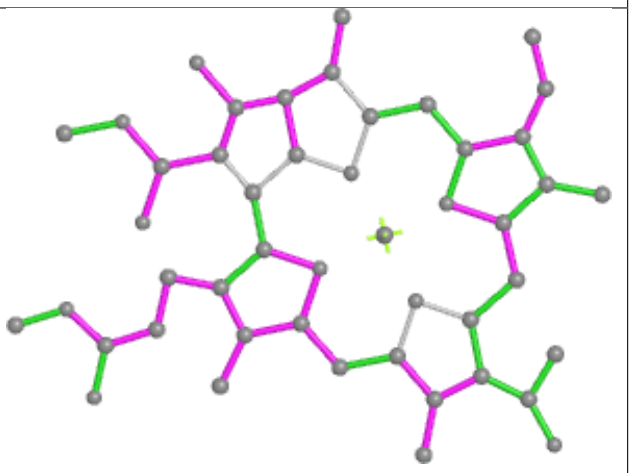


Rings

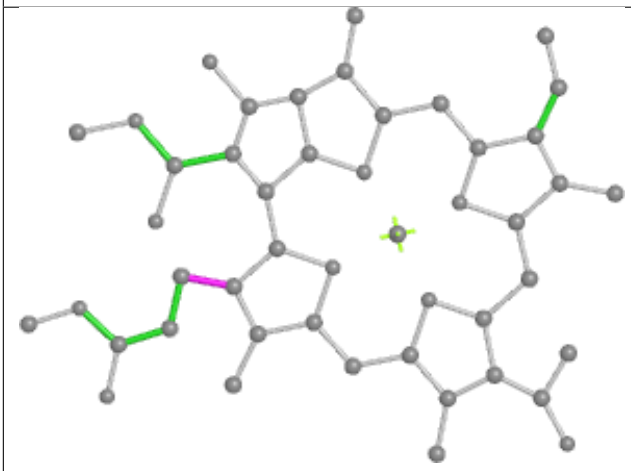
Ligand BCL 6 36



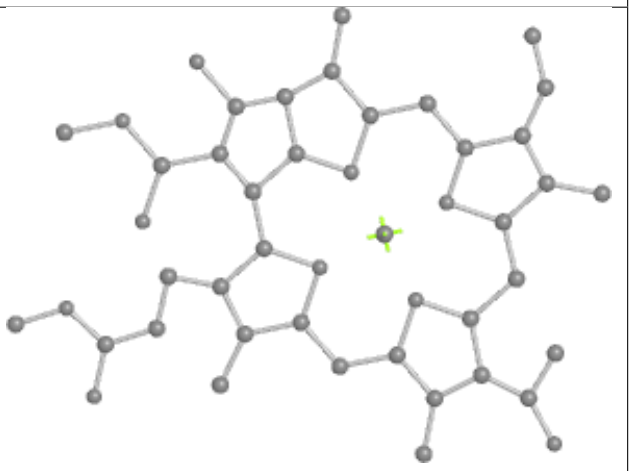
Bond lengths



Bond angles

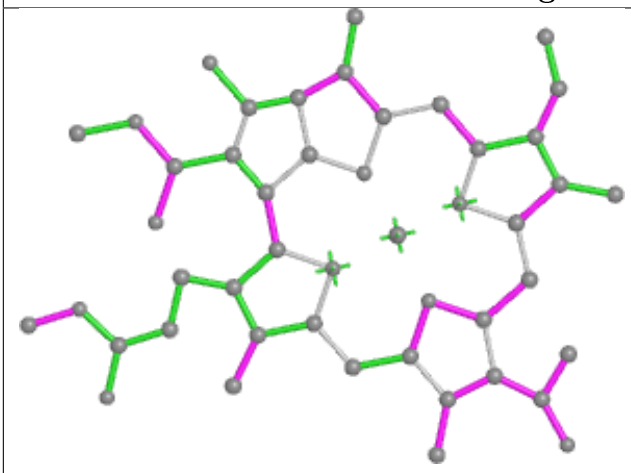


Torsions

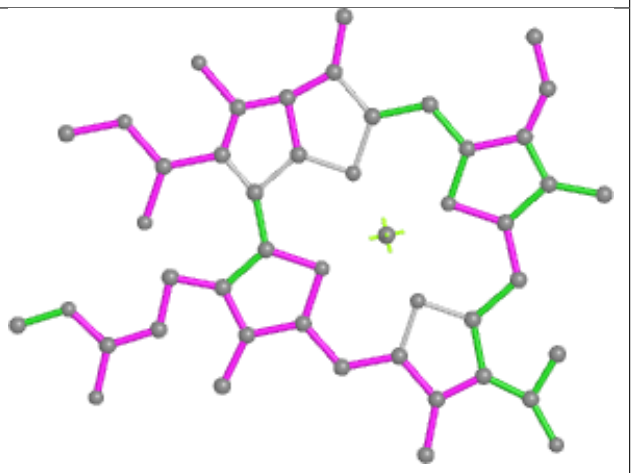


Rings

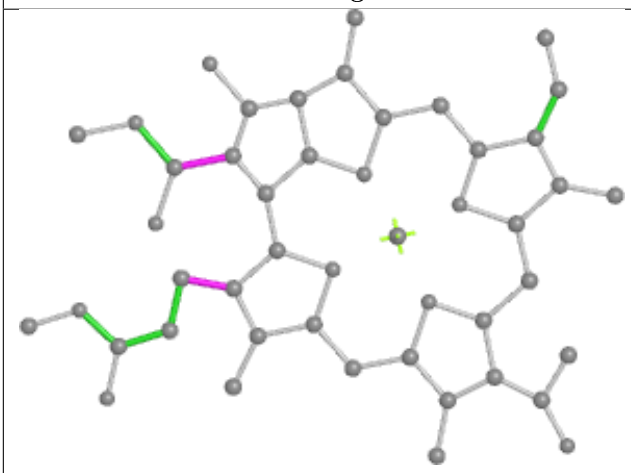
Ligand BCL 8 36



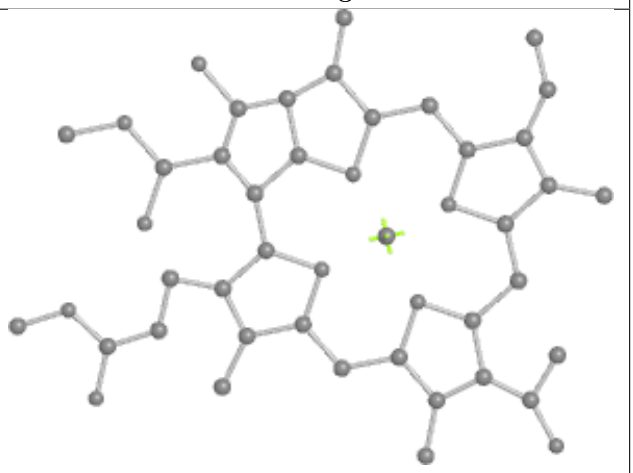
Bond lengths



Bond angles

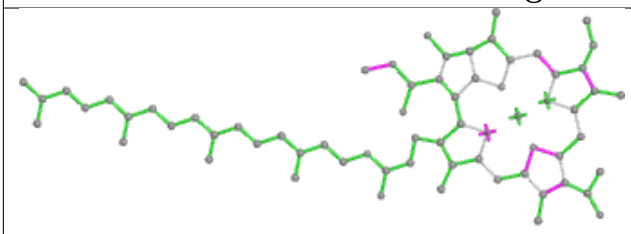


Torsions

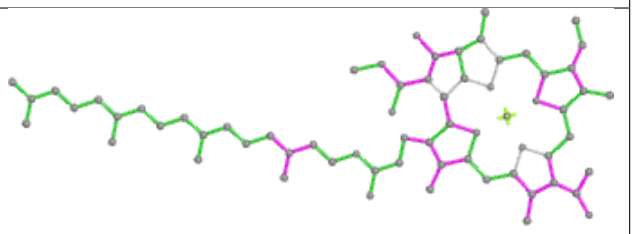


Rings

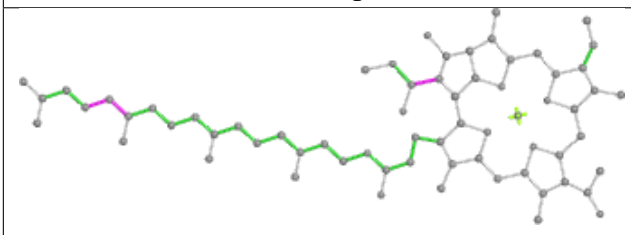
Ligand BCL B 304



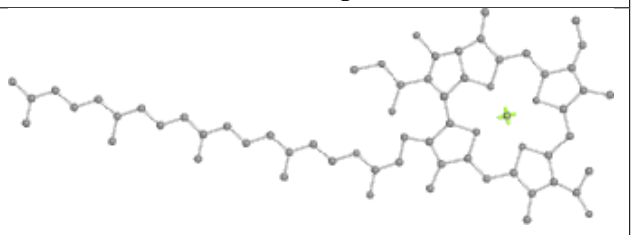
Bond lengths



Bond angles

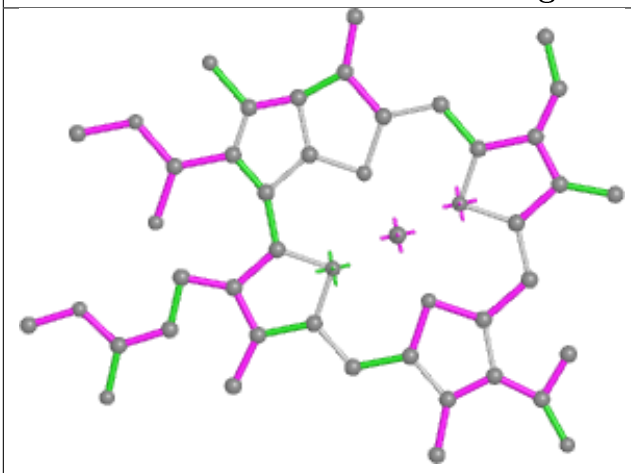


Torsions

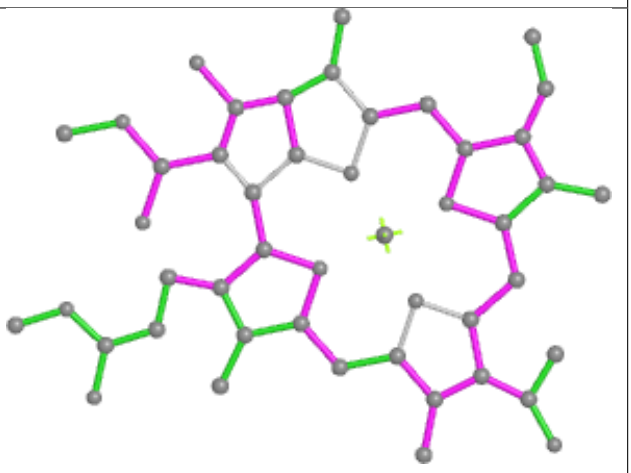


Rings

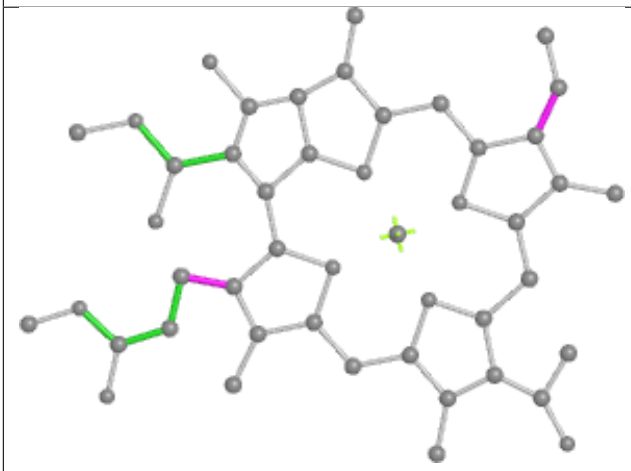
Ligand BCL 1 38



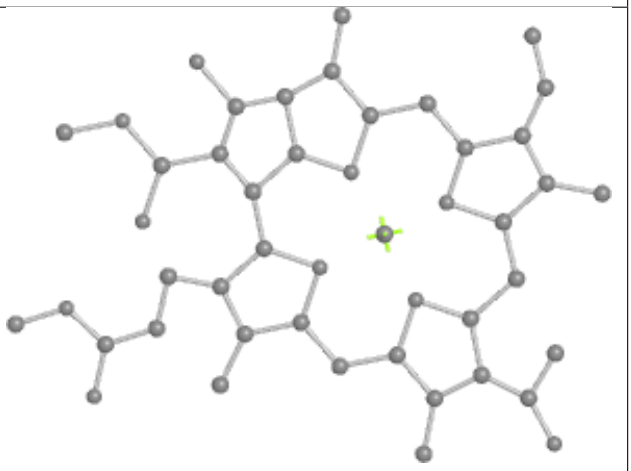
Bond lengths



Bond angles

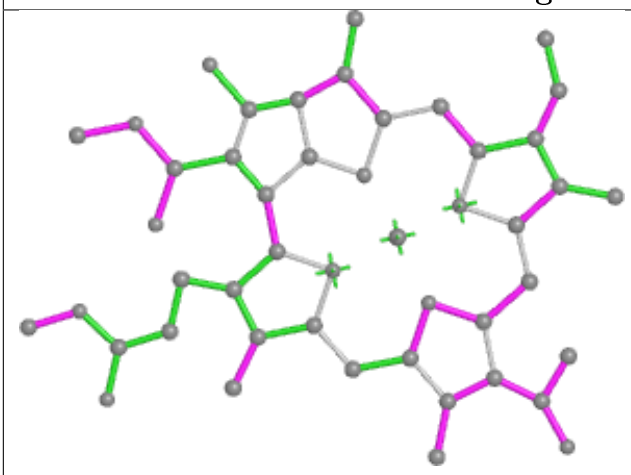


Torsions

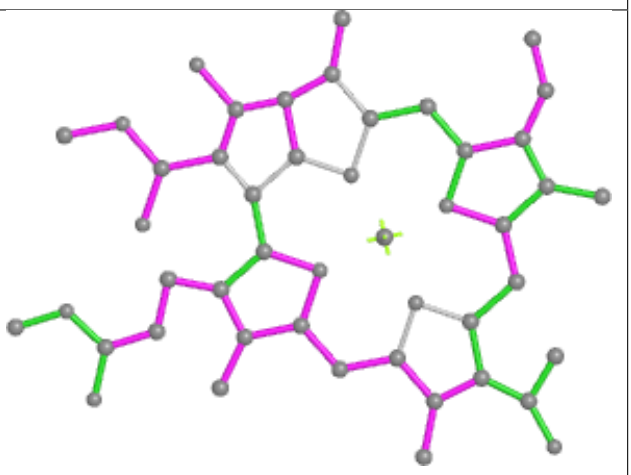


Rings

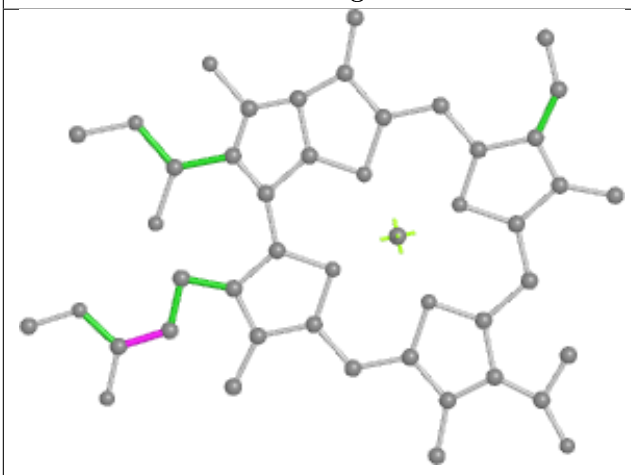
Ligand BCL P 38



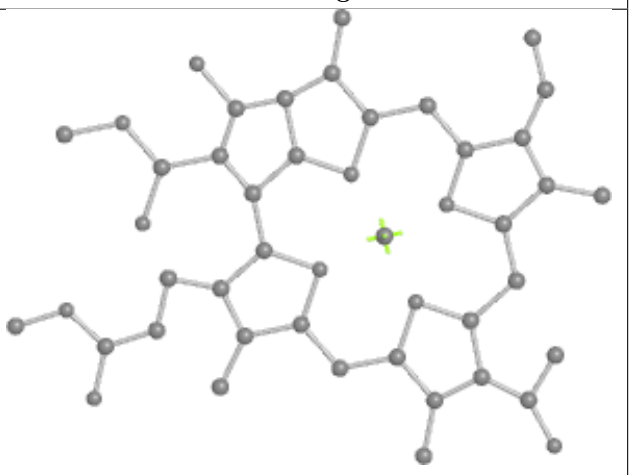
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	0/281	-	-	-	-
2	B	0/302	-	-	-	-
3	C	0/241	-	-	-	-
4	1	0/26	-	-	-	-
4	3	0/26	-	-	-	-
4	5	0/26	-	-	-	-
4	7	0/26	-	-	-	-
4	D	0/26	-	-	-	-
4	F	0/26	-	-	-	-
4	H	0/26	-	-	-	-
4	J	0/26	-	-	-	-
4	L	0/26	-	-	-	-
4	N	0/26	-	-	-	-
4	P	0/26	-	-	-	-
4	R	0/26	-	-	-	-
4	T	0/26	-	-	-	-
4	V	0/26	-	-	-	-
4	X	0/26	-	-	-	-
4	Z	0/26	-	-	-	-
5	2	0/30	-	-	-	-
5	4	0/30	-	-	-	-
5	6	0/30	-	-	-	-
5	8	0/30	-	-	-	-
5	E	0/30	-	-	-	-
5	G	0/30	-	-	-	-
5	I	0/30	-	-	-	-
5	K	0/30	-	-	-	-
5	M	0/30	-	-	-	-
5	O	0/30	-	-	-	-
5	Q	0/30	-	-	-	-
5	S	0/30	-	-	-	-
5	U	0/30	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
5	W	0/30	-	-	-	-
5	Y	0/30	-	-	-	-
All	All	0/1690	-	-	-	-

There are no RSRZ outliers to report.

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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BCL	5	38	47/66	0.52	0.75	198,198,198,198	0
7	BPH	A	401	65/65	0.52	0.69	198,198,198,198	0
7	BPH	B	402	65/65	0.57	0.74	198,198,198,198	0
6	BCL	U	36	47/66	0.57	0.42	198,198,198,198	0
6	BCL	S	36	47/66	0.60	0.58	198,198,198,198	0
6	BCL	P	39	47/66	0.62	0.35	198,198,198,198	0
6	BCL	Y	37	47/66	0.63	0.57	198,198,198,198	0
6	BCL	A	302	66/66	0.64	0.78	198,198,198,198	0
6	BCL	B	304	66/66	0.65	0.67	198,198,198,198	0
6	BCL	M	36	47/66	0.66	0.40	198,198,198,198	0
6	BCL	F	4	47/66	0.66	0.89	198,198,198,198	0
6	BCL	8	36	47/66	0.66	0.81	198,198,198,198	0
6	BCL	V	38	47/66	0.66	0.56	198,198,198,198	0
6	BCL	J	8	47/66	0.67	0.30	198,198,198,198	0
6	BCL	R	38	47/66	0.67	0.36	198,198,198,198	0
6	BCL	T	38	47/66	0.67	0.34	198,198,198,198	0
6	BCL	7	38	47/66	0.67	0.44	198,198,198,198	0

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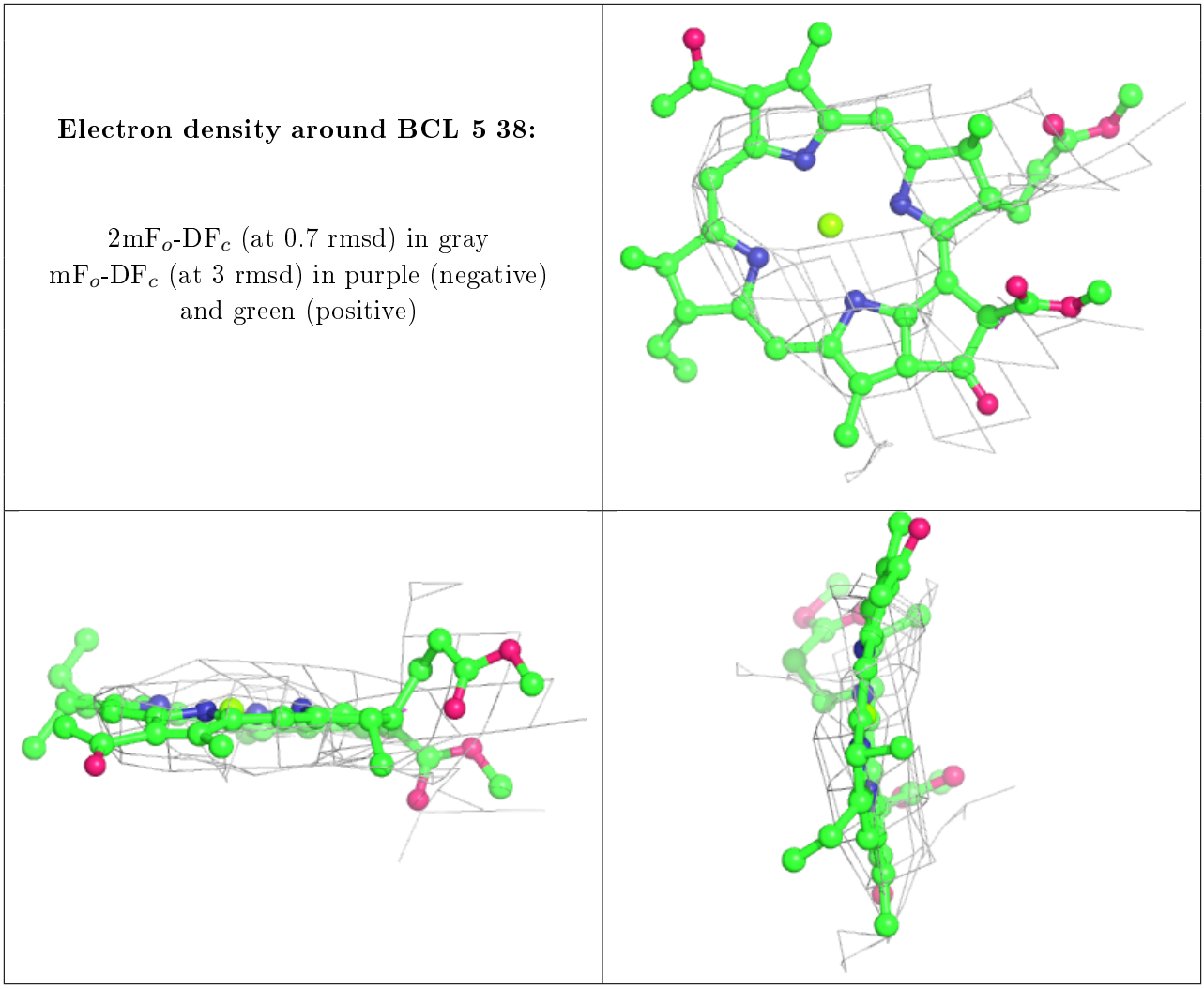
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BCL	D	2	47/66	0.68	0.50	198,198,198,198	0
6	BCL	E	1	47/66	0.68	0.40	198,198,198,198	0
6	BCL	I	5	47/66	0.70	0.46	198,198,198,198	0
6	BCL	P	38	47/66	0.70	0.27	198,198,198,198	0
6	BCL	1	38	47/66	0.71	0.44	198,198,198,198	0
6	BCL	K	36	47/66	0.71	0.37	198,198,198,198	0
6	BCL	3	39	47/66	0.72	0.33	198,198,198,198	0
6	BCL	A	301	66/66	0.72	0.54	198,198,198,198	0
6	BCL	L	10	47/66	0.73	0.37	198,198,198,198	0
6	BCL	6	36	47/66	0.73	0.42	198,198,198,198	0
6	BCL	B	303	66/66	0.73	0.70	198,198,198,198	0
6	BCL	H	6	47/66	0.76	0.27	198,198,198,198	0
6	BCL	W	36	47/66	0.78	0.67	198,198,198,198	0
6	BCL	N	38	47/66	0.79	0.22	198,198,198,198	0
6	BCL	Y	36	47/66	0.79	0.32	198,198,198,198	0
6	BCL	3	38	47/66	0.80	0.24	198,198,198,198	0
6	BCL	N	11	47/66	0.81	0.22	198,198,198,198	0
6	BCL	G	3	47/66	0.82	0.43	198,198,198,198	0
6	BCL	2	36	47/66	0.83	0.52	198,198,198,198	0
8	FE	B	500	1/1	0.94	0.63	198,198,198,198	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.

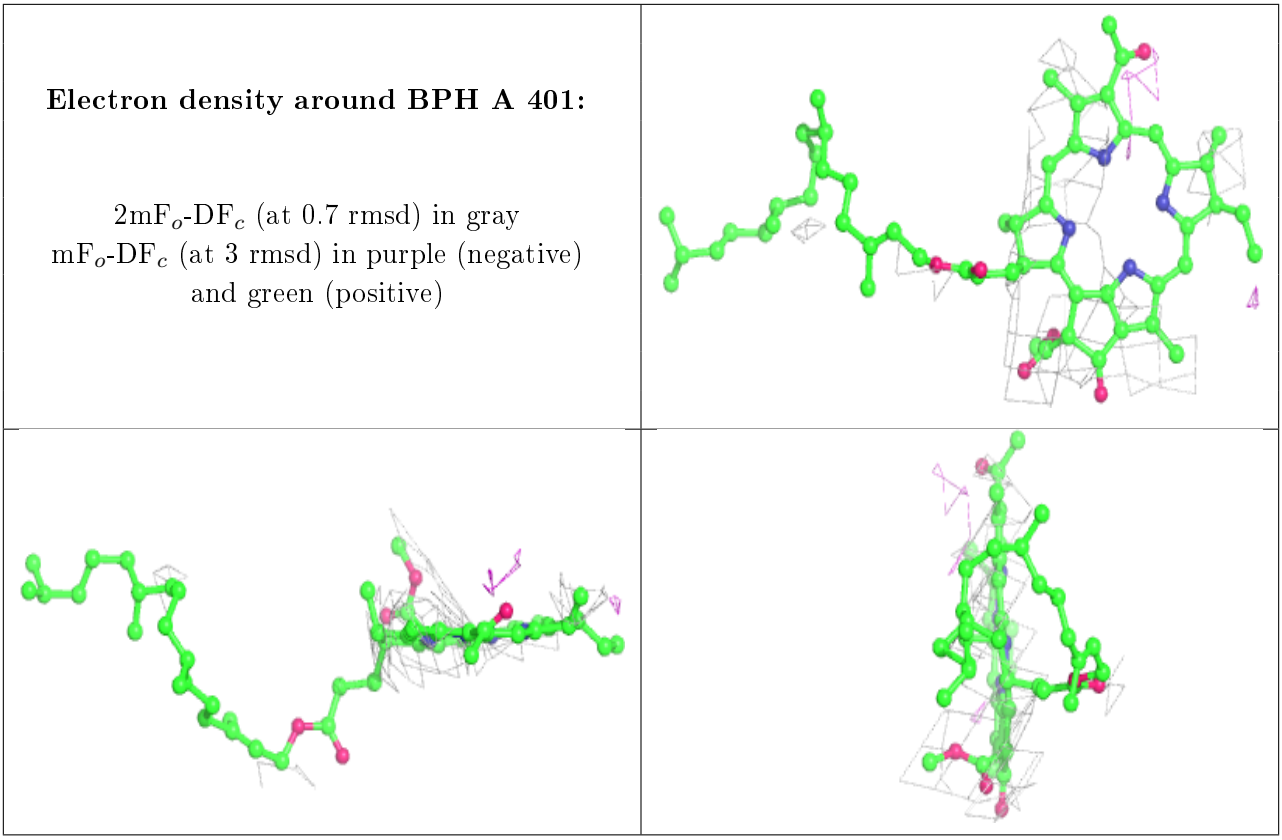
Electron density around BCL 5 38:

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



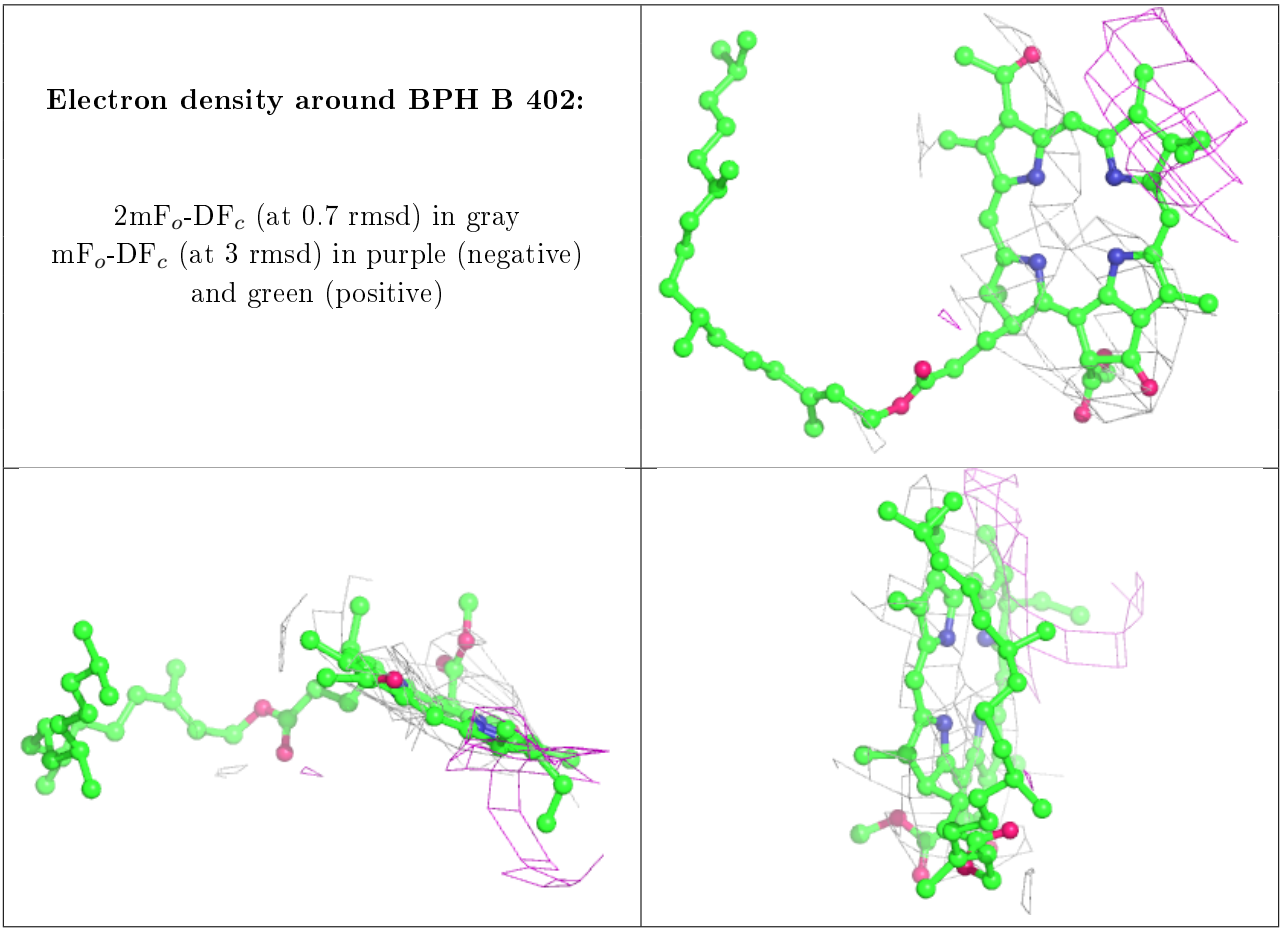
Electron density around BPH A 401:

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



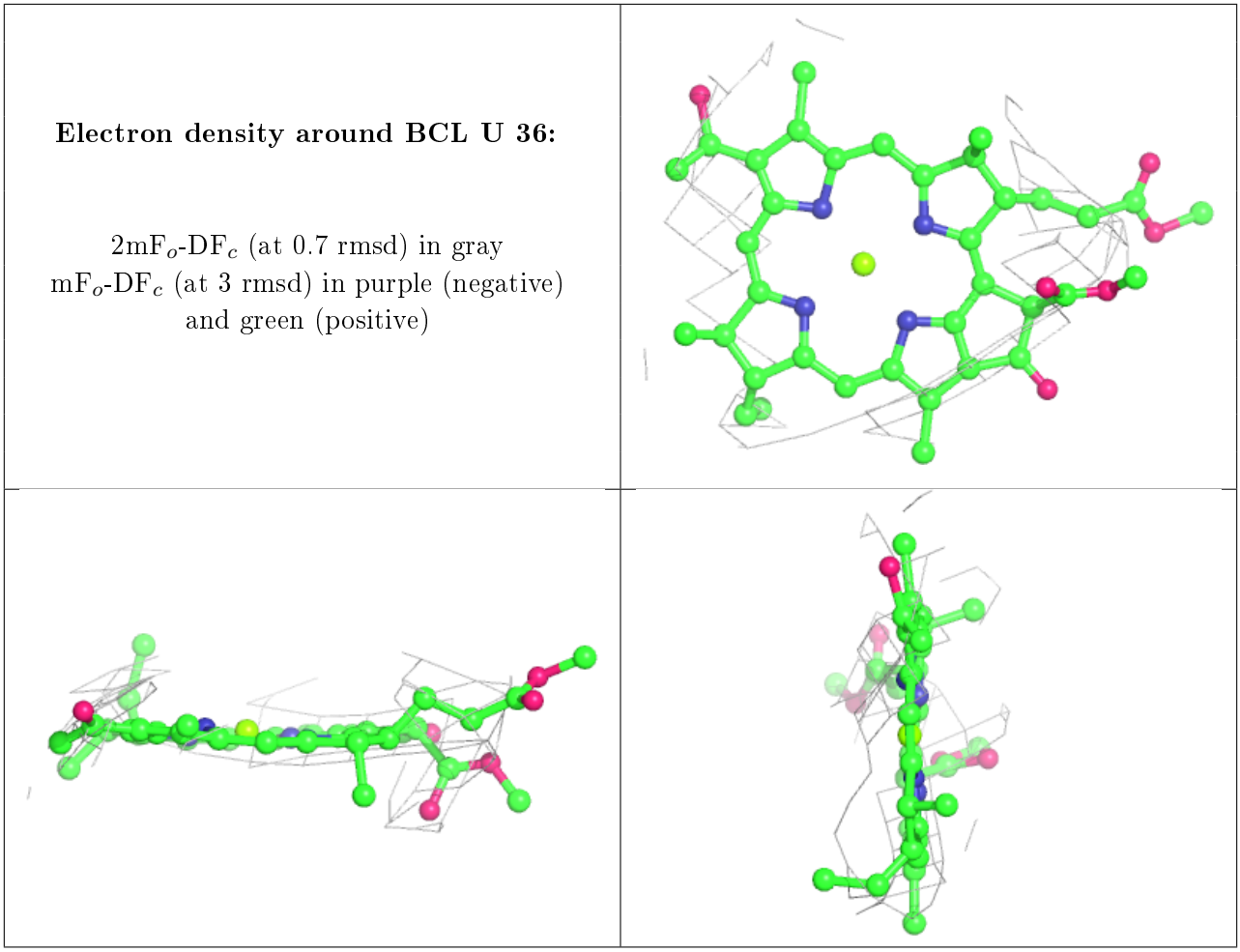
Electron density around BPH B 402:

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



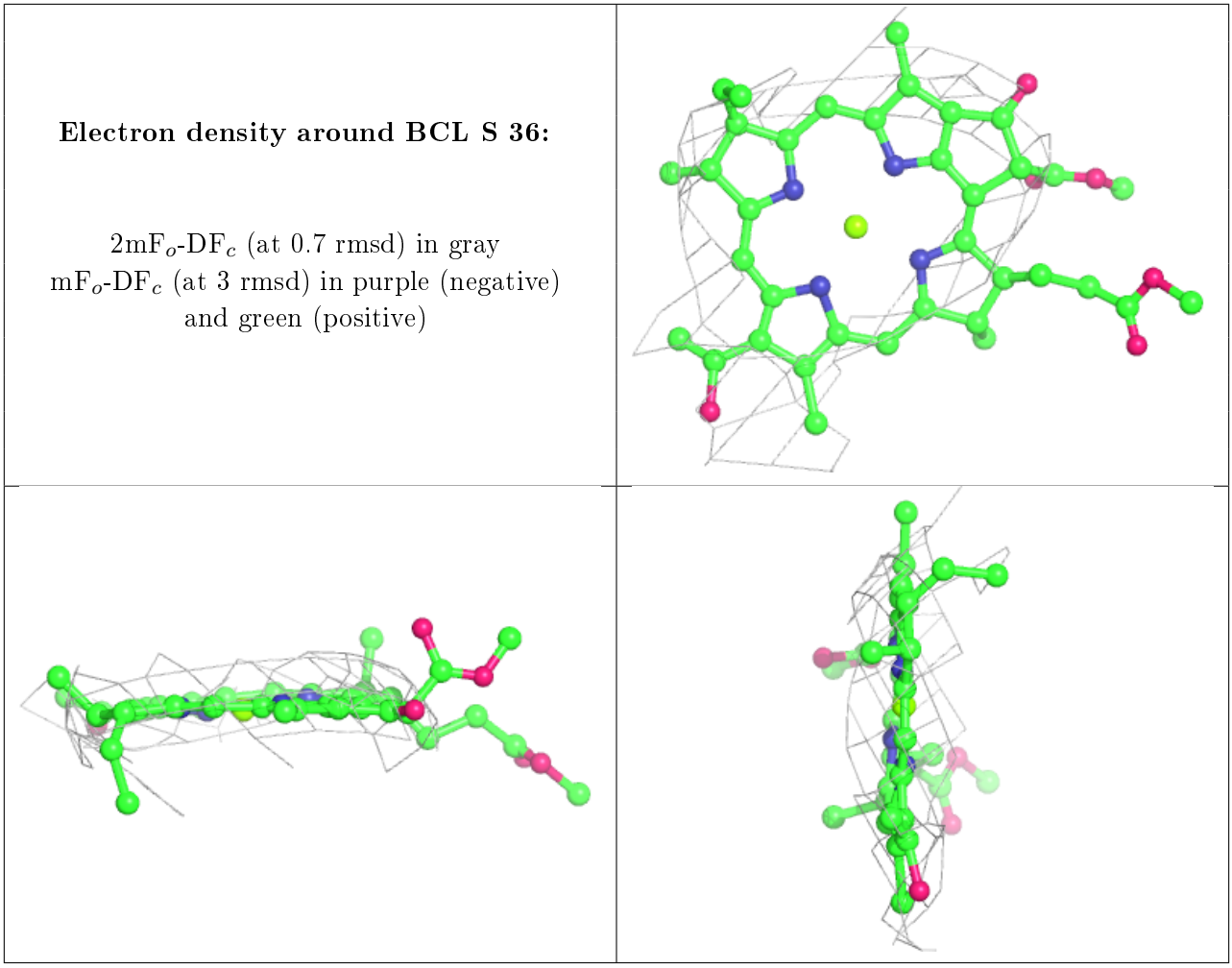
Electron density around BCL U 36:

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



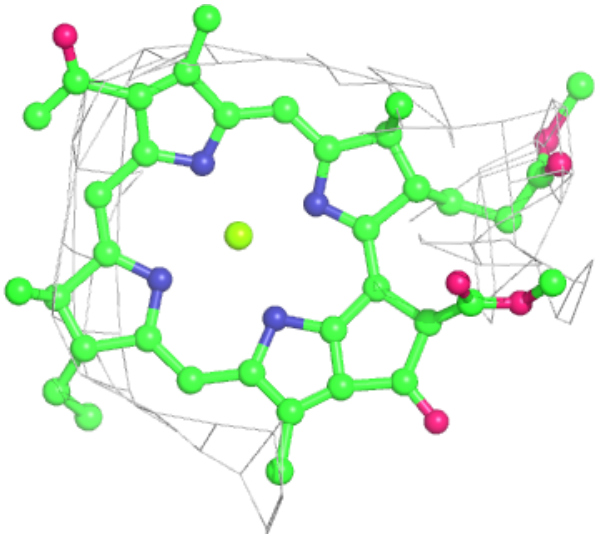
Electron density around BCL S 36:

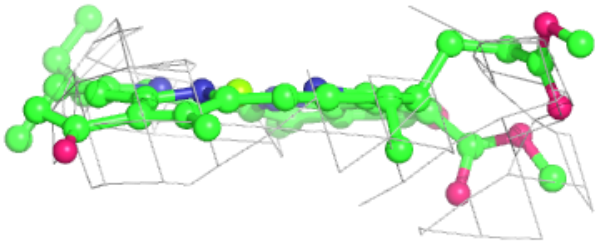
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

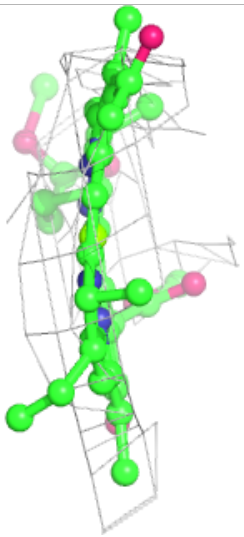


Electron density around BCL P 39:

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

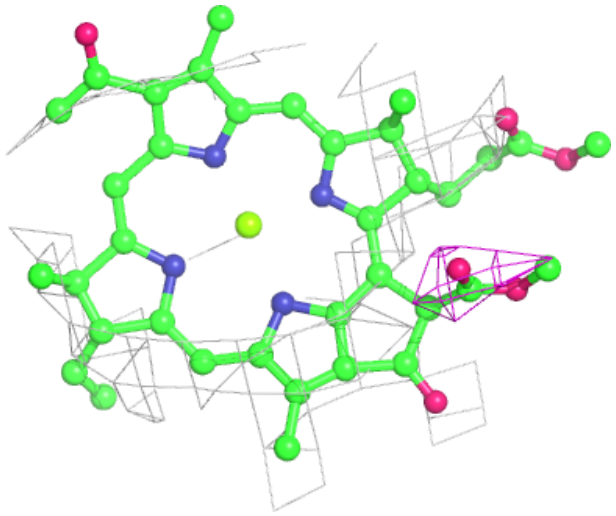


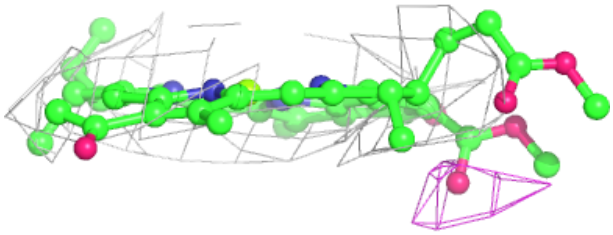


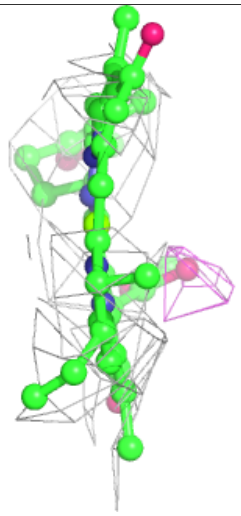


Electron density around BCL Y 37:

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

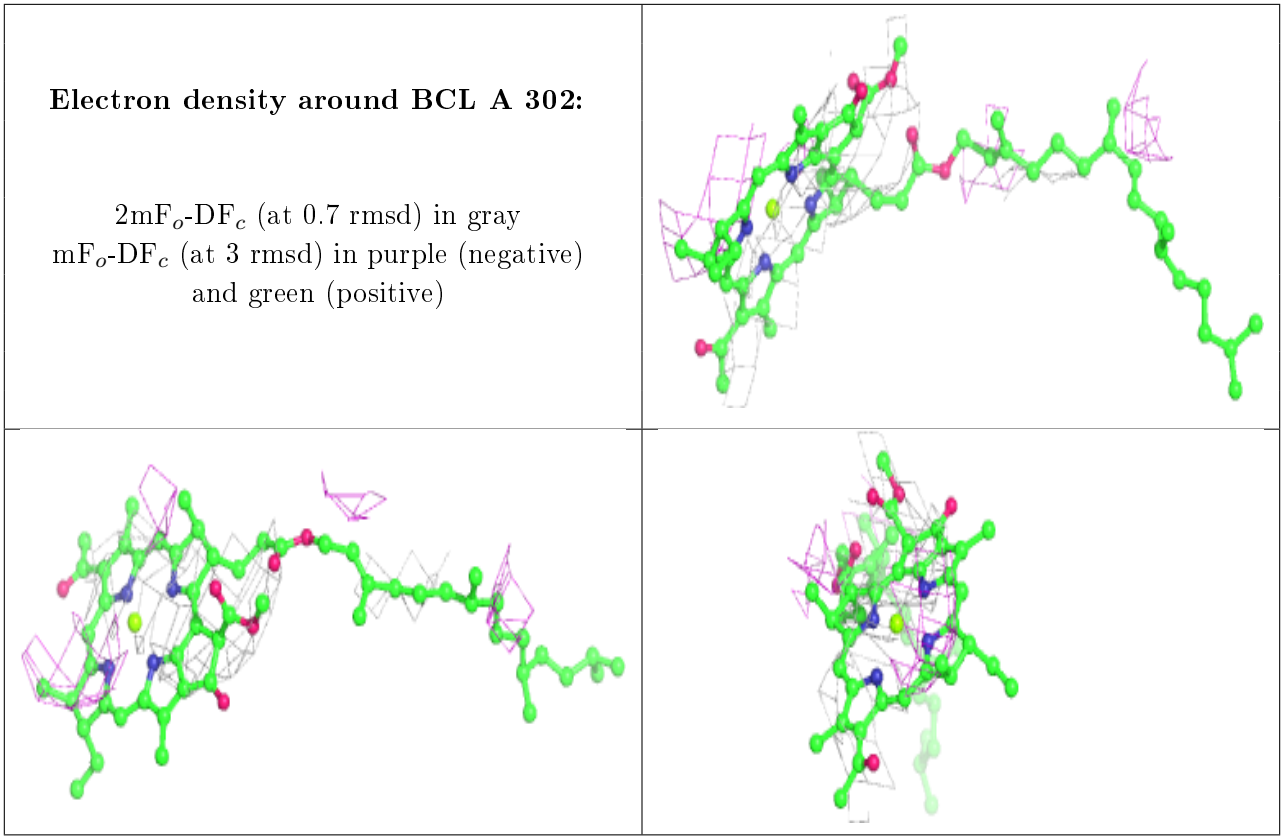






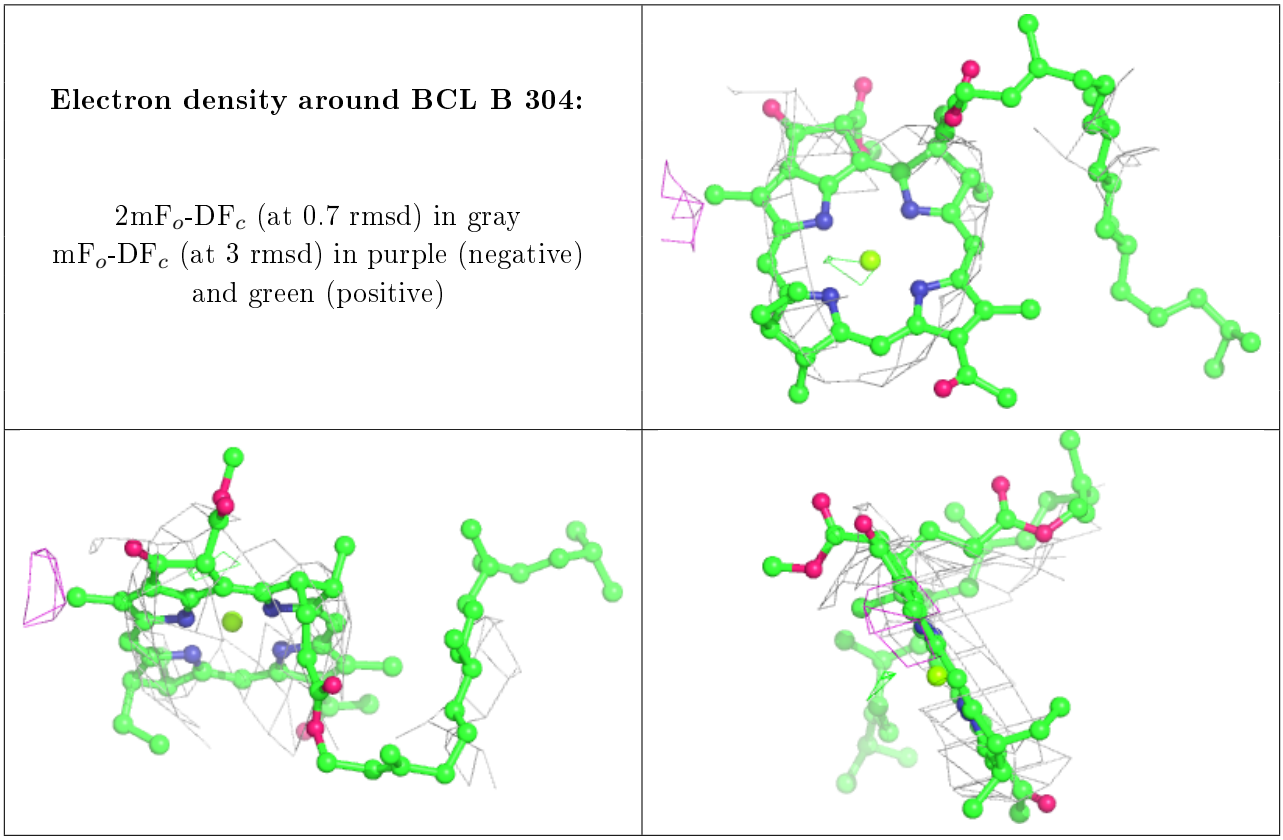
Electron density around BCL A 302:

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



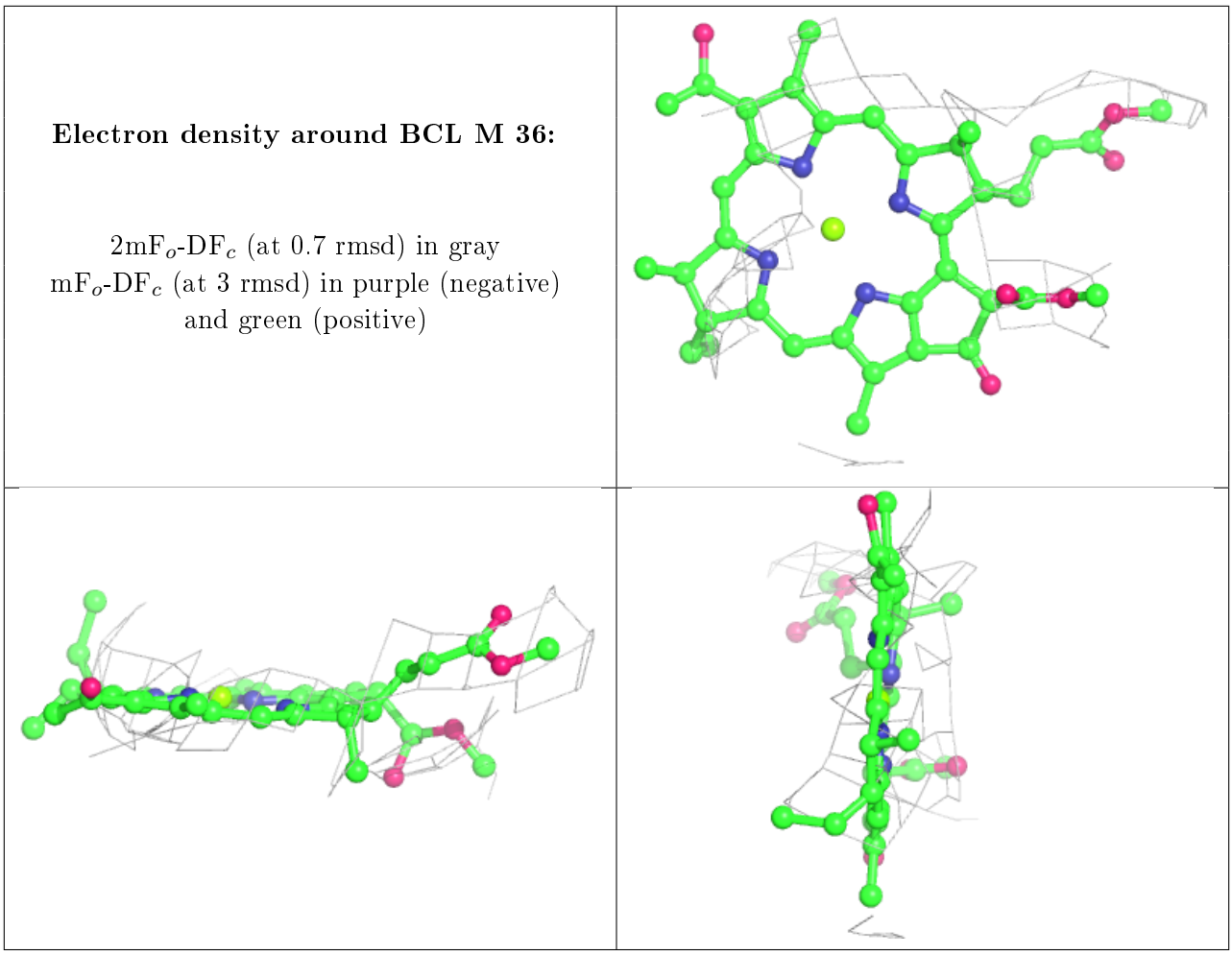
Electron density around BCL B 304:

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



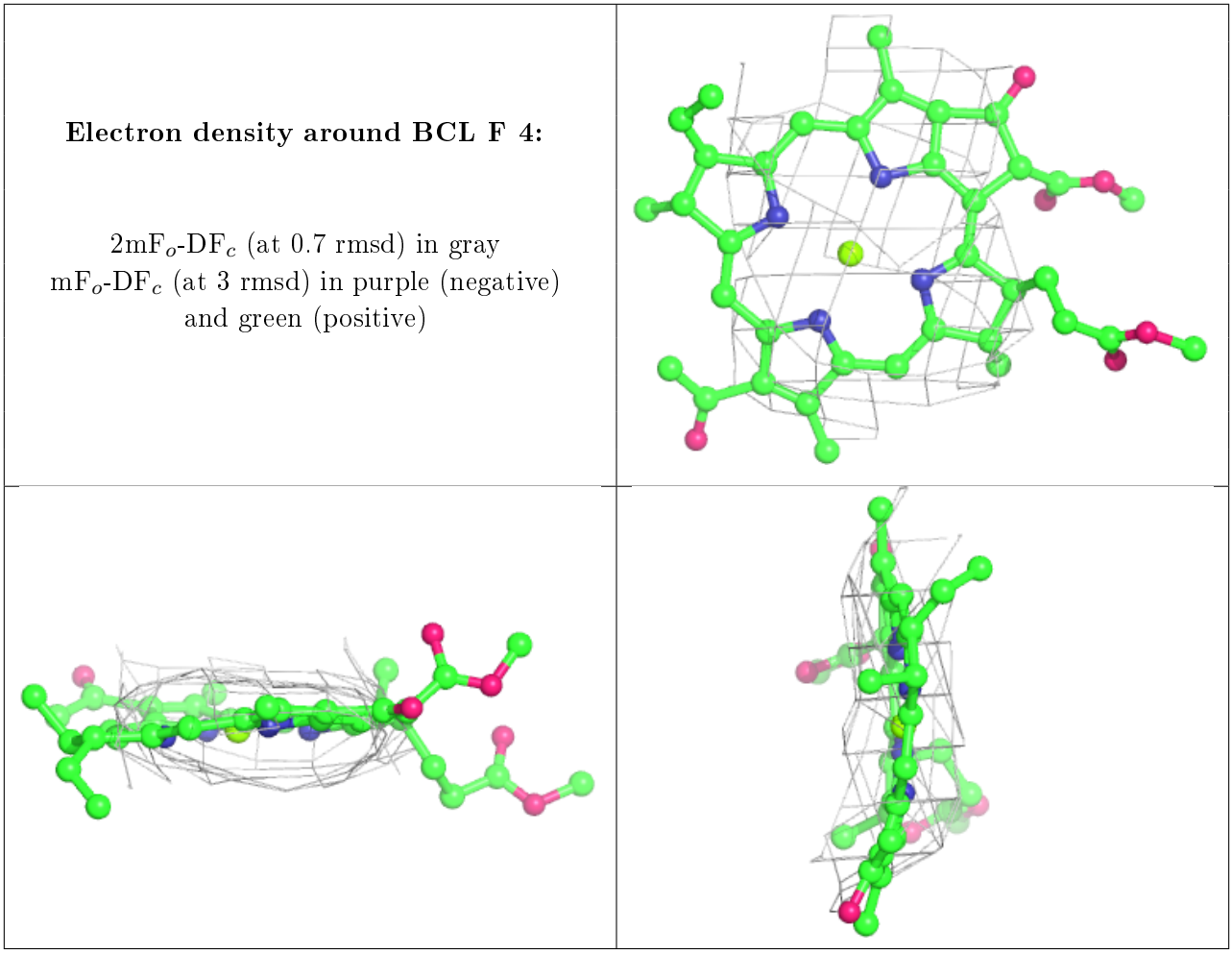
Electron density around BCL M 36:

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



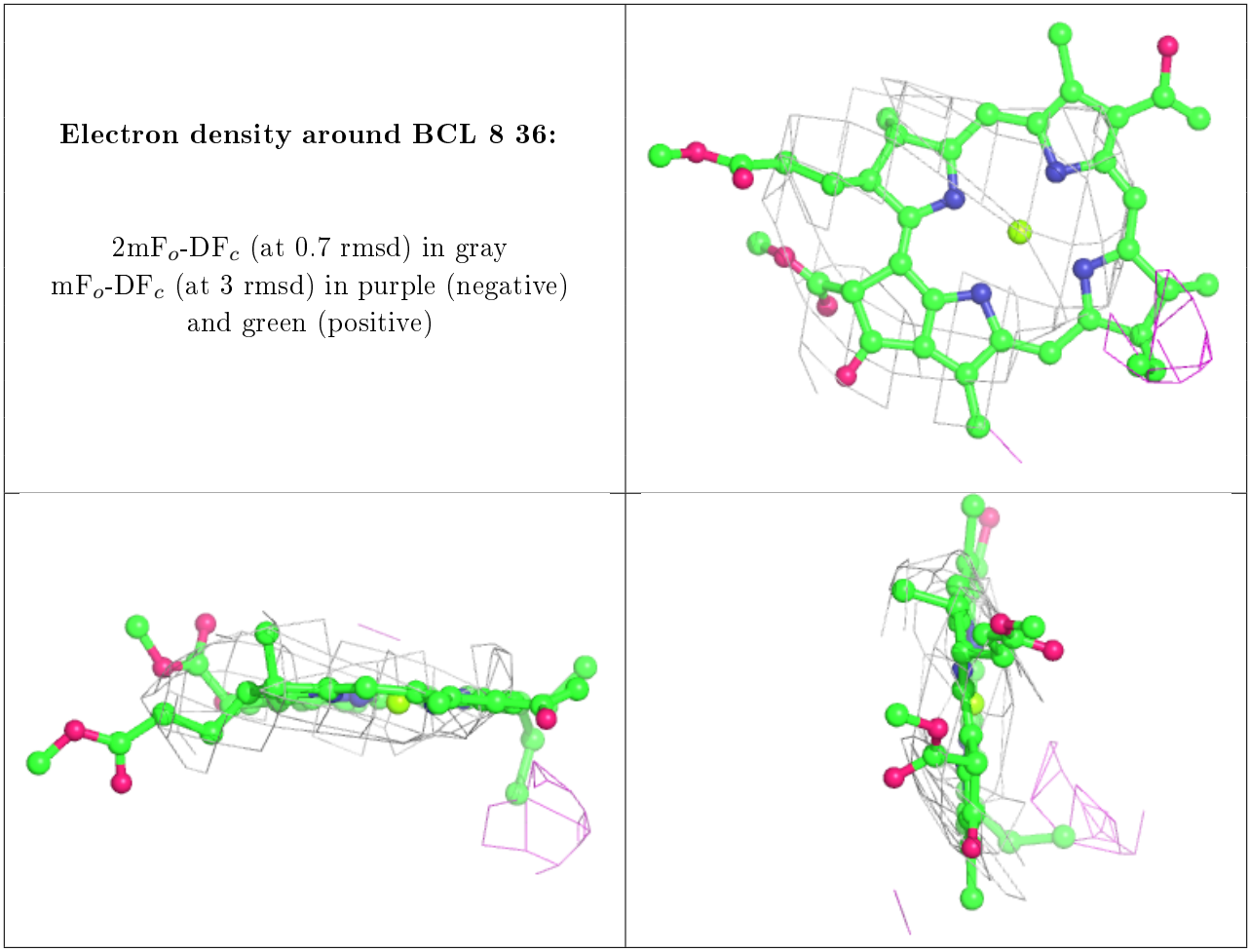
Electron density around BCL F 4:

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



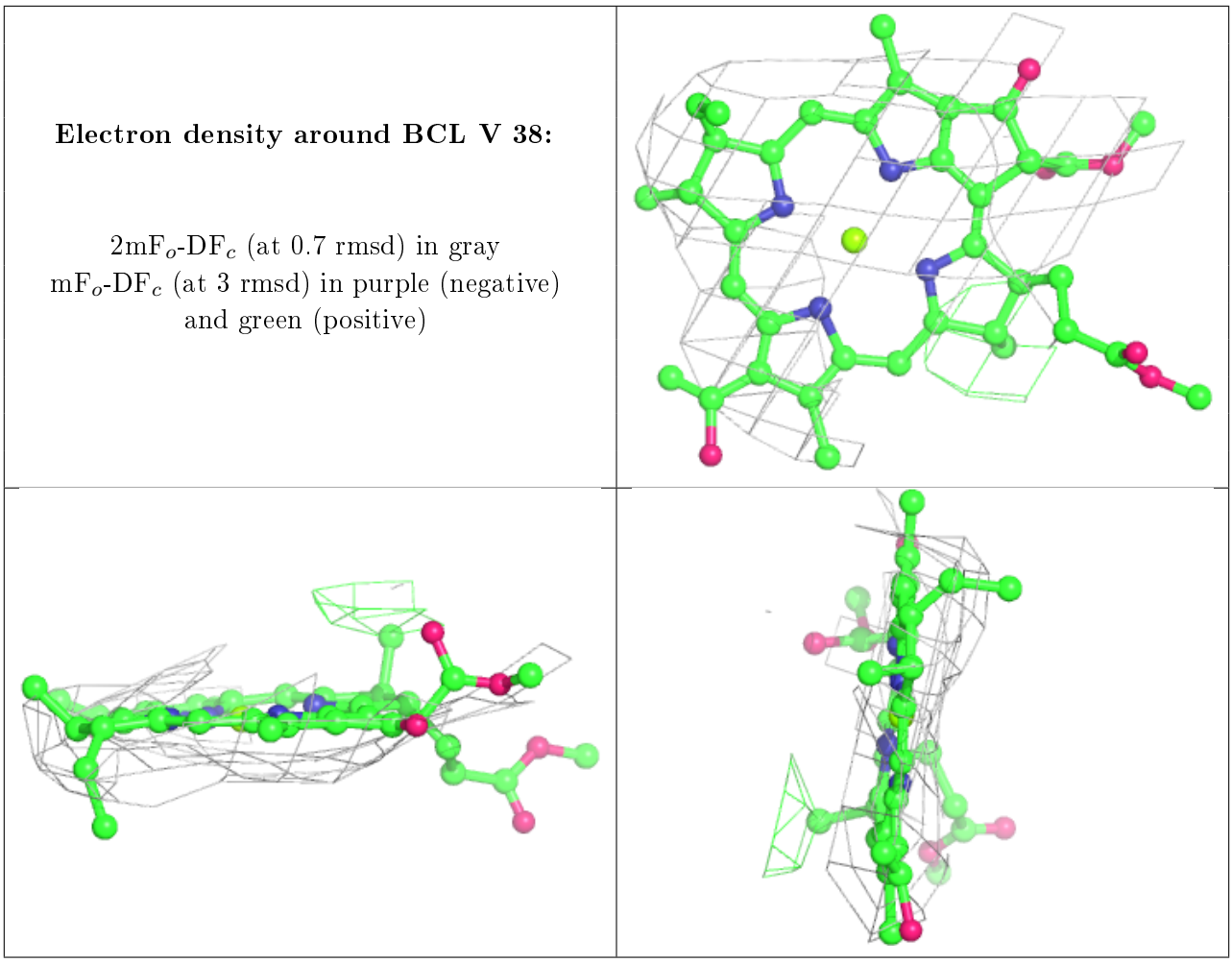
Electron density around BCL 8 36:

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



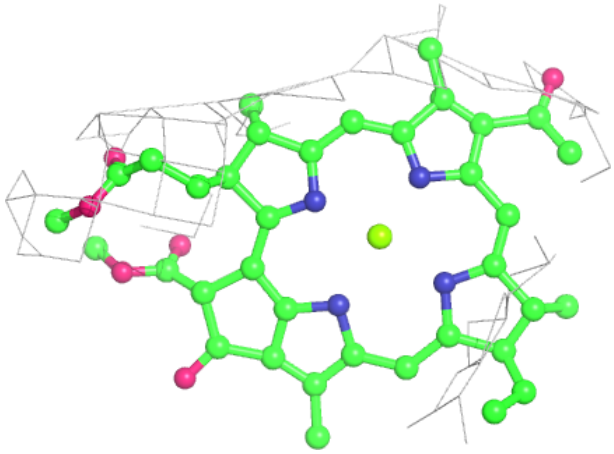
Electron density around BCL V 38:

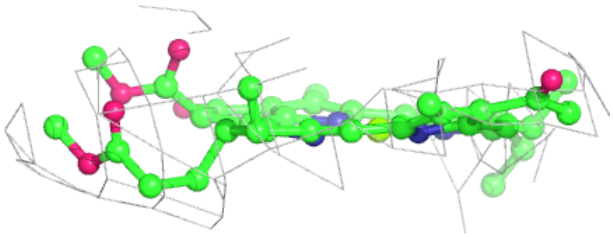
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

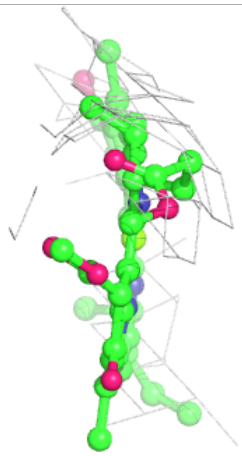


Electron density around BCL J 8:

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

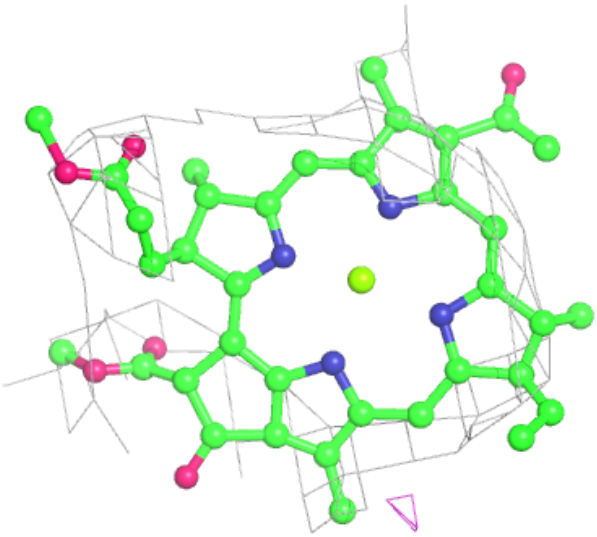


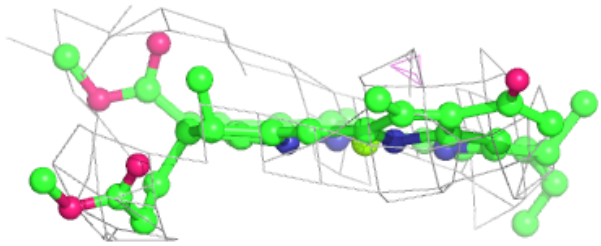


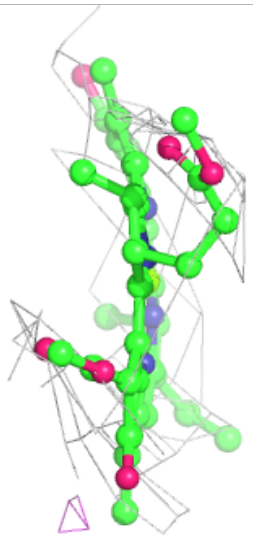


Electron density around BCL R 38:

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

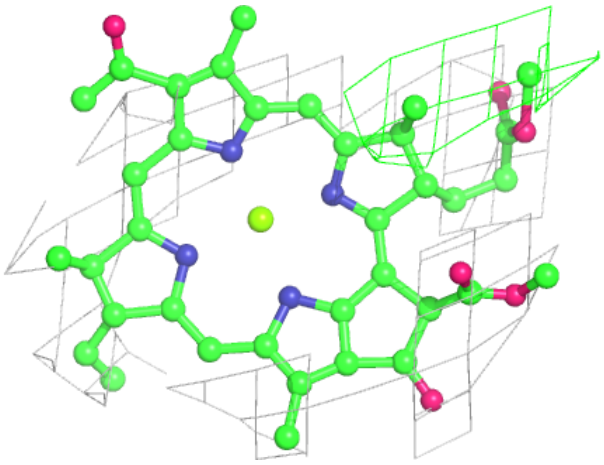


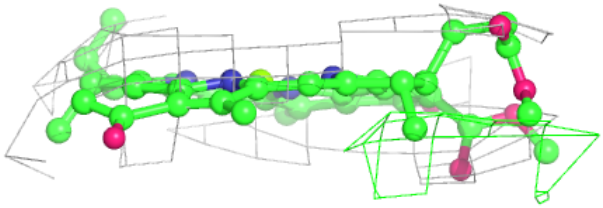


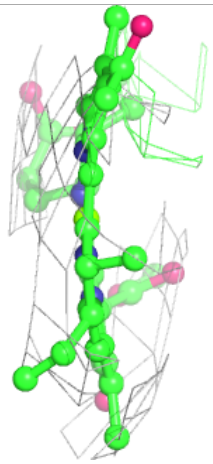


Electron density around BCL T 38:

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

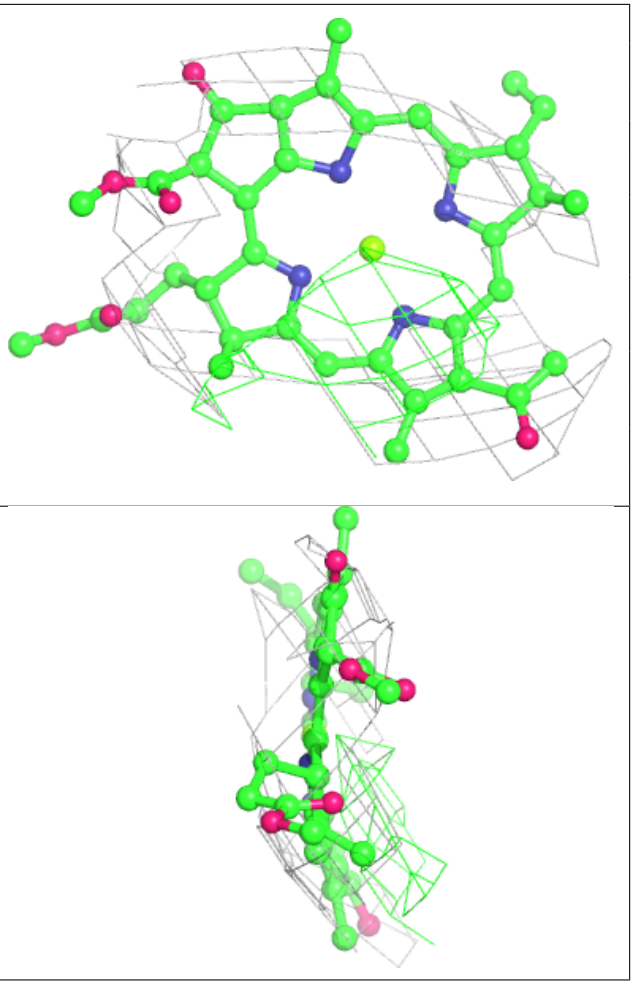


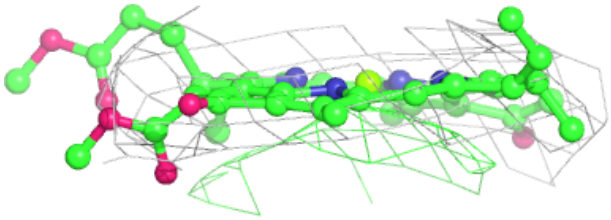




Electron density around BCL 7 38:

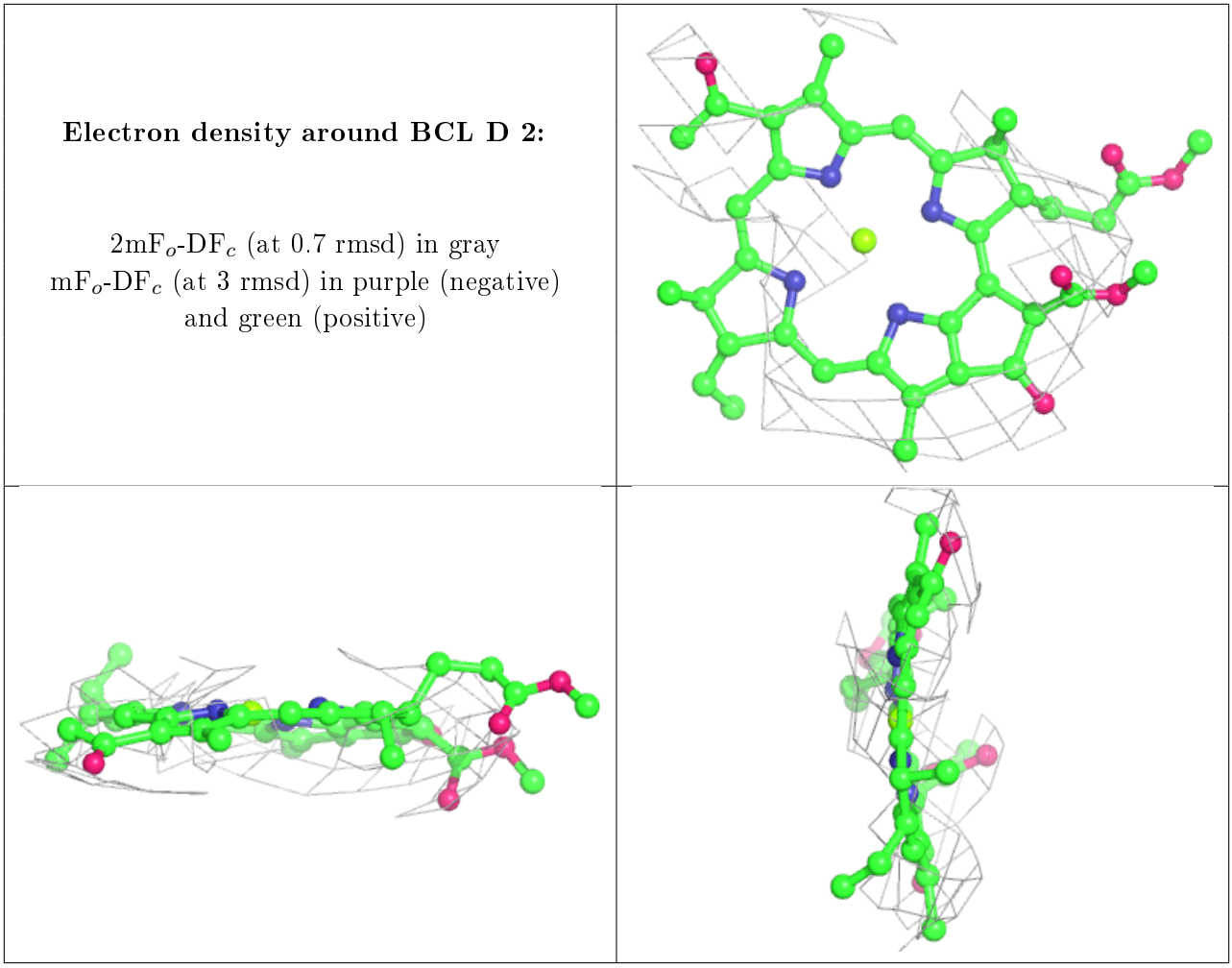
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





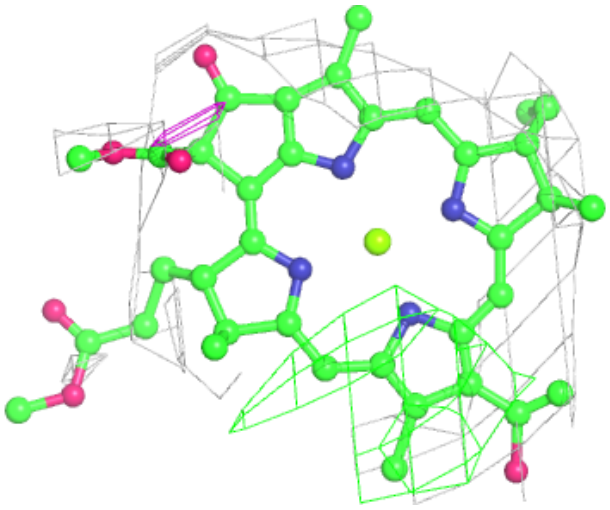
Electron density around BCL D 2:

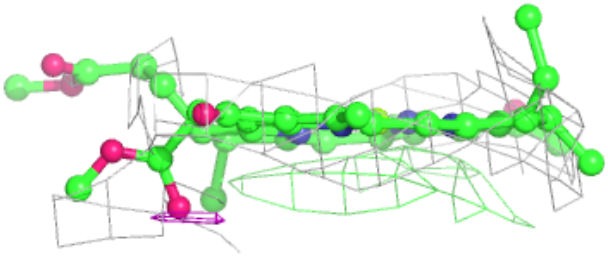
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

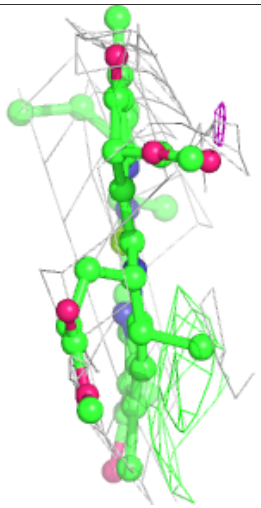


Electron density around BCL E 1:

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

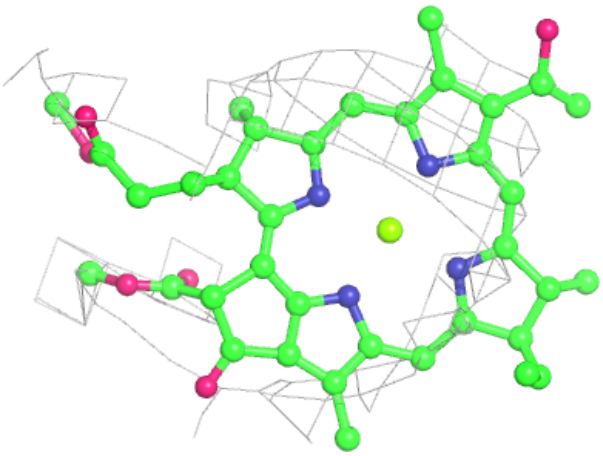


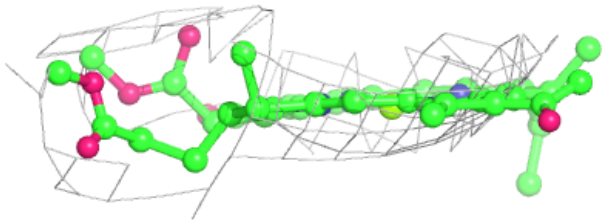


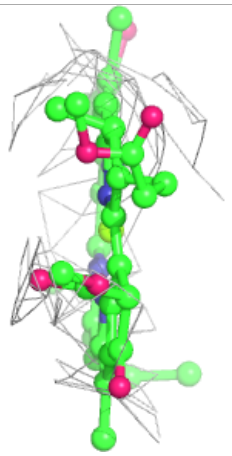


Electron density around BCL I 5:

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

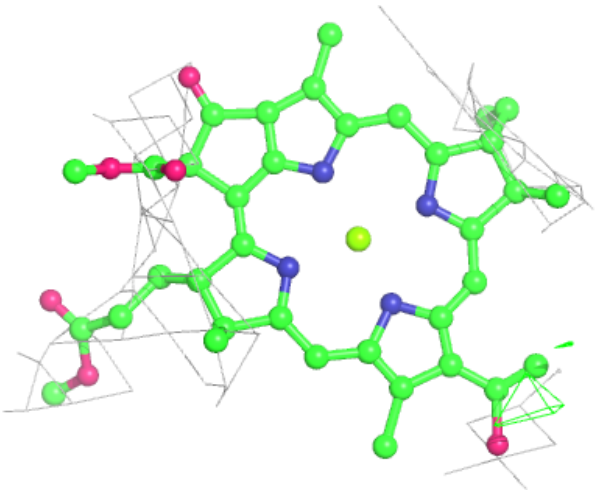


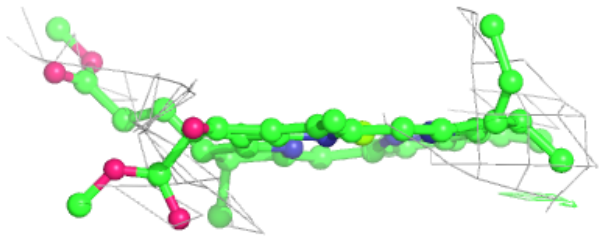


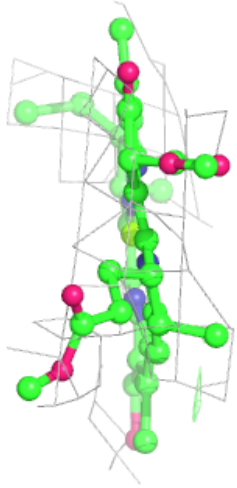


Electron density around BCL P 38:

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

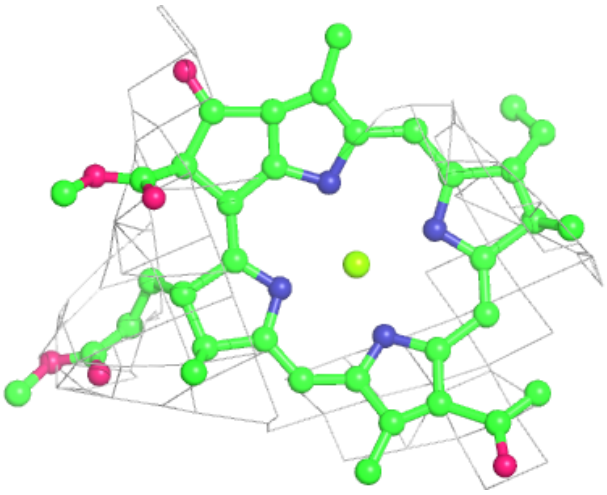


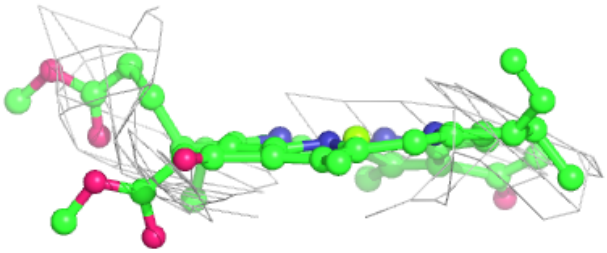


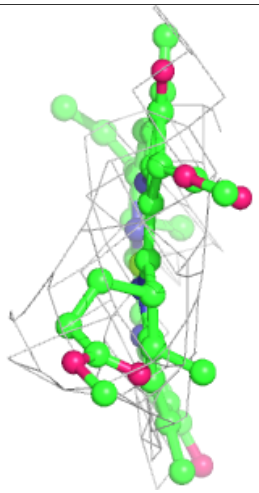


Electron density around BCL 1 38:

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

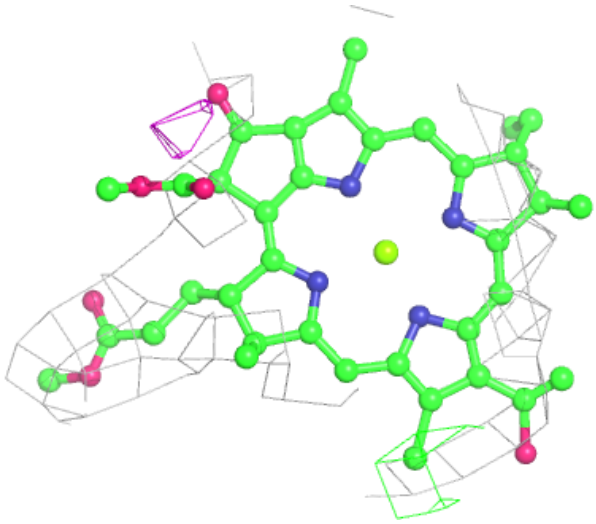


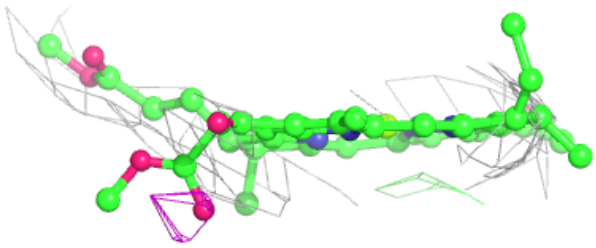


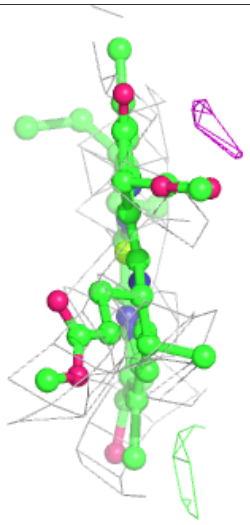


Electron density around BCL K 36:

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

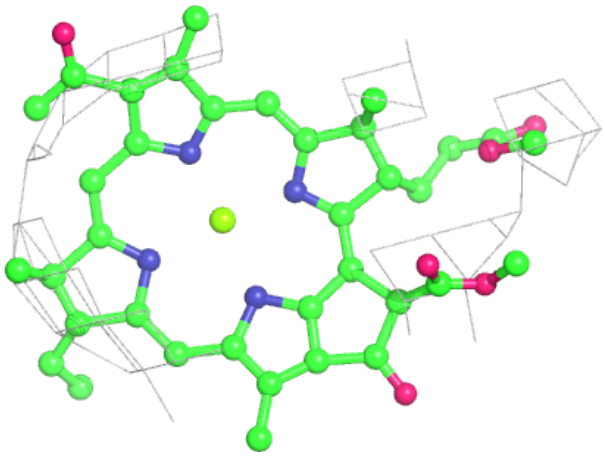


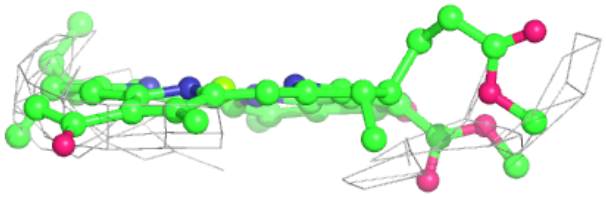


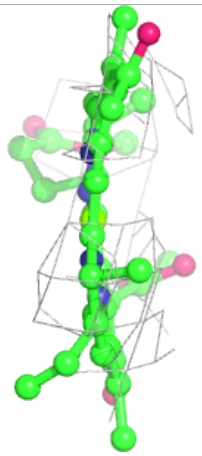


Electron density around BCL 3 39:

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

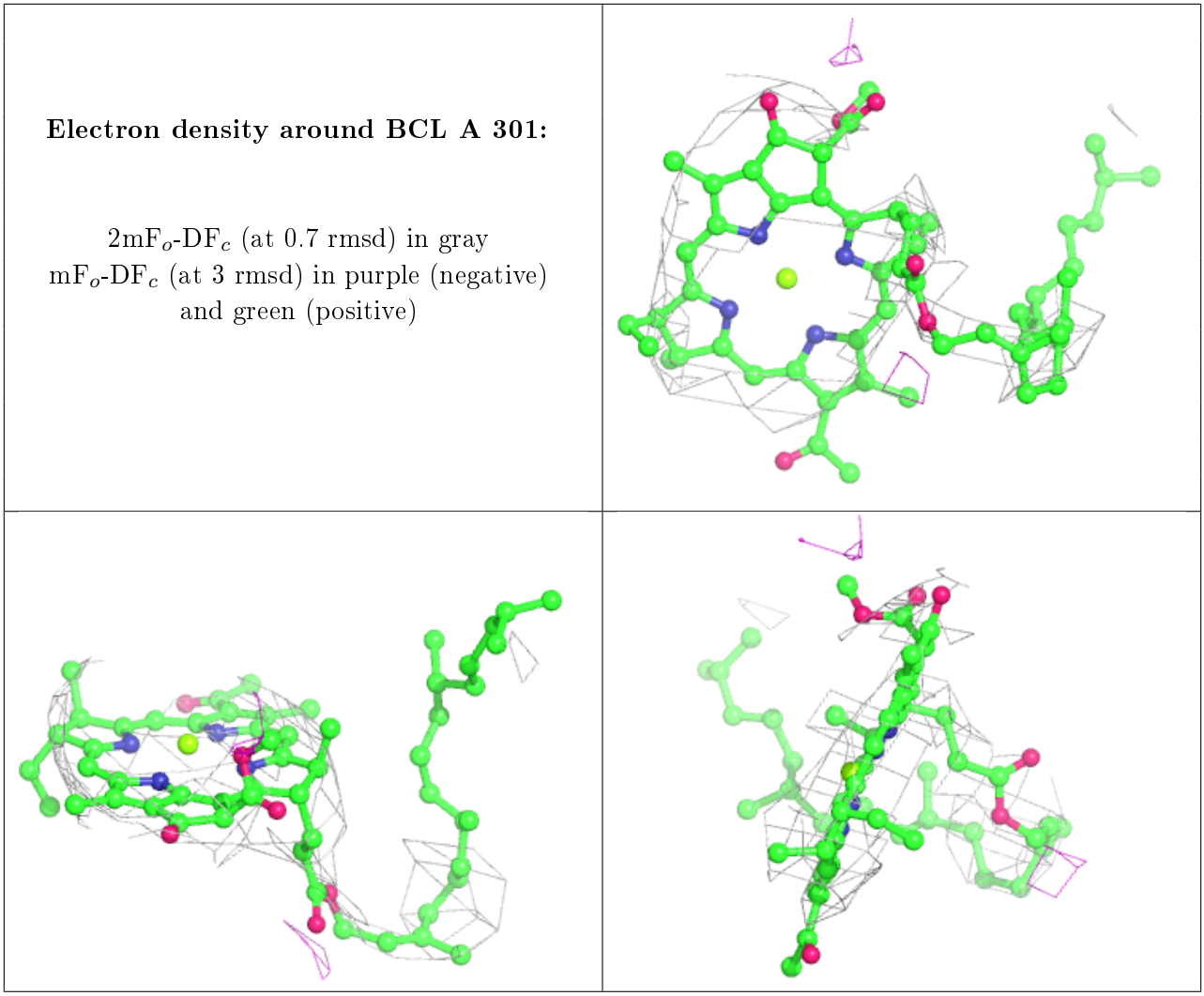






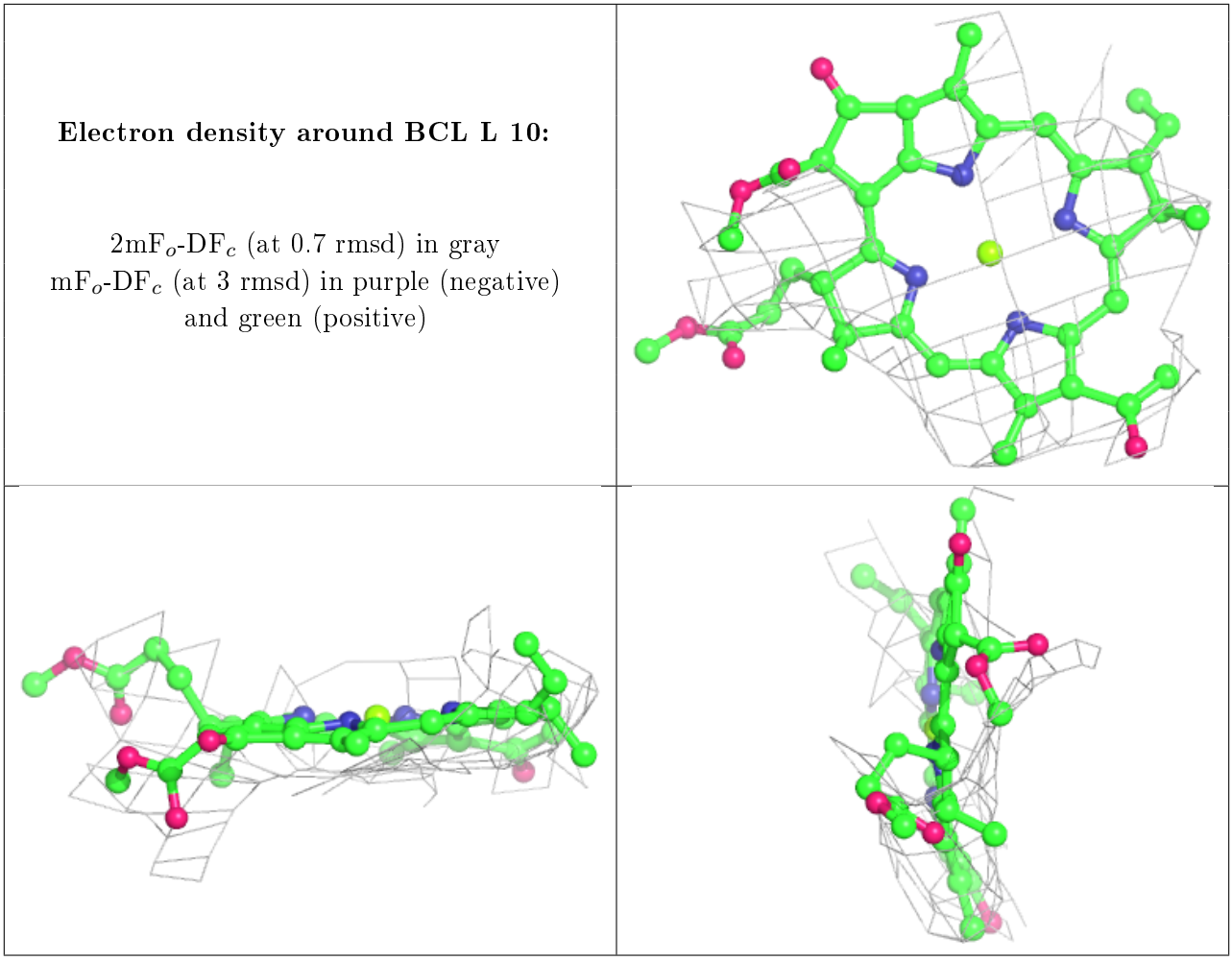
Electron density around BCL A 301:

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



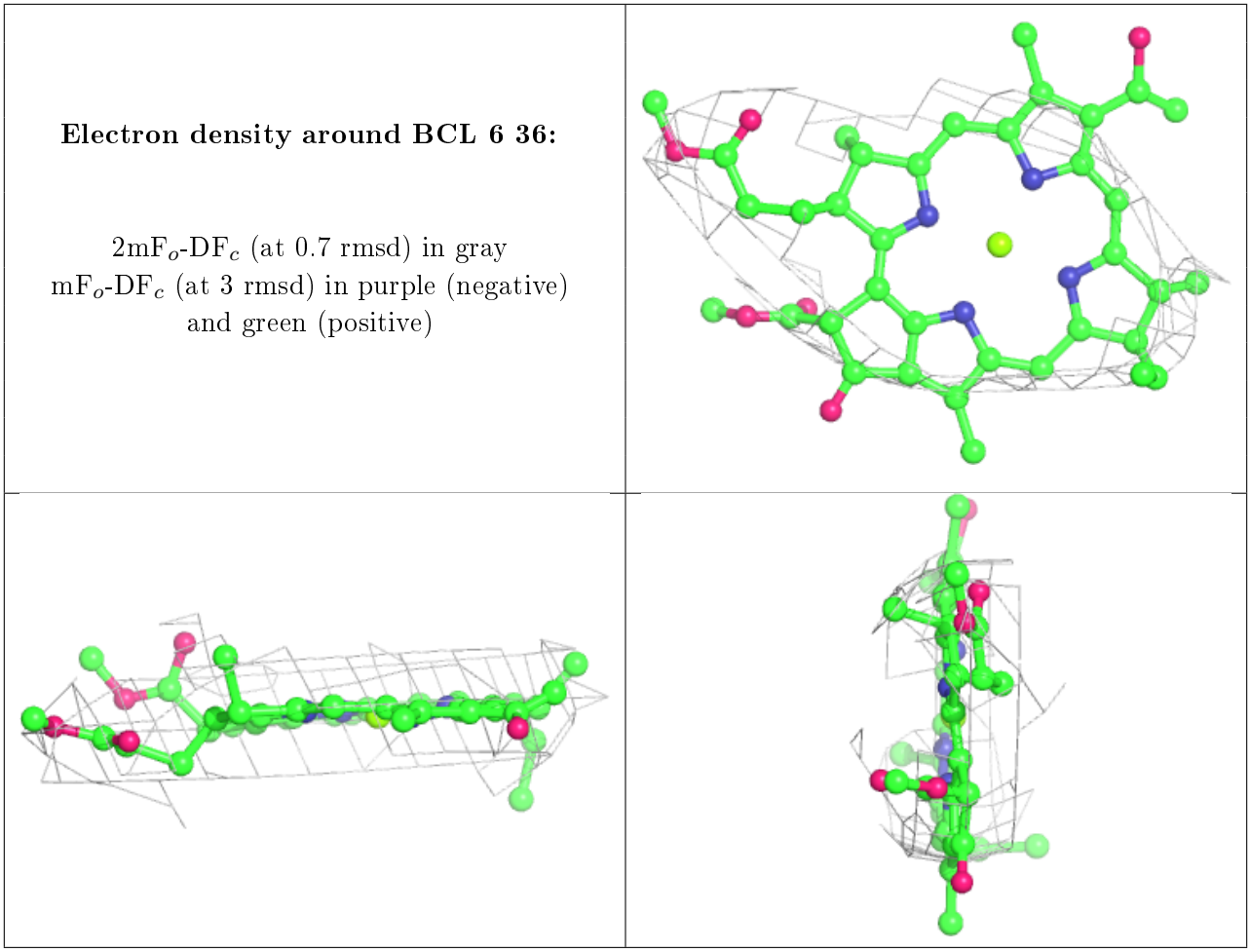
Electron density around BCL L 10:

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



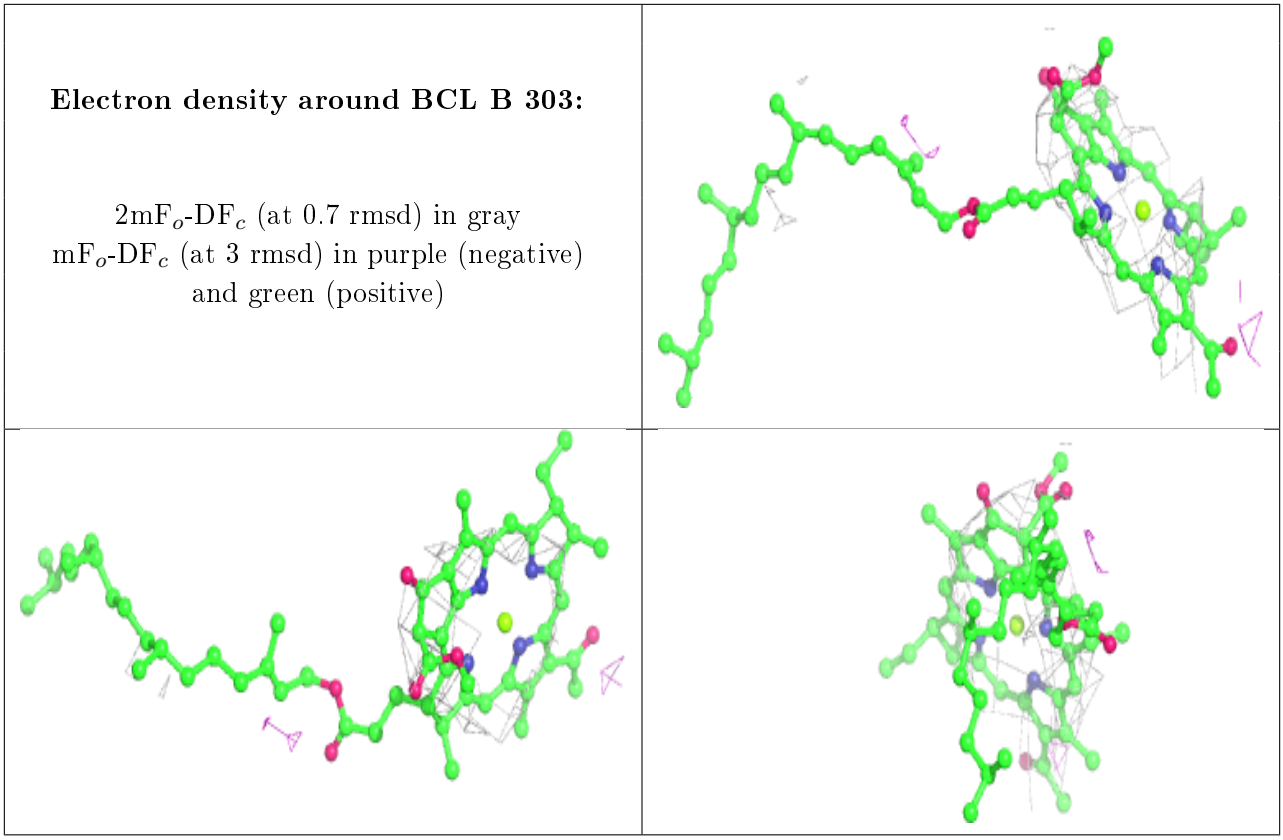
Electron density around BCL 6 36:

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



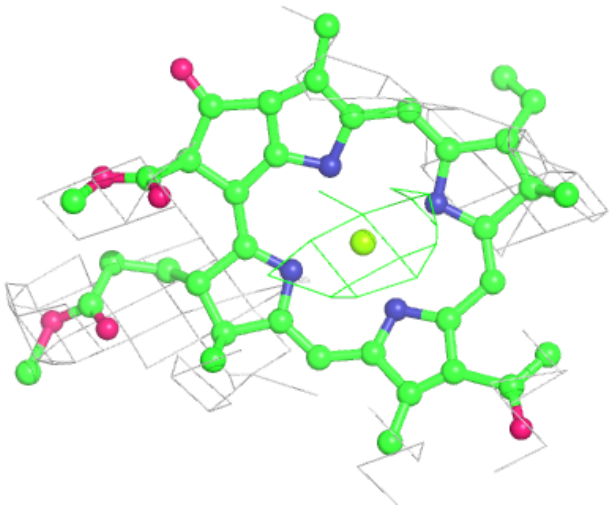
Electron density around BCL B 303:

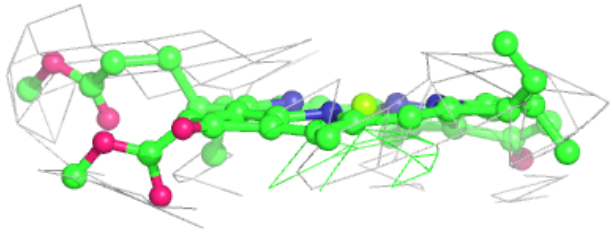
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

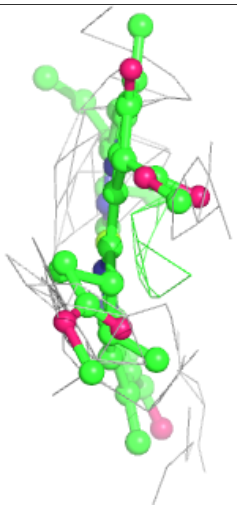


Electron density around BCL H 6:

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

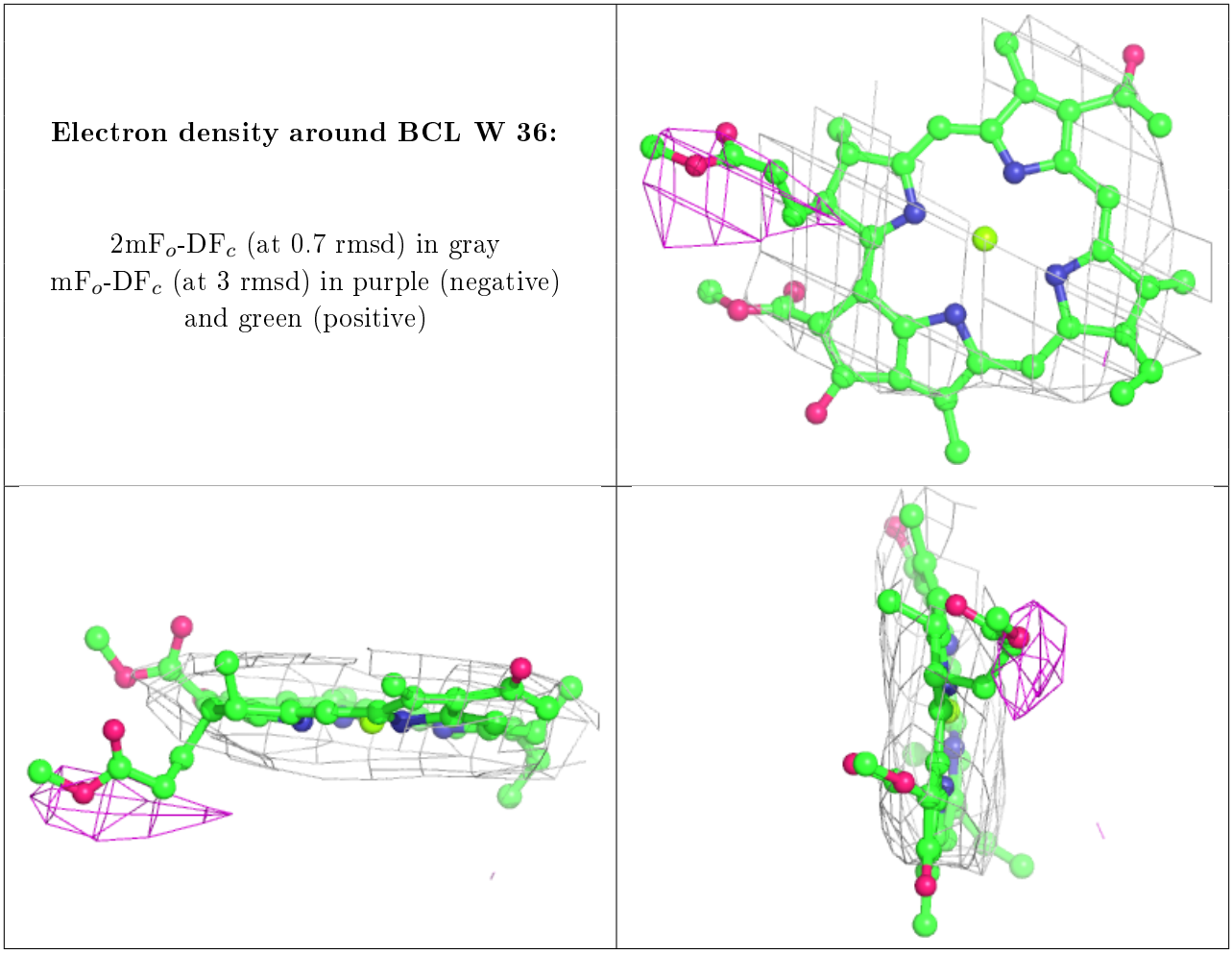






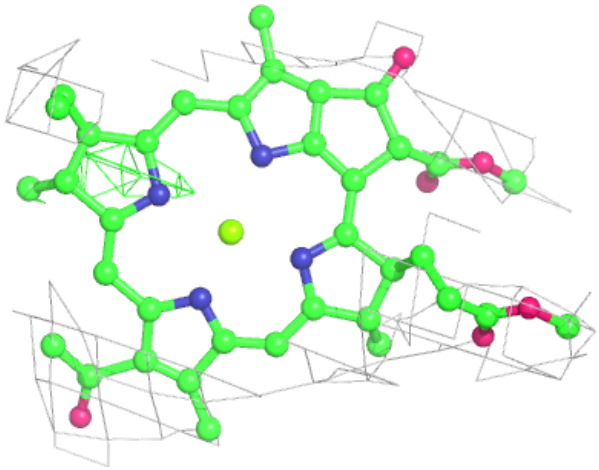
Electron density around BCL W 36:

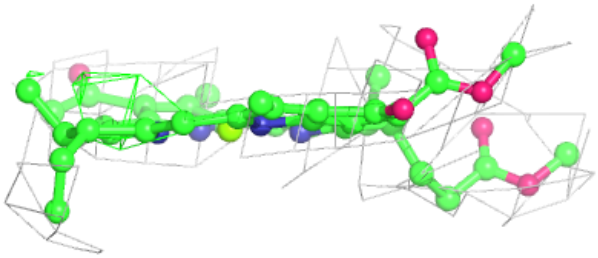
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

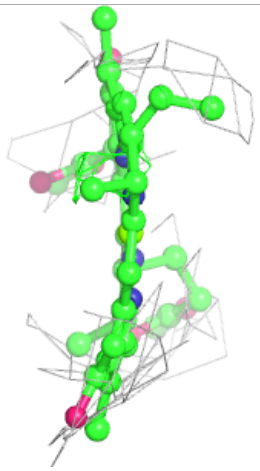


Electron density around BCL N 38:

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

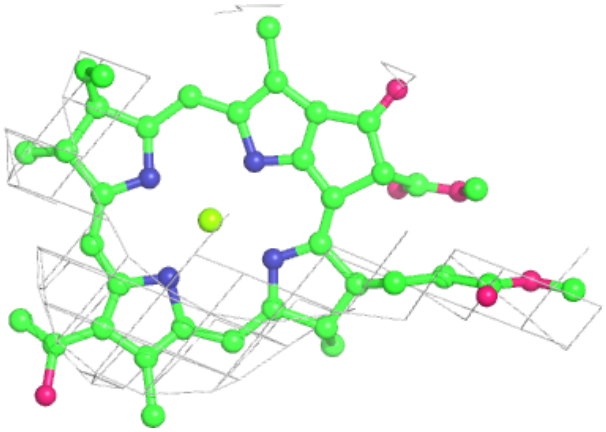


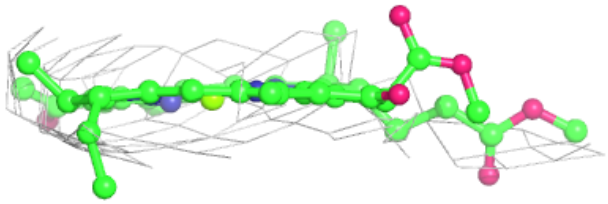


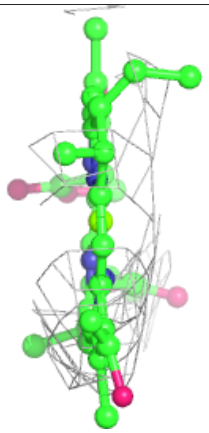


Electron density around BCL Y 36:

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

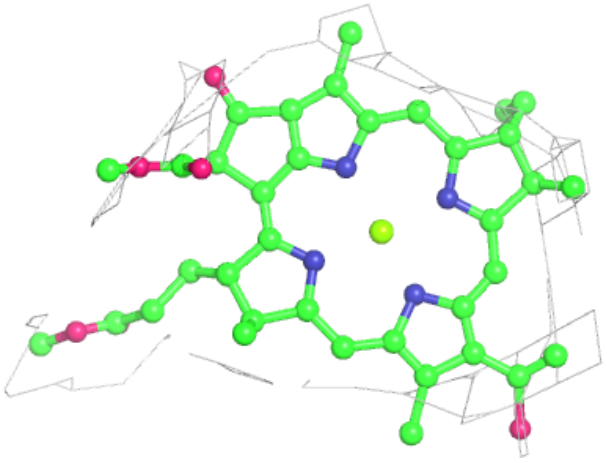


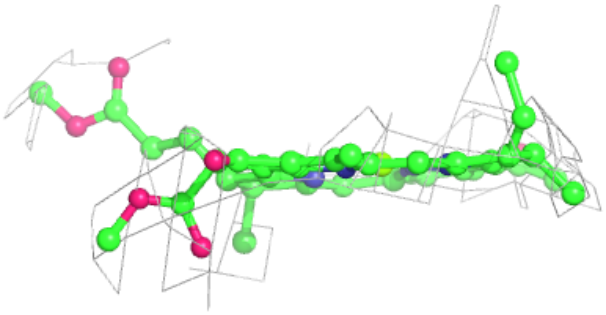


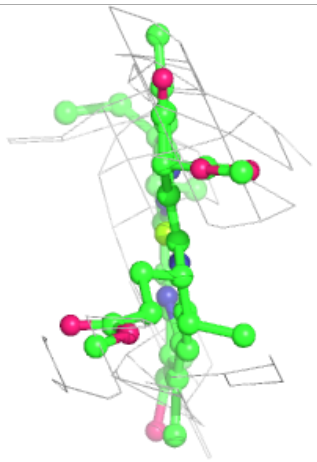


Electron density around BCL 3 38:

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

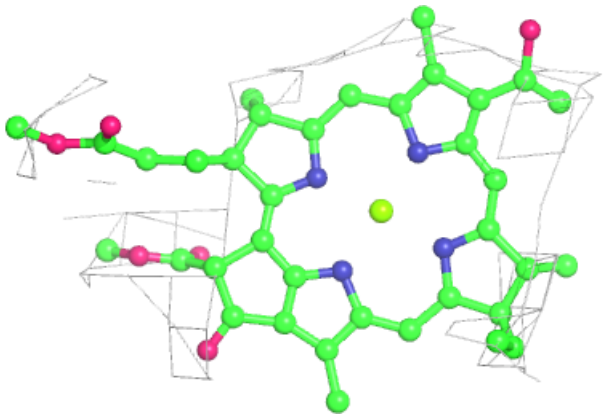


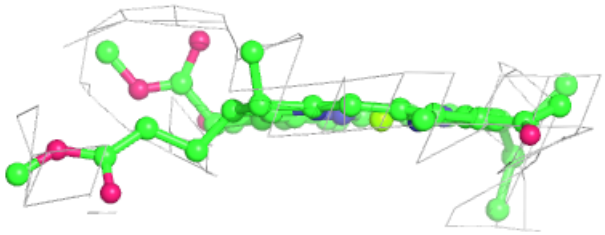


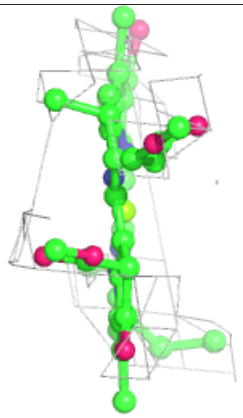


Electron density around BCL N 11:

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

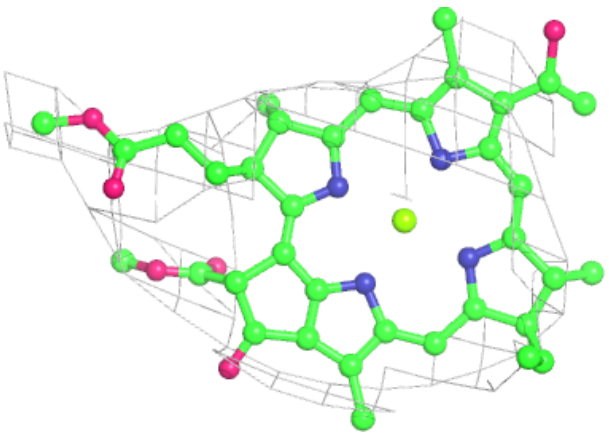


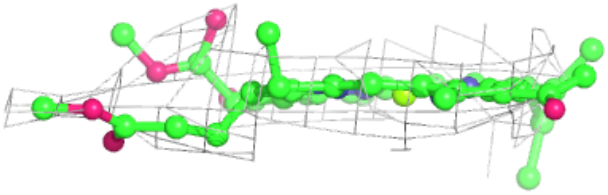


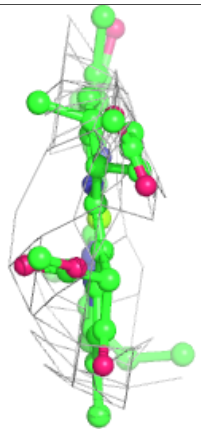


Electron density around BCL G 3:

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

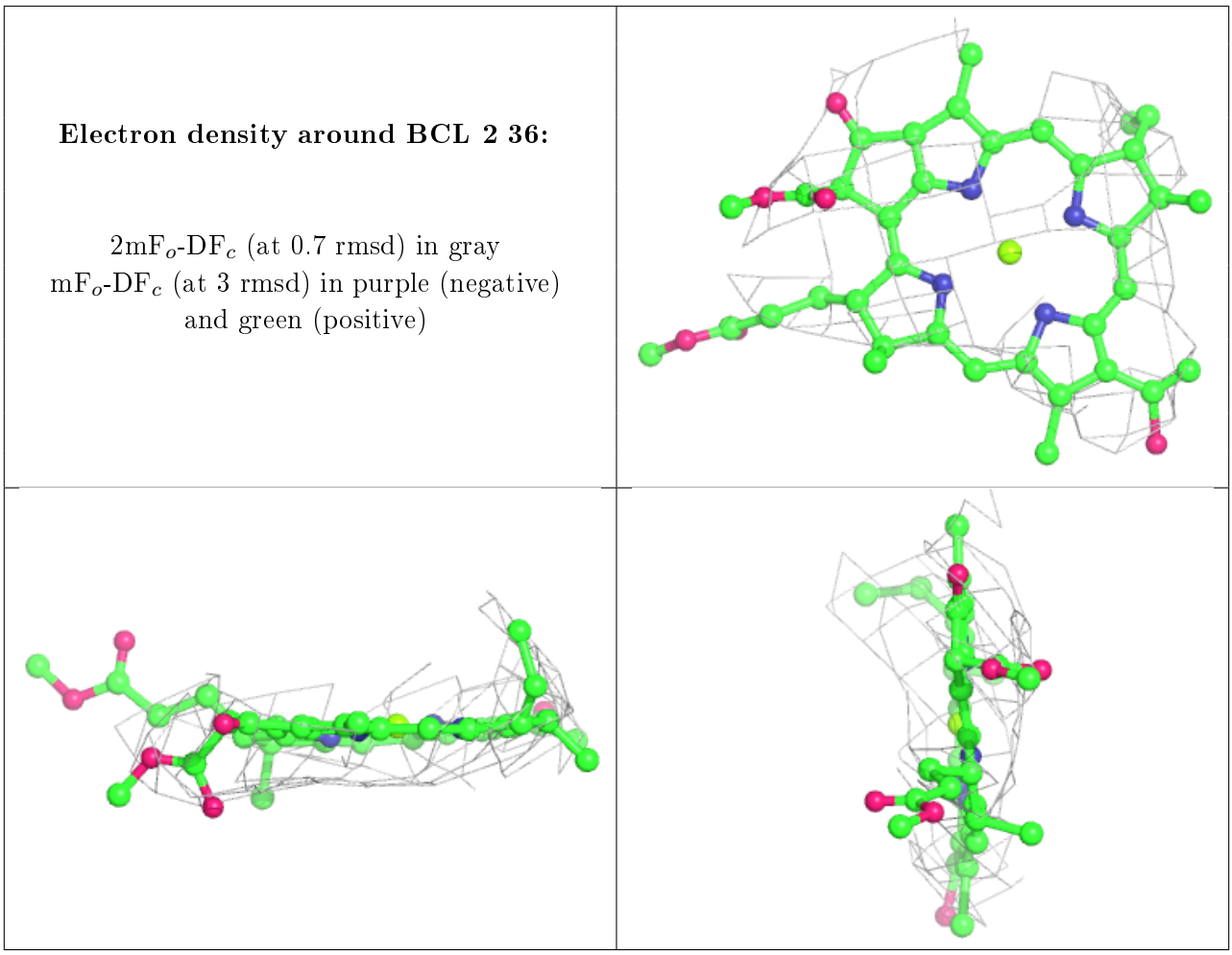






Electron density around BCL 2 36:

$2mF_o$-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.