Bond precision: \( C-C = 0.0033 \text{ Å} \)

Wavelength: 0.71073 Å

Cell:
- \( a = 9.9440(4) \) Å
- \( b = 9.3620(4) \) Å
- \( c = 18.5299(7) \) Å
- \( \alpha = 90 \)°
- \( \beta = 95.626(3) \)°
- \( \gamma = 90 \)°

Temperature: 150 K

Volume: \( 1716.75(12) \) Å\(^3\)

Space group: \( P\ 21/c \)

Hall group: \(-P\ 2ybc\)

Moiety formula: \( \text{C}_{12}\ H_{18}\ Cl\ Cu\ N_{4}\ O,\ B\ F_{4}\)

Sum formula: \( \text{C}_{12}\ H_{18}\ B\ Cl\ Cu\ F_{4}\ N_{4}\ O\)

\( \text{Mr} = 420.11 \)

\( \text{Dx, g cm}^{-3} = 1.625 \)

\( Z = 4 \)

\( \mu = 1.475 \)

\( F_{000} = 852.0 \)

\( F_{000}' = 854.27 \)

\( h,k,l, \max = 12,12,24 \)

\( \text{Tmin', Tmax} = 0.370, 0.642 \)

\( \text{Correction method} = \text{MULTI-SCAN} \)

\( \text{Data completeness} = 0.999 \)

\( \theta(\text{max}) = 27.483 \)

\( R(\text{reflections}) = 0.0334(3327) \)

\( w R^2(\text{reflections}) = 0.0858(3931) \)

\( S = 1.050 \)

\( \text{Npar} = 249 \)

The following ALERTS were generated. Each ALERT has the format

**test-name_ALERT_alert-type_alert-level**

Click on the hyperlinks for more details of the test.

### Alert level C

**PLAT244_ALERT_4_C** Low 'Solvent' Ueq as Compared to Neighbors of B1 Check

**PLAT712_ALERT_1_C** ANGLE Unknown or Inconsistent Label ............ F3BB Check

**PLAT712_ALERT_1_C** ANGLE Unknown or Inconsistent Label ............ F3BB Check

**PLAT712_ALERT_1_C** ANGLE Unknown or Inconsistent Label ............ F3BB Check

**PLAT712_ALERT_1_C** ANGLE Unknown or Inconsistent Label ............ F3BB Check

**PLAT712_ALERT_1_C** ANGLE Unknown or Inconsistent Label ............ F3BB Check

**PLAT712_ALERT_1_C** ANGLE Unknown or Inconsistent Label ............ F3BB Check

**PLAT712_ALERT_1_C** ANGLE Unknown or Inconsistent Label ............ F3BB Check

### Alert level G

**PLAT063_ALERT_4_G** Crystal Size Likely too Large for Beam Size .... 0.70 mm

**PLAT302_ALERT_4_G** Anion/Solvent/Minor-Residue Disorder (Resd 2) 60% Note

**PLAT883_ALERT_1_G** No Info/Value for _atom_sites_solution_primary. Please Do!

**PLAT910_ALERT_3_G** Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation); however, if you intend to submit to Acta Crystallographica Section C or E or IUCrData, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the Notes for Authors of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

Datablock 1 - ellipsoid plot
Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry