

## Datablock: 2

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Bond precision: C-C = 0.0034 A Wavelength=0.71073  
Cell: a=10.1820(6) b=8.6362(6) c=18.7170(11)  
alpha=90 beta=95.178(5) gamma=90  
Temperature 293 K  
:  
Calculated Reported  
Volume 1639.14(18) 1639.14(19)  
Space group P 21/c P 21/c  
Hall group -P 2ybc -P 2ybc  
Moiety formula C12 H18 Cl Cu N5 O4 ?  
Sum formula C12 H18 Cl Cu N5 O4  
Mr 395.31 395.30  
Dx,g cm-3 1.602 1.602  
Z 4 4  
Mu (mm-1) 1.522 1.522  
F000 812.0 812.0  
F000' 814.13  
h,k,lmax 13,11,24 12,11,24  
Nref 3752 3657  
Tmin,Tmax 0.760,0.859 0.681,1.000  
Tmin' 0.587  
Correction method= # Reported T Limits: Tmin=0.681  
Tmax=1.000 AbsCorr = MULTI-SCAN  
Data completeness= 0.975 Theta(max)= 27.484  
R(reflections)= 0.0346( 2788) wR2(reflections)= 0.0872( 3657)  
S = 1.034 Npar= 212

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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.

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### ● Alert level C

<a href="#">PLAT230_ALERT_2_C</a>	Hirshfeld Test Diff for 01 --C8 .	5.1 s.u.
<a href="#">PLAT241_ALERT_2_C</a>	High 'MainMol' Ueq as Compared to Neighbors of	02 Check
<a href="#">PLAT242_ALERT_2_C</a>	Low 'MainMol' Ueq as Compared to Neighbors of	N5 Check
<a href="#">PLAT911_ALERT_3_C</a>	Missing FCF Refl Between Thmin & STh/L= 0.600	2 Report

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### ● Alert level G

<a href="#">PLAT199_ALERT_1_G</a>	Reported _cell_measurement_temperature ..... (K)	293 Check
<a href="#">PLAT200_ALERT_1_G</a>	Reported _diffrn_ambient_temperature ..... (K)	293 Check
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Cu1 (II) .	2.23 Info
<a href="#">PLAT883_ALERT_1_G</a>	No Info/Value for _atom_sites_solution_primary .	Please Do !
<a href="#">PLAT910_ALERT_3_G</a>	Missing # of FCF Reflection(s) Below Theta(Min).	3 Note
<a href="#">PLAT912_ALERT_4_G</a>	Missing # of FCF Reflections Above STh/L= 0.600	76 Note
<a href="#">PLAT978_ALERT_2_G</a>	Number C-C Bonds with Positive Residual Density.	2 Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check
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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.

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

## Datablock 2 - ellipsoid plot

