

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

**Datablock: shelx**

Bond precision:	C-C = 0.0051 A	Wavelength=1.54178	
Cell:	a=15.6899 (5)	b=10.7161 (3)	c=11.3062 (4)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	1900.96(11)	1900.96(11)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C18 H26 Cu N4 O4	?
Sum formula	C18 H26 Cu N4 O4	C18 H26 Cu N4 O4
Mr	425.98	425.97
Dx, g cm-3	1.488	1.488
Z	4	4
Mu (mm-1)	1.897	1.897
F000	892.0	892.0
F000'	886.52	
h, k, lmax	18, 12, 13	18, 12, 13
Nref	1742	1721
Tmin, Tmax	0.746, 0.767	0.658, 0.753
Tmin'	0.519	

Correction method= # Reported T Limits: Tmin=0.658 Tmax=0.753  
AbsCorr = MULTI-SCAN

Data completeness= 0.988                      Theta (max)= 68.325

R(reflections)= 0.0475( 1696)	wR2(reflections)= 0.1402( 1721)
S = 1.143	Npar= 126

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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 B

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for C7 --C8 . 8.7 s.u.

**Author Response: Some of the atoms were not ideally shaped due to thermal disorder. However, this doesn't indicate an incorrect atom-type assignment.**

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#### Alert level C

PLAT415\_ALERT\_2\_C Short Inter D-H..H-X H2 ..H8 . 2.14 Ang.  
x,1-y,-1/2+z = 7\_565 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.746 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 18 Report  
5 1 0, 3 1 1, 0 0 2, 0 2 2, 1 2 2, 2 0 2,  
0 2 3, 0 0 4, 0 2 4, 1 0 4, 2 0 4, 1 1 5,  
2 1 5, 0 0 6, 1 0 6, 1 1 6, 2 1 6, 1 1 7,  
PLAT934\_ALERT\_3\_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check  
0 2 0,

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#### Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 1 Report  
H2  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Cu1 (II) . 2.31 Info  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT899\_ALERT\_4\_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note  
1 1 0, 2 0 0,  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 1 Note  
PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 1 Note  
2 0 0,  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 7.20 Note  
Predicted wR2: Based on SigI\*\*2 1.95 or SHELX Weight 12.74  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 6 Info

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

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

