

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 4

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Bond precision:	C-C = 0.0051 A	Wavelength=0.71073
Cell:	a=10.8070(6)	b=17.7249(13)      c=13.4503(7)
	alpha=90	beta=91.991(5)      gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	2574.9(3)	2574.9(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H30 Cu N4 O6	2(C14 H15 Cu0.5 N2 O3)
Sum formula	C28 H30 Cu N4 O6	C28 H30 Cu N4 O6
Mr	582.11	582.10
Dx,g cm-3	1.502	1.502
Z	4	4
Mu (mm-1)	0.900	0.900
F000	1212.0	1212.0
F000'	1213.76	
h,k,lmax	15,24,18	15,23,18
Nref	7557	6603
Tmin,Tmax	0.947,0.956	0.560,1.000
Tmin'	0.638	

Correction method= # Reported T Limits: Tmin=0.560 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.874      Theta(max)= 30.073

R(reflections)= 0.0563( 3330)      wR2(reflections)= 0.1274( 6603)

S = 0.986      Npar= 363

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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.



### Alert level C

PLAT352_ALERT_3_C	Short	N-H (X0.87,N1.01A)	N3	- H3	.	0.74 Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond	C11	- C110	.	1.53 Ang.



### Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1 --N3 .	5.1 s.u.
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O4	109.7 Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact C110 ..C210	3.13 Ang.
	x,y,z =	1_555 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II) .	2.03 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu2 (II) .	2.05 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !

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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  
 2 **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

2 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  
 1 ALERT type 3 Indicator that the structure quality may be low  
 0 ALERT type 4 Improvement, methodology, query or suggestion  
 2 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.

Datablock 4 - ellipsoid plot

