

# 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: yn45

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Bond precision:    C-C = 0.0051 Å                      Wavelength=1.54184

Cell:                      a=23.4161(3)              b=13.2985(1)              c=7.2391(1)  
                            alpha=90                      beta=90                      gamma=90  
Temperature:              100 K

	Calculated	Reported
Volume	2254.25(5)	2254.25(5)
Space group	C m c 21	C m c 21
Hall group	C 2c -2	C 2c -2
Moiety formula	C17 H18 Cu N4 O8 S2, 2(H2 O)	C17 H18 Cu N4 O8 S2, 2(H2 O)
Sum formula	C17 H22 Cu N4 O10 S2	C17 H22 Cu N4 O10 S2
Mr	570.06	570.04
Dx, g cm-3	1.680	1.680
Z	4	4
Mu (mm-1)	3.670	3.670
F000	1172.0	1172.0
F000'	1170.31	
h,k,lmax	28,15,8	28,15,8
Nref	2089[ 1137]	1940
Tmin,Tmax	0.738,0.802	0.639,1.000
Tmin'	0.660	

Correction method= # Reported T Limits: Tmin=0.639 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.71/0.93                      Theta(max)= 67.491

R(reflections)= 0.0321( 1926)                      wR2(reflections)= 0.0822( 1940)

S = 1.031                                      Npar= 175

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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

PLAT090\_ALERT\_3\_C Poor Data / Parameter Ratio (Zmax > 18) ..... 6.50 Note

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### Alert level G

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report  
PLAT142\_ALERT\_4\_G s.u. on b - Axis Small or Missing ..... 0.00010 Ang.  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O1S ..C1 2.99 Ang.  
1-x,y,z = 4\_655 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 2 Note  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Cu1 (II) . 2.20 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  
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 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  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

# start Validation Reply Form

\_vrf\_PLAT090\_yn45

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PROBLEM: Poor Data / Parameter Ratio (Zmax > 18) ..... 6.50 Note

RESPONSE: ...

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# end Validation Reply Form

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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.

