

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

Bond precision:	C-C = 0.0051 A	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

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 10/08/2020; check.def file version of 19/03/2021

