

# 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: s

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Bond precision:    C-C = 0.0116 A                      Wavelength=0.71073

Cell:                      a=7.2491(14)                      b=9.1431(18)                      c=12.370(3)  
                                    alpha=107.40(3)                      beta=92.38(3)                      gamma=102.99(3)

Temperature:            293 K

	Calculated	Reported
Volume	757.1(3)	757.1(3)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C20 H22 Cu N10 O2 S2	?
Sum formula	C20 H22 Cu N10 O2 S2	C20 H22 Cu N10 O2 S2
Mr	562.15	562.14
Dx,g cm-3	1.233	1.233
Z	1	1
Mu (mm-1)	0.891	0.891
F000	289.0	289.0
F000'	289.64	
h,k,lmax	8,10,14	8,10,14
Nref	2675	2637
Tmin,Tmax	0.759,0.807	0.907,1.000
Tmin'	0.759	

Correction method= # Reported T Limits: Tmin=0.907 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.986                      Theta(max)= 25.000

R(reflections)= 0.0978( 2261)                      wR2(reflections)= 0.3286( 2637)

S = 1.138                                      Npar= 162

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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**

PLAT094\_ALERT\_2\_B Ratio of Maximum / Minimum Residual Density .... 5.15 Report  
PLAT601\_ALERT\_2\_B Structure Contains Solvent Accessible VOIDS of . 188 Ang3

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**Alert level C**

DIFMX01\_ALERT\_2\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
  \_refine\_diff\_density\_max given = 2.601  
  Test value = 2.175  
DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
  The relevant atom site should be identified.  
RFACR01\_ALERT\_3\_C The value of the weighted R factor is > 0.25  
  Weighted R factor given 0.329  
PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.33 Report  
PLAT097\_ALERT\_2\_C Large Reported Max. (Positive) Residual Density 2.60 eA-3  
PLAT341\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0116 Ang.

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**Alert level G**

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 1 Info  
PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF Please Do !  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large. 0.18 Report  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large. 5.93 Why ?  
PLAT093\_ALERT\_1\_G No su's on H-positions, refinement reported as . mixed Check  
PLAT154\_ALERT\_1\_G The su's on the Cell Angles are Equal ..... 0.0300 Degree  
PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check  
PLAT200\_ALERT\_1\_G Reported \_diffn\_ambient\_temperature ..... (K) 293 Check  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 3 Do !  
  N1 -CU1 -N1 -C1 12.00 0.00 2.665 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 6 Do !  
  N1 -CU1 -N1 -C5 6.00 0.00 2.665 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 7 Do !  
  N2 -CU1 -N2 -C7 15.00 0.00 2.665 1.555 1.555 1.555  
PLAT710\_ALERT\_4\_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 28 Do !  
  CU1 -N2 -C7 -S1 -136.00 37.00 1.555 1.555 1.555  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Cu1 (II) ..... 2.36 Note  
PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
5 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*, 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 21/04/2015; check.def file version of 09/03/2015**

