checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_8v00498_0m_a

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: cu_8v00498_0m_a

```
Bond precision:   C-C = 0.0025 A              Wavelength=1.54178

Cell:             a=9.143(5)      b=9.617(8)           c=15.379(7)
                  alpha=90        beta=103.96(3)       gamma=90
Temperature:      100 K

                  Calculated                Reported
Volume            1312.3(14)                1312.4(14)
Space group       P 21/n                    P 1 21/n 1
Hall group        -P 2yn                    -P 2yn
Moiety formula    C15 H10 N2 O4 S           C15 H10 N2 O4 S
Sum formula       C15 H10 N2 O4 S           C15 H10 N2 O4 S
Mr                314.31                    314.31
Dx,g cm-3         1.591                     1.591
Z                 4                         4
Mu (mm-1)         2.404                     2.404
F000              648.0                     648.0
F000'             651.36
h,k,lmax          11,11,18                  11,11,18
Nref              2496                      2493
Tmin,Tmax         0.794,0.908               0.588,0.753
Tmin'             0.649

Correction method= # Reported T Limits: Tmin=0.588 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.999        Theta(max)= 70.229

R(reflections)= 0.0308( 2200)     wR2(reflections)= 0.0780( 2493)

S = 1.044                 Npar= 199
```

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

```
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C1      - C2      .       1.53 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     2.560 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600         3 Report
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Alert level G

```
PLAT432_ALERT_2_G Short Inter X...Y Contact  O4      ..C1             2.82 Ang.
                                     1/2-x,-1/2+y,1/2-z  =     2_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O4      ..C2             2.90 Ang.
                                     1/2-x,-1/2+y,1/2-z  =     2_545 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        9 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
   3 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

   1 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
   2 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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 05/12/2020; check.def file version of 05/12/2020