checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:  C-C = 0.0036 A          Wavelength=0.71073

Cell:           a=15.1231(9)    b=26.5571(15)       c=12.1855(6)
                alpha=90        beta=100.591(2)     gamma=90
Temperature:    200 K

                Calculated                Reported
Volume          4810.6(5)                 4810.6(5)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C22 H17 Cu I2 N5 O S      C22 H17 Cu I2 N5 O S
Sum formula     C22 H17 Cu I2 N5 O S      C22 H17 Cu I2 N5 O S
Mr              716.82                    716.80
Dx,g cm-3       1.980                     1.979
Z               8                         8
Mu (mm-1)       3.586                     3.586
F000            2744.0                    2744.0
F000'           2740.71
h,k,lmax        23,40,18                  23,40,18
Nref            18348                     18325
Tmin,Tmax       0.530,0.699               0.567,0.747
Tmin'           0.483

Correction method= # Reported T Limits: Tmin=0.567 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 33.145

R(reflections)= 0.0297( 15514)    wR2(reflections)= 0.0734( 18325)

S = 1.067                 Npar= 577
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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

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PLAT480_ALERT_4_C Long H...A H-Bond Reported H13C     ..I1       .       3.18 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H16      ..I1       .       3.14 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H22      ..I4       .       3.31 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H23      ..I3       .       3.26 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H24      ..S1       .       2.94 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H35A     ..I2       .       3.30 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H35C     ..I2       .       3.31 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H36B     ..I2       .       3.32 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.234 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).        10 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        10 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..         1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.76A   From I3             1.70 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.68A   From I4             1.65 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H35A            -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H35B            -0.37 eA-3
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Alert level G

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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.72 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1      --S1       .       10.5 s.u.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C13 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C14 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C35 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C36 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.35 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2       (II)      .       2.36 Info
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          4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         8 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         5 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
  16 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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
  13 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.

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

Datablock shelx - ellipsoid plot