checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mk1094

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: mk1094

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Bond precision:   C-C = 0.0098 A           Wavelength=0.71073

Cell:             a=24.916(2)      b=9.3586(9)        c=9.3255(9)
                  alpha=90         beta=92.291(3)     gamma=90
Temperature:      296 K

                  Calculated                 Reported
Volume            2172.8(3)                  2172.8(4)
Space group       P 21/c                     P 21/c
Hall group        -P 2ybc                    -P 2ybc
Moiety formula    C16 H32 Cu N6 O4           ?
Sum formula       C16 H32 Cu N6 O4           C16 H32 Cu N6 O4
Mr                436.03                     436.01
Dx,g cm-3         1.333                      1.333
Z                 4                          4
Mu (mm-1)         1.037                      1.037
F000              924.0                      924.0
F000'             925.57
h,k,lmax          31,11,11                   31,11,11
Nref              4457                       4439
Tmin,Tmax                                    0.527,0.745
Tmin'

Correction method= # Reported T Limits: Tmin=0.527 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.996        Theta(max)= 26.418

R(reflections)= 0.0671( 3222)     wR2(reflections)= 0.1546( 4439)

S = 1.090                    Npar= 307
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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 C

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PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...      Please Check
PLAT054_ALERT_1_C Medium   Crystal Dimension Missing (or Error) ...      Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...      Please Check
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range       5.6 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range      10.0 Ratio
PLAT245_ALERT_2_C U(iso) H1         Smaller than U(eq) N1       by      0.016 Ang**2
PLAT245_ALERT_2_C U(iso) H3         Smaller than U(eq) N3       by      0.021 Ang**2
PLAT245_ALERT_2_C U(iso) H4         Smaller than U(eq) N4       by      0.022 Ang**2
PLAT245_ALERT_2_C U(iso) H6         Smaller than U(eq) N6       by      0.024 Ang**2
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cu1      0.081 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00975 Ang.
PLAT352_ALERT_3_C Short  N-H (X0.87,N1.01A)  N1       - H1       .      0.76 Ang.
PLAT352_ALERT_3_C Short  N-H (X0.87,N1.01A)  N4       - H4       .      0.72 Ang.
PLAT352_ALERT_3_C Short  N-H (X0.87,N1.01A)  N6       - H6       .      0.74 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N1       --H1       .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N3       --H3       .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N4       --H4       .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N6       --H6       .     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     4.939 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         9 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....        5 Note
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.       0 Info
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      10 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        3 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     8.75 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records        1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        3 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records        1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )     22% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      14 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      27 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        9 Note
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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
  22 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  12 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
  11 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 06/01/2019; check.def file version of 19/12/2018