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

```
Bond precision:   C-C = 0.0043 A           Wavelength=0.71073

Cell:             a=11.7258(13)     b=12.8692(14)      c=12.6384(14)
                  alpha=90          beta=96.173(2)     gamma=90
Temperature:      273 K

                 Calculated                  Reported
Volume           1896.1(4)                   1896.1(4)
Space group      P 21/n                      P 21/n
Hall group       -P 2yn                      -P 2yn
Moiety formula   C36 H30 Cu2 N6 O12, 4(H2 O) ?
Sum formula      C36 H38 Cu2 N6 O16          C36 H38 Cu2 N6 O16
Mr               937.82                      937.80
Dx,g cm-3        1.643                       1.643
Z                2                           2
Mu (mm-1)        1.206                       1.206
F000             964.0                       964.0
F000'            965.74
h,k,lmax         13,15,15                    13,15,15
Nref             3337                        3306
Tmin,Tmax        0.785,0.810                 0.794,0.817
Tmin'            0.785

Correction method= # Reported T Limits: Tmin=0.794 Tmax=0.817
AbsCorr = ?

Data completeness= 0.991            Theta(max)= 25.009

R(reflections)= 0.0376( 2929)                    wR2(reflections)=
                                                 0.1003( 3306)
S = 1.089                  Npar= 275
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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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PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.61 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O4       --C7       .        7.0 s.u.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.406 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         31 Report
                   2  0  0,  12  5  0, -12  3  1, -13  4  1,  -5  9  1,   7  9  1,
                   8 11  1,  -4  6  2,  -5  7  2,   8 10  2,   8 11  3,  -4  9  4,
                  -3  9  4,  -5 10  4,  -4 10  4,  -5 11  4,  -4 10  5,  -2 11  5,
                  -1  7  6,  -2  9  6,  -2 10  6,  -1 10  6,   6 10  6,  -3 12  6,
                  -7  3  7,   0 10  7,   0 11  7,   1  0  9,  -4  0 12,  -6  0 14,
                  -5  1 14,
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          2 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          5 Report
              H1B   H2A   H2B   H3A   H3B
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        273 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
              H2 O
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.26 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         10 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated   and Succeeded by SHELXL     2019/3 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        77% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
              -12  3  1,  -5 10  4, -13  4  1,   6 10  6,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.8 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       50.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.993 Note
              Predicted wR2: Based on SigI**2  3.35 or SHELX Weight  9.21
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 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
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
23 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  7 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
  6 ALERT type 4 Improvement, methodology, query or suggestion
  4 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 11/11/2024; check.def file version of 11/11/2024

Datablock shelx - ellipsoid plot