checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rf1148

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: rf1148

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Bond precision:    C-C = 0.0102 A            Wavelength=0.71073

Cell:            a=11.7640(8)     b=15.6015(10)        c=14.7695(11)
                 alpha=90         beta=99.030(4)       gamma=90
Temperature:     100 K

                   Calculated                 Reported
Volume           2677.1(3)                  2677.1(3)
Space group      P 21/c                     P 21/c
Hall group       -P 2ybc                    -P 2ybc
Moiety formula   C22 H32 Cl Cu N4 O2, F6 P  C22 H32 Cl Cu N4 O2, F6 P
Sum formula      C22 H32 Cl Cu F6 N4 O2 P   C22 H32 Cl Cu F6 N4 O2 P
Mr               628.49                     628.47
Dx,g cm-3        1.559                      1.559
Z                4                          4
Mu (mm-1)        1.045                      1.045
F000             1292.0                     1292.0
F000'            1294.94
h,k,lmax         14,19,18                   14,19,18
Nref             5263                       5058
Tmin,Tmax        0.829,0.910                0.810,0.932
Tmin'            0.829

Correction method= # Reported T Limits: Tmin=0.810 Tmax=0.932
AbsCorr = MULTI-SCAN

Data completeness= 0.961         Theta(max)= 26.000

R(reflections)= 0.0826( 3742)     wR2(reflections)= 0.1916( 5058)

S = 1.177                    Npar= 381
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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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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.970 Why?
PLAT213_ALERT_2_C Atom C10             has ADP max/min Ratio .....         3.4 oblate
PLAT213_ALERT_2_C Atom C11             has ADP max/min Ratio .....         3.8 oblate
PLAT213_ALERT_2_C Atom C16             has ADP max/min Ratio .....         3.8 oblate
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.01019 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......       9.264 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......       2.272 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         145 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H21B             -0.36 eA-3
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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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        5 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT   Unusually Large    32.30 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT244_ALERT_4_G Low     'Solvent' Ueq as Compared to Neighbors of       P7 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       57% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  Cl1B     ..C10            3.25 Ang.
                                  x,1/2-y,1/2+z  =       4_566 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       30 Note
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        50 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...       18 Note
PLAT954_ALERT_1_G Reported (CIF) and Actual (FCF) Kmax Differ by .        1 Units
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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
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   2 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
   7 ALERT type 3 Indicator that the structure quality may be low
   5 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 03/05/2019; check.def file version of 29/04/2019