checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 13138

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: 13138**

Bond precision: C-C = 0.0020 Å  Wavelength=0.71073

Cell:  
a=7.5467(3)  b=12.7659(6)  c=17.0298(8)  
alpha=90  beta=102.574(2)  gamma=90

Temperature: 100 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>1601.31(12)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/n</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2yn</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C14 H16 Cl2 Cu N4 O2</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C14 H16 Cl2 Cu N4 O2</td>
</tr>
<tr>
<td>Mr</td>
<td>406.76</td>
</tr>
<tr>
<td>Dx,g cm-3</td>
<td>1.687</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm-1)</td>
<td>1.711</td>
</tr>
<tr>
<td>F000</td>
<td>828.0</td>
</tr>
<tr>
<td>F000’</td>
<td>830.67</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>10,17,22</td>
</tr>
<tr>
<td>Nref</td>
<td>3981</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.413,0.599</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.375</td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.453 Tmax=0.628  
AbsCorr = MULTI-SCAN

Data completeness= 1.000   Theta(max)= 28.313

R(reflections)= 0.0240( 3779)     wR2(reflections)= 0.0672(3981)

S = 1.000   Npar= 213

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

PLAT480_ALERT_4_C Long H...A H-Bond Reported H1 .. CL1 .. 2.92 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H8 .. CL1 .. 2.93 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H3A2 .. CL1 .. 2.95 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cul -- CL1 .. 6.0 su
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ............ 6 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cul (II) ...... 2.14 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............. 1 Note

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
6 ALERT level G = General information/check it is not something unexpected

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, 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 21/06/2015; check.def file version of 21/06/2015

Datablock 13138 - ellipsoid plot