**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 15115_sq

**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: 15115_sq**

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0080 Å</th>
<th>Wavelength=0.71073</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td>a=10.0766(16)</td>
<td>b=33.708(6)</td>
</tr>
<tr>
<td>alpha=90</td>
<td>beta=91.135(2)</td>
<td>gamma=90</td>
</tr>
<tr>
<td>Temperature:</td>
<td>100 K</td>
<td></td>
</tr>
<tr>
<td>Volume</td>
<td>3772.6(11)</td>
<td>3772.6(11)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/n</td>
<td>P 21/n</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2yn</td>
<td>-P 2yn</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C33 H26 Cu2 N9 O4, B F4</td>
<td>C33 H26 Cu2 N9 O4, B F4</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C33 H26 B Cu2 F4 N9 O4</td>
<td>C33 H26 B Cu2 F4 N9 O4</td>
</tr>
<tr>
<td>Mr</td>
<td>826.54</td>
<td>826.52</td>
</tr>
<tr>
<td>Dx, g cm^{-3}</td>
<td>1.455</td>
<td>1.455</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm^{-1})</td>
<td>1.195</td>
<td>1.195</td>
</tr>
<tr>
<td>F000</td>
<td>1672.0</td>
<td>1672.0</td>
</tr>
<tr>
<td>F000’</td>
<td>1675.25</td>
<td></td>
</tr>
<tr>
<td>h,k,l_{max}</td>
<td>13,44,14</td>
<td>13,44,14</td>
</tr>
<tr>
<td>Nref</td>
<td>8900</td>
<td>8831</td>
</tr>
<tr>
<td>Tmin,T_{max}</td>
<td>0.818,0.866</td>
<td>0.701,0.870</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.682</td>
<td></td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.701 Tmax=0.870
AbsCorr = MULTI-SCAN

Data completeness= 0.992

Theta(max)= 27.761

R(reflections)= 0.0844( 7272)
wr2(reflections)= 0.1953( 8831)

S = 1.184  Npar= 577

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 A
0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
12 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Alert level B
PLAT420_ALERT_2_B D-H Without Acceptor O1S  -  H1SA ..  Please Check
PLAT420_ALERT_2_B D-H Without Acceptor O1S  -  H1SB ..  Please Check

Alert level C
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ............... 0.0080 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2A .. O1C .. 2.62 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1B .. F4D' .. 2.64 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1B .. O1S .. 2.65 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2C .. F2D' .. 2.60 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ...... 7.649 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ...... 2.704 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 6 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check
PLAT975_ALERT_2_C Check Calcd Residual Density 1.07A From O1C 0.57 eA-3

Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 14 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 27.80 Why ?
PLAT302_ALERT_4_G Anion/Solvent Disorder ............... Percentage = 100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 1.69) in Resd. # 2 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 1.82) in Resd. # 3 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms ( 1.50) in Resd. # 4 Check
PLAT665_ALERT_4_G Structure Contains Solvent Accessible VOIDS of . 250 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .......... 12 Note
PLAT880_ALERT_3_G Number of Least-Squares Restraints ............. 574 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 64 Note
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