# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision:   C-C = 0.0013 A                Wavelength=0.71073

Cell:           a=7.8673(5)          b=11.0031(7)        c=11.7131(6)
                alpha=82.325(2)    beta=89.994(2)    gamma=81.179(2)
Temperature:    100 K

|                | Calculated | Reported |
|----------------|------------|----------|
| Volume         | 992.76(10) | 992.76(10) |
| Space group    | P -1 | P -1 |
| Hall group     | -P 1 | -P 1 |
| Moiety formula | C36 H20 Br3.77 Cl8 Cu2 N4 | C36 H20 Br3.77 Cl8 Cu2 N4 |
| Sum formula    | C36 H20 Br3.77 Cl8 Cu2 N4 | C36 H20 Br3.77 Cl8 Cu2 N4 |
| Mr             | 1220.83 | 1220.83 |
| Dx,g cm-3      | 2.042 | 2.041 |
| Z              | 1 | 1 |
| Mu (mm-1)      | 5.443 | 5.438 |
| F000           | 590.1 | 590.0 |
| F000'          | 591.03 | |
| h,k,lmax       | 15,21,23 | 15,21,23 |
| Nref           | 16613 | 16169 |
| Tmin,Tmax      | 0.240,0.337 | 0.338,0.447 |
| Tmin'          | 0.143 | |

Correction method= # Reported T Limits: Tmin=0.338 Tmax=0.447
AbsCorr = EMPIRICAL

Data completeness= 0.973          Theta(max)= 45.293

R(reflections)= 0.0250( 13645)     wR2(reflections)= 0.0671( 16169)

S = 1.062                    Npar= 245

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 B
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..        4 Check

> **Author Response: This error refers to (2 -9 4), (-5 7 5), (5 -8 7) and (-6 -1 7)
> outliers, which have been likely over-corrected for absorption. Due to surface
> roughness and black crystal colour, applying a reliable analytical correction was
> impossible. Including or not these outliers out of 16169 symmetry-independent
> reflections in the data set do not change significantly the spherical atoms
> outcomes.**

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### 🟡 Alert level C
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..    Please Check

> **Author Response: The presence of non-integer number of atoms is
> consistent with the fractional occupance of the bromine atom BR1.**

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### ⚪ Alert level G
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...    Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Br1       --Cu        .      29.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu        --N1        .       8.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu        --N2        .       9.5 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )        3% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1 )     73.77 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl1       ..Cl12           3.27 Ang.
                                             -1+x,1+y,-1+z  =      1_464 Check
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       444 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        7 Info

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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
   1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  11 **ALERT level G** = General information/check it is not something unexpected

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

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# checkCIF publication errors

## Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
           empty.

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 0 ALERT level A = Data missing that is essential or data in wrong format
 1 ALERT level G = General alerts. Data that may be required is missing
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**Publication of your CIF**

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

**PLATON version of 22/12/2019; check.def file version of 13/12/2019**