checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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 = 0.0072 A           Wavelength=0.71073

Cell:          a=7.706(5)         b=10.274(5)        c=13.666(5)
               alpha=93.846(5)   beta=92.271(5)   gamma=107.216(5)
Temperature:   293 K

                  Calculated                    Reported
Volume            1029.1(9)                     1029.1(9)
Space group       P -1                          P -1
Hall group        -P 1                          -P 1
                  C9 H9 Cl3 Cu N O4, C6 H16
Moiety formula    N                             C15 H25 Cl3 Cu N2 O4

Sum formula       C15 H25 Cl3 Cu N2 O4          C15 H25 Cl3 Cu N2 O4
Mr                467.27                        467.26
Dx,g cm-3         1.508                         1.508
Z                 2                             2
Mu (mm-1)         1.471                         1.471
F000              482.0                         482.0
F000'             483.67
h,k,lmax          10,13,18                      10,13,18
Nref              5053                          4604
Tmin,Tmax         0.650,0.802                   4.900,
Tmin'             0.637

Correction method= # Reported T Limits: Tmin=4.900 Tmax=*****
AbsCorr = NUMERICAL

Data completeness= 0.911            Theta(max)= 28.162

R(reflections)= 0.0399( 1758)       wR2(reflections)= 0.0688( 4604)

S = 0.684                    Npar= 233
```

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 B
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low ..   38% Check
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low .   0.940 Why?

🟡 Alert level C
GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
            outside the range 0.80 <> 2.00
            Goodness of fit given =   0.684
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
            Rint given   0.126
PLAT223_ALERT_4_C Solv./Anion Resd 2   H   Ueq(max)/Ueq(min) Range   6.7 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O2 Check
PLAT245_ALERT_2_C U(iso) H22   Smaller than U(eq) N2   by   0.016 Ang**2
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.00722 Ang.
PLAT761_ALERT_1_C CIF Contains no X-H Bonds ....   Please Check
PLAT762_ALERT_1_C CIF Contains no X-Y-H or H-Y-H Angles ....   Please Check

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⚪ Alert level G
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ....   0.126 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT153_ALERT_1_G The s.u.'s on the Cell Axes   are Equal ..(Note)   0.005 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.005 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)   293 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #   2 Note
             C6 H16 N
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1   (II)   .   2.01 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters   2 Info
PLAT883_ALERT_1_G No Info for _atom_sites_solution_primary ....   Please Do !

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

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

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checkCIF publication errors

🔴 Alert level A

```
PUBL006_ALERT_1_A  _publ_requested_journal is missing
           e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
           Abstract of paper in English.
```

⚪ Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
           empty.
```

```
3 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
```

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 level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
```

```
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

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 18/02/2019; check.def file version of 18/02/2019

Datablock I - ellipsoid plot