# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) nos014_150k

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: nos014_150k

Bond precision:   C-C = 0.0094 A           Wavelength=1.34143

Cell:          a=27.6940(16)     b=15.9902(7)         c=7.8753(6)
               alpha=90          beta=102.343(5)      gamma=90
Temperature:   150 K

|                  | Calculated          | Reported            |
|------------------|---------------------|---------------------|
| Volume           | 3406.8(4)           | 3406.8(4)           |
| Space group      | C 2/c               | C 1 2/c 1           |
| Hall group       | -C 2yc              | -C 2yc              |
| Moiety formula   | C35 H30 Cu2 F N3 O8 | C35 H30 Cu2 F N3 O8 |
| Sum formula      | C35 H30 Cu2 F N3 O8 | C35 H30 Cu2 F N3 O8 |
| Mr               | 766.72              | 766.70              |
| Dx,g cm-3        | 1.495               | 1.495               |
| Z                | 4                   | 4                   |
| Mu (mm-1)        | 7.083               | 7.077               |
| F000             | 1568.0              | 1568.0              |
| F000'            | 1549.31             |                     |
| h,k,lmax         | 34,20,9             | 34,19,9             |
| Nref             | 3604                | 3531                |
| Tmin,Tmax        | 0.199,0.280         | 0.012,0.083         |
| Tmin'            | 0.127               |                     |

Correction method= # Reported T Limits: Tmin=0.012 Tmax=0.083
AbsCorr = MULTI-SCAN

Data completeness= 0.980          Theta(max)= 57.942

R(reflections)= 0.0907( 2854)     wR2(reflections)= 0.2590( 3531)

S = 1.151                 Npar= 227

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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PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................   0.26 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference F1      --C15    .     0.16 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00942 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......  4.849 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600      9 Report
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## Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...      1 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension      1 Info
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large   0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large  15.02 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group     C2/c  I2/a Note
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records      1 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1        (II)    .     2.14 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      6 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600     57 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...      2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      3 Info
PLAT984_ALERT_1_G The  C-f'=    0.0148 Deviates from the B&C-Value  0.0137 Check
PLAT984_ALERT_1_G The Cu-f'=   -2.9183 Deviates from the B&C-Value -2.7974 Check
PLAT984_ALERT_1_G The  F-f'=    0.0600 Deviates from the B&C-Value  0.0583 Check
PLAT984_ALERT_1_G The  N-f'=    0.0253 Deviates from the B&C-Value  0.0241 Check
PLAT984_ALERT_1_G The  O-f'=    0.0412 Deviates from the B&C-Value  0.0389 Check
PLAT985_ALERT_1_G The Cu-f"=    3.6937 Deviates from the B&C-Value  3.6876 Check
PLAT985_ALERT_1_G The  F-f"=    0.0411 Deviates from the B&C-Value  0.0400 Check
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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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

   8 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
   5 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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.

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**PLATON version of 16/07/2020; check.def file version of 12/07/2020**