checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait ..

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) elaf023

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
Please wait while processing ....            Interpreting this report
```

Structure factor report

Datablock: elaf023

```
Bond precision:      C-C = 0.0031 A              Wavelength=0.71073
Cell:        a=16.5043(12)   b=17.7857(12)   c=7.1311(6)
             alpha=90        beta=96.241(3)   gamma=90
Temperature: 100 K
                   Calculated                 Reported
Volume             2080.9(3)                  2080.9(3)
Space group        P 21/c                     P 21/c
Hall group         -P 2ybc                    -P 2ybc
Moiety formula     C18 H20 Cl Cu N5 O S, C H4 O    C18 H20 Cl Cu N5 O S, C H4 O
Sum formula        C19 H24 Cl Cu N5 O2 S      C19 H24 Cl Cu N5 O2 S
Mr                 485.49                     485.48
Dx,g cm-3          1.550                      1.550
Z                  4                          4
Mu (mm-1)          1.305                      1.305
F000               1004.0                     1004.0
F000'              1006.62
h,k,lmax           23,25,10                   23,25,10
Nref               6171                       5986
Tmin,Tmax          0.910,0.949                0.780,0.950
Tmin'              0.770
Correction method= # Reported T Limits: Tmin=0.780
Tmax=0.950 AbsCorr = MULTI-SCAN
Data completeness= 0.970        Theta(max)= 30.192
R(reflections)= 0.0368( 4621)     wR2(reflections)= 0.0913( 5986)
S = 1.022          Npar= 264
```

```
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
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   9 Report

🔘 Alert level G
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   2 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical   ? Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1   --S1   .   6.0 s.u.
PLAT398_ALERT_2_G Deviating C-O-C   Angle From 120 for O1   108.4 Degree

```
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      174 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        9 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        7 Info
```

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 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.
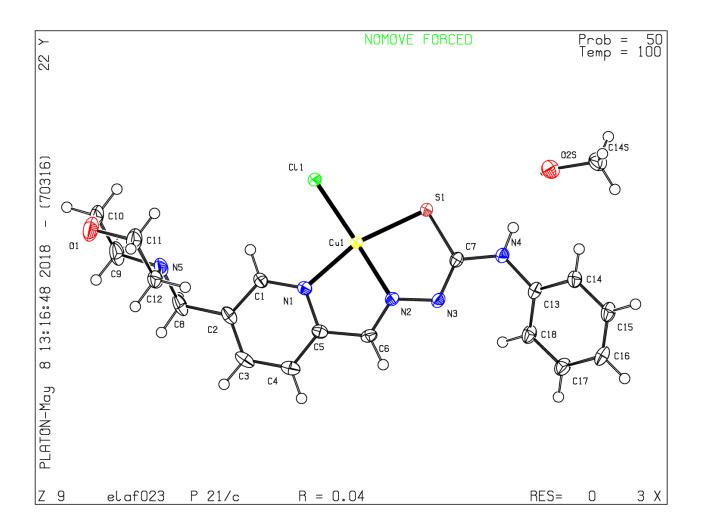
Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 23/04/2018; check.def file version of 23/04/2018

Datablock elaf023 - ellipsoid plot

Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry