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: ad50

```
Bond precision:   C-C = 0.0083 A            Wavelength=0.71073

Cell:             a=12.7818(16)    b=13.6298(16)        c=14.5042(19)
                  alpha=90         beta=94.530(17)      gamma=90
Temperature:      293 K

                  Calculated                Reported
Volume            2518.9(5)                 2518.9(5)
Space group       P 21/n                    P 21/n
Hall group        -P 2yn                    ?
Moiety formula    C16 H25 Cu N6 O14 Pr      ?
Sum formula       C16 H25 Cu N6 O14 Pr      C16 H25 Cu N6 O14 Pr
Mr                729.88                    729.87
Dx,g cm-3         1.925                     1.925
Z                 4                         4
Mu (mm-1)         2.835                     2.835
F000              1452.0                    1452.0
F000'             1453.11
h,k,lmax          15,16,17                  15,16,17
Nref              4420                      4423
Tmin,Tmax         0.335,0.868               0.633,0.995
Tmin'             0.309

Correction method= # Reported T Limits: Tmin=0.633 Tmax=0.995
AbsCorr = PSI-SCANS

Data completeness= 1.001         Theta(max)= 24.970

R(reflections)= 0.0363( 3129)     wR2(reflections)= 0.0984( 4423)

S = 1.010                 Npar= 359
```

```
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.
```

```
WEIGH01_ALERT_1_C  Extra text has been found in the
           _refine_ls_weighting_scheme field. This should be in the
           _refine_ls_weighting_details field.
           Weighting scheme given as calc w=1/[\s^2^(Fo^2^)+(0.0659P)^2^+1.0581
           Weighting scheme identified as calc
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      O7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     O12 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     O13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Pr Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      N6 Check
PLAT314_ALERT_2_C Small Angle for H2O: Metal-O4     -H42      .      88.96 Degree
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00831 Ang.
```

```
ABSTY01_ALERT_1_G  Extra text has been found in the _exptl_absorpt_correction_type
           field, which should be only a single keyword. A literature
           citation should be included in the _exptl_absorpt_process_details
           field.
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)      293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pr     --O7      .       5.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pr     --O12     .       6.3 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Cu     (II)     .      2.39 Info
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found    Please Check
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2016 Note
```

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

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

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_WEIGH01_ad50
;
PROBLEM: Extra text has been found in the
RESPONSE: ...
;
_vrf_PLAT241_ad50
;
PROBLEM: High    'MainMol' Ueq as Compared to Neighbors of      O7 Check
RESPONSE: ...
;
_vrf_PLAT242_ad50
;
PROBLEM: Low     'MainMol' Ueq as Compared to Neighbors of      Pr Check
RESPONSE: ...
```

```
;
_vrf_PLAT314_ad50
;
PROBLEM: Small Angle for H2O: Metal-O4     -H42      .        88.96 Degree
RESPONSE: ...
;
_vrf_PLAT342_ad50
;
PROBLEM: Low Bond Precision on  C-C Bonds ...............     0.00831 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

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 13/08/2017; check.def file version of 12/12/2017