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: ad26

```
Bond precision:   C-C = 0.0045 A              Wavelength=0.71073

Cell:           a=10.0995(8)        b=10.1606(14)    c=9.0768(10)
                alpha=114.210(11)   beta=91.365(8)   gamma=94.020(9)
Temperature:    293 K

                  Calculated                 Reported
Volume            846.01(18)                 846.01(16)
Space group       P -1                       P -1
Hall group        -P 1                       ?
                  C28 H40 Cu2 N8 O2, 2(C H4
Moiety formula                               ?
                  O)
Sum formula       C30 H48 Cu2 N8 O4          C30 H48 Cu2 N8 O4
Mr                711.86                      711.84
Dx,g cm-3         1.397                       1.397
Z                 1                           1
Mu (mm-1)         1.303                       1.303
F000              374.0                       374.0
F000'             374.74
h,k,lmax          12,12,11                    12,12,11
Nref              3682                        3682
Tmin,Tmax         0.562,0.771                 0.894,0.999
Tmin'             0.551

Correction method= # Reported T Limits: Tmin=0.894 Tmax=0.999
AbsCorr = PSI-SCAN

Data completeness= 1.000          Theta(max)= 26.970

R(reflections)= 0.0248( 2905)     wR2(reflections)= 0.0655( 3682)

S = 1.115                    Npar= 201
```

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
PLAT230_ALERT_2_B Hirshfeld Test Diff for   C6   --C7   .   13.5 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for   C6   --C9   .   26.7 s.u.
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu   --O1_a   .   22.0 s.u.

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🟡 Alert level C
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^)+(0.0235P)^2^+0.3357
            Weighting scheme identified as calc
PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced ....   Please Do !
PLAT230_ALERT_2_C Hirshfeld Test Diff for   O1   --N1   .   5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C5   --C6   .   7.0 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C5 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C6 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.7 Note
PLAT412_ALERT_2_C Short Intra XH3 .. XHn   H4A   ..H5B   ..   1.88 Ang.

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⚪ Alert level G
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF   Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...   2 Units
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) Cu   --N3   .   5.4 s.u.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C3 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C4 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu   (II)   .   2.34 Info
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found   Please Check
PLAT881_ALERT_1_G No Datum for _diffrn_reflns_av_R_equivalents ...   Please Do !
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL   2016 Note

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

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

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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_ad26
;
PROBLEM: Extra text has been found in the
```

```
RESPONSE: ...
;
_vrf_PLAT155_ad26
;
PROBLEM: The Triclinic Unitcell is NOT Reduced ..........    Please Do !
RESPONSE: ...
;
_vrf_PLAT230_ad26
;
PROBLEM: Hirshfeld Test Diff for   O1      --N1      .        5.1 s.u.
RESPONSE: ...
;
_vrf_PLAT241_ad26
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of      C5 Check
RESPONSE: ...
;
_vrf_PLAT242_ad26
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of      C6 Check
RESPONSE: ...
;
_vrf_PLAT250_ad26
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.7 Note
RESPONSE: ...
;
_vrf_PLAT412_ad26
;
PROBLEM: Short Intra XH3 .. XHn   H4A    ..H5B     ..       1.88 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

NOMOVE FORCED

Prob = 50
Temp = 293

26 Y

PLATON-Feb 2 14:41:50 2018 - (70316)

Z -62   ad26   P -1   R = 0.02   RES= 0 -106 X