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: 180416h

```
Bond precision:  C-C = 0.0223 A           Wavelength=0.71073

Cell:          a=8.7871(7)       b=12.5399(11)    c=27.800(2)
               alpha=94.077(2)   beta=96.539(1)   gamma=103.400(3)
Temperature:   298 K
```

	Calculated	Reported
Volume	2945.4(4)	2945.4(4)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C54 H42 Cu4 N14 O10 [+ solvent]	?
Sum formula	C54 H42 Cu4 N14 O10 [+ solvent]	C54 H42 Cu4 N14 O10
Mr	1301.22	1301.18
Dx,g cm-3	1.467	1.467
Z	2	2
Mu (mm-1)	1.492	1.492
F000	1320.0	1320.0
F000'	1322.98	
h,k,lmax	10,14,33	10,14,33
Nref	10397	9998
Tmin,Tmax	0.706,0.776	0.547,0.786
Tmin'	0.498	

```
Correction method= # Reported T Limits: Tmin=0.547 Tmax=0.786
AbsCorr = MULTI-SCAN

Data completeness= 0.962          Theta(max)= 25.020

R(reflections)= 0.1091( 5017)     wR2(reflections)= 0.3205( 9998)

S = 0.968                 Npar= 798
```

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
```
PLAT341_ALERT_3_B Low Bond Precision on  C-C Bonds ...............    0.02227 Ang.
PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ...       ! Note
```

🟡 Alert level C
```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .    0.962 Why?
PLAT082_ALERT_2_C High R1 Value ...................................    0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................    0.32 Report
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu3       --N9       .     5.1 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu2       --N8          0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu4       --N12         0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O7        --N13         0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O8        --N13         0.25 Ang.
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of     O5 Check
PLAT362_ALERT_2_C Short   C(sp3)-C(sp2) Bond  C2      - C3       .    1.37 Ang.
PLAT362_ALERT_2_C Short   C(sp3)-C(sp2) Bond  C5      - C6       .    1.39 Ang.
PLAT369_ALERT_2_C Long    C(sp2)-C(sp2) Bond  C37     - C42      .    1.54 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor        N2      --H2B      Please Check
PLAT420_ALERT_2_C D-H Without Acceptor        N4      --H4B      Please Check
```

⚪ Alert level G
```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension       1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF   Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       4 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large    0.19 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as   mixed Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for   O5        --N13      .     6.4 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )      7% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C10      -C17        1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C22      -C29        1.44 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C34      -C41        1.47 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C22      -C29       0.17 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C34      -C41       0.22 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C46      -C53       0.16 Ang.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....     C6 Check
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O7'     146.6 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  O9        ..C52        2.92 Ang.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure    207 A**3
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed      ! Info
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   2018 Note
```

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

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 ALERT type 2 Indicator that the structure model may be wrong or deficient
  4 ALERT type 3 Indicator that the structure quality may be low
  8 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 30/01/2018; check.def file version of 30/01/2018

O Y

PLATON-Apr 19 13:29:17 2018 - (70316)

Z 169   180416h   P-1   R = 0.11   RES=   O   -83 X