checkCIF/PLATON report

Structure factors have been supplied for datablock(s) crl119

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: crl119

```
Bond precision:  O- C = 0.0040 A         Wavelength=0.71073

Cell:             a=9.987(4)     b=5.658(3)         c=11.581(5)
                  alpha=90       beta=99.68(1)      gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	645.1(5)	645.0(5)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C8 H16 Cu N6 O4	?
Sum formula	C8 H16 Cu N6 O4	C8 H16 Cu N6 O4
Mr	323.82	323.81
Dx,g cm-3	1.667	1.667
Z	2	2
Mu (mm-1)	1.714	1.714
F000	334.0	334.0
F000’	334.75	
h,k,lmax	13,7,15	13,7,15
Nref	1724	1663
Tmin,Tmax	0.669,0.773	0.669,0.773
Tmin’	0.592	

```
Correction method= # Reported T Limits: Tmin=0.669 Tmax=0.773
AbsCorr = MULTI-SCAN

Data completeness= 0.965          Theta(max)= 29.000

R(reflections)= 0.0383( 1217)     wR2(reflections)= 0.1724( 1663)

S = 0.668                 Npar= 98
```

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

```
PLAT352_ALERT_3_B Short   N-H (X0.87,N1.01A)  N1     -   H1     ..       0.59 Ang.
```

Alert level C

```
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      0.668
PLAT352_ALERT_3_C Short   N-H (X0.87,N1.01A)  N2     -   H2     ..       0.67 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N1     --  H1     ...     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N2     --  H2     ...     Please Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2     ..  O2      ..       2.64 Ang.
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Note
```

Alert level G

```
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         61 Note
```

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

   1 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
   2 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 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_GOODF01_crl119
;
PROBLEM: The least squares goodness of fit parameter lies
RESPONSE: ...
;
_vrf_PLAT352_crl119
;
PROBLEM: Short   N-H (X0.87,N1.01A)  N2     -   H2     ..       0.67 Ang.
RESPONSE: ...
;
_vrf_PLAT420_crl119
;
PROBLEM: D-H Without Acceptor       N1     --  H1     ...     Please Check
RESPONSE: ...
;
_vrf_PLAT480_crl119
;
PROBLEM: Long H...A H-Bond Reported H2     ..  O2      ..       2.64 Ang.
RESPONSE: ...
;
_vrf_PLAT978_crl119
;
```

```
PROBLEM: Number C-C Bonds with Positive Residual Density.          0 Note
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 27/03/2017; check.def file version of 24/03/2017

Datablock crl119 - ellipsoid plot