checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

```
Bond precision:  C-C = 0.0068 A          Wavelength=0.71073

Cell:             a=7.018(3)     b=20.472(8)        c=13.619(6)
                  alpha=90       beta=99.25(3)      gamma=90
Temperature:      296 K
```

	Calculated	Reported
Volume	1931.2(14)	1931.3(13)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P2ybc
Moiety formula	C17 H13 Br Cl Cu N3 O6	?
Sum formula	C17 H13 Br Cl Cu N3 O6	C17 H13 Br Cl Cu N3 O6
Mr	534.20	534.20
Dx,g cm-3	1.837	1.837
Z	4	4
Mu (mm-1)	3.379	3.379
F000	1060.0	1060.0
F000’	1061.17	
h,k,lmax	9,27,18	9,27,18
Nref	5137	4864
Tmin,Tmax	0.487,0.738	0.524,0.751
Tmin’	0.471	

```
Correction method= # Reported T Limits: Tmin=0.524 Tmax=0.751
AbsCorr = INTEGRATION

Data completeness= 0.947          Theta(max)= 28.970

R(reflections)= 0.0570( 2812)     wR2(reflections)= 0.1777( 4864)

S = 0.951                 Npar= 274
```

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

```
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low .      0.947 Note
PLAT480_ALERT_4_B Long H...A H-Bond Reported H5     ..  BR1      ..       3.46 Ang.
PLAT480_ALERT_4_B Long H...A H-Bond Reported H5     ..  BR1      ..       3.46 Ang.
PLAT480_ALERT_4_B Long H...A H-Bond Reported H5     ..  BR1      ..       3.46 Ang.
PLAT480_ALERT_4_B Long H...A H-Bond Reported H5     ..  BR1      ..       3.46 Ang.
PLAT480_ALERT_4_B Long H...A H-Bond Reported H5     ..  BR1      ..       3.46 Ang.
PLAT480_ALERT_4_B Long H...A H-Bond Reported H5     ..  BR1      ..       3.46 Ang.
PLAT480_ALERT_4_B Long H...A H-Bond Reported H5     ..  BR1      ..       3.46 Ang.
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as integration
PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) ........     Please Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O6 Check
PLAT245_ALERT_2_C U(iso) H1      Smaller than U(eq) C4      by ...      0.014 AngSq
PLAT245_ALERT_2_C U(iso) H5      Smaller than U(eq) C7      by ...      0.024 AngSq
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C12    -C17           1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0068 Ang.
PLAT352_ALERT_3_C Short   N-H (X0.87,N1.01A)  N3     -   H6      ..       0.74 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H9     ..  O7       ..       2.62 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1     ..  O8       ..       2.95 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1     ..  O8       ..       2.95 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1     ..  O8       ..       2.95 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1     ..  O8       ..       2.95 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.207 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         10 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....          1 Check
PLAT977_ALERT_2_C Check the Negative Difference Density on      H6      -0.31 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
```

Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.          2 Note
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        Cl2 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1     (II)     .....      2.43 Info
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2016 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        260 Note
```

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

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

checkCIF publication errors

Alert level A

```
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. 'Acta Crystallographica Section C'
```

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

```
   1 ALERT level A = Data missing that is essential or data in wrong format
   1 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock I - ellipsoid plot