checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20wd_wvz_wd1_4bt_0ma

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: 20wd_wvz_wd1_4bt_0ma

```
Bond precision:    C-C = 0.0037 A            Wavelength=0.71073

Cell:          a=17.2800(7)     b=4.4056(2)           c=11.8697(4)
               alpha=90         beta=91.019(2)        gamma=90
Temperature:   150 K

                   Calculated                   Reported
Volume             903.48(6)                    903.48(6)
Space group        P 21/c                       P 1 21/c 1
Hall group         -P 2ybc                      -P 2ybc
Moiety formula     C8 H8 Br N3 O                C8 H8 Br N3 O
Sum formula        C8 H8 Br N3 O                C8 H8 Br N3 O
Mr                 242.07                       242.08
Dx,g cm-3          1.780                        1.780
Z                  4                            4
Mu (mm-1)          4.511                        4.511
F000               480.0                        480.0
F000'              479.04
h,k,lmax           21,5,14                      21,5,14
Nref               1804                         1774
Tmin,Tmax          0.425,0.697                  0.540,0.745
Tmin'              0.384

Correction method= # Reported T Limits: Tmin=0.540 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.983          Theta(max)= 26.131

R(reflections)= 0.0323( 1443)      wR2(reflections)= 0.0725( 1774)

S = 1.038                   Npar= 118
```

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 C

```
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......       2.727 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          16 Report
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         3 Report
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br1       ..Br1            3.52 Ang.
                                             2-x,-y,2-z  =     3_757 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        13 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         3 Info
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 16/07/2020; check.def file version of 12/07/2020

NOMOVE FORCED

Prob = 50
Temp = 150

33 Y

PLATON-Jul 24 16:45:47 2020 - (70316)

Z 148   20wd_wvz_wP 1 21/c 1   R = 0.03

RES=   0 -121 X