checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2

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: 2

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Bond precision:   C-C = 0.0117 A              Wavelength=0.71073

Cell:             a=10.1265(2)      b=15.3814(2)        c=14.2252(2)
                  alpha=90          beta=92.268(1)      gamma=90
Temperature:      120 K

                  Calculated                 Reported
Volume            2213.98(6)                 2213.98(6)
Space group       P 21                       P 1 21 1
Hall group        P 2yb                      P 2yb
Moiety formula    C27 H55 Br5 Cs2 N O13 Sb   C12 H24 Cs O6, Br5 Sb, C15
                                             H31 Cs N O7
Sum formula       C27 H55 Br5 Cs2 N O13 Sb   C27 H55 Br5 Cs2 N O13 Sb
Mr                1388.80                    1388.84
Dx,g cm-3         2.083                      2.083
Z                 2                          2
Mu (mm-1)         6.808                      6.808
F000              1328.0                     1328.0
F000'             1323.23
h,k,lmax          15,23,21                   15,23,21
Nref              16341[ 8433]               14990
Tmin,Tmax                                    0.940,0.940
Tmin'

Correction method= # Reported T Limits: Tmin=0.940 Tmax=0.940
AbsCorr = SPHERE

Data completeness= 1.78/0.92       Theta(max)= 32.747

R(reflections)= 0.0416( 13948)     wR2(reflections)= 0.0978( 14990)

S = 1.047                    Npar= 445
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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
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.01167 Ang.

⚪ Alert level G
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .   0.067 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT153_ALERT_1_G The s.u.'s on the Cell Axes   are Equal ..(Note)   0.0002 Ang.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1   --Br1   .   9.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1   --Br2   .   5.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sb1   --Br3   .   6.0 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   3 Note
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Sb1   --Cs02   ..   4.25 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Sb1   (III)   .   2.76 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..   ! Info
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   440 Note
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by   1 Check

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

   3 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
   2 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 22/04/2020; check.def file version of 09/03/2020

Datablock 2 - ellipsoid plot