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: I

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Bond precision:   As- O = 0.0079 A        Wavelength=0.71073

Cell:           a=34.442(7)     b=5.5044(11)         c=15.292(3)
                alpha=90        beta=100.625(9)      gamma=90
Temperature:    293 K

                Calculated                  Reported
Volume          2849.4(10)                  2849.4(10)
Space group     C 2/c                       C 1 2/c 1
Hall group      -C 2yc                      -C 2yc
Moiety formula  As2 Bi6 O15 Zn              ?
Sum formula     As2 Bi6 O15 Zn              As2 Bi6 O15 Zn1
Mr              1709.11                     1709.10
Dx,g cm-3       7.968                       7.965
Z               8                           8
Mu (mm-1)       80.182                      80.183
F000            5712.0                      5712.0
F000'           5542.58
h,k,lmax        42,6,19                     42,6,19
Nref            2948                        2921
Tmin,Tmax       0.004,0.056                 0.216,0.745
Tmin'           0.000

Correction method= # Reported T Limits: Tmin=0.216 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.991          Theta(max)= 26.510

R(reflections)= 0.0318( 2676)     wR2(reflections)= wR= 0.0414(
                                  2921)

S = 1.880               Npar= 143
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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 A**
PLAT213_ALERT_2_A Atom As2   has ADP max/min Ratio .....   5.6 prolat

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🟠 **Alert level B**
PLAT213_ALERT_2_B Atom Bi1   has ADP max/min Ratio .....   4.4 oblate

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🟡 **Alert level C**
PLAT213_ALERT_2_C Atom As1   has ADP max/min Ratio .....   3.3 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1   O   Ueq(max)/Ueq(min) Range   3.9 Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   3.8 Note

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⚪ **Alert level G**
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF   Please Do !
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)   293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   8 Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found   Please Check

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   1 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
   3 **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
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   1 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 11/08/2016; check.def file version of 04/08/2016

NOMOVE FORCED

Prob = 50
Temp = 293

C 1 2/c 1   R = 0.03   RES=   0   -8 X