checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

```
Bond precision:    C-C = 0.0090 A            Wavelength=0.71073

Cell:              a=14.0504(3)     b=14.0504(3)      c=21.4176(5)
                   alpha=90         beta=90           gamma=120
Temperature:       120 K

                   Calculated                Reported
Volume             3661.7(2)                 3661.69(19)
Space group        R -3                      R -3
Hall group         -R 3                      -R 3
Moiety formula     C24 H48 Ba Br6 Cs O12 Sb, 2(C12 H24 Ba0.5 Cs0.5 O6),
                   1.782(C3 H7 N O)          Br6 Sb1, 1.783(C3 H7 N O)
Sum formula        C29.35 H60.47 Ba Br6 Cs   C29.35 H60.48 Ba Br6 Cs
                   N1.78 O13.78 Sb           N1.78 O13.78 Sb
Mr                 1530.28                   1530.44
Dx,g cm-3          2.082                     2.082
Z                  3                         3
Mu (mm-1)          7.055                     7.055
F000               2193.8                    2194.0
F000'              2186.11
h,k,lmax           20,20,30                  20,20,30
Nref               2492                      2495
Tmin,Tmax                                    0.465,0.477
Tmin'

Correction method= # Reported T Limits: Tmin=0.465 Tmax=0.477
AbsCorr = SPHERE

Data completeness= 1.001          Theta(max)= 30.502

R(reflections)= 0.0381( 2127)     wR2(reflections)= 0.0802( 2495)

S = 1.182                    Npar= 82
```

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

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ      Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..       Please Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of          O1 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............        0.009 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......        4.819 Check
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⚪ Alert level G

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PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ      Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...      Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT   Unusually Large      33.99 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Sb1        --Br1      .     37.3 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Ba1        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cs1        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        12% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )       3.56 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn       H1B      ..H7C       .     2.10 Ang.
                                  2/3+y,4/3-x+y,4/3-z  =     14_566 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         12 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Sb1        (III)     .     2.72 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

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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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   3 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
   3 ALERT type 3 Indicator that the structure quality may be low
   7 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

NOMOVE FORCED

Prob = 50
Temp = 120

PLATON-May 28 07:27:04 2020 - (70316)

59 Y

Z -94   1   R -3   R = 0.04   RES=   0   95 X