checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ysb2o4br

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: ysb2o4br

```
Bond precision:   Sb- O = 0.0113 A         Wavelength=0.71069

Cell:              a=8.9654(6)      b=7.8023(5)          c=7.7961(5)
                   alpha=90         beta=91.398(3)       gamma=90
Temperature:       293 K

                 Calculated                 Reported
Volume           545.18(6)                  545.18(6)
Space group      P 21/c                     P21/c
Hall group       -P 2ybc                    ?
Moiety formula   O8 Sb4 Y2, 2(Br)           ?
Sum formula      Br2 O8 Sb4 Y2              Br O4 Sb2 Y
Mr               952.66                     476.32
Dx,g cm-3        5.803                      5.803
Z                2                          4
Mu (mm-1)        27.639                     27.639
F000             832.0                      832.0
F000'            815.80
h,k,lmax         11,10,10                   11,10,10
Nref             1239                       1220
Tmin,Tmax        0.565,0.759                0.299,0.687
Tmin'            0.496

Correction method= # Reported T Limits: Tmin=0.299 Tmax=0.687
AbsCorr = NUMERICAL

Data completeness= 0.985            Theta(max)= 27.390

R(reflections)= 0.0603( 740)                    wR2(reflections)=
                                                0.1287( 1220)
S = 0.986                  Npar= 74
```

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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.92A From Sb1 2.82 eA-3

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.132
PLAT199_ALERT_1_C Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_C Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT213_ALERT_2_C Atom O1 has ADP max/min Ratio ..... 3.3 prolat
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 13.665 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.830 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.76A From Sb2 1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.69A From Sb1 -1.70 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Sb1 1.14 eA-3

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 !
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.132 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Sb1 (III) . 2.89 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Sb2 (III) . 2.71 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Y (III) . 3.02 Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL/ 2018 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 19 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **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
4 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
5 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 13/07/2021; check.def file version of 13/07/2021

Datablock ysb2o4br - ellipsoid plot