checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CaLiSb

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: CaLiSb

```
Bond precision:    = 0.0000 A                    Wavelength=0.71073

Cell:            a=7.6428(10)       b=4.6324(6)       c=8.2923(11)
                 alpha=90           beta=90           gamma=90
Temperature:     200 K

                 Calculated                  Reported
Volume           293.59(7)                   293.58(7)
Space group      P n m a                     Pnma
Hall group       -P 2ac 2n                   ?
Moiety formula   Sb, Ca, Li                  CaLiSb
Sum formula      Ca Li Sb                    Ca Li Sb
Mr               168.78                      168.77
Dx,g cm-3        3.819                       3.818
Z                4                           4
Mu (mm-1)        10.780                      10.780
F000             296.0                       296.0
F000'            294.64
h,k,lmax         10,6,10                     10,6,10
Nref             392                         392
Tmin,Tmax        0.602,0.724                 0.604,0.724
Tmin'            0.578

Correction method= MULTI-SCAN

Data completeness= 1.000           Theta(max)= 27.940

R(reflections)= 0.0123( 364)       wR2(reflections)= 0.0303( 392)

S = 1.155                    Npar= Npar = 20
```

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 G**
```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF      Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ      Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical        ? 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
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 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
   0 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock CaLiSb - ellipsoid plot