checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Eu3Li4Sb4

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: Eu3Li4Sb4

Bond precision: Sb-Sb = 0.0008 A Wavelength=0.71073

Cell:
   a=4.7680(7) b=7.3856(10) c=15.656(2)
   alpha=90   beta=90   gamma=90
Temperature: 200 K

   Calculated   Reported
Volume   551.32(13) 551.33(13)
Space group   I m m m   Immm
Hall group   -I 2 2   ?
Moiety formula Eu3 Sb4, 4(Li) Eu3Li4Sb4
Sum formula   Eu3 Li4 Sb4   Eu3 Li4 Sb4
Mr   970.71   970.64
Dx,g cm-3   5.847   5.847
Z   2   2
Mu (mm-1)   26.369   26.369
F000   810.0   810.0
F000’   804.91
h,k,lmax   6,9,20   6,9,20
Nref   414   415
Tmin,Tmax   0.596,0.590   0.582,0.693
Tmin’   0.584

Correction method= MULTI-SCAN

Data completeness= 1.002   Theta(max)= 28.060
R(reflections)= 0.0161( 380)   wr2(reflections)= 0.0365( 415)
S = 1.057   Npar= Npar = 23

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.
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 Eu3Li4Sb4 - ellipsoid plot

Prob = 50
Temp = 200

Z -89 Eu3Li4Sb4 Imm m R = 0.02 RES = 0 -96 X