

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: finabs4

Bond precision: N- B = 0.0120 A Wavelength=1.54184

Cell: a=14.9980(3) b=10.4896(2) c=11.0167(2)
 alpha=90 beta=90 gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	1733.18(6)	1733.18(6)
Space group	C m c 21	C m c 21
Hall group	C 2c -2	C 2c -2
Moiety formula	C9 H29 B N Sb Si2	C9 H29 B N Sb Si2
Sum formula	C9 H29 B N Sb Si2	C9 H29 B N Sb Si2
Mr	340.08	340.07
Dx,g cm-3	1.303	1.303
Z	4	4
Mu (mm-1)	13.728	13.728
F000	696.0	696.0
F000'	699.04	
h,k,lmax	17,12,13	17,12,13
Nref	1591[842]	1418
Tmin,Tmax	0.052,0.094	0.048,0.295
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.048 Tmax=0.295
AbsCorr = ANALYTICAL

Data completeness= 1.68/0.89 Theta(max)= 66.512

R(reflections)= 0.0242(1401) wR2(reflections)= 0.0554(1418)

S = 1.046 Npar= 85

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

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 9.91 Note



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size	0.64 mm
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints	2 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 5 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 1 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
 3 ALERT type 4 Improvement, methodology, query or suggestion
 0 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 29/01/2015; check.def file version of 29/01/2015

