

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: fin

No errors found in this datablock

Bond precision: N- C = 0.0052 A Wavelength=1.54178

Cell: a=20.2849(10) b=11.6491(6) c=10.5383(4)
 alpha=90 beta=90 gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	2490.2(2)	2490.2(2)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C6 H23 B2 N2 Sb	C6 H23 B2 N2 Sb
Sum formula	C6 H23 B2 N2 Sb	C6 H23 B2 N2 Sb
Mr	266.64	266.63
Dx,g cm-3	1.423	1.422
Z	8	8
Mu (mm-1)	17.182	17.182
F000	1072.0	1072.0
F000'	1073.96	
h,k,lmax	25,14,13	25,14,12
Nref	2532	2483
Tmin,Tmax	0.070,0.649	0.170,0.664
Tmin'	0.007	

Correction method= # Reported T Limits: Tmin=0.170 Tmax=0.664
AbsCorr = ANALYTICAL

Data completeness= 0.981 Theta(max)= 74.057

R(reflections)= 0.0370(1893) wR2(reflections)= 0.1115(2483)

S = 1.055 Npar= 125

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.

