

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo

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: mo

Bond precision: C-C = 0.0027 Å

Wavelength=0.71073

Cell: a=8.2625(2) b=8.2880(2) c=8.6339(2)
 alpha=101.745(2) beta=96.091(2) gamma=111.755(2)
Temperature: 123 K

	Calculated	Reported
Volume	526.81(2)	526.81(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C7 H16 B N2 Sb	?
Sum formula	C7 H16 B N2 Sb	C7 H16 B N2 Sb
Mr	260.79	260.78
Dx,g cm-3	1.644	1.644
Z	2	2
Mu (mm-1)	2.565	2.565
F000	256.0	256.0
F000'	254.88	
h,k,lmax	11,11,12	11,11,12
Nref	3239	3223
Tmin,Tmax	0.709,0.860	0.719,0.884
Tmin'	0.565	

Correction method= # Reported T Limits: Tmin=0.719 Tmax=0.884
AbsCorr = GAUSSIAN

Data completeness= 0.995

Theta(max)= 30.565

R(reflections)= 0.0211(2840)

wR2(reflections)= 0.0605(3223)

S = 1.062

Npar= 129

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	3.09	Report
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600		5 Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal	0.00200	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of >Sb1A is Constrained at	0.800	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <Sb1B is Constrained at	0.200	Check
PLAT301_ALERT_3_G	Main Residue Disorder Percentage =	9	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Th(Min) ...	4	Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	7	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
4 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.

Datablock mo - ellipsoid plot

