

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: N- C = 0.0060 A Wavelength=1.54178

Cell: a=9.4332(2) b=6.8542(1) c=22.3341(3)
 alpha=90 beta=92.300(2) gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	1442.89(4)	1442.89(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C6 H24 B2 N2 P, I	C6 H24 B2 N2 P, I
Sum formula	C6 H24 B2 I N2 P	C6 H24 B2 I N2 P
Mr	303.76	303.76
Dx,g cm-3	1.398	1.398
Z	4	4
Mu (mm-1)	18.176	18.174
F000	608.0	608.0
F000'	609.27	
h,k,lmax	11,8,26	11,8,26
Nref	2539	2530
Tmin,Tmax	0.183,0.241	0.214,0.402
Tmin'	0.068	

Correction method= ANALYTICAL

Data completeness= 0.996 Theta(max)= 66.440

R(reflections)= 0.0407(2159) wR2(reflections)= 0.1113(2530)

S = 1.064 Npar= 133

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

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	?
PLAT128_ALERT_4_G	Alternate Setting of Space-group P21/c 	P21/n
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2

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
 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
 1 ALERT type 3 Indicator that the structure quality may be low
 2 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.

1 **ALERT level A** = Data missing that is essential or data in wrong format
 0 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```

# start Validation Reply Form
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
# end Validation Reply Form

```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock I - ellipsoid plot

