

# checkCIF/PLATON report

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

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: I

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Bond precision:	N- B = 0.0060 A	Wavelength=0.71073
Cell:	a=10.8435(3)	b=7.1547(1)      c=11.9395(4)
	alpha=90	beta=112.021(4)      gamma=90
Temperature:	123 K	
	Calculated	Reported
Volume	858.71(5)	858.71(5)
Space group	P 2/c	P 2/c
Hall group	-P 2yc	-P 2yc
Moiety formula	C6 H28 B3 N2 P2, I	C6 H28 B3 N2 P2, I
Sum formula	C6 H28 B3 I N2 P2	C6 H28 B3 I1 N2 P2
Mr	349.57	349.57
Dx,g cm-3	1.352	1.352
Z	2	2
Mu (mm-1)	2.025	2.025
F000	352.0	352.0
F000'	351.51	
h,k,lmax	15,10,16	14,9,16
Nref	2519	2284
Tmin,Tmax	0.742,0.856	0.724,0.904
Tmin'	0.622	

Correction method= ANALYTICAL

Data completeness= 0.907      Theta(max)= 30.050

R(reflections)= 0.0332( 2024)      wR2(reflections)= 0.0825( 2284)

S = 1.057      Npar= 88

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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.

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### Alert level C

PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	B1
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	N1
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ...		2.3

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### Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF	? Do !
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....		5

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 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  
0 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## checkCIF publication errors

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### 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.

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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

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### 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 a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

```

# 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.

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**PLATON version of 01/06/2013; check.def file version of 24/05/2013**

Datablock I - ellipsoid plot

