

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

Bond precision: C-C = 0.0033 Å Wavelength=1.54178

Cell: a=16.5779(2) b=6.2048(1) c=14.2632(1)
 alpha=90 beta=90 gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	1467.15(3)	1467.15(3)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C15 H21 B N P	C15 H21 B N P
Sum formula	C15 H21 B N P	C15 H21 B N P
Mr	257.11	257.11
Dx, g cm-3	1.164	1.164
Z	4	4
Mu (mm-1)	1.488	1.488
F000	552.0	552.0
F000'	554.35	
h, k, lmax	19, 7, 16	19, 7, 16
Nref	2586[1352]	2364
Tmin, Tmax	0.866, 0.900	0.860, 0.925
Tmin'	0.802	

Correction method= ANALYTICAL

Data completeness= 1.75/0.91 Theta(max)= 66.511

R(reflections)= 0.0261(2317) wR2(reflections)= 0.0706(2364)

S = 1.031 Npar= 214

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 B

Crystal system given = orthorhombic

PLAT019_ALERT_1_B _diffn_measured_fraction_theta_full/_max < 1.0 0.973 Report

Author Response: In the same time data below $d > 0.841\text{\AA}$ are complete (99.5%, see _diffn_measured_fraction_theta_max) according to the IUCr requirements

 Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 6.30 Note

Author Response: It is simply not true! We have 2364 refls to 214 parameters that gives us $2364/214=11.0$, not 6.3!

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.595 4 Report

Author Response: They are hidden in the beam stop.

PLAT915_ALERT_3_C Low Friedel Pair Coverage 82 %

Author Response: Absolute structure determination was not one of our goals.

 Alert level G

PLAT143_ALERT_4_G su on c - Axis Small or Missing 0.00010 Ang.

PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still 97 %

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 1 **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

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

