

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) xs2259a

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: xs2259a

Bond precision: C-C = 0.0047 Å Wavelength=0.71073

Cell: a=12.2301 (5) b=10.3563 (4) c=12.8772 (4)
alpha=90 beta=100.128 (4) gamma=90

Temperature: 110 K

	Calculated	Reported
Volume	1605.59(11)	1605.59(11)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H15 N3 Pd	C22 H15 N3 Pd
Sum formula	C22 H15 N3 Pd	C22 H15 N3 Pd
Mr	427.77	427.77
Dx, g cm ⁻³	1.770	1.770
Z	4	4
Mu (mm ⁻¹)	1.166	1.166
F000	856.0	856.0
F000'	852.24	
h, k, lmax	15,13,16	15,13,16
Nref	3693	3695
Tmin, Tmax	0.900, 0.966	0.880, 1.000
Tmin'	0.900	

Correction method= # Reported T Limits: Tmin=0.880 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 1.001 Theta (max) = 27.499

R(reflections)= 0.0334(2920) wR2 (reflections)=
0.0719(3695)
S = 1.032 Npar= 235

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**

PLAT420_ALERT_2_C D-H Bond Without Acceptor N2 --H2A . Please Check

 **Alert level G**

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	1 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1 (II) .	1.82 Info
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	3.3 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	4 Info

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

0 **ALERT level B** = A potentially serious problem, consider carefully

1 **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

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

2 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT420_xs2259a
;
PROBLEM: D-H Bond Without Acceptor N2 --H2A . Please Check
RESPONSE: ...
;
# end Validation Reply Form
```

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* or *IUCrData*, 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.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock xs2259a - ellipsoid plot

