

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: PdCl₂L₁₂

Bond precision: C-C = 0.0082 A Wavelength=0.71073

Cell: a=23.9383(7) b=10.5614(3) c=31.7091(9)
 alpha=90 beta=111.457(1) gamma=90

Temperature: 193 K

	Calculated	Reported
Volume	7461.1(4)	7461.1(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C54 H66 Cl2 P2 Pd	?
Sum formula	C54 H66 Cl2 P2 Pd	C54 H66 Cl2 P2 Pd
Mr	954.31	954.30
Dx,g cm-3	1.274	1.274
Z	6	6
Mu (mm-1)	0.579	0.579
F000	3000.0	3000.0
F000'	2997.82	
h,k,lmax	29,13,39	29,13,39
Nref	15247	15118
Tmin,Tmax	0.673,0.955	0.687,0.955
Tmin'	0.660	

Correction method= # Reported T Limits: Tmin=0.687 Tmax=0.955
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 26.372

R(reflections)= 0.0556(12427) wR2(reflections)= 0.1336(15118)

S = 1.160 Npar= 799

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**

PLAT234_ALERT_4_C	Large Hirshfeld Difference C16	-- C17 ..	0.17 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C5 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C12 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C39 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C53 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C4 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C13 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C40 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C49 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.00816 Ang.

● **Alert level G**

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		2 Report
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size ...		0.70 mm
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		18.85 Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pd1 -- C11 ..		7.0 s.u.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		12 Note

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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
10 **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
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 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.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

