

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) EB6xRT

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: EB6xRT

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Bond precision:	C-C = 0.0035 A	Wavelength=0.62000
Cell:	a=15.157(3)	b=13.336(3)      c=17.127(3)
	alpha=90	beta=112.74(3)      gamma=90
Temperature:	298 K	
	Calculated	Reported
Volume	3192.8(13)	3192.8(13)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C34 H33 N P Pd, Cl O4	C34 H33 N P Pd, Cl O4
Sum formula	C34 H33 Cl N O4 P Pd	C34 H33 Cl N O4 P Pd
Mr	692.43	692.43
Dx, g cm <sup>-3</sup>	1.441	1.441
Z	4	4
Mu (mm <sup>-1</sup> )	0.516	0.516
F000	1416.0	1416.0
F000'	1411.57	
h, k, lmax		23, 21, 26
Nref		14031
Tmin, Tmax	0.970, 0.990	
Tmin'	0.950	

Correction method= Not given

Data completeness=      Theta(max)= 31.086

R(reflections)= 0.0351( 11737)

wR2(reflections)=  
0.1150( 14031)

S = 1.041

Npar= 381

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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

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C4\_2 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Pd\_1 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Cl\_2 Check  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including Cl\_5 0.117 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 23 Report  
0 2 0, 1 1 0, 3 0 0, 1 1 1, 1 3 1, 3 6 1,  
5 6 1, -1 0 2, 0 1 2, 2 0 2, -2 1 3, 0 2 3,  
-2 4 4, 0 0 4, 1 0 4, 2 0 4, 0 0 8, 1 0 10,  
-6 4 13, -7 0 14, -4 0 14, -4 1 14, -4 6 14,  
PLAT913\_ALERT\_3\_C Missing # of Very Strong Reflections in FCF .... 4 Note  
0 2 0, 3 0 0, 2 0 2, 0 0 4,

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### Alert level G

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report  
PLAT092\_ALERT\_4\_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.62000 Ang.  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 1 Report  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Pd\_1 --C\_2 . 8.0 s.u.  
PLAT244\_ALERT\_4\_G Low 'Solvent' Ueq as Compared to Neighbors of Cl\_5 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 75 Note  
O4\_5 Cl\_5 O1\_5 O3\_5 O2\_5 Pd\_1 C4\_3 H4\_3  
C5\_3 H5\_3 C6\_3 H6\_3 C9\_3 C3\_3 H3\_3 C8\_3  
C7\_3 H7\_3 C1\_3 H1\_3 C2\_3 H2\_3 P\_4 C12\_4  
H12\_4 C11\_4 H11\_4 C10\_4 H10\_4 C9\_4 H9\_4 C8\_4  
H8\_4 C7\_4 C1\_4 C6\_4 H6\_4 C5\_4 H5\_4 C4\_4  
H4\_4 C3\_4 H3\_4 C2\_4 H2\_4 C13\_4 C14\_4 H14\_4  
C15\_4 H15\_4 C16\_4 H16\_4 C17\_4 H17\_4 C18\_4 H18\_4  
C1\_2 H1\_2 C2\_2 H2A\_2 H2B\_2 C3\_2 H3A\_2 H3B\_2  
C4\_2 H4A\_2 H4B\_2 C5\_2 H5A\_2 H5B\_2 C6\_2 H6A\_2  
H6B\_2 N\_2 C\_2  
PLAT790\_ALERT\_4\_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note  
C1 O4  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 6 Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note  
1 0 0,  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 1157 Note  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 14 Note  
3 0 0, 0 0 4, 0 2 0, -2 4 4, 2 0 2, 0 1 2,  
0 2 3, 1 0 0, 1 1 0, 1 1 1, 1 3 1, -2 1 3,  
5 6 1, 3 6 1,  
PLAT950\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units  
PLAT952\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Lmax Differ. 2 Units  
PLAT956\_ALERT\_1\_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units  
PLAT958\_ALERT\_1\_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 2 Units  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 10 Info  
PLAT992\_ALERT\_5\_G Repd & Actual \_reflns\_number\_gt Values Differ by 5 Check

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0	<b>ALERT level A</b>	= Most likely a serious problem - resolve or explain
0	<b>ALERT level B</b>	= A potentially serious problem, consider carefully
7	<b>ALERT level C</b>	= Check. Ensure it is not caused by an omission or oversight
18	<b>ALERT level G</b>	= General information/check it is not something unexpected
3	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
9	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
6	ALERT type 4	Improvement, methodology, query or suggestion
3	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* 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.

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**PLATON version of 14/11/2023; check.def file version of 14/09/2023**

