

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) EB44

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: EB44

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Bond precision:      C-C = 0.0029 Å      Wavelength=0.62000

Cell:                      a=19.569(4)              b=9.821(2)              c=17.575(4)  
                                alpha=90              beta=90              gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	3377.7(12)	3377.7(12)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C35 H37 N O3 P Pd, Cl O4	C35 H37 N O3 P Pd, Cl O4
Sum formula	C35 H37 Cl N O7 P Pd	C35 H37 Cl N O7 P Pd
Mr	756.48	756.47
Dx, g cm <sup>-3</sup>	1.488	1.488
Z	4	4
Mu (mm <sup>-1</sup> )	0.497	0.497
F000	1552.0	1552.0
F000'	1547.66	
h, k, lmax	32, 16, 29	32, 15, 27
Nref	16377[ 8403]	15352
Tmin, Tmax	0.971, 0.990	
Tmin'	0.952	

Correction method= Not given

Data completeness= 1.83/0.94      Theta(max)= 31.097

R(reflections)= 0.0252( 14379)

wR2(reflections)=  
0.0660( 15352)

S = 1.062

Npar= 467

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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 G

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	10	Note
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.62000	Ang.
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pd_1 --C_2 .	5.9	s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 2 )	2.91	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )	2.09	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2B_5 ..C2_4 .	3.01	Ang.
	x,y,z =	1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	88	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	Cl O4		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3	Note
	Cl O4		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	11	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	361	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax 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.	6	Info

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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  
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
19 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 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  
10 ALERT type 4 Improvement, methodology, query or suggestion  
1 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.

