

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) EB52

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: EB52

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Bond precision:	C-C = 0.0027 Å	Wavelength=0.62000
Cell:	a=12.091 (2)	b=12.295 (2)      c=12.729 (3)
	alpha=82.90 (3)	beta=82.85 (3)      gamma=89.24 (3)
Temperature:	100 K	
	Calculated	Reported
Volume	1863.2 (6)	1863.0 (7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C41 H43 N O3 P Pd, Cl O4	C41 H43 N O3 P Pd, Cl O4
Sum formula	C41 H43 Cl N O7 P Pd	C41 H43 Cl N O7 P Pd
Mr	834.58	834.58
Dx, g cm <sup>-3</sup>	1.488	1.488
Z	2	2
Mu (mm <sup>-1</sup> )	0.457	0.457
F000	860.0	860.0
F000'	857.84	
h, k, lmax		20, 20, 21
Nref		16033
Tmin, Tmax	0.973, 0.991	
Tmin'	0.955	
Correction method=	Not given	
Data completeness=		Theta(max)= 31.172
R(reflections)= 0.0431 ( 13563)		wR2(reflections)= 0.1214 ( 16033)
S = 1.085	Npar= 519	

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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

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & Sth/L= 0.600 33 Report  
7 1 0, -8-10 1, 10 -4 1, 9 -3 2, 9 -2 2, 9 0 2,  
7 7 2, 13 -5 3, 8 -4 3, 13 -4 3, 8 -2 3, 8 -1 3,  
9 -1 3, 8 0 3, 9 0 3, -3 -8 4, 12 -5 4, 12 -4 4,  
12 -3 4, 9 -2 4, 12 -2 4, 14 -1 4, -5 7 4, 1 4 5,  
10 -4 6, 11 -1 6, 0 9 6, 11 -2 7, 10 -1 7, 13 -1 8,  
13 0 8, 12 -2 9, 12 -1 9,  
PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.69Ang From Pd\_1 2.17 eA-3  
PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.60Ang From Pd\_1 -1.79 eA-3

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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.  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree  
PLAT175\_ALERT\_4\_G The CIF-Embedded .res File Contains SAME Records 1 Report  
PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 2 Report  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Pd\_1 --C\_2 . 7.4 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 ) 3.27 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 3 ) 1.73 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 100 Note  
Pd\_1 N\_2 C\_2 C1\_2 C2\_2 H2A\_2 H2B\_2 C3\_2  
H3A\_2 H3B\_2 C4\_2 H4A\_2 H4B\_2 C5\_2 H5\_2 C6\_2  
H6A\_2 H6B\_2 C7\_2 H7\_2 C8\_2 H8A\_2 H8B\_2 C9\_2  
H9\_2 C10\_2 H10A\_2 H10B\_2 C1A\_5 O1A\_5 O2A\_5 O3A\_5  
O4A\_5 C1B\_5 O1B\_5 O2B\_5 O3B\_5 O4B\_5 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 C9\_4 H9\_4 C8\_4 H8\_4  
C7\_4 C1\_4 C6\_4 H6\_4 C5\_4 H5\_4 C4\_4 C3\_4  
H3\_4 C2\_4 H2\_4 C13\_4 C14\_4 H14\_4 C15\_4 H15\_4  
C16\_4 C17\_4 H17\_4 C18\_4 H18\_4 Oa\_4 Ca\_4 Ha1\_4  
Ha2\_4 Ha3\_4 Oc\_4 Cc\_4 Hc1\_4 Hc2\_4 Hc3\_4 Ob\_4  
Cb\_4 Hb1\_4 Hb2\_4 Hb3\_4  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 49 Note  
PLAT899\_ALERT\_4\_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above Sth/L= 0.600 2102 Note  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 2 Note  
9 0 3, 1 4 5,  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 3.9 Low  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 8 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

3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

18 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

6 ALERT type 2 Indicator that the structure model may be wrong or deficient

3 ALERT type 3 Indicator that the structure quality may be low

10 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* 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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