

# checkCIF/PLATON report

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: dl184ef1

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Bond precision:    C-C = 0.0088 A                      Wavelength=0.71073

Cell:                      a=16.0741(5)              b=12.4076(4)              c=19.9806(5)  
                            alpha=90                      beta=90                      gamma=90

Temperature:              180 K

	Calculated	Reported
Volume	3985.0(2)	3985.0(2)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C28 H60 Cl4 N4 P2 Pd2	C28 H60 Cl4 N4 P2 Pd2
Sum formula	C28 H60 Cl4 N4 P2 Pd2	C28 H60 Cl4 N4 P2 Pd2
Mr	869.34	869.34
Dx,g cm-3	1.449	1.449
Z	4	4
Mu (mm-1)	1.274	1.274
F000	1784.0	1784.0
F000'	1779.53	
h,k,lmax	19,15,24	19,15,24
Nref	3784	3782
Tmin,Tmax	0.759,0.892	0.739,0.890
Tmin'	0.682	

Correction method= MULTI-SCAN

Data completeness= 0.999                      Theta(max)= 25.680

R(reflections)= 0.0420( 2735)              wR2(reflections)= 0.1199( 3782)

S = 1.099                      Npar= 189

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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

PLAT222_ALERT_3_C	Large Non-Solvent	H	Ueq(max)/Ueq(min) ...	3.10	Ratio
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Pd1	-- Cl2 ..	5.23	su
PLAT242_ALERT_2_C	Check Low		Ueq as Compared to Neighbors for		C5
PLAT342_ALERT_3_C	Low Bond Precision on		C-C Bonds (x 1000) Ang ..		9
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd.	#			1
	C28 H60 Cl4 N4 P2 Pd2				

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**Alert level G**

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large.

7.42

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0 **ALERT level A** = In general: serious problem  
0 **ALERT level B** = Potentially serious problem  
5 **ALERT level C** = Check and explain  
1 **ALERT level G** = General alerts; check

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  
2 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

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### **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.**

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**PLATON version of 13/08/2009; check.def file version of 12/08/2009**

