checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: jod1382s

Bond precision: C-C = 0.0073 A Wavelength=0.71073

Cell: **a=12.9357(11)** **b=11.9801(12)** **c=13.0750(11)**
alpha=90 **beta=100.862(2)** **gamma=90**
Temperature: **100 K**

	Calculated	Reported
Volume	1989.9(3)	1989.9(3)
Space group	P 21	P2(1)
Hall group	P 2yb	?
Moiety formula	C36 H47 I N O4 P Pd, C H Cl3	?
Sum formula	C37 H48 Cl3 I N O4 P Pd	C37 H48 Cl3 I N O4 P Pd
Mr	941.38	941.38
Dx,g cm-3	1.571	1.571
Z	2	2
Mu (mm-1)	1.522	1.522
F000	948.0	948.0
F000'	946.44	
h,k,lmax	17,16,17	17,16,17
Nref	5389[10300]	9421
Tmin,Tmax	0.848,0.885	0.772,0.888
Tmin'	0.715	

Correction method= MULTI-SCAN

Data completeness= 1.75/0.91 **Theta(max)= 28.710**

R(reflections)= 0.0422(9000) **wR2(reflections)= 0.0911(9421)**

S = 1.097 **Npar= 434**

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 B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 1
PLAT221_ALERT_2_B Large Solvent/Anion Cl Ueq(max)/Ueq(min) ... 5.00 Ratio

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Alert level C

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PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          4
PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H01A   ...          ?
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Alert level G

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HYDTR01_ALERT_1_G  Extra text has been found in the _refine_ls_hydrogen_treatment fi
           Explanatory text should be in the _publ_section_refinement field.
           Hydrogen treatment given as NH2 free, rigid methyls, others riding
           Hydrogen treatment identified as  riding
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
           _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max           28.71
          From the CIF: _reflns_number_total               9421
          Count of symmetry unique reflns         5389
          Completeness (_total/calc)            174.82%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured      4032
          Fraction of Friedel pairs measured     0.748
          Are heavy atom types Z>Si present        yes
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....          8
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of         C99
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................        100 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          2
PLAT791_ALERT_4_G Note: The Model has Chirality at C7     (Verify)          S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         12
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

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

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 16/02/2011; check.def file version of 16/02/2011

Datablock jod1382s - ellipsoid plot