checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ds6y2_0m

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: ds6y2_0m

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Bond precision:  C-C = 0.0081 A          Wavelength=0.71073

Cell:            a=14.425(5)    b=6.913(2)          c=15.918(5)
                 alpha=90       beta=102.100(6)     gamma=90
Temperature:     293 K

                Calculated                Reported
Volume          1552.1(9)                 1552.1(9)
Space group     P 21/n                    P 1 21/n 1
Hall group      -P 2yn                    -P 2yn
Moiety formula  C15 H16 N2 O5 Pd, H2 O    C15 H16 N2 O5 Pd, H2 O
Sum formula     C15 H18 N2 O6 Pd          C15 H18 N2 O6 Pd
Mr              428.71                    428.71
Dx,g cm-3       1.835                     1.835
Z               4                         4
Mu (mm-1)       1.231                     1.231
F000            864.0                     864.0
F000'           860.41
h,k,lmax        21,10,23                  20,10,23
Nref            5458                      5123
Tmin,Tmax       0.744,0.985               0.800,1.000
Tmin'           0.650

Correction method= # Reported T Limits: Tmin=0.800 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.939          Theta(max)= 32.143

R(reflections)= 0.0548( 2645)     wR2(reflections)= 0.1746( 5123)

S = 0.894                 Npar= 247
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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.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field. Absorption correction given as multi-scan

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

PLAT222_ALERT_3_C	Non-Solvent Resd 1	H Uiso(max)/Uiso(min) Range	5.6	Ratio
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N2	Check
PLAT245_ALERT_2_C	U(iso) H2	Smaller than U(eq) N2 by ...	0.016	AngSq
PLAT245_ALERT_2_C	U(iso) H11	Smaller than U(eq) C11 by ...	0.019	AngSq
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.00808	Ang.
PLAT350_ALERT_3_C	Short C-H (X0.96,N1.08A)	C10 - H10 ..	0.82	Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A)	C11 - H11 ..	1.11	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance		7.303	Check
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.58A From O6	-0.73	eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.65A From O6	-0.60	eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.85A From O6	-0.56	eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.67A From O6	-0.52	eA-3

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		2	Report
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.		5	Note
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)		293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)		293	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		313	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density		3	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 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* 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.

PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock ds6y2_0m - ellipsoid plot