checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_1658

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: exp_1658

```
Bond precision:  C-C = 0.0056 A          Wavelength=1.54184

Cell:            a=34.2146(5)     b=15.9294(2)     c=14.1391(2)
                 alpha=90         beta=90          gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	7706.07(18)	7706.06(18)
Space group	I b a 2	I b a 2
Hall group	I 2 -2c	I 2 -2c
Moiety formula	C49 H43 N3 O2 Pd	C49 H43 N3 O2 Pd
Sum formula	C49 H43 N3 O2 Pd	C49 H43 N3 O2 Pd
Mr	812.26	812.26
Dx,g cm-3	1.400	1.400
Z	8	8
Mu (mm-1)	4.231	4.232
F000	3360.0	3360.0
F000’	3369.33	
h,k,lmax	40,18,16	40,18,16
Nref	6794[3555]	5342
Tmin,Tmax	0.688,0.655	0.673,1.000
Tmin’	0.624	

```
Correction method= # Reported T Limits: Tmin=0.673 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.50/0.79      Theta(max)= 66.568

R(reflections)= 0.0233( 5020)     wR2(reflections)= 0.0586( 5342)

S = 1.038                 Npar= 503
```

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

```
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       7.07 Note
```

Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         1 Report
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C48 Check
PLAT792_ALERT_1_G Model has Chirality at C15         (Polar  SPGR)         R Verify
PLAT792_ALERT_1_G Model has Chirality at C16         (Polar  SPGR)         R Verify
PLAT792_ALERT_1_G Model has Chirality at C19         (Polar  SPGR)         R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1       (II)      .      2.04 Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       90% Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage       55 %
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        3 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
   1 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 03/06/2021; check.def file version of 02/06/2021

Datablock exp_1658 - ellipsoid plot