checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_2204_sq

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_2204_sq

```
Bond precision:   C-C = 0.0081 A          Wavelength=1.54184

Cell:             a=15.7666(5)     b=13.1945(3)         c=15.9606(5)
                  alpha=90         beta=114.654(3)      gamma=90
Temperature:      100 K
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	Calculated	Reported
Volume	3017.65(17)	3017.65(16)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C64 H53 Br N6 Pd2 [+ solvent]	C64 H53 Br N6 Pd2
Sum formula	C64 H53 Br N6 Pd2 [+ solvent]	C64 H53 Br N6 Pd2
Mr	1198.82	1198.83
Dx,g cm-3	1.319	1.319
Z	2	2
Mu (mm-1)	5.900	5.900
F000	1212.0	1212.0
F000'	1213.80	
h,k,lmax	18,15,18	18,15,18
Nref	5345	5344
Tmin,Tmax	0.517,0.554	0.343,1.000
Tmin'	0.293	

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Correction method= # Reported T Limits: Tmin=0.343 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 66.599
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R(reflections)= 0.0516(4563)

wR2(reflections)= 0.1513(5344)

S = 1.079 Npar= 340

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

```
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00812 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         2 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.06Ang From N2      .      -0.43 eA-3
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1      --N3       .       5.2 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Br1        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5         Constrained at       0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        1% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C23 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure       146 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1       (II)      .      2.29 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         6 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       81% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       1.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         2 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
  4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 14 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
  6 ALERT type 3 Indicator that the structure quality may be low
  5 ALERT type 4 Improvement, methodology, query or suggestion
  1 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.

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock exp_2204_sq - ellipsoid plot