checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_2202

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_2202

Bond precision: C-C = 0.0096 A Wavelength=1.54184

Cell: a=15.5587(8) b=13.3543(5) c=15.9419(8)
alpha=90 beta=113.942(6) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3027.3(3)	3027.3(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C64 H52 Br2 N6 Pd2, 2(C H Cl3)	C64 H52 Br2 N6 Pd2, 2(C H Cl3)
Sum formula	C66 H54 Br2 Cl6 N6 Pd2	C66 H54 Br2 Cl6 N6 Pd2
Mr	1516.45	1516.47
Dx,g cm-3	1.664	1.664
Z	2	2
Mu (mm-1)	9.147	9.146
F000	1512.0	1512.0
F000'	1517.03	
h,k,lmax	18,15,18	18,15,18
Nref	5342	5338
Tmin,Tmax	0.167,0.401	0.120,1.000
Tmin'	0.043	

Correction method= # Reported T Limits: Tmin=0.120 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 66.589

R(reflections)= 0.0648(4847) wR2(reflections)= 0.1751(5338)

S = 1.013 Npar= 386

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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.05Ang From Pd1 2.60 eA-3
PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.05Ang From Pd1 2.52 eA-3

Alert level C

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of Cl1 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of Cl0A Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of Cl2 Check
PLAT336_ALERT_2_C Long Bond Distance for ..... C33 -Cl1 1.960 Ang.
PLAT336_ALERT_2_C Long Bond Distance for ..... C33A -Cl0A 1.874 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00962 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 4 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.91Ang From Br1 2.17 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.07Ang From Cl1 1.66 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.22Ang From Br1 1.65 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.91Ang From Pd1 -1.62 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.00Ang From Cl2 -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.92Ang From Br1 -1.53 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.92Ang From Pd1 -1.51 eA-3

Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 13.46 Why ?
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 25% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 1 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1 (II) . 2.29 Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 87% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 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

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_2202 - ellipsoid plot