checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_2635_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_2635_sq

```
Bond precision:   C-C = 0.0174 A          Wavelength=1.54184

Cell:           a=15.9679(12)      b=20.0928(15)     c=24.0357(17)
                alpha=71.862(7)    beta=71.330(7)    gamma=86.857(6)
Temperature:    100 K
```

	Calculated	Reported
Volume	6934.2(10)	6934.2(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C128 H106 N12 Pd4 [+ solvent]	C128 H106 N12 Pd4
Sum formula	C128 H106 N12 Pd4 [+ solvent]	C128 H106 N12 Pd4
Mr	2237.86	2237.84
Dx,g cm-3	1.072	1.072
Z	2	2
Mu (mm-1)	4.455	4.455
F000	2284.0	2284.0
F000'	2290.27	
h,k,lmax	19,23,28	19,23,28
Nref	24479	24470
Tmin,Tmax	0.395,0.800	0.254,1.000
Tmin'	0.228	

```
Correction method= # Reported T Limits: Tmin=0.254 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 66.600
```

R(reflections)= 0.0861(13613)

wR2(reflections)= 0.2438(24470)

S = 0.960 Npar= 1321

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	4.4	Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.6	Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N5 --C23 .	0.16	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C47 --C48 .	0.17	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C58 --C62 .	0.19	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C59 --C60 .	0.16	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C70 --C73 .	0.16	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C75 --C76 .	0.16	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C110 --C115 .	0.22	Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C44	Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	C111	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C97	Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C110	Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.0174	Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C10 - C65 .	1.53	Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C19 - C74 .	1.53	Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C24 - C82 .	1.53	Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...	-0.565	Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595	9	Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.07Ang From Pd2	1.68	eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.10Ang From Pd4	1.64	eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.02Ang From Pd3	1.53	eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.18Ang From Pd3	1.51	eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Pd3	1.08	eA-3

Alert level G

PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety	C89	Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure	!	Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1 (II) .	2.33	Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd2 (II) .	2.25	Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd3 (II) .	2.35	Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd4 (II) .	2.37	Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
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	39%	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	2	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
0 **ALERT level B** = A potentially serious problem, consider carefully
24 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected

```
  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 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
 10 ALERT type 4 Improvement, methodology, query or suggestion
  4 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 18/11/2022; check.def file version of 18/11/2022

Datablock exp_2635_sq - ellipsoid plot