checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pd8as3-1

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: pd8as3-1

```
Bond precision:  Pd-As = 0.0015 A        Wavelength=0.71073

Cell:             a=7.4261(4)     b=7.4261(4)     c=10.3097(9)
                  alpha=90        beta=90         gamma=120
Temperature:      293 K

                Calculated                Reported
Volume          492.38(8)                 492.38(7)
Space group     P -3                      P -3
Hall group      -P 3                      -P 3
Moiety formula  As3 Pd8                   ?
Sum formula     As3 Pd8                   As3 Pd8
Mr              1075.96                   1075.96
Dx,g cm-3       10.886                    10.886
Z               3                         3
Mu (mm-1)       36.277                    36.277
F000            1401.0                    1401.0
F000'           1377.99
h,k,lmax        9,9,13                    9,9,13
Nref            831                       833
Tmin,Tmax       0.130,0.337               0.527,1.000
Tmin'           0.023

Correction method= # Reported T Limits: Tmin=0.527 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.002          Theta(max)= 28.497

R(reflections)= 0.0341( 699)      wR2(reflections)= 0.0571( 833)

S = 0.994                 Npar= 51
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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 A

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 2.42A From Pd1 4.19 eA-3

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		2.25	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density		3.79	eA-3
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.830	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.05A From Pd6	1.91	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.90A From Pd4	1.78	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.78A From Pd3	1.78	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.05A From Pd2	1.71	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.40A From Pd4	1.53	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.18A From As3	1.51	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.43A From As3	-1.57	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.30A From Pd1	-1.56	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.83A From Pd5	-1.51	eA-3

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
0 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 22/12/2019; check.def file version of 13/12/2019

Datablock pd8as3-1 - ellipsoid plot