

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: jod991s

Bond precision: C-C = 0.0027 Å Wavelength=0.71073

Cell: a=10.1328(9) b=8.1803(7) c=31.117(3)
 alpha=90 beta=92.022(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2577.7(4)	2577.7(4)
Space group	P 21/n	P 2(1)/n
Hall group	-P 2yn	?
Moiety formula	C27 H33 Br N O2 P Pd	?
Sum formula	C27 H33 Br N O2 P Pd	C27 H33 Br N O2 P Pd
Mr	620.81	620.82
Dx,g cm-3	1.600	1.600
Z	4	4
Mu (mm-1)	2.356	2.356
F000	1256.0	1256.0
F000'	1251.66	
h,k,lmax	13,11,41	13,11,41
Nref	6641	6278
Tmin,Tmax	0.680,0.889	0.717,0.891
Tmin'	0.537	

Correction method= MULTI-SCAN

Data completeness= 0.945 Theta(max)= 28.680

R(reflections)= 0.0247(5731) wR2(reflections)= 0.0578(6278)

S = 1.048 Npar= 311

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

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Pd1 -- Br1 .. 13.00 su

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.16

PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) ... 5.50 Ratio

PLAT413_ALERT_2_C	Short Inter XH3 .. XHn	H9B	..	H28A	..	2.12 Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor	N1	-	H01A	...	?
PLAT420_ALERT_2_C	D-H Without Acceptor	N1	-	H01B	...	?

● Alert level G

HYDTR01_ALERT_1_G Extra text has been found in the `_refine_ls_hydrogen_treatment` field. Explanatory text should be in the `_publ_section_refinement` field.

Hydrogen treatment given as NH2 free with SADI, rigid methyls, other Hydrogen treatment identified as riding

PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	1
PLAT128_ALERT_4_G	Alternate Setting of Space-group P21/c	P21/n
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	2

0 **ALERT level A** = In general: serious problem
1 **ALERT level B** = Potentially serious problem
5 **ALERT level C** = Check and explain
4 **ALERT level G** = General alerts; check

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
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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*, 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 22/10/2010; check.def file version of 11/10/2010

