

# checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

## Datablock: jod101ssq

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Bond precision: C-C = 0.0037 A Wavelength=0.71073  
Cell: a=27.304(3) b=11.2118(11) c=31.402(3)  
alpha=90 beta=90 gamma=90  
Temperature: 100 K

	Calculated	Reported
Volume	9613.0(17)	9613.2(16)
Space group	P b c a	P bca
Hall group	-P 2ac 2ab	?
Moiety formula	C42 H42 Br N3 O2 Pd, C4 H10 O, C H Cl3	?
Sum formula	C47 H53 Br Cl3 N3 O3 Pd	C47 H53 Br Cl3 N3 O3 Pd
Mr	1000.57	1000.58
Dx,g cm-3	1.383	1.383
Z	8	8
Mu (mm-1)	1.425	1.425
F000	4096.0	4096.0
F000'	4090.52	
h,k,lmax	36,15,42	36,15,42
Nref	12457	12032
Tmin,Tmax	0.670,0.843	0.722,0.848
Tmin'	0.637	

Correction method= MULTI-SCAN

Data completeness= 0.966 Theta(max)= 28.730


R(reflections)= 0.0421( 10253) wR2(reflections)= 0.0911( 12032)

S = 1.128 Npar= 539


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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.

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 **Alert level A**  
PLAT601\_ALERT\_2\_A Structure Contains Solvent Accessible VOIDS of . 215.00 A\*\*3

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 **Alert level C**  
PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) Pd1 -- Br1 .. 6.00 su

PLAT232\_ALERT\_2\_C Hirshfeld Test Diff (M-X) Pd1 -- C41 .. 5.67 su  
PLAT420\_ALERT\_2\_C D-H Without Acceptor N1 - H01A ... ?  
PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C99

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● **Alert level G**

HYDTR01\_ALERT\_1\_G Extra text has been found in the \_refine\_ls\_hydrogen\_treatment fi  
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

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large. 10.31

PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints ..... 9

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 2

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1 **ALERT level A** = In general: serious problem

0 **ALERT level B** = Potentially serious problem

4 **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

1 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

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Datablock jod101ssq - ellipsoid plot

