

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: joe6912s

Bond precision: C-C = 0.0037 A Wavelength=0.71073

Cell: a=8.8675(7) b=13.5117(11) c=15.0521(12)
 alpha=68.116(2) beta=79.424(2) gamma=75.791(2)

Temperature: 100 K

	Calculated	Reported
Volume	1613.8(2)	1613.8(2)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C34 H33 Br N O2 P Pd, C H2 Cl2	?
Sum formula	C35 H35 Br Cl2 N O2 P Pd	C35 H35 Br Cl2 N O2 P Pd
Mr	789.81	789.82
Dx,g cm-3	1.625	1.625
Z	2	2
Mu (mm-1)	2.062	2.062
F000	796.0	796.0
F000'	794.46	
h,k,lmax	11,18,20	11,18,20
Nref	8336	7568
Tmin,Tmax	0.781,0.940	0.829,0.941
Tmin'	0.597	

Correction method= MULTI-SCAN

Data completeness= 0.908 Theta(max)= 28.710

R(reflections)= 0.0289(7000) wR2(reflections)= 0.0727(7568)

S = 1.035 Npar= 398

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.

[IMAGE] Alert level C

PLAT420_ALERT_2_C D-H Without Acceptor	N1	-	H01A	...	?
PLAT420_ALERT_2_C D-H Without Acceptor	N1	-	H01B	...	?

[IMAGE] 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 others
Hydrogen treatment identified as riding

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3
PLAT005_ALERT_5_G	No <code>_iucr_refine_instructions_details</code> in CIF	?
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal	0.00200 Deg.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pd1 -- Br1 ..	32.0 su
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	2
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	1

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
1 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*, 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.

Datablock joe6912s - ellipsoid plot

[IMAGE]