

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: isu60_sp1

Bond precision:	C-C = 0.0060 A	Wavelength=0.71073
Cell:	a=17.7668(11) b=17.2559(11) c=15.0620(8)	alpha=90 beta=113.482(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	4235.3(4)	4235.3(4)
Space group	P 21/c	P 2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C84 H78 Br2 N2 O4 P2 Pd2, 3.72(C H2 Cl2), 0.28(C H2 Cl), 0.2	?
Sum formula	C88 H86 Br2 Cl8 N2 O4 P2 Pd2	C88 H86 Br2 Cl8 N2 O4 P2 Pd2
Mr	1953.73	1953.75
Dx,g cm-3	1.532	1.532
Z	2	2
Mu (mm-1)	1.709	1.709
F000	1976.0	1976.0
F000'	1974.20	
h,k,lmax	23,23,20	23,23,20
Nref	10587	10566
Tmin,Tmax	0.750,0.843	0.836,0.901
Tmin'	0.723	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 28.350

R(reflections)= 0.0492(8399) wR2(reflections)= 0.1288(10566)

S = 1.032 Npar= 509

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

PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent					3
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

RADNT01_ALERT_1_G Extra text has been found in the `_diffrn_radiation_type` field. Radiation given as high brilliance microfocus sealed tube MoK\alpha Radiation identified as Mo K\alpha

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					12
PLAT005_ALERT_5_G	No <code>_iucr_refine_instructions_details</code> in the CIF					?
PLAT007_ALERT_5_G	Note: Number of Unrefined D-H Atoms					1
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.					17.77
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pd1 -- Br1 ..					12.3 su
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of					C92
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder					100 Perc.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels					2
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .					1.11 Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					80
	CL1' -C91 -CL1 1.555 1.555 1.555					25.70 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					87
	CL2 -C91 -CL2' 1.555 1.555 1.555					7.10 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					88
	CL1' -CL1 -C91 1.555 1.555 1.555					32.20 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					89
	CL1' -CL1 -C91' 1.555 1.555 1.555					41.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					90
	C91 -CL1 -C91' 1.555 1.555 1.555					21.70 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					91
	C91 -CL2 -C91' 1.555 1.555 1.555					23.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					92
	C91 -C91' -CL1' 1.555 1.555 1.555					39.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					96
	CL1' -C91' -CL1 1.555 1.555 1.555					21.30 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					100
	C91 -CL1' -C91' 1.555 1.555 1.555					30.00 Deg.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints					9

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

2 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
13 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

