

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dm1603

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: dm1603

Bond precision:	C-C = 0.0112 Å	Wavelength=0.71073
Cell:	a=20.957(5) b=8.1726(17) c=22.929(5)	
	alpha=90 beta=106.623(3) gamma=90	
Temperature:	100 K	
	Calculated	Reported
Volume	3763.0(14)	3763.1(14)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C43 H45 Br N5 Pd, Br	C43 H45 Br N5 Pd, Br
Sum formula	C43 H45 Br2 N5 Pd	C43 H45 Br2 N5 Pd
Mr	898.04	898.06
Dx,g cm-3	1.585	1.585
Z	4	4
Mu (mm-1)	2.655	2.655
F000	1816.0	1816.0
F000'	1810.23	
h,k,lmax	25,10,28	25,10,28
Nref	7387	7389
Tmin,Tmax	0.775,0.948	0.613,1.000
Tmin'	0.654	

Correction method= # Reported T Limits: Tmin=0.613 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.997

R(reflections)= 0.0694(5351) wR2(reflections)= 0.1683(7389)

S = 1.089 Npar= 468

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

PLAT220_ALERT_2_C	Non-Solvent Resd 1	C	Ueq(max)/Ueq(min) Range	3.8	Ratio
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.01125	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance		3.750	Check
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.			0	Note



Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large		34.16	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pd1	-- Br1	..	13.4	s.u.

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
2 **ALERT level G** = General information/check it is not something unexpected
- 0 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
2 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
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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.

