

# 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: joe124\_1

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Bond precision:    C-C = 0.0066 Å                      Wavelength=1.54184

Cell:                      a=29.001(2)              b=9.2274(7)              c=19.9745(16)  
                                    alpha=90                      beta=102.373(7)              gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	5221.1(7)	5221.1(7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	?
Moiety formula	C28 H29 Br N2 O2 Pd	?
Sum formula	C28 H29 Br N2 O2 Pd	C28 H29 Br N2 O2 Pd
Mr	611.83	611.84
Dx,g cm <sup>-3</sup>	1.557	1.557
Z	8	8
Mu (mm <sup>-1</sup> )	7.736	7.736
F000	2464.0	2464.0
F000'	2464.97	
h,k,lmax	36,11,25	35,11,24
Nref	5360	5145
Tmin,Tmax	0.454,0.793	0.524,0.837
Tmin'	0.294	

Correction method= ANALYTICAL

Data completeness= 0.960                      Theta(max)= 74.800

R(reflections)= 0.0479( 4453)                      wR2(reflections)= 0.1370( 5145)

S = 1.040                                      Npar= 318

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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 C

PLAT245_ALERT_2_C	U(iso) H01B	Smaller than U(eq) N1	by ...	0.012 AngSq
PLAT250_ALERT_2_C	Large U3/U1	Ratio for Average U(i,j) Tensor	....	2.1
PLAT420_ALERT_2_C	D-H Without Acceptor	N1	- H01B ...	?

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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

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF ....	?
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	9.06
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pd1 -- Br1 ..	15.5 su
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	2
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	1

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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  
3 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 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

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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*, 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.

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