

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp\_2188\_sq\_sq

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: exp\_2188\_sq\_sq

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Bond precision:      C-C = 0.0103 Å      Wavelength=1.54184

Cell:                      a=15.8106(14)                      b=11.2102(10)                      c=17.812(3)  
                              alpha=90                      beta=105.385(11)                      gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	3043.9(7)	3043.8(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C64 H54 N6 O Pd [+ solvent]	C64 H54 N6 O Pd
Sum formula	C64 H54 N6 O Pd [+ solvent]	C64 H54 N6 O Pd
Mr	1029.53	1029.53
Dx, g cm <sup>-3</sup>	1.123	1.123
Z	2	2
Mu (mm <sup>-1</sup> )	2.781	2.781
F000	1068.0	1068.0
F000'	1070.90	
h, k, lmax	18, 13, 21	18, 13, 21
Nref	5380	5374
Tmin, Tmax	0.602, 0.757	0.540, 1.000
Tmin'	0.546	

Correction method= # Reported T Limits: Tmin=0.540 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 66.587

R(reflections)= 0.0900( 3484)

wR2(reflections)=  
0.2829( 5374)

S = 1.054

Npar= 377

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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

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....	0.28	Report
PLAT213_ALERT_2_C	Atom C27 has ADP max/min Ratio .....	3.6	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C9 --C10	5.6	s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C24	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C23	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.2	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.01033	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	4.599	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.193	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	6	Report

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### Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	9	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.15	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of N3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1A Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2A Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C32 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C32A Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	8%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1A ..C13	2.89	Ang.
	x, 3/2-y, 1/2+z =	4_576	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1A ..C7	2.94	Ang.
	x, 3/2-y, 1/2+z =	4_576	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1A ..C8	2.98	Ang.
	x, 3/2-y, 1/2+z =	4_576	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2A ..C9	2.91	Ang.
	1-x, -1/2+y, 1/2-z =	2_645	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2A ..C14	2.93	Ang.
	1-x, -1/2+y, 1/2-z =	2_645	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2A ..C8	3.00	Ang.
	1-x, -1/2+y, 1/2-z =	2_645	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure .....	!	Info
PLAT793_ALERT_4_G	Model has Chirality at C32 (Centro SPGR)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	77	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	36%	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	1.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	4	Check

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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

11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

25 **ALERT level G** = General information/check it is not something unexpected

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

15 ALERT type 2 Indicator that the structure model may be wrong or deficient

9 ALERT type 3 Indicator that the structure quality may be low

11 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* 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.

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