

# checkCIF/PLATON report

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: isu451si

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Bond precision:    C-C = 0.0038 A                      Wavelength=0.71073

Cell:                      a=15.9002(14)            b=12.8403(11)            c=27.037(3)  
                            alpha=90                      beta=107.076(2)            gamma=90

Temperature:            100 K

	Calculated	Reported
Volume	5276.6(9)	5276.7(8)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C29 H29 I N P Pd	?
Sum formula	C29 H29 I N P Pd	C29 H29 I N P Pd
Mr	655.80	655.80
Dx,g cm-3	1.651	1.651
Z	8	8
Mu (mm-1)	1.951	1.951
F000	2592.0	2592.0
F000'	2581.72	
h,k,lmax	21,17,36	21,16,36
Nref	6745	6445
Tmin,Tmax	0.697,0.746	0.629,0.758
Tmin'	0.683	

Correction method= MULTI-SCAN

Data completeness= 0.956                      Theta(max)= 28.570

R(reflections)= 0.0273( 6063)                      wR2(reflections)= 0.0577( 6445)

S = 1.116                                      Npar= 300

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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 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 rigid methyls others riding  
Hydrogen treatment identified as riding

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large.                      12.78

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0 **ALERT level A** = In general: serious problem  
0 **ALERT level B** = Potentially serious problem  
0 **ALERT level C** = Check and explain  
2 **ALERT level G** = General alerts; check

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 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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### **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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**PLATON version of 22/10/2010; check.def file version of 11/10/2010**

