

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: joc272s_squeezed

Bond precision: C-C = 0.0027 A Wavelength=0.71073

Cell: a=10.7469(9) b=12.5246(11) c=12.5931(11)
 alpha=79.641(2) beta=82.117(2) gamma=81.423(2)

Temperature: 100 K

	Calculated	Reported
Volume	1638.1(2)	1638.1(2)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C32 H36 N O6 P Pd	?
Sum formula	C32 H36 N O6 P Pd	C32 H36 N O6 P Pd
Mr	667.99	667.99
Dx,g cm-3	1.354	1.354
Z	2	2
Mu (mm-1)	0.656	0.656
F000	688.0	688.0
F000'	686.49	
h,k,lmax	14,16,17	14,16,16
Nref	8444	7684
Tmin,Tmax	0.843,0.949	0.754,0.949
Tmin'	0.843	

Correction method= MULTI-SCAN

Data completeness= 0.910 Theta(max)= 28.690

R(reflections)= 0.0257(7272) wR2(reflections)= 0.0629(7684)

S = 1.049 Npar= 390

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 B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s)	1
PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of .	181 A**3

● **Alert level C**

PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min) ...	3.2 Ratio
PLAT222_ALERT_3_C	Large Non-Solvent	H	Uiso(max)/Uiso(min) ..	4.9 Ratio

● **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, ordered methyls rigid
Hydrogen treatment identified as riding

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	24
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained Atom Sites	41
PLAT005_ALERT_5_G	No <code>_iucr_refine_instructions_details</code> in CIF	?
PLAT154_ALERT_1_G	The <code>su</code> 's on the Cell Angles are Equal	0.00200 Deg.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pd1 -- N1 ..	6.3 su
PLAT301_ALERT_3_G	Note: Main Residue Disorder	5 Perc.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	5
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	23
	01 -C5 -O1' 1.555 1.555 1.555	12.00 Deg.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	342

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

2 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
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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 18/07/2011; check.def file version of 04/07/2011

