

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: ip1019a

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=23.4555(19) b=7.7080(4) c=12.3813(10)
 alpha=90 beta=97.962(9) gamma=90

Temperature: 213 K

	Calculated	Reported
Volume	2216.9(3)	2216.9(3)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C20 H24 N6 Pd S2	?
Sum formula	C20 H24 N6 Pd S2	C20 H24 N6 Pd S2
Mr	518.99	518.97
Dx,g cm ⁻³	1.555	1.555
Z	4	4
Mu (mm ⁻¹)	1.044	1.044
F000	1056.0	1056.0
F000'	1053.23	
h,k,lmax	30,10,16	30,10,16
Nref	2679	2662
Tmin,Tmax	0.694,0.959	0.717,0.967
Tmin'	0.652	

Correction method= NUMERICAL

Data completeness= 0.994 Theta(max)= 27.990

R(reflections)= 0.0235(2143) wR2(reflections)= 0.0454(2662)

S = 0.841 Npar= 180

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

ABSTY02_ALERT_1_C An `_exptl_absorpt_correction_type` has been given without a literature citation. This should be contained in the `_exptl_absorpt_process_details` field.
Absorption correction given as numerical

PLAT350_ALERT_3_C	Short C-H Bond (0.96A)	C1	-	H1B	...	0.83	Ang.
PLAT391_ALERT_3_C	Deviating Methyl C2			H-C-H Bond Angle	101	Deg.
PLAT420_ALERT_2_C	D-H Without Acceptor	N3	-	H3N	...	?	

● **Alert level G**

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF	?
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms	in Heavy-Atom Struct.	11

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

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
2 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

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 05/11/2012; check.def file version of 05/11/2012

