

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pddtnm\_0m

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: pddtnm\_0m

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Bond precision:    C-C = 0.0038 A                      Wavelength=0.71069

Cell:              a=8.971(5)              b=9.039(5)              c=11.497(5)  
                    alpha=76.613(5)      beta=89.317(5)      gamma=69.446(5)

Temperature:      298 K

	Calculated	Reported
Volume	846.8(8)	846.7(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C12 H11 Cl4 N3 Pd S2	?
Sum formula	C12 H11 Cl4 N3 Pd S2	C12 H11 Cl4 N3 Pd S2
Mr	509.56	509.56
Dx,g cm-3	1.998	1.999
Z	2	2
Mu (mm-1)	1.970	1.970
F000	500.0	500.0
F000'	499.77	
h,k,lmax	11,12,15	11,12,15
Nref	4220	3884
Tmin,Tmax	0.660,0.821	0.607,0.746
Tmin'	0.497	

Correction method= # Reported T Limits: Tmin=0.607 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.920                      Theta(max)= 28.320

R(reflections)= 0.0256( 3662)              wR2(reflections)= 0.0650( 3884)

S = 1.039                                      Npar= 199

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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

PLAT213_ALERT_2_C	Atom Cl3	has ADP max/min Ratio	....	3.7	prolat
PLAT220_ALERT_2_C	Non-Solvent	Resd 1 Cl	Ueq(max)/Ueq(min) Range	4.1	Ratio
PLAT250_ALERT_2_C	Large U3/U1	Ratio for Average U(i,j)	Tensor	....	2.1 Note
PLAT431_ALERT_2_C	Short Inter HL..A	Contact Cl4	..S2	.	3.42 Ang.
		2-x,2-y,-z =		2_775	Check
PLAT911_ALERT_3_C	Missing FCF Refl	Between Thmin & STh/L=	0.600		14 Report

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### ● Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell	Angles are Equal	..(Note)	0.005	Degree
PLAT432_ALERT_2_G	Short Inter X...Y	Contact Cl1	..Cl	3.19	Ang.
		1-x,2-y,1-z =		2_676	Check
PLAT794_ALERT_5_G	Tentative Bond Valency	for Pd	(II)	.	2.11 Info
PLAT912_ALERT_4_G	Missing # of FCF	Reflections Above STh/L=	0.600		323 Note
PLAT978_ALERT_2_G	Number C-C Bonds	with Positive Residual	Density.		7 Info

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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
- 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 5 **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* 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.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

Datablock pdtdtnm\_0m - ellipsoid plot

