

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_70427b

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: mo\_70427b

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Bond precision:	C-C = 0.0107 Å	Wavelength=0.71073	
Cell:	a=13.2082(11)	b=24.654(2)	c=25.224(2)
	alpha=90	beta=90	gamma=90
Temperature:	173 K		
	Calculated	Reported	
Volume	8213.8(12)	8213.8(12)	
Space group	P b c a	P b c a	
Hall group	-P 2ac 2ab	-P 2ac 2ab	
Moiety formula	C28 H40 B20 N4 Pd2 S2	?	
Sum formula	C28 H40 B20 N4 Pd2 S2	C28 H40 B20 N4 Pd2 S2	
Mr	925.76	925.76	
Dx,g cm-3	1.497	1.497	
Z	8	8	
Mu (mm-1)	1.007	1.007	
F000	3680.0	3680.0	
F000'	3666.62		
h,k,lmax	17,32,32	17,31,32	
Nref	9456	9410	
Tmin,Tmax	0.818,0.834	0.628,0.746	
Tmin'	0.818		

Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.995      Theta(max)= 27.532

R(reflections)= 0.0614( 6341)      wR2(reflections)= 0.1632( 9410)

S = 1.105      Npar= 513

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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

CRYSC01\_ALERT\_1\_C The word below has not been recognised as a standard identifier.  
block

CRYSC01\_ALERT\_1\_C No recognised colour has been given for crystal colour.

PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.01067	Ang.
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600	23 Report
PLAT971_ALERT_2_C	Check Calcd Residual Density 0.84A From Pd2	2.00	eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density 1.86A From C28	1.85	eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density 1.00A From Pd2	1.75	eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density 0.83A From Pd1	1.72	eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density 2.23A From C23	1.69	eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density 0.99A From Pd1	1.69	eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density 0.99A From Pd2	1.53	eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Note

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### ● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	28.41	Why ?
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C2	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C10	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C11	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C2 ..	1.63	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C3 ..	1.50	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C10 - C11 ..	1.65	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C10 - C12 ..	1.51	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	20 Note

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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  
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
14 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
18 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  
3 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

