

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_70304b

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_70304b

Bond precision:	C-C = 0.0176 A	Wavelength=0.71073
Cell:	a=11.185(3)	b=18.389(6) c=19.122(6)
	alpha=80.688(5)	beta=79.836(5) gamma=85.532(5)
Temperature:	173 K	
	Calculated	Reported
Volume	3815(2)	3815(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C35 H40 B10 N P2 Pd S	?
Sum formula	C35 H40 B10 N P2 Pd S	C35 H40 B10 N P2 Pd S
Mr	783.18	783.18
Dx,g cm-3	1.364	1.363
Z	4	4
Mu (mm-1)	0.653	0.653
F000	1596.0	1596.0
F000'	1593.67	
h,k,lmax	13,22,23	13,22,23
Nref	15000	14832
Tmin,Tmax	0.882,0.901	0.585,0.746
Tmin'	0.593	

Correction method= # Reported T Limits: Tmin=0.585 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 26.000

R(reflections)= 0.0826(9641) wR2(reflections)= 0.2852(14832)

S = 1.032 Npar= 927

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

PLAT411_ALERT_2_B Short Inter H...H Contact H13A .. H7' . 1.99 Ang.

Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.29 Report
PLAT213_ALERT_2_C Atom N1 has ADP max/min Ratio 3.2 prolat
PLAT213_ALERT_2_C Atom B7 has ADP max/min Ratio 3.3 oblate
PLAT213_ALERT_2_C Atom N2 has ADP max/min Ratio 3.1 prolat
PLAT213_ALERT_2_C Atom C39 has ADP max/min Ratio 3.5 prolat
PLAT213_ALERT_2_C Atom B14 has ADP max/min Ratio 3.3 oblate
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 4.1 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 2 H Uiso(max)/Uiso(min) Range 4.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C14 -- C15 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30 -- C31 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference B8 -- B12 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2 -- C39 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C57 -- C58 .. 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference B18 -- B22 .. 0.18 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C57 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C53 Check
PLAT330_ALERT_2_C Large Average Phenyl C-C Dist. C4' -C9' 1.41 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01758 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C2 - H2 .. 1.12 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C37 - H37 .. 1.12 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H57 .. H57 . 2.05 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 7.896 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.074 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 161 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 10 Check
PLAT971_ALERT_2_C Check Calcd Residual Density 0.78A From Pd2 2.21 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.77A From Pd2 -1.90 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.85A From Pd1 -1.58 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H4 -0.52 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H14A -0.54 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H19 -0.33 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H44 -0.37 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H46B -0.31 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H48 -0.44 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H49 -0.34 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Note

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 15 Report
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size 0.80 mm
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.16 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 23.19 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.005 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1).. 12 % Note
PLAT303_ALERT_2_G Full Occupancy H-Atom H4 with # Connections 2.00 Check
PLAT303_ALERT_2_G Full Occupancy H-Atom H14A with # Connections 2.00 Check
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 C36 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C37 Check

PLAT367_ALERT_2_G Long?	C(sp?)-C(sp?) Bond	C1	-	C2	..	1.62 Ang.
PLAT367_ALERT_2_G Long?	C(sp?)-C(sp?) Bond	C1	-	C3	..	1.54 Ang.
PLAT367_ALERT_2_G Long?	C(sp?)-C(sp?) Bond	C36	-	C37	..	1.64 Ang.
PLAT367_ALERT_2_G Long?	C(sp?)-C(sp?) Bond	C36	-	C38	..	1.53 Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				93 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600				7 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File	...				3 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 38 ALERT type 2 Indicator that the structure model may be wrong or deficient
 11 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT084_mo_70304b
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.29 Report
RESPONSE: ...
;
_vrf_PLAT213_mo_70304b
;
PROBLEM: Atom N1 has ADP max/min Ratio ..... 3.2 prolat
RESPONSE: ...
;
_vrf_PLAT220_mo_70304b
;
PROBLEM: Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
RESPONSE: ...
;
_vrf_PLAT222_mo_70304b
;
PROBLEM: Non-Solvent Resd 2 H Uiso(max)/Uiso(min) Range 4.2 Ratio
RESPONSE: ...
;
_vrf_PLAT234_mo_70304b
;
PROBLEM: Large Hirshfeld Difference C14 -- C15 .. 0.17 Ang.
RESPONSE: ...
;
_vrf_PLAT241_mo_70304b
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of C57 Check
RESPONSE: ...
;
_vrf_PLAT242_mo_70304b
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of C53 Check
RESPONSE: ...
;
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_vrf_PLAT330_mo_70304b
;
PROBLEM: Large Average Phenyl C-C Dist. C4' -C9' 1.41 Ang.
RESPONSE: ...
;
_vrf_PLAT342_mo_70304b
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.01758 Ang.
RESPONSE: ...
;
_vrf_PLAT351_mo_70304b
;
PROBLEM: Long C-H (X0.96,N1.08A) C2 - H2 .. 1.12 Ang.
RESPONSE: ...
;
_vrf_PLAT411_mo_70304b
;
PROBLEM: Short Inter H...H Contact H57 .. H57 . 2.05 Ang.
RESPONSE: ...
;
_vrf_PLAT906_mo_70304b
;
PROBLEM: Large K value in the Analysis of Variance ..... 7.896 Check
RESPONSE: ...
;
_vrf_PLAT911_mo_70304b
;
PROBLEM: Missing # FCF Refl Between THmin & STh/L= 0.600 161 Report
RESPONSE: ...
;
_vrf_PLAT918_mo_70304b
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) . 10 Check
RESPONSE: ...
;
_vrf_PLAT971_mo_70304b
;
PROBLEM: Check Calcd Residual Density 0.78A From Pd2 2.21 eA-3
RESPONSE: ...
;
_vrf_PLAT972_mo_70304b
;
PROBLEM: Check Calcd Residual Density 0.77A From Pd2 -1.90 eA-3
RESPONSE: ...
;
_vrf_PLAT977_mo_70304b
;
PROBLEM: Check the Negative Difference Density on H4 -0.52 eA-3
RESPONSE: ...
;
_vrf_PLAT978_mo_70304b
;
PROBLEM: Number C-C Bonds with Positive Residual Density. 0 Note
RESPONSE: ...
;
# end Validation Reply Form

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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.

