

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) iEB44

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: iEB44

Bond precision:	C-C = 0.0042 A	Wavelength=0.62000
Cell:	a=19.544 (4) alpha=90	b=9.842 (2) beta=90
Temperature:	100 K	c=17.561 (4) gamma=90
	Calculated	Reported
Volume	3377.9 (12)	3377.9 (12)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C35 H37 N O3 P Pd, Cl O4	C35 H37 N O3 P Pd, Cl O4
Sum formula	C35 H37 Cl N O7 P Pd	C35 H37 Cl N O7 P Pd
Mr	756.48	756.47
Dx, g cm ⁻³	1.487	1.488
Z	4	4
Mu (mm ⁻¹)	0.497	0.497
F000	1552.0	1552.0
F000'	1547.66	
h, k, lmax	32, 16, 29	30, 16, 29
Nref	16358 [8394]	15086
Tmin, Tmax	0.971, 0.990	
Tmin'	0.952	
Correction method= Not given		
Data completeness=	1.80/0.92	Theta(max)= 31.093
R(reflections)=	0.0332 (13238)	wR2(reflections)=
S =	1.083	0.0861 (15086)
	Npar= 467	

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

PLAT213_ALERT_2_C	Atom C4_2	has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1 H Uiso(max)/Uiso(min) Range	4.3	Ratio
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #		1	Note
	C35 H37 N O3 P Pd			
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	6	Report



Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu			
	not performed for this radiation type.			
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		10	Note
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.62000 Ang.		
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records		1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Pd_1 --C_2	.	7.2	s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)		2.63	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)		2.37	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O2B_5 ..C2_4	.	3.00	Ang.
	x,y,z =		1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		88	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		11	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	513	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		14	Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ		2	Units
PLAT956_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Hmax Differ		2	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		6	Info

- 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
17 **ALERT level G** = General information/check it is not something unexpected

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
9 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.

