

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision:	C-C = 0.0051 Å	Wavelength=0.71069
Cell:	a=15.216(3) b=4.8276(8) c=19.590(3)	
	alpha=90 beta=107.160(4) gamma=90	
Temperature:	296 K	
	Calculated	Reported
Volume	1375.0(4)	1375.0(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H13 Co O5 P, H2 O	?
Sum formula	C13 H15 Co O6 P	C13 H15 Co1 O6 P1
Mr	357.15	357.20
Dx,g cm-3	1.725	1.716
Z	4	4
Mu (mm-1)	1.389	1.389
F000	732.0	732.0
F000'	734.14	
h,k,lmax	23,7,30	23,7,30
Nref	5394	5348
Tmin,Tmax	0.849,0.881	0.883,1.000
Tmin'	0.520	

Correction method= # Reported T Limits: Tmin=0.883 Tmax=1.000
AbsCorr = NUMERICAL

Data completeness= 0.991 Theta(max)= 33.470

R(reflections)= 0.0462(3811) wR2(reflections)= wR= 0.0877(5348)

S = 1.720 Npar= 191

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**

PLAT420_ALERT_2_B	D-H Without Acceptor	O4	--	H104	...	Please Check
PLAT780_ALERT_1_B	Coordinates do not Form a Properly Connected Set					Please Do !

 **Alert level G**

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension					1 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF					Please Do !
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Col	--	O3	..		6.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Col	--	O6	..		5.7 s.u.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels					15 Note
PLAT793_ALERT_4_G	The Model has Chirality at C1		(Centro SPGR)			R Verify
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found					Please Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
3 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* 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 19/11/2015; check.def file version of 17/11/2015

