

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: abssph

No errors found in this datablock

Bond precision:	C-C = 0.0052 A	Wavelength=1.54180
Cell:	a=18.6430(3) b=10.35933(15) c=15.7607(2)	
	alpha=90 beta=111.8802(18) gamma=90	
Temperature:	123 K	
	Calculated	Reported
Volume	2824.59(8)	2824.60(8)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C8 H16 Cl4 O2 V, C6 H28 B3 N2 P2	C8 H16 Cl4 O2 V, C6 H28 B3 N2 P2
Sum formula	C14 H44 B3 Cl4 N2 O2 P2 V	C14 H44 B3 Cl4 N2 O2 P2 V
Mr	559.62	559.62
Dx, g cm-3	1.316	1.316
Z	4	4
Mu (mm-1)	7.588	7.588
F000	1176.0	1176.0
F000'	1186.34	
h,k,lmax	23,12,19	22,12,19
Nref	5627	5459
Tmin,Tmax	0.189,0.613	0.209,1.000
Tmin'	0.086	

Correction method= MULTI-SCAN

Data completeness= 0.970 Theta(max)= 72.837

R(reflections)= 0.0461(3998) wR2(reflections)= 0.1128(5459)

S = 0.956 Npar= 299

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*, 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.

