

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) platon

No syntax errors found. CIF dictionary Interpreting this report

Datablock: platon

Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=16.345(7) b=6.288(3) c=19.938(8)
 alpha=90 beta=96.169(7) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	2037.3(15)	2037.3(15)
Space group	P 2/c	P2/c
Hall group	P 2yc	?
Moiety formula	C23 H24 N O3 P	?
Sum formula	C23 H24 N O3 P	C23 H24 N O3 P
Mr	393.40	393.40
Dx,g cm-3	1.283	1.283
Z	4	4
Mu (mm-1)	0.158	0.158
F000	832.0	832.0
F000'	832.75	
h,k,lmax	19,7,23	19,7,23
Nref	3599	3597
Tmin,Tmax	0.963,0.978	0.963,0.978
Tmin'	0.963	

Correction method= EMPIRICAL

Data completeness= 0.999 Theta(max)= 25.000

R(reflections)= 0.0487(2999) wR2(reflections)= 0.1315(3597)

S = 1.099 Npar= 257

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

PLAT906_ALERT_3_C Large K value in the Analysis of Variance 6.507
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.595 2

● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF	?
PLAT093_ALERT_1_G	No su's on H-positions,	refinement reported as	mixed
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C6 -- C7 ..	5.3 su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C7 -- C8 ..	5.8 su
PLAT909_ALERT_3_G	Percentage of Observed Data at Theta(Max)	still	70 %

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
0 ALERT type 4 Improvement, methodology, query or suggestion
1 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*, 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 24/04/2013; check.def file version of 23/04/2013

