

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) APP

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: APP

Bond precision:	C-C = 0.0056 Å	Wavelength=0.71073
Cell:	a=8.4373(2)	b=14.9917(3) c=46.2319(8)
	alpha=90	beta=94.494(1) gamma=90
Temperature:	296 K	
	Calculated	Reported
Volume	5829.9(2)	5829.9(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C60 H60 N9 O6 P3	C60 H60 N9 O6 P3
Sum formula	C60 H60 N9 O6 P3	C60 H60 N9 O6 P3
Mr	1096.08	1096.08
Dx, g cm ⁻³	1.249	1.249
Z	4	4
Mu (mm ⁻¹)	0.160	0.160
F000	2304.0	2304.0
F000'	2306.07	
h, k, lmax	10, 19, 59	10, 19, 59
Nref	12710	12686
Tmin, Tmax	0.972, 0.984	0.591, 0.746
Tmin'	0.969	

Correction method= # Reported T Limits: Tmin=0.591 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.999

R(reflections)= 0.0782(8108)	wR2(reflections)=
S = 1.075	0.2024(12686)
Npar= 769	

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

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 7.2 Ratio

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_B Large Hirshfeld Difference C29 --C30 . 0.27 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.



Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.1 Ratio

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.3 Ratio

PLAT234_ALERT_4_C Large Hirshfeld Difference N4 --C7 . 0.24 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_C Large Hirshfeld Difference N4 --C8 . 0.23 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_C Large Hirshfeld Difference N8 --C48 . 0.20 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_C Large Hirshfeld Difference C8 --C9 . 0.22 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_C Large Hirshfeld Difference C19 --C20 . 0.23 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

19 ALERT type 2 Indicator that the structure model may be wrong or deficient
10 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
2 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 18/05/2022; check.def file version of 17/05/2022

