checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1tBuNC

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: 1tBuNC

Bond precision: C-C = 0.0026 A Wavelength=0.71073

Cell: a=19.9406(6) b=8.6565(2) c=20.1247(6)
alpha=90 beta=116.119(4) gamma=90
Temperature: 103 K

	Calculated	Reported
Volume	3119.10(18)	3119.10(18)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C31 H49 Al N P	C31 H49 Al N P
Sum formula	C31 H49 Al N P	C31 H49 Al N P
Mr	493.66	493.66
Dx,g cm-3	1.051	1.051
Z	4	4
Mu (mm-1)	0.134	0.134
F000	1080.0	1080.0
F000’	1080.94	
h,k,lmax	23,10,24	23,10,24
Nref	5652	5641
Tmin,Tmax	0.975,0.989	0.816,1.000
Tmin’	0.970	

Correction method= # Reported T Limits: Tmin=0.816 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.245

R(reflections)= 0.0381(5020) wR2(reflections)= 0.1028(5641)

S = 1.035 Npar= 322

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

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       3.05 Report
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        4.4 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        4.4 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N1       --C28      .        5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C1       --C2       .        5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C1       --C3       .        5.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C1       --C4       .        6.1 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         11 Report
```

Alert level G

```
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Al1      --C27      .        8.8 s.u.
PLAT328_ALERT_4_G Possible Missing H on sp3? Phosphorus ..........         P1 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT898_ALERT_4_G Second Reported H-M Symbol in CIF Ignored ......          ! Check
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        80% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...         2 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         9 Info
```

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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 07/08/2019; check.def file version of 30/07/2019

Datablock 1tBuNC - ellipsoid plot