checkCIF/PLATON report

No syntax errors found.   **CIF dictionary**   **Interpreting this report**

Datablock: new

```
Bond precision:   C-C = 0.0041 A              Wavelength=0.71073

Cell:            a=7.3041(8)      b=17.5360(18)        c=14.2346(13)
                 alpha=90         beta=95.204(3)       gamma=90
Temperature:     296 K

                 Calculated                  Reported
Volume           1815.7(3)                   1815.7(3)
Space group      P 21                        P2(1)
Hall group       P 2yb                       ?
Moiety formula   C18 H25 B2 N3               ?
Sum formula      C18 H25 B2 N3               C18 H25 B2 N3
Mr               305.03                      305.03
Dx,g cm-3        1.116                       1.116
Z                4                           4
Mu (mm-1)        0.065                       0.065
F000             656.0                       656.0
F000'            656.18
h,k,lmax         9,22,18                     9,22,18
Nref             4138[ 8007]                 4128
Tmin,Tmax        0.987,0.988                 0.987,0.988
Tmin'            0.987

Correction method= MULTI-SCAN

Data completeness= 1.00/0.52       Theta(max)= 27.100

R(reflections)= 0.0437( 3490)      wR2(reflections)= 0.1168( 4128)

S = 1.060                   Npar= 425
```

```
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**
PLAT222_ALERT_3_C Large Non-Solvent   H   Ueq(max)/Ueq(min) ...   3.17 Ratio

---

⚪ **Alert level G**
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
            correct. If it is not, please give the correct count in the

```
  _publ_section_exptl_refinement section of the submitted CIF.
  From the CIF: _diffrn_reflns_theta_max           27.10
  From the CIF: _reflns_number_total               4128
  Count of symmetry unique reflns        4138
  Completeness (_total/calc)          99.76%
  TEST3: Check Friedels for noncentro structure
  Estimate of Friedel pairs measured           0
  Fraction of Friedel pairs measured     0.000
  Are heavy atom types Z>Si present         no
```

```
  0 ALERT level A = In general: serious problem
  0 ALERT level B = Potentially serious problem
  1 ALERT level C = Check and explain
  1 ALERT level G = General alerts; check

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  0 ALERT type 2 Indicator that the structure model may be wrong or deficient
  1 ALERT type 3 Indicator that the structure quality may be low
  1 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
```

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 13/08/2009; check.def file version of 12/08/2009