checkCIF/PLATON report

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

Datablock: jn07_0m

Bond precision: C-C = 0.0038 A   Wavelength=0.71073

Cell: a=20.7504(8)   b=7.9455(3)   c=13.4383(4)
               alpha=90   beta=100.245(2)   gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	2180.28(14)	2180.28(13)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C21 H37 N O, H2 O	?
Sum formula	C21 H39 N O2	C21 H39 N O2
Mr	337.53	337.53
Dx,g cm-3	1.028	1.028
Z	4	4
Mu (mm-1)	0.064	0.064
F000	752.0	752.0
F000'	752.29	
h,k,lmax	24,9,16	24,9,16
Nref	3863	3846
Tmin,Tmax	0.992,0.994	0.858,0.968
Tmin'	0.987	

Correction method= EMPIRICAL

Data completeness= 0.996   Theta(max)= 25.060

R(reflections)= 0.0473(1361)   wR2(reflections)= 0.1543(3846)

S = 0.767   Npar= 225

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
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections too Low ....   35 Perc.

🟡 Alert level C
ABSTY02_ALERT_1_C   An _exptl_absorpt_correction_type has been given without
        a literature citation. This should be contained in the

```
                    _exptl_absorpt_process_details field.
                    Absorption correction given as empirical
GOODF01_ALERT_2_C   The least squares goodness of fit parameter lies
                    outside the range 0.80 <> 2.00
                    Goodness of fit given =      0.767
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.04
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #         2
                    H2 O
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   0 ALERT level A = In general: serious problem
   1 ALERT level B = Potentially serious problem
   4 ALERT level C = Check and explain
   0 ALERT level G = General alerts; check

   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
   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
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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 22/10/2010; check.def file version of 11/10/2010

Datablock jn07_0m - ellipsoid plot