checkCIF/PLATON report

No syntax errors found. [CIF dictionary] [Interpreting this report]

Datablock: jn07_0m

Bond precision:  C–C = 0.0038 Å  Wavelength=0.71073

Cell:  

\[
\begin{align*}
\text{a} & = 20.7504(8) \\
\text{b} & = 7.9455(3) \\
\text{c} & = 13.4383(4) \\
\text{alpha} & = 90 \\
\text{beta} & = 100.245(2) \\
\text{gamma} & = 90
\end{align*}
\]

Temperature:  296 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>2180.28(14)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/c</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2ybc</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C21 H37 N O, H2 O</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C21 H39 N O2</td>
</tr>
<tr>
<td>Mr</td>
<td>337.53</td>
</tr>
<tr>
<td>Dx,g cm⁻³</td>
<td>1.028</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>0.064</td>
</tr>
<tr>
<td>F₀₀₀</td>
<td>752.0</td>
</tr>
<tr>
<td>F₀₀₀’</td>
<td>752.29</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>24,9,16</td>
</tr>
<tr>
<td>Nref</td>
<td>3863</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.992,0.994</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.987</td>
</tr>
</tbody>
</table>

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

\[ \text{test-name}_\text{ALERT}_\text{alert-type}_\text{alert-level} \]

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_absorp_correction_type has been given without a literature citation. This should be contained in the
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

PLAT190_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 2

H2 O

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

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