checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: i13605

Bond precision: C-C = 0.0019 AWavelength=0.71073

Cell: a=9.6885•1, b=15.3367•3, c=15.1186•2, gamma=90

alpha=90 beta=97.993•1,

Temperature: 100 K

Calculated Reported Volume 2224.64•6, 2224.64•6, P 1 21/n 1 Space group P 21/n

Hall group -P 2yn -P 2yn

Moiety formula C22 H38 B N3 C22 H38 B N3 Sum formula C22 H38 B N3 C22 H38 B N3

Mr 355.36 355.36 Dx,g cm-3 1.061 1.061 Ζ 4 4 Mu •mm-1, 0.062 0.062 784.0 F000 784.0

F000' 784.22

h,k,lmax 12,19,19 12,19,19 Nref 5097 5073 Tmin,Tmax 0.979,0.983 0.906, 0.970

Tmin' 0.979

Correction method= MULTI-SCAN

Data completeness= 0.995 Theta•max,= 27.480

R•reflections,= 0.0456• 4136, wR2•reflections,= 0.1229• 5073,

S = 0.779Npar= 243

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

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00 Goodness of fit given = 0.779