

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: d127a

Bond precision: C-C = 0.0030 A

Wavelength=0.71073

Cell: a=11.8598(10) b=5.6497(4) c=18.4376(15)
 alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1235.40(17)	1235.40(17)
Space group	P n a 21	Pna2(1)
Hall group	P 2c -2n	?
Moiety formula	C16 H13 N3	?
Sum formula	C16 H13 N3	C16 H13 N3
Mr	247.29	247.29
Dx,g cm-3	1.330	1.330
Z	4	4
Mu (mm-1)	0.081	0.081
F000	520.0	520.0
F000'	520.17	
h,k,lmax	15,7,23	15,7,23
Nref	2824[1456]	2598
Tmin,Tmax	0.981,0.988	0.970,0.988
Tmin'	0.970	

Correction method= MULTI-SCAN

Data completeness= 1.78/0.92 Theta(max)= 27.450

R(reflections)= 0.0499(2464) wR2(reflections)= 0.1299(2598)

S = 1.082 Npar= 172

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.

Datablock d127a - ellipsoid plot

