



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_3504_autored

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: exp_3504_autored

Bond precision:	C-C = 0.0016 Å	Wavelength=1.54184
Cell:	a=11.4378 (1) alpha=90	b=10.3941 (1) beta=105.994 (1)
Temperature:	110 K	c=12.9963 (1) gamma=90
	Calculated	Reported
Volume	1485.26 (2)	1485.26 (2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H17 N O3	C16 H17 N O3
Sum formula	C16 H17 N O3	C16 H17 N O3
Mr	271.31	271.30
Dx, g cm ⁻³	1.213	1.213
Z	4	4
Mu (mm ⁻¹)	0.683	0.683
F000	576.0	576.0
F000'	577.79	
h, k, lmax	14, 13, 16	14, 13, 16
Nref	3132	3105
Tmin, Tmax	0.854, 0.928	0.710, 1.000
Tmin'	0.837	

Correction method= # Reported T Limits: Tmin=0.710 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991

Theta(max)= 76.877

R(reflections)= 0.0357(2766)

wR2(reflections)=
0.0965(3105)

S = 1.041

Npar= 184

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 G

PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing	0.00010 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing	0.00010 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	27 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value	5.704 Note
Predicted wR2: Based on SigI**2 1.69 or SHELX Weight	9.27 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	10 Info

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

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

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

