

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: 413tong_0m

Bond precision: C-C = 0.0058 Å Wavelength=0.71073

Cell: a=9.7094(5) b=10.2557(5) c=12.1003(6)
 alpha=105.243(2) beta=107.468(2) gamma=93.009(2)
Temperature: 100 K

	Calculated	Reported
Volume	1097.55(10)	1097.55(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C33 H19 N O3	C33 H19 N O3
Sum formula	C33 H19 N O3	C33 H19 N O3
Mr	477.49	477.49
Dx, g cm ⁻³	1.445	1.445
Z	2	2
Mu (mm ⁻¹)	0.093	0.093
F000	496.0	496.0
F000'	496.22	
h, k, lmax	12, 12, 15	12, 12, 15
Nref	4526	4317
Tmin, Tmax	0.993, 0.996	0.654, 0.745
Tmin'	0.989	

Correction method= # Reported T Limits: Tmin=0.654 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.954 Theta(max)= 26.465

R(reflections)= 0.0722(2780)	wR2(reflections)=
S = 1.123	0.2440(4317)
Npar= 334	

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

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75

_refine_diff_density_min given = -0.622

Test value = -0.600

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.965 Why?

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -0.62 eA-3

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00578 Ang.

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C26 - C27 . 1.53 Ang.

PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note

C33 H19 N O3



Alert level G

PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF Please Check

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 12 Note

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 2 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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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. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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* or *IUCrData*, 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.

