

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I5

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: I5

| | | | |
|-----------------|----------------|--------------------|-------------|
| Bond precision: | C-C = 0.0028 A | Wavelength=1.54178 | |
| Cell: | a=11.471(4) | b=8.269(3) | c=12.518(4) |
| | alpha=90 | beta=96.155(14) | gamma=90 |
| Temperature: | 296 K | | |
| | Calculated | Reported | |
| Volume | 1180.5(7) | 1180.5(7) | |
| Space group | P 21/c | P21/c | |
| Hall group | -P 2ybc | ? | |
| Moiety formula | C14 H14 N2 O | C14 H14 N2 O | |
| Sum formula | C14 H14 N2 O | C14 H14 N2 O | |
| Mr | 226.27 | 226.27 | |
| Dx,g cm-3 | 1.273 | 1.273 | |
| Z | 4 | 4 | |
| Mu (mm-1) | 0.650 | 0.619 | |
| F000 | 480.0 | 456.0 | |
| F000' | 481.37 | | |
| h,k,lmax | 13,9,14 | 13,9,14 | |
| Nref | 1999 | 1929 | |
| Tmin,Tmax | 0.867,0.878 | 0.867,0.878 | |
| Tmin' | 0.867 | | |

Correction method= # Reported T Limits: Tmin=0.867 Tmax=0.878
AbsCorr = MULTI-SCAN

Data completeness= 0.965 Theta(max)= 64.690

R(reflections)= 0.0570(1742) wR2(reflections)= 0.1676(1929)

S = 1.067 Npar= 156

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**

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies
outside the range 0.99 <> 1.01
Calculated value of mu = 0.650
Value of mu given = 0.619

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5863

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.965 Note
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 4.98 %
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT230_ALERT_2_C Hirshfeld Test Diff for C12 -- C13 .. 5.1 s.u.
PLAT420_ALERT_2_C D-H Without Acceptor N16 -- H16A ... Please Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.586 71 Report
PLAT977_ALERT_2_C Check the Negative Difference Density on H16B -0.40 eA-3

● **Alert level G**

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still 84 %
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 5 Note

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

5 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
5 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 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. 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.

PLATON version of 08/07/2016; check.def file version of 05/07/2016

