checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_345

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_345

Bond precision: C-C = 0.0045 A   Wavelength=0.71073

Cell: a=17.093(2)   b=6.9475(10)   c=18.529(3)
                   alpha=90   beta=90   gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	2200.4(5)	2200.4(5)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C12 H12 N2 O	C12 H12 N2 O
Sum formula	C12 H12 N2 O	C12 H12 N2 O
Mr	200.24	200.24
Dx,g cm-3	1.209	1.209
Z	8	8
Mu (mm-1)	0.079	0.079
F000	848.0	848.0
F000'	848.33	
h,k,lmax	24,9,26	24,9,24
Nref	3352	3012
Tmin,Tmax	0.975,0.991	0.263,1.000
Tmin'	0.963	

Correction method= # Reported T Limits: Tmin=0.263 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.899   Theta(max)= 30.491

R(reflections)= 0.0662(1010)   wR2(reflections)=
                                                 0.2241(3012)

S = 0.937   Npar= 143

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 B
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low ..   34% Check

Alert level C
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C10   --C11   .   5.3 s.u.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.00455 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...   -0.141 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   2.526 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).   5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   14 Report

Alert level G
PLAT012_ALERT_1_G No   _shelx_res_checksum Found in CIF ......   Please Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   297 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   7 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.   2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.   2 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   0 Info

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

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  3 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
  1 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. 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 06/07/2023; check.def file version of 30/06/2023

NOMOVE FORCED

Prob = 50
Temp = 295

-11 Y

PLATON-Sep 8 12:50:20 2023 - (60723)

Z -55   exp_345   P b c a   R = 0.07   RES= 0 -90 X