checkCIF/PLATON report

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: test1_a

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Bond precision:    C-C = 0.0064 A              Wavelength=0.71073

Cell:              a=10.7002(11)      b=6.0652(7)         c=11.8500(12)
                   alpha=90           beta=99.659(3)      gamma=90
Temperature:       126 K

                   Calculated                   Reported
Volume             758.15(14)                   758.15(14)
Space group        P 21                         P 1 21 1
Hall group         P 2yb                        P 2yb
Moiety formula     C13 H25 N O5                 C13 H25 N O5
Sum formula        C13 H25 N O5                 C13 H25 N O5
Mr                 275.34                       275.34
Dx,g cm-3          1.206                        1.206
Z                  2                            2
Mu (mm-1)          0.092                        0.092
F000               300.0                        300.0
F000'              300.16
h,k,lmax           12,7,14                      12,7,14
Nref               2667[ 1472]                  2586
Tmin,Tmax          0.989,0.992                  0.507,0.745
Tmin'              0.950

Correction method= # Reported T Limits: Tmin=0.507 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.76/0.97        Theta(max)= 25.007
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R(reflections)= 0.0525(2515)

wR2(reflections)= 0.1366(2586)

S = 1.157   Npar= 180

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

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STRVA01_ALERT_4_C           Flack test results are meaningless.
          From the CIF: _refine_ls_abs_structure_Flack     0.000
          From the CIF: _refine_ls_abs_structure_Flack_su     0.600
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .     0.974 Why?
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.00644 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     2.037 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).     7 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=     0.595     32 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....     17 Note
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..     1 Check
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............     2 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .     0.600 Report
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O3     .     107.5 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........     37 Note
PLAT791_ALERT_4_G Model has Chirality at C007       (Sohnke SpGr)     R Verify
PLAT791_ALERT_4_G Model has Chirality at C009       (Sohnke SpGr)     R Verify
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 with s.u.     0.60 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still     93% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File     1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     4.6 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.     0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 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
   9 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 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.

PLATON version of 19/02/2022; check.def file version of 19/02/2022