checkCIF/PLATON report

Structure factors have been supplied for datablock(s) angel1

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: angel1

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Bond precision:   C-C = 0.0080 A          Wavelength=0.71073

Cell:             a=6.5034(9)     b=20.107(3)          c=9.4107(13)
                  alpha=90        beta=108.768(6)      gamma=90
Temperature:      296 K

                 Calculated                Reported
Volume           1165.2(3)                 1165.1(3)
Space group      P 21/c                    P 21/c
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C12 H15 N O2              C12 H15 N O2
Sum formula      C12 H15 N O2              C12 H15 N O2
Mr               205.25                    205.25
Dx,g cm-3        1.170                     1.170
Z                4                         4
Mu (mm-1)        0.080                     0.080
F000             440.0                     440.0
F000'            440.20
h,k,lmax         5,17,8                    5,17,8
Nref             786                       785
Tmin,Tmax        0.978,0.983               0.978,0.983
Tmin'            0.978

Correction method= # Reported T Limits: Tmin=0.978 Tmax=0.983
AbsCorr = MULTI-SCAN

Data completeness= 0.999           Theta(max)= 17.848

R(reflections)= 0.0451( 609)                    wR2(reflections)=
                                                0.1162( 785)
S = 1.068                  Npar= 143
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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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4312

Author Response: This alarm is due to the crystal diffracting weakly at high angle.

PLAT088_ALERT_3_A Poor Data / Parameter Ratio ..... 5.49 Note

Author Response: The alarm of poor data / parameter ratio is due to the crystal which diffracted quite weakly at high angle.

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for C8 --C9 . 5.5 s.u.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C9 Check
PLAT245_ALERT_2_C U(iso) H1N Smaller than U(eq) N1 by 0.012 Ang**2
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.008 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.548 Check

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? 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 65% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.8 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

2 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **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
4 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
0 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 12/09/2022; check.def file version of 09/08/2022

Datablock angel1 - ellipsoid plot