checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_613F22_LT_0m_a

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: cu_613F22_LT_0m_a

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Bond precision:  C-C = 0.0025 A          Wavelength=1.54178

Cell:            a=7.8377(5)    b=16.5237(11)      c=12.3065(8)
                 alpha=90       beta=99.120(2)     gamma=90
Temperature:     150 K

                Calculated                Reported
Volume          1573.64(18)               1573.64(18)
Space group     P 21                      P 21
Hall group      P 2yb                     P 2yb
Moiety formula  C34 H56 O7                ?
Sum formula     C34 H56 O7                C34 H56 O7
Mr              576.79                    576.78
Dx,g cm-3       1.217                     1.217
Z               2                         2
Mu (mm-1)       0.664                     0.664
F000            632.0                     632.0
F000'           633.85
h,k,lmax        9,20,14                   9,20,14
Nref            5970[ 3096]               5925
Tmin,Tmax       0.691,0.762               0.680,0.773
Tmin'           0.627

Correction method= # Reported T Limits: Tmin=0.680 Tmax=0.773
AbsCorr = MULTI-SCAN

Data completeness= 1.91/0.99      Theta(max)= 70.142

R(reflections)= 0.0280( 5858)     wR2(reflections)= 0.0749( 5925)

S = 1.046                 Npar= 467
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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 C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ..... 6.61 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 4 Note

Alert level G

PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.63 mm
PLAT791_ALERT_4_G Model has Chirality at C3 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C9 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C11 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C14 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C16 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C19 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C20 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C24 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C25 (Sohnke SpGr) S Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 19 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 1 Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
11 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 08/07/2020; check.def file version of 17/06/2020

Datablock cu_613F22_LT_0m_a - ellipsoid plot