checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_22172_auto

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_22172_auto

```
Bond precision:   C-C = 0.0047 A           Wavelength=1.54184

Cell:              a=8.1497(3)      b=12.7732(5)      c=29.0573(10)
                   alpha=90         beta=90           gamma=90
Temperature:       100 K

                 Calculated                  Reported
Volume           3024.80(19)                 3024.80(19)
Space group      P 21 21 21                  P 21 21 21
Hall group       P 2ac 2ab                   P 2ac 2ab
Moiety formula   C35 H44 O5                  C35 H44 O5
Sum formula      C35 H44 O5                  C35 H44 O5
Mr               544.70                      544.70
Dx,g cm-3        1.196                       1.196
Z                4                           4
Mu (mm-1)        0.621                       0.621
F000             1176.0                      1176.0
F000'            1179.39
h,k,lmax         9,15,34                     9,15,34
Nref             5339[ 3049]                 5319
Tmin,Tmax        0.963,0.988                 0.760,1.000
Tmin'            0.940

Correction method= # Reported T Limits: Tmin=0.760 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.74/1.00        Theta(max)= 66.589

R(reflections)= 0.0459( 4682)                wR2(reflections)=
                                             0.1206( 5319)
S = 1.099                  Npar= 365
```

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

```
PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ...      3.000 Sigma
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00474 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
              C35 H44 O5
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595          4 Report
                6  0  3,   0 11  6,   0 11  7,   0 12 10,
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
              H1
PLAT791_ALERT_4_G Model has Chirality at C8         (Sohncke SpGr)          R Verify
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        68% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
                0  0  2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         16 Note
               -7  1  7,  -7  4 22,  -6  1 23,  -6  1 24,  -6  2 24,  -1 12  7,
                0 11  6,   0 11  7,   0 12 10,   1 12  8,   1 12  9,   2 13 11,
                3 14  8,   6  0  3,   8  1 19,   9  5  6,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.088 Note
              Predicted wR2: Based on SigI**2  5.78 or SHELX Weight 10.97
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          6 Info
```

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 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 22/08/2024; check.def file version of 21/08/2024

Datablock exp_22172_auto - ellipsoid plot