checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 22094_agf34

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: 22094_agf34

```
Bond precision:   C-C = 0.0018 A          Wavelength=1.54184

Cell:             a=13.4802(2)     b=11.2809(1)        c=9.1821(1)
                  alpha=90         beta=90.983(1)      gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           1396.11(3)                1396.11(3)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C14 H15 F3 N2 O           C14 H15 F3 N2 O
Sum formula      C14 H15 F3 N2 O           C14 H15 F3 N2 O
Mr               284.28                    284.28
Dx,g cm-3        1.352                     1.352
Z                4                         4
Mu (mm-1)        0.978                     0.978
F000             592.0                     592.0
F000'            594.23
h,k,lmax         15,12,10                  15,12,10
Nref             2226                      2224
Tmin,Tmax        0.889,0.925               0.702,1.000
Tmin'            0.889

Correction method= # Reported T Limits: Tmin=0.702 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 62.490

R(reflections)= 0.0302( 2041)                wR2(reflections)=
                                             0.0777( 2224)
S = 1.074                 Npar= 188
```

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

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5752
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.575 2 Report

Alert level G

PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..... 0.00010 Ang.
PLAT793_ALERT_4_G Model has Chirality at C1 (Centro SPGR) R Verify
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 87% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 125.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 11 Info

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

0 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
3 ALERT type 3 Indicator that the structure quality may be low
2 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 22094_agf34 - ellipsoid plot

