checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3-57-1

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: 3-57-1

```
Bond precision:   C-C = 0.0055 A          Wavelength=0.71073

Cell:           a=9.3415(10)      b=10.0623(13)     c=19.6690(17)
                alpha=81.197(9)   beta=78.568(8)    gamma=63.180(12)
Temperature:    150 K

                 Calculated                Reported
Volume           1612.9(3)                 1612.9(3)
Space group      P -1                      P -1
Hall group       -P 1                      -P 1
Moiety formula   C16 H23 F N2 O            C16 H23 F N2 O
Sum formula      C16 H23 F N2 O            C16 H23 F N2 O
Mr               278.36                    278.36
Dx,g cm-3        1.146                     1.146
Z                4                         4
Mu (mm-1)        0.080                     0.080
F000             600.0                     600.0
F000'            600.27
h,k,lmax         11,11,23                  11,11,23
Nref             5670                      5670
Tmin,Tmax        0.989,0.992               0.224,1.000
Tmin'            0.988

Correction method= # Reported T Limits: Tmin=0.224 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 24.999

R(reflections)= 0.0871( 4092)                wR2(reflections)=
                                             0.2326( 5670)
S = 1.056                  Npar= 377
```

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

```
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C22 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00554 Ang.
PLAT352_ALERT_3_C Short  N-H (X0.87,N1.01A)  N2       - H2       .       0.76 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C7       - C8       .       1.53 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     17.358 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.170 Check
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 ..............          1 Report
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        44% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.9 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
```

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
6 **ALERT level G** = General information/check it is not something unexpected

0 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
8 ALERT type 3 Indicator that the structure quality may be low
0 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 06/07/2023; check.def file version of 30/06/2023

Datablock 3-57-1 - ellipsoid plot