checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I_Fo23_INVERT_v01

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: I_Fo23_INVERT_v01

```
Bond precision:   C-C = 0.0048 A          Wavelength=0.71073

Cell:             a=4.9556(2)     b=5.6718(3)         c=19.6250(15)
                  alpha=90        beta=96.618(6)      gamma=90
Temperature:      294 K

                 Calculated                Reported
Volume           547.93(6)                 547.93(6)
Space group      P n                       P n
Hall group       P -2yac                   P -2yac
Moiety formula   C13 H8 F3 N O             C13 H8 F3 N O
Sum formula      C13 H8 F3 N O             C13 H8 F3 N O
Mr               251.20                    251.20
Dx,g cm-3        1.523                     1.523
Z                2                         2
Mu (mm-1)        0.132                     0.132
F000             256.0                     256.0
F000'            256.18
h,k,lmax         6,7,25                    6,7,25
Nref             2571[ 1289]               1600
Tmin,Tmax        0.980,0.987               0.982,0.995
Tmin'            0.947

Correction method= # Reported T Limits: Tmin=0.982 Tmax=0.995
AbsCorr = ANALYTICAL

Data completeness= 1.24/0.62        Theta(max)= 27.693

R(reflections)= 0.0376( 1334)                wR2(reflections)=
                                             0.0789( 1600)
S = 1.094                Npar= 167
```

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

```
STRVA01_ALERT_4_C           Flack parameter is too small
          From the CIF: _refine_ls_abs_structure_Flack   -1.500
          From the CIF: _refine_ls_abs_structure_Flack_su    0.800
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........       7.38 Note
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F12      --C12      .        5.5 s.u.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C21      -C26      .       1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00477 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.248 Check
```

Alert level G

```
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      0.800 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         56 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage         29 %
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.20 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.5 Low
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
6 **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
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock I_Fo23_INVERT_v01 - ellipsoid plot