checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I_Fo24_MOLBANK_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_Fo24_MOLBANK_v01

```
Bond precision:   C-C = 0.0047 A          Wavelength=0.71073

Cell:             a=5.6756(3)     b=4.9829(2)         c=19.3064(12)
                  alpha=90        beta=91.197(5)      gamma=90
Temperature:      294 K
```

	Calculated	Reported
Volume	545.88(5)	545.88(5)
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	1.528	1.528
Z	2	2
Mu (mm-1)	0.132	0.132
F000	256.0	256.0
F000'	256.18	
h,k,lmax	7,6,25	7,6,24
Nref	2550[1278]	1799
Tmin,Tmax	0.942,0.991	0.933,0.991
Tmin'	0.884	

```
Correction method= # Reported T Limits: Tmin=0.933 Tmax=0.991
AbsCorr = ANALYTICAL

Data completeness= 1.41/0.71        Theta(max)= 27.676

R(reflections)= 0.0377( 1615)                    wR2(reflections)=
                                                 0.0942( 1799)
S = 1.042                  Npar= 168
```

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   -0.500
          From the CIF: _refine_ls_abs_structure_Flack_su    0.700
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........       7.16 Note
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F12      --C12      .        5.5 s.u.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00469 Ang.
```

Alert level G

```
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      0.700 Report
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..       0.93 mm
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
               0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         73 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage         47 %
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .      0.10 Check
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 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
9 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 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 29/11/2023; check.def file version of 14/09/2023

Datablock I_Fo24_MOLBANK_v01 - ellipsoid plot