checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20251022_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: 20251022_auto

```
Bond precision:   C-C = 0.0024 A          Wavelength=0.71073

Cell:             a=19.5061(8)     b=7.0805(2)          c=24.9807(11)
                  alpha=90         beta=111.708(5)      gamma=90
Temperature:      298 K

                 Calculated                  Reported
Volume           3205.5(2)                   3205.5(2)
Space group      I 2/a                       I 1 2/a 1
Hall group       -I 2ya                      -I 2ya
Moiety formula   C16 H15 F N2 O4 S           C16 H15 F N2 O4 S
Sum formula      C16 H15 F N2 O4 S           C16 H15 F N2 O4 S
Mr               350.36                      350.36
Dx,g cm-3        1.452                       1.452
Z                8                           8
Mu (mm-1)        0.236                       0.236
F000             1456.0                      1456.0
F000'            1457.77
h,k,lmax         27,10,35                    26,9,34
Nref             4881                        4077
Tmin,Tmax        0.893,0.914                 0.437,1.000
Tmin'            0.868

Correction method= # Reported T Limits: Tmin=0.437 Tmax=1.000
AbsCorr = MULTI-SCAN
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Data completeness= 0.835 Theta(max)= 30.482

R(reflections)= 0.0403(3151) wR2(reflections)= 0.1117(4077)

S = 1.089 Npar= 219

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
-8 0 4, 0 0 16,

Alert level G

PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]= 2.25 Note
0 0 2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 768 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
0 0 16, -8 0 4,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.7 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.533 Note
Predicted wR2: Based on SigI**2 3.16 or SHELX Weight 10.26 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 7 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **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
1 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 20/06/2026; check.def file version of 19/06/2026

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duplicate check

No duplication found

Datablock 20251022_auto - ellipsoid plot

