checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: a

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Bond precision:  C-C = 0.0040 A          Wavelength=0.71073

Cell:          a=9.7735(3)         b=12.0104(4)   c=13.4634(5)
               alpha=106.275(1)    beta=90        gamma=90.065(2)
Temperature:   296 K

                Calculated                Reported
Volume          1517.05(9)                1517.05(9)
Space group     P -1                      P-1
Hall group      -P 1                      ?
Moiety formula  C18 H10 F4 O3             ?
Sum formula     C18 H10 F4 O3             C18 H10 F4 O3
Mr              350.26                    350.26
Dx,g cm-3       1.534                     1.534
Z               4                         4
Mu (mm-1)       0.136                     0.136
F000            712.0                     712.0
F000'           712.56
h,k,lmax        12,15,17                  12,15,17
Nref            6980                      6625
Tmin,Tmax       0.966,0.981               0.965,0.981
Tmin'           0.965

Correction method= # Reported T Limits: Tmin=0.965 Tmax=0.981
AbsCorr = EMPIRICAL

Data completeness= 0.949          Theta(max)= 27.510

R(reflections)= 0.0951( 4737)     wR2(reflections)= 0.2929( 6625)

S = 1.049                 Npar= 451
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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 B

SYMMS02_ALERT_1_B Two angles should be 90 for a monoclinic cell
Cell 9.7735 12.0104 13.4634
Angles 106.2750 90.0000 90.0650

Author Response: Although the two angles are almost 90, the cell is not monoclinic. The checking program PLATON did not find a symmetry higher than triclinic. If t data was averaged in a monoclinic space group C2/c setting, the Rint is equal t but any fragment of the structure is not determined.

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low . 0.950 Note

Author Response: We made several attempts to obtain better quality data for this structure, after a number of attempts of data collection, the reported one is found to be the best one.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as empirical
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
identifier.
clourless
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.29 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.13 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 0.81 eA-3

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.19 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with P-1 Check
PLAT145_ALERT_4_G s.u. on beta Small or Missing ..... 0.0000 Degree
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C36 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C35 Check
PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C25 -C30 1.44 Ang.
PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C8 -C13 1.45 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C25 -C30 0.16 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C8 -C13 0.17 Ang.
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 2 Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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

  8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  9 ALERT type 2 Indicator that the structure model may be wrong or deficient
  2 ALERT type 3 Indicator that the structure quality may be low
  3 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
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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 24/11/2016; check.def file version of 23/11/2016

Datablock a - ellipsoid plot