checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_ydg_lcf_11_0m_a

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: mo_ydg_lcf_11_0m_a

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Bond precision:   C-C = 0.0065 A          Wavelength=0.71073

Cell:              a=7.5369(3)      b=12.4354(7)      c=14.8372(7)
                   alpha=90         beta=90           gamma=90
Temperature:       303 K

                 Calculated                Reported
Volume           1390.61(12)               1390.61(12)
Space group      P 21 21 21                P 21 21 21
Hall group       P 2ac 2ab                 P 2ac 2ab
Moiety formula   C10 H12 Br F N6 O3        C10 H12 Br F N6 O3
Sum formula      C10 H12 Br F N6 O3        C11 H12 Br F N5 O3
Mr               363.16                    361.17
Dx,g cm-3        1.735                     1.725
Z                4                         4
Mu (mm-1)        2.988                     2.986
F000             728.0                     724.0
F000'            727.18
h,k,lmax         9,16,19                   9,16,19
Nref             3190[ 1842]               3182
Tmin,Tmax        0.549,0.658               0.583,0.746
Tmin'            0.392

Correction method= # Reported T Limits: Tmin=0.583 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.73/1.00        Theta(max)= 27.505

R(reflections)= 0.0382( 2604)                wR2(reflections)=
                                             0.0966( 3182)
S = 0.947                  Npar= 192
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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 C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..      1.99 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0065 Ang.
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Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C11 H12 Br1 F1 N5 O3
           Atom count from _chemical_formula_moiety:C10 H12 Br1 F1 N6 O3
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C11 H12 Br1 F1 N5 O3
           Atom count from the _atom_site data:  C10 H12 Br1 F1 N6 O3
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C11 H12 Br F N5 O3
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         44.00     40.00    4.00
          H         48.00     48.00    0.00
          Br         4.00      4.00    0.00
          F          4.00      4.00    0.00
          N         20.00     24.00   -4.00
          O         12.00     12.00    0.00
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          6 Report
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O2       .      109.6 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  Br1      ..C2       .       3.33 Ang.
                                          1-x,1/2+y,3/2-z  =      3_656 Check
PLAT791_ALERT_4_G Model has Chirality at C1          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C5          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C8          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C9          (Sohnke SpGr)          R Verify
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 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
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  4 ALERT type 2 Indicator that the structure model may be wrong or deficient
  1 ALERT type 3 Indicator that the structure quality may be low
  4 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. 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 12/09/2022; check.def file version of 09/08/2022

Datablock mo_ydg_lcf_11_0m_a - ellipsoid plot