checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_AlMe_0m

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_AlMe_0m

```
Bond precision:  C-C = 0.0082 A          Wavelength=0.71073

Cell:          a=7.354(4)        b=7.723(4)       c=12.601(6)
               alpha=94.767(7)   beta=98.204(7)   gamma=115.566(6)
Temperature:   100 K

                 Calculated                Reported
Volume           630.6(6)                  630.6(5)
Space group      P -1                      P -1
Hall group       -P 1                      -P 1
Moiety formula   C10 H20 Al N2 S2          C10 H21 Al N2 S2
Sum formula      C10 H20 Al N2 S2          C10 H21 Al N2 S2
Mr               259.38                    260.39
Dx,g cm-3        1.366                     1.371
Z                2                         2
Mu (mm-1)        0.463                     0.463
F000             278.0                     280.0
F000'            278.67
h,k,lmax         8,9,15                    8,9,15
Nref             2346                      2333
Tmin,Tmax        0.989,0.991
Tmin'            0.977

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

Data completeness= 0.994          Theta(max)= 25.495

R(reflections)= 0.0733( 1437)     wR2(reflections)= 0.1386( 2333)

S = 1.250                 Npar= 138
```

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

```
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 multi-scan
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       1.01 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT234_ALERT_4_C Large Hirshfeld Difference C1     --  C2      ..       0.16 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.5 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0082 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.867 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         13 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Note
```

Alert level G

```
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:C10 H21 Al1 N2 S2
           Atom count from the _atom_site data:  C10 H20 Al1 N2 S2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C10 H21 Al N2 S2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         20.00     20.00    0.00
          H         42.00     40.00    2.00
          Al         2.00      2.00    0.00
          N          4.00      4.00    0.00
          S          4.00      4.00    0.00
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT793_ALERT_4_G The Model has Chirality at N1      (Centro SPGR)          S Verify
PLAT793_ALERT_4_G The Model has Chirality at N2      (Centro SPGR)          R Verify
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          7 Note
```

---

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

   7 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
   3 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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_ABSTY02_mo_AlMe_0m
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
```

```
_vrf_PLAT041_mo_AlMe_0m
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT043_mo_AlMe_0m
;
PROBLEM: Calculated and Reported Mol. Weight Differ by ..       1.01 Check
RESPONSE: ...
;
_vrf_PLAT068_mo_AlMe_0m
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)...     Please Check
RESPONSE: ...
;
_vrf_PLAT234_mo_AlMe_0m
;
PROBLEM: Large Hirshfeld Difference C1     --  C2      ..       0.16 Ang.
RESPONSE: ...
;
_vrf_PLAT250_mo_AlMe_0m
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.5 Note
RESPONSE: ...
;
_vrf_PLAT340_mo_AlMe_0m
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............     0.0082 Ang.
RESPONSE: ...
;
_vrf_PLAT906_mo_AlMe_0m
;
PROBLEM: Large K value in the Analysis of Variance ......      2.867 Check
RESPONSE: ...
;
_vrf_PLAT911_mo_AlMe_0m
;
PROBLEM: Missing # FCF Refl Between THmin & STh/L=  0.600         13 Report
RESPONSE: ...
;
_vrf_PLAT978_mo_AlMe_0m
;
PROBLEM: Number C-C Bonds with Positive Residual Density.          0 Note
RESPONSE: ...
;
# end Validation Reply Form
```

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 27/03/2017; check.def file version of 24/03/2017

Datablock mo_AlMe_0m - ellipsoid plot