checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

```
Bond precision:    C-C = 0.0063 A              Wavelength=0.71073

Cell:              a=18.512(3)       b=27.014(4)        c=7.4371(12)
                   alpha=90          beta=90            gamma=90
Temperature:       296 K

                   Calculated                 Reported
Volume             3719.2(10)                 3719.2(10)
Space group        P c c n                    P c c n
Hall group         -P 2ab 2ac                 -P 2ab 2ac
Moiety formula     C18 H20 N4 O S [+ solvent] C18 H20 N4 O S
Sum formula        C18 H20 N4 O S [+ solvent] C18 H20 N4 O S
Mr                 340.44                     340.44
Dx,g cm-3          1.216                      1.216
Z                  8                          8
Mu (mm-1)          0.185                      0.185
F000               1440.0                     1440.0
F000'              1441.45
h,k,lmax           24,35,9                    23,34,9
Nref               4283                       4014
Tmin,Tmax          0.955,0.978                0.662,0.746
Tmin'              0.955

Correction method= # Reported T Limits: Tmin=0.662 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.937            Theta(max)= 27.526
```

R(reflections)= 0.0757(1934)

wR2(reflections)= 0.2646(4014)

S = 1.052   Npar= 220

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

```
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..      48% Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................    0.26 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range     3.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range     4.4 Ratio
PLAT241_ALERT_2_C High  'MainMol' Ueq as Compared to Neighbors of       N4 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of      C15 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of      C17 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00633 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond C15     - C16     .     1.42 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn    H16A    ..H16A    .     2.10 Ang.
                                    1/2-x,3/2-y,z  =      2_565 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N2      --H2      .    Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    7.789 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    2.048 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600        6 Report
            22  0  0, 22  2  0,  0 30  0,  1 31  0,  0 32  0,  2 32  0,
```

⚪ Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      2 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms       3 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       2 Report
            H1      H2
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large    0.14 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records       1 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par   0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar   0.0020 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure     100 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       4 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed       ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       2 Note
            1  1  0,  0  2  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600     259 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........   5.518 Note
            Predicted wR2: Based on SigI**2  4.80 or SHELX Weight 25.15
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       0 Info
```

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

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 ALERT type 2 Indicator that the structure model may be wrong or deficient
 11 ALERT type 3 Indicator that the structure quality may be low
  5 ALERT type 4 Improvement, methodology, query or suggestion
  2 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 15/07/2024; check.def file version of 15/07/2024