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: 4

```
Bond precision:   C-C = 0.0081 A          Wavelength=0.71073

Cell:               a=17.629(2)      b=7.8704(11)      c=18.671(2)
                    alpha=90         beta=90           gamma=90
Temperature:        100 K

                 Calculated                  Reported
Volume           2590.6(5)                   2590.6(6)
Space group      P b c a                     P b c a
Hall group       -P 2ac 2ab                  -P 2ac 2ab
Moiety formula   C15 H14 N2 O S              C15 H14 N2 O S
Sum formula      C15 H14 N2 O S              C15 H14 N2 O S
Mr               270.34                      270.34
Dx,g cm-3        1.386                       1.386
Z                8                           8
Mu (mm-1)        0.242                       0.242
F000             1136.0                      1136.0
F000'            1137.38
h,k,lmax         20,9,22                     20,9,22
Nref             2285                        2283
Tmin,Tmax        0.966,0.990                 0.532,0.746
Tmin'            0.962

Correction method= # Reported T Limits: Tmin=0.532 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.999           Theta(max)= 25.020

R(reflections)= 0.1202( 1745)                wR2(reflections)=
                                             0.1762( 2283)
S = 1.254                  Npar= 174
```

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

PLAT082_ALERT_2_C High R1 Value ..... 0.12 Report
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00807 Ang.

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
H1
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 13.76 Why ?
PLAT793_ALERT_4_G Model has Chirality at C8 (Centro SpGr) S Verify

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **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
1 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. 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 22/08/2024; check.def file version of 21/08/2024

Datablock 4 - ellipsoid plot

