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: 1

```
Bond precision:    C-C = 0.0092 A              Wavelength=0.71073

Cell:            a=4.6973(8)         b=11.160(2)        c=11.554(2)
                 alpha=67.350(5)     beta=82.509(4)     gamma=87.050(5)
Temperature:     296 K

                 Calculated                   Reported
Volume           554.20(17)                   554.18(18)
Space group      P 1                          P 1
Hall group       P 1                          P 1
Moiety formula   C25 H20 N4 O4 S2             ?
Sum formula      C25 H20 N4 O4 S2             C25 H20 N4 O4 S2
Mr               504.57                       504.57
Dx,g cm-3        1.512                        1.512
Z                1                            1
Mu (mm-1)        0.284                        0.284
F000             262.0                        262.0
F000'            262.35
h,k,lmax         5,13,13                      5,13,13
Nref             3950[ 1975]                  3606
Tmin,Tmax        0.986,0.992                  0.960,0.991
Tmin'            0.958

Correction method= # Reported T Limits: Tmin=0.960 Tmax=0.991
AbsCorr = MULTI-SCAN

Data completeness= 1.83/0.91        Theta(max)= 25.062

                                               wR2(reflections)=
R(reflections)= 0.0434( 2953)                  0.1108( 3606)

S = 1.062                   Npar= 325
```

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

```
STRVA01_ALERT_4_C            Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack      0.500
          From the CIF: _refine_ls_abs_structure_Flack_su   12.000
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........      6.08 Note
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.    C1        -C6      .      1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.00924 Ang.
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⚪ Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............      1 Report
               H4
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .   0.500 Note
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical      ? Check
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =      3 Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....    C10 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged  Please Check
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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
   7 ALERT level G = General information/check it is not something unexpected

   2 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
   2 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 13/12/2023; check.def file version of 13/12/2023