checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

```
Bond precision:   C-C = 0.0052 A            Wavelength=0.71073

Cell:           a=6.6021(5)        b=7.5617(7)        c=8.1001(7)
                alpha=110.521(8)   beta=100.869(7)   gamma=99.006(7)
Temperature:    293 K

                  Calculated                    Reported
Volume           360.87(6)                      360.87(6)
Space group      P 1                            P 1
Hall group       P 1                            P 1
Moiety formula   C8 H13 N5, 2(C N S)            C8 H13 N5, 2(N C S)
Sum formula      C10 H13 N7 S2                  C10 H13 N7 S2
Mr               295.39                         295.39
Dx,g cm-3        1.359                          1.359
Z                1                              1
Mu (mm-1)        0.367                          0.367
F000             154.0                          154.0
F000'            154.28
h,k,lmax         8,10,10                        8,10,10
Nref             3784[ 1892]                    2846
Tmin,Tmax        0.838,0.943                    0.924,1.000
Tmin'            0.820

Correction method= # Reported T Limits: Tmin=0.924 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.50/0.75      Theta(max)= 28.911

R(reflections)= 0.0348( 2560)      wR2(reflections)= 0.0887( 2846)

S = 1.027                   Npar= 193
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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

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PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of          C9 Check
PLAT242_ALERT_2_C Low     'MainMol' Ueq as Compared to Neighbors of         C10 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00517 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor        N1      --  H1A    ...    Please Check
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage         63 %
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         8 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         3 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)       293 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2 Note
          C N S
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        10 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       231 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 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
```

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 13/08/2017; check.def file version of 27/07/2017