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: fe0145_a

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Bond precision:    C-C = 0.0037 A           Wavelength=0.71073

Cell:              a=26.796(16)      b=8.141(3)         c=18.666(8)
                   alpha=90          beta=103.29(4)     gamma=90
Temperature:       100 K

                   Calculated                Reported
Volume             3963(3)                   3963(3)
Space group        C 2/c                     C 2/c
Hall group         -C 2yc                    -C 2yc
Moiety formula     C9 H25 B10 Cl2 N2 Sb      C9 H25 B10 Cl2 N2 Sb
Sum formula        C9 H25 B10 Cl2 N2 Sb      C9 H25 B10 Cl2 N2 Sb
Mr                 462.07                    462.06
Dx,g cm-3          1.549                     1.549
Z                  8                         8
Mu (mm-1)          1.655                     1.656
F000               1824.0                    1824.0
F000'              1821.91
h,k,lmax           33,10,23                  33,10,23
Nref               4061                      4034
Tmin,Tmax          0.804,0.876               0.697,0.773
Tmin'              0.780

Correction method= # Reported T Limits: Tmin=0.697 Tmax=0.773
AbsCorr = NUMERICAL

Data completeness= 0.993          Theta(max)= 26.372

R(reflections)= 0.0255( 3813)     wR2(reflections)= 0.0602( 4034)

S = 1.185                Npar= 224
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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 B**
PLAT410_ALERT_2_B Short Intra H...H Contact H4A   ..H7A   .   1.88 Ang.
                                             x,y,z =   1_555 Check

⬤ **Alert level C**
PLAT420_ALERT_2_C D-H Without Acceptor   N2   --H2A   .   Please Check

⬤ **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 Uij Restrained non-H Atoms ...   21 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   8.07 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records   1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records   1 Report
PLAT343_ALERT_2_G Unusual sp?   Angle Range in Main Residue for   C2 Check
PLAT343_ALERT_2_G Unusual sp?   Angle Range in Main Residue for   C3 Check
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C1   - C2   .   1.51 Ang.
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C2   - C3   .   1.63 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   8 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   541 Note

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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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 18/02/2019; check.def file version of 18/02/2019