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: ww

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Bond precision:    C-C = 0.0025 A              Wavelength=0.71073

Cell:              a=7.8192(16)       b=8.8800(18)       c=9.0142(18)
                   alpha=83.14(3)     beta=65.27(3)      gamma=81.67(3)
Temperature:       293 K

                   Calculated                  Reported
Volume             561.3(2)                    561.3(2)
Space group        P -1                        P-1
Hall group         -P 1                        ?
Moiety formula     C16 H22 Mn N4 O10, 2(H2 O)  ?
Sum formula        C16 H26 Mn N4 O12           C16 H26 Mn N4 O12
Mr                 521.35                      521.35
Dx,g cm-3          1.542                       1.542
Z                  1                           1
Mu (mm-1)          0.657                       0.657
F000               271.0                       271.0
F000'              271.49
h,k,lmax           10,11,11                    10,11,11
Nref               2582                        2559
Tmin,Tmax          0.877,0.888                 0.880,0.891
Tmin'              0.877

Correction method= # Reported T Limits: Tmin=0.880 Tmax=0.891
AbsCorr = MULTI-SCAN

Data completeness= 0.991            Theta(max)= 27.460

R(reflections)= 0.0381( 2467)       wR2(reflections)= 0.0969( 2559)

S = 1.061                   Npar= 151
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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        Mn1 Check
PLAT420_ALERT_2_C D-H Without Acceptor        N2      --  H2B     ...    Please Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        9 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF    Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        7 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical        ? Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as    mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.03 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)      293 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        5 Do !
          N1  -MN1 -N1  -C5      1.00  0.00  2.675  1.555  1.555  1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       10 Do !
          N1  -MN1 -N1  -C1     17.00  0.00  2.675  1.555  1.555  1.555
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        6 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        6 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL     2014 Note
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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
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 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
   2 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*, 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 19/11/2015; check.def file version of 17/11/2015