checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ganr109_0m_a

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: ganr109_0m_a

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Bond precision:   C-C = 0.0054 A          Wavelength=0.71073

Cell:           a=11.3848(7)       b=13.2226(8)      c=17.9690(9)
                alpha=81.733(2)    beta=82.039(2)    gamma=66.802(2)
Temperature:    100 K

                Calculated                  Reported
Volume          2450.5(2)                   2450.5(2)
Space group     P -1                        P -1
Hall group      -P 1                        -P 1
Moiety formula  C45 H63 B N4 O2 Zn, C6 H14  C45 H63 B N4 O2 Zn, C6 H14
Sum formula     C51 H77 B N4 O2 Zn          C51 H77 B N4 O2 Zn
Mr              854.37                      854.34
Dx,g cm-3       1.158                       1.158
Z               2                           2
Mu (mm-1)       0.542                       0.542
F000            924.0                       924.0
F000'           924.84
h,k,lmax        14,17,23                    14,17,23
Nref            11306                       11269
Tmin,Tmax       0.968,0.973                 0.647,0.746
Tmin'           0.968

Correction method= # Reported T Limits: Tmin=0.647 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.997           Theta(max)= 27.551

R(reflections)= 0.0574( 8159)                wR2(reflections)=
                                             0.1565( 11269)
S = 1.037                  Npar= 550
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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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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C47 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4    Please Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...    -1.075 Report
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         8 Note
               1  0  0,   0  1  0,   1  1  0,   0 -1  1,   0  0  1,   1  0  1,
               0  1  1,   1  1  1,
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Alert level G

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PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.002 Degree
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C30 Check
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O1       .     106.0 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O2       .     105.6 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         3 Note
              C01J    H01A    H01B
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        29 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.6 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     2.332 Note
              Predicted wR2: Based on SigI**2  6.71 or SHELX Weight 15.10
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         2 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
  10 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 22/08/2024; check.def file version of 21/08/2024

Datablock ganr109_0m_a - ellipsoid plot