checkCIF/PLATON report

Structure factors have been supplied for datablock(s) LFF3-Zn

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: LFF3-Zn

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Bond precision:  C-C = 0.0036 A          Wavelength=1.54184

Cell:            a=12.8594(4)    b=14.7599(4)       c=11.4301(4)
                 alpha=90        beta=91.303(3)     gamma=90
Temperature:     173 K

                Calculated                Reported
Volume          2168.91(12)               2168.91(12)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C18 H18 N4 O12 Zn2, H2 O  ?
Sum formula     C18 H20 N4 O13 Zn2        C18 H20 N4 O13 Zn2
Mr              631.16                    631.12
Dx,g cm-3       1.933                     1.933
Z               4                         4
Mu (mm-1)       3.477                     3.477
F000            1280.0                    1280.0
F000'           1271.70
h,k,lmax        15,17,13                  15,17,13
Nref            4084                      3951
Tmin,Tmax       0.692,0.706               0.953,1.000
Tmin'           0.565

Correction method= # Reported T Limits: Tmin=0.953 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.967          Theta(max)= 69.726

R(reflections)= 0.0306( 3369)     wR2(reflections)= 0.0819( 3951)

S = 1.040                 Npar= 334
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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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PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.977 Why?
PLAT716_ALERT_1_C H...A   Unknown or Inconsistent Label ..........          . Check
PLAT716_ALERT_1_C H...A   Unknown or Inconsistent Label ..........          . Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         89 Report
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         10 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn2      --O3       .        5.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn2      --O4       .       19.5 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       2.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2       (II)      .       2.03 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         44 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          9 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
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   3 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
   4 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 22/04/2020; check.def file version of 09/03/2020

Datablock LFF3-Zn - ellipsoid plot