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

Bond precision: C-C = 0.0078 A Wavelength=0.71073

Cell: a=11.421(2) b=9.2213(17) c=15.188(3)
alpha=90 beta=106.112(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1536.7(5)	1536.7(5)
Space group	P 21	P21
Hall group	P 2yb	?
Moiety formula	C32 H32 N4 O7 Zn, H2 O	?
Sum formula	C32 H34 N4 O8 Zn	C32 H34 Cu0 N4 O8 Zn
Mr	668.02	668.00
Dx,g cm-3	1.444	1.444
Z	2	2
Mu (mm-1)	0.857	0.857
F000	696.0	696.0
F000’	696.87	
h,k,lmax	15,12,20	15,12,20
Nref	7613[4039]	5465
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 1.35/0.72 Theta(max)= 28.260

R(reflections)= 0.0439(4217) wR2(reflections)= 0.1156(5465)

S = 1.005 Npar= 411

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 Low .......      0.962 Note
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given .     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       9.83 Note
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range       3.2 Ratio
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C14 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.0078 Ang.
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Alert level G

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CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C32 H34 Cu0 N4 O8 Zn
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         64.00     64.00    0.00
          H         68.00     68.00    0.00
          Cu         2.00      0.00    2.00
          N          8.00      8.00    0.00
          O         16.00     16.00    0.00
          Zn         2.00      2.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension .......         2 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         3 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn1    --  O6      ..       6.9 su
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C10 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C21 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         1 Do !
            O5  -ZN1 -O1  -C11   123.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        10 Do !
            N4  -ZN1 -N3  -C32   145.00  1.40   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        15 Do !
            N4  -ZN1 -N3  -C28   -35.40  1.90   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        21 Do !
            N3  -ZN1 -N4  -C23    13.30  1.90   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        26 Do !
            N3  -ZN1 -N4  -C27  -172.40  1.50   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        30 Do !
            O1  -ZN1 -O5  -C22  -127.00  2.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        36 Do !
            O7  -ZN1 -O6  -C22   -42.00  4.00   1.555   1.555   1.555   2.555
PLAT791_ALERT_4_G The Model has Chirality at C8      .............         S Verify
PLAT791_ALERT_4_G The Model has Chirality at C19     .............         S Verify
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
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  20 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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  3 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
 12 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 20/08/2014; check.def file version of 18/08/2014

Datablock ww - ellipsoid plot