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: MUF-91-3h-41pc

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Bond precision:  = 0.0000 A              Wavelength=0.71080

Cell:              a=17.119(2)      b=17.119(2)      c=17.119(2)
                   alpha=90         beta=90          gamma=90
Temperature:       100 K
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	Calculated	Reported
Volume	5016.9(18)	5016.9(18)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	2(C8.45 H4.83 N0.50 O1.53 Zn0.47)	1(C84 H48 N6 O13 Zn4), 1(C17.42 H9.95 O5.39 Zn1.66)
Sum formula	C16.90 H9.66 N O3.06 Zn0.94	C101.41 H57.95 N6 O18.39 Zn5.66
Mr	337.43	2024.60
Dx,g cm-3	0.670	0.670
Z	6	1
Mu (mm-1)	0.699	0.699
F000	1025.3	1025.0
F000’	1027.25	
h,k,lmax	17,17,17	17,17,17
Nref	1051[591]	1046
Tmin,Tmax		0.622,0.746
Tmin’		

```
Correction method= # Reported T Limits: Tmin=0.622 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.77/1.00      Theta(max)= 20.816

R(reflections)= 0.1752( 882)      wR2(reflections)= 0.4698( 1046)

S = 2.253                 Npar= 99
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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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5000
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ..... 0.47 Report

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Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.6701 Check
PLAT082_ALERT_2_B High R1 Value ..... 0.18 Report
PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) ..... 5.97 Note
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C14 Check
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C34 Check
PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

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Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 2.253
RADNW01_ALERT_1_C The radiation wavelength lies outside the expected range
for the supplied radiation type. Expected range 0.71065-0.71075
Wavelength given = 0.71080
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.620
From the CIF: _refine_ls_abs_structure_Flack_su 0.018
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
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
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT087_ALERT_2_C Unsatisfactory S value (Too High) ..... 2.25 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O1 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . ZN0A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O2 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C10 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C11 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C12 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C13 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C14 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . N1 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C15 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C16 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C17 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C18 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C19 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C20 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C21 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . ZN1 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O3 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . O4 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C30 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C31 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C32 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C33 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C34 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O1 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . ZN0A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O2 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C10 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C11 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C12 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C13 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C14 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . N1 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C15 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C16 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C17 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C18 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C19 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C20 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C21 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . ZN1 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O3 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . O4 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C30 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C31 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C32 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C33 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C34 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O1 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . ZN0A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O2 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C10 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C11 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C12 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C13 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C14 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . N1 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C15 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C16 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C17 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C18 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C19 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C20 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C21 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . ZN1 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O3 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . O4 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C30 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C31 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C32 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C33 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C34 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Zn1 0.110 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 0.62 Check

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Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C101.41 H57.95 N6 O18.39 Zn5.66
Atom count from the _atom_site data: C77.33380 H52.96375 N6.004520 O8
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 1

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          From the CIF: _chemical_formula_sum  C101.41 H57.95 N6 O18.39 Zn5.66
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        101.42     77.34   24.08
          H         57.95     52.97    4.99
          N          6.00      6.00    0.00
          O         18.39      8.54    9.85
          Zn         5.66      0.94    4.72
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         16 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       6.00 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         11 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          5 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Zn0A       Constrained at     0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at     0.0417 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1         Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20        Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21        Constrained at       0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  1        15.78 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C13      ..C15             2.75 Ang.
                                                      z,y,x  =     24_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  N1       ..C15             2.40 Ang.
                                                      z,y,x  =     24_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15             3.18 Ang.
                                                   1-x,y,1-z  =      9_656 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15             3.18 Ang.
                                                      z,y,x  =     24_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15             3.18 Ang.
                                                   1-z,y,1-x  =     23_656 Check
PLAT607_ALERT_4_G VOID Test Skipped Due to Severe Disorder .....          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........         1 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        32 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       177 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
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  2 ALERT level A = Most likely a serious problem - resolve or explain
  6 ALERT level B = A potentially serious problem, consider carefully
 83 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 49 ALERT level G = General information/check it is not something unexpected

 14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 16 ALERT type 2 Indicator that the structure model may be wrong or deficient
  5 ALERT type 3 Indicator that the structure quality may be low
105 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 07/08/2019; check.def file version of 30/07/2019

Datablock MUF-91-3h-41pc - ellipsoid plot