checkCIF/PLATON report

Structure factors have been supplied for datablock(s) muf-91-15h-68pc

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-91-15h-68pc

Bond precision: = 0.0000 A Wavelength=0.95372

Cell: a=17.076(11) b=17.076(11) c=17.076(11)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4979(10)	4979(10)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	2(C9.37 H5.35 N0.50 O1.82 Zn0.56)	C84 H48 N6 O13 Zn4, C28.369 H16.211 O8.781 Zn2.702
Sum formula	C18.73 H10.70 N O3.63 Zn1.12	C112.37 H64.21 N6 O21.78 Zn6.70
Mr	381.03	2284.80
Dx,g cm-3	0.762	0.762
Z	6	1
Mu (mm-1)	1.826	1.799
F000	1156.3	1156.0
F000'	1156.39	
h,k,lmax	17,17,17	17,17,16
Nref	1033[581]	1031
Tmin,Tmax		0.524,0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.524 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.77/1.00 Theta(max)= 28.449

R(reflections)= 0.1803(815) wR2(reflections)= 0.5023(1031)

S = 2.316 Npar= 33

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 =    0.4995
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ...................       0.50 Report
PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of .       1597 Ang**3
```

Alert level B

```
PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 .........     0.7625 Check
PLAT082_ALERT_2_B High R1 Value ..................................       0.18 Report
PLAT971_ALERT_2_B Check Calcd Resid. Dens.  1.92Ang From O1              2.74 eA-3
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on      Zn0A       1.60 eA-3
```

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 =      2.316
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.553
          From the CIF: _refine_ls_abs_structure_Flack_su    0.014
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) ..............       2.32 Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       3.34 Report
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Zn1      0.150 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .       0.55 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.499          3 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          4 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      13.54 Check
```

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:C112.37 H64.21 N6 O21.78 Zn6.7
           Atom count from the _atom_site data:  C81.65399 H56.11199 N6 O10.12580
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
              not performed for this radiation type.
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
          From the CIF: _chemical_formula_sum  C112.37 H64.21 N6 O21.78 Zn6.70
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        112.37     81.65   30.72
          H         64.21     56.11    8.10
          N          6.00      6.00    0.00
          O         21.78     10.13   11.65
          Zn         6.70      1.12    5.58
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         10 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         19 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     6.0000 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
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.95372 Ang.
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          3 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          3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 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  )      17.59 Check
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing).        C14 Check
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing).        C34 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C13      ..C15      .       2.74 Ang.
                                                    z,y,x  =     24_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  N1       ..C15      .       2.39 Ang.
                                                    z,y,x  =     24_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15      .       3.17 Ang.
                                                 1-x,y,1-z  =      9_656 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15      .       3.17 Ang.
                                                    z,y,x  =     24_555 Check
```

```
PLAT432_ALERT_2_G Short Inter X...Y Contact  C14      ..C15      .       3.17 Ang.
                                                1-z,y,1-x  =     23_656 Check
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 .............    93 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still     34% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).     4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....     2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File     3 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .     1 Units
PLAT984_ALERT_1_G The  O-f'=    0.0218 Deviates from the B&C-Value   0.0205 Check
PLAT984_ALERT_1_G The Zn-f'=   -0.1382 Deviates from the B&C-Value  -0.1517 Check
PLAT985_ALERT_1_G The Zn-f"=    2.4327 Deviates from the B&C-Value   2.3734 Check
```

---

3 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
60 **ALERT level G** = General information/check it is not something unexpected

16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
21 ALERT type 2 Indicator that the structure model may be wrong or deficient
10 ALERT type 3 Indicator that the structure quality may be low
34 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_THETM01_muf-91-15h-68pc
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: ...
;
_vrf_PLAT084_muf-91-15h-68pc
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................       0.50 Report
RESPONSE: ...
;
_vrf_PLAT601_muf-91-15h-68pc
;
PROBLEM: Unit Cell Contains Solvent Accessible VOIDS of .       1597 Ang**3
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 20/01/2022; check.def file version of 19/01/2022

Datablock muf-91-15h-68pc - ellipsoid plot