checkCIF/PLATON report

Structure factors have been supplied for datablock(s) muf-91-9h-51pc

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-91-9h-51pc

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Bond precision:   = 0.0000 A              Wavelength=0.95372

Cell:               a=17.172(8)      b=17.172(8)      c=17.172(8)
                    alpha=90         beta=90          gamma=90
Temperature:        100 K
```

	Calculated	Reported
Volume	5064(7)	5064(7)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	C13.19 H7.54 N0.75 O2.46 Zn0.76	C84 H48 N6 O13 Zn4, C21.478 H12.273 O6.648 Zn2.046
Sum formula	C13.19 H7.54 N0.75 O2.46 Zn0.76	C105.48 H60.27 N6 O19.65 Zn6.05
Mr	265.18	2121.51
Dx,g cm-3	0.696	0.696
Z	8	1
Mu (mm-1)	1.618	1.600
F000	1073.8	1074.0
F000'	1073.93	
h,k,lmax	12,12,12	12,12,12
Nref	453[263]	446
Tmin,Tmax		0.426,0.746
Tmin'		

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Correction method= # Reported T Limits: Tmin=0.426 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.98        Theta(max)= 20.632
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R(reflections)= 0.2016(354)

wR2(reflections)= 0.4467(446)

S = 1.987 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 = 0.3695
PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of . 1654 Ang**3

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.6957 Check
PLAT082_ALERT_2_B High R1 Value ..... 0.20 Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.45 Report
PLAT260_ALERT_2_B Large Average Ueq of Residue Including Zn1 0.310 Check

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Alert level C

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 0.030
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.977 Why?
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
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.79 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.0 Note
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 0.62 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.369 2 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check
PLAT926_ALERT_1_C Reported and Calculated R1 Differ by ..... 0.0014 Check
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by ..... 0.0049 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 16.84 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:C105.48 H60.27 N6 O19.65 Zn6.05
Atom count from the _atom_site data: C78.94800 H54.14400 N6 O9.135 Zn
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 C105.48 H60.27 N6 O19.65 Zn6.05

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	105.48	78.95	26.53
H	60.27	54.14	6.13
N	6.00	6.00	0.00
O	19.65	9.14	10.51
Zn	6.05	1.01	5.04

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 ...	18	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	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 ...	8.0000	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	2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	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)	24.69	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 C14 ..C15 .	3.19	Ang.
	1-z,y,1-x =	23_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C14 ..C15 .	3.19	Ang.
	1-x,y,1-z =	9_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 #	31	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	75	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	61%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note

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PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         2 Note
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
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  15 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  56 ALERT level G = General information/check it is not something unexpected

  16 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
  12 ALERT type 3 Indicator that the structure quality may be low
  34 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.

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-91-9h-51pc
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: ...
;
_vrf_PLAT601_muf-91-9h-51pc
;
PROBLEM: Unit Cell Contains Solvent Accessible VOIDS of .       1654 Ang**3
RESPONSE: ...
;
# end Validation Reply Form
```

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

Datablock muf-91-9h-51pc - ellipsoid plot