

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) muf-91-12h-71pc

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-91-12h-71pc

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Bond precision: = 0.0000 Å Wavelength=0.71075

Cell: a=17.159 (5) b=17.159 (5) c=17.159 (5)  
alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	5052 (4)	5052 (5)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	C14.22 H8.12 N0.75 O2.78 Zn0.85	C84 H48 N6 O13 Zn4, C29.757 H17.004 O9.211 Zn2.834
Sum formula	C14.22 H8.12 N0.75 O2.78 Zn0.85	C113.76 H65 N6 O22.21 Zn6.83
Mr	289.70	2317.67
Dx, g cm-3	0.762	0.762
Z	8	1
Mu (mm-1)	0.836	0.836
F000	1172.0	1172.0
F000'	1174.42	
h, k, lmax	15,15,15	15,15,15
Nref	800 [ 454 ]	803
Tmin, Tmax		0.457, 0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.457 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.77/1.00 Theta (max)= 18.835

R(reflections)= 0.1634( 577)  
S = 1.706  
Npar= 34

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wR2 (reflections)=  
0.4055( 803)

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.

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#### 🔴 Alert level A

THETM01\_ALERT\_3\_A The value of sine(theta\_max)/wavelength is less than 0.550  
Calculated sin(theta\_max)/wavelength = 0.4542  
PLAT245\_ALERT\_2\_A U(iso) H13 Smaller than U(eq) N1 by 0.202 Ang\*\*2  
PLAT601\_ALERT\_2\_A Unit Cell Contains Solvent Accessible VOIDS of . 1647 Ang\*\*3

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#### 🟡 Alert level B

PLAT031\_ALERT\_4\_B Refined Extinction Parameter Within Range of ... 1.500 Sigma  
PLAT049\_ALERT\_1\_B Calculated Density Less Than 1.0 gcm-3 ..... 0.7618 Check  
PLAT082\_ALERT\_2\_B High R1 Value ..... 0.16 Report  
PLAT084\_ALERT\_3\_B High wR2 Value (i.e. > 0.25) ..... 0.41 Report  
PLAT934\_ALERT\_3\_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check  
PLAT987\_ALERT\_1\_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please 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 0.320  
From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 0.050  
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  
PLAT250\_ALERT\_2\_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.8 Note  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including Zn1 0.256 Check  
PLAT329\_ALERT\_4\_C Carbon Atom Hybridisation Unclear for ..... C13 Check  
PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check  
PLAT927\_ALERT\_1\_C Reported and Calculated wR2 Differ by ..... -0.0024 Check  
PLAT939\_ALERT\_3\_C Large Value of Not (SHELXL) Weight Optimized S . 44.42 Check  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.90Ang From O1 . 0.68 eA-3

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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: C113.7599 H65 N6 O22.21 Zn6.83  
Atom count from the \_atom\_site data: C82.18200 H56.496 N6 O10.31919 Z  
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 C113.76 H65 N6 O22.21 Zn6.83  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif	sites	diff		
C	113.76	82.18		31.58		
H	65.00	56.50		8.50		
N	6.00	6.00		0.00		
O	22.21	10.32		11.89		
Zn	6.83	1.14		5.69		
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
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	)	26.72	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-x,y,1-z	=	9_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C14	..C15	.	3.19	Ang.
			1-z,y,1-x	=	23_656	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....				1	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...				6.70	Deg.
	N1 -C13 -H13 1_555 1_555 1_555 .....	#			13	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...				10.90	Deg.
	C13 -N1 -H13 1_555 1_555 1_555 .....	#			14	Check
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 !
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

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3 <b>ALERT level A</b> = Most likely a serious problem - resolve or explain
6 <b>ALERT level B</b> = A potentially serious problem, consider carefully
13 <b>ALERT level C</b> = Check. Ensure it is not caused by an omission or oversight
52 <b>ALERT level G</b> = General information/check it is not something unexpected

13 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
9 ALERT type 3 Indicator that the structure quality may be low
37 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-91-12h-71pc
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
```

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RESPONSE: ...
;
_vrf_PLAT245_muf-91-12h-71pc
;
PROBLEM: U(iso) H13      Smaller than U(eq) N1      by      0.202 Ang**2
RESPONSE: ...
;
_vrf_PLAT601_muf-91-12h-71pc
;
PROBLEM: Unit Cell Contains Solvent Accessible VOIDS of .      1647 Ang**3
RESPONSE: ...
;
# end Validation Reply Form

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

Datablock muf-91-12h-71pc - ellipsoid plot

