

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) muf-91-1h-12pc

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-91-1h-12pc

Bond precision:	= 0.0000 A	Wavelength=0.71075
Cell:	a=17.036(12)	b=17.036(12) c=17.036(12)
	alpha=90	beta=90 gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	4944(10)	4944(10)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	2(C7.43 H4.25 N0.50 O1.22 Zn0.38)	C84 H48 N6 O13 Zn4, C5.23 H2.988 O1.619 Zn0.498
Sum formula	C14.87 H8.50 N O2.44 Zn0.75	C89.23 H50.99 N6 O14.62 Zn4.50
Mr	289.20	1735.19
Dx, g cm ⁻³	0.583	0.583
Z	6	1
Mu (mm ⁻¹)	0.567	0.567
F000	880.3	880.0
F000'	881.89	
h, k, lmax	12, 12, 12	12, 12, 11
Nref	402[235]	395
Tmin, Tmax		0.595, 0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.595 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 1.68/0.98

Theta(max)= 14.701

R(reflections)= 0.1956(256)

wR2(reflections)=
0.4628(395)

S = 1.627

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 = 0.3571

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) 0.46 Report

PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of . 1599 Ang**3

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 0.5828 Check

PLAT082_ALERT_2_B High R1 Value 0.20 Report

PLAT260_ALERT_2_B Large Average Ueq of Residue Including Zn1 0.419 Check

PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.131

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: _refine_ls_abs_structure_Flack 0.310

From the CIF: _refine_ls_abs_structure_Flack_su 0.090

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.131 Report

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.970 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) 6.94 Note

PLAT220_ALERT_2_C NonSolvent Resd 1 Zn Ueq(max)/Ueq(min) Range 3.1 Ratio

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.2 Note

PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for C13 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.549 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.079 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.357 3 Report

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 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 . 10.63 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: C89.22999 H50.99 N6 O14.62 Zn4.5

Atom count from the _atom_site data: C72.546 H46.48799 N6 O6.790899 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 C89.23 H50.99 N6 O14.62 Zn4.50

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	89.23	72.55	16.68
H	50.99	46.49	4.50
N	6.00	6.00	0.00
O	14.62	6.79	7.83
Zn	4.50	0.75	3.75

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
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 ...	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
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	2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of Zn0A	0.1667	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C11	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H20	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21	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)	13.78	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 N1 ..C15 .	2.44	Ang.
	1-x, -y, z =	3_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact N1 ..C14 .	2.99	Ang.
	1-x, -y, z =	3_655	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 #	32	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	81	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	35%	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
PLAT930_ALERT_2_G	FCF-based Twin Law (7-5 5) Est.d BASF	0.60	Check
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2	Note
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	1	Units

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

15 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 ALERT type 2 Indicator that the structure model may be wrong or deficient
 16 ALERT type 3 Indicator that the structure quality may be low
 36 ALERT type 4 Improvement, methodology, query or suggestion
 1 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-91-1h-12pc
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: ...
;
_vrf_PLAT084_muf-91-1h-12pc
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.46 Report
RESPONSE: ...
;
_vrf_PLAT601_muf-91-1h-12pc
;
PROBLEM: Unit Cell Contains Solvent Accessible VOIDS of . 1599 Ang**3
RESPONSE: ...
;
# end Validation Reply Form
```

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

