checkCIF/PLATON report

Structure factors have been supplied for datablock(s) muf-92-3h-42pc

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-92-3h-42pc

```
Bond precision:   O- C = 0.0005 A          Wavelength=0.71075

Cell:               a=17.146(7)      b=17.146(7)      c=17.146(7)
                    alpha=90         beta=90          gamma=90
Temperature:        100 K
```

	Calculated	Reported
Volume	5041(6)	5041(6)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	C7 H4 N0.50 O1.08 Zn0.33, 2(C0.74 H0.47 N0.05 O0.23 Zn0.07)	C84 H48 N6 O13 Zn4, C17.56 H11.284 N1.254 O5.435 Zn1.672
Sum formula	C8.47 H4.94 N0.60 O1.54 Zn0.47	C101.56 H59.28 N7.25 O18.44 Zn5.67
Mr	170.74	2046.75
Dx,g cm-3	0.675	0.674
Z	12	1
Mu (mm-1)	0.699	0.698
F000	1038.0	1037.0
F000'	1040.01	
h,k,lmax	13,13,13	13,13,13
Nref	563[324]	558
Tmin,Tmax		0.577,0.746
Tmin'		

```
Correction method= # Reported T Limits: Tmin=0.577 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.99        Theta(max)= 16.465
```

R(reflections)= 0.1840(433)

wR2(reflections)= 0.4146(558)

S = 1.745 Npar= 66

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 = 0.3988
PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of . 1549 Ang**3

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 ..... 0.6749 Check
PLAT082_ALERT_2_B High R1 Value ..... 0.18 Report
PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.41 Report
PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) ..... 4.85 Note
PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

---

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.550
From the CIF: _refine_ls_abs_structure_Flack_su 0.060
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
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C4A Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O3A Check
PLAT245_ALERT_2_C U(iso) H7A Smaller than U(eq) N9A by 0.049 Ang**2
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.5 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Zn2A 0.283 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Zn2B 0.227 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for ..... C7A Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 0.55 Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 10.91 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:C101.56 H59.28 N7.25 O18.44 Zn5.
Atom count from the _atom_site data: C92.64 H57.86399 N6.624 O18.46 Z
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 C101.56 H59.28 N7.25 O18.44 Zn5.67
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	101.56	92.64	8.92
H	59.28	57.86	1.42
N	7.25	6.62	0.63
O	18.44	18.46	-0.02
Zn	5.67	2.35	3.32

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 14 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 25 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 4 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 ... 12.0000 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 2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 12 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 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 2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Zn2A Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N9A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A Constrained at 0.25 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 81% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing). C8A Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 3 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 6.70 Deg.
N9A -C7A -H7A 1_555 1_555 1_555 ..... # 15 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 10.90 Deg.
C7A -N9A -H7A 1_555 1_555 1_555 ..... # 16 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 24 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 120 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 .... 3 Note

```
   2 ALERT level A = Most likely a serious problem - resolve or explain
   5 ALERT level B = A potentially serious problem, consider carefully
  17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  48 ALERT level G = General information/check it is not something unexpected

  12 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
  34 ALERT type 4 Improvement, methodology, query or suggestion
   3 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-92-3h-42pc
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: ...
;
_vrf_PLAT601_muf-92-3h-42pc
;
```

```
PROBLEM: Unit Cell Contains Solvent Accessible VOIDS of .       1549 Ang**3
RESPONSE: ...
;
# end Validation Reply Form
```

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

Datablock muf-92-3h-42pc - ellipsoid plot