checkCIF/PLATON report

Structure factors have been supplied for datablock(s) muf-92-3h-50pc

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-50pc

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Bond precision:   O- C = 0.0002 A          Wavelength=0.71075

Cell:               a=17.141(3)      b=17.141(3)      c=17.141(3)
                    alpha=90         beta=90          gamma=90
Temperature:        100 K
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	Calculated	Reported
Volume	5036(3)	5036(3)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	12(C7 H4 N0.50 O1.08 Zn0.33), C21 H13.49 N1.51 O6.50 Zn2	C84 H48 N6 O13 Zn4, C21.011 H13.501 N1.501 O6.503 Zn2.001
Sum formula	C105 H61.49 N7.51 O19.50 Zn6	C105.01 H61.50 N7.50 O19.50 Zn6
Mr	2132.66	2132.45
Dx,g cm-3	0.703	0.703
Z	1	1
Mu (mm-1)	0.739	0.738
F000	1080.1	1080.0
F000'	1082.21	
h,k,lmax	13,13,13	13,13,13
Nref	563[324]	558
Tmin,Tmax		0.663,0.746
Tmin'		

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Correction method= # Reported T Limits: Tmin=0.663 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.99        Theta(max)= 16.470
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R(reflections)= 0.1551(502)

wR2(reflections)= 0.3708(558)

S = 1.861 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 = 0.3989
PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of . 1540 Ang**3

Alert level B

PLAT049_ALERT_1_B	Calculated Density Less Than 1.0 gcm-3	0.7032 Check
PLAT082_ALERT_2_B	High R1 Value	0.16 Report
PLAT084_ALERT_3_B	High wR2 Value (i.e. > 0.25)	0.37 Report
PLAT090_ALERT_3_B	Poor Data / Parameter Ratio (Zmax > 18)	4.85 Note
PLAT245_ALERT_2_B	U(iso) H7A Smaller than U(eq) N9A by	0.089 Ang**2
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 0.438
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
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C4A Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.1 Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Zn2A 0.227 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Zn2B 0.205 Check
PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for	C7A Check
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	2 Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	36.71 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:C105.01 H61.5 N7.5 O19.5 Zn6
Atom count from the _atom_site data: C96 H59.73600 N6.756 O19.5 Zn2.6
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 C105.01 H61.50 N7.50 O19.50 Zn6
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	105.01	96.00	9.01
H	61.50	59.74	1.76
N	7.50	6.76	0.74
O	19.50	19.50	0.00
Zn	6.00	2.67	3.33

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
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
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 2) 100% Note
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing). C8A Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C7B ..C8B . 2.40 Ang.
1-x,-y,z = 3_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C7B ..C7B . 3.16 Ang.
1-x,-y,z = 3_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C7B ..C7B . 3.16 Ang.
1-x,-1+z,1-y = 5_646 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C8B ..C8B . 1.51 Ang.
1-x,-y,z = 3_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C8B ..N9B . 2.80 Ang.
1-x,-1+z,1-y = 5_646 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C8B ..N9B . 2.80 Ang.
1-x,-y,z = 3_655 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 3 Note

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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  #         23 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 !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        73% 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
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  2 ALERT level A = Most likely a serious problem - resolve or explain
  6 ALERT level B = A potentially serious problem, consider carefully
 14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 55 ALERT level G = General information/check it is not something unexpected

 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 17 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
  3 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-92-3h-50pc
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: ...
;
_vrf_PLAT601_muf-92-3h-50pc
;
PROBLEM: Unit Cell Contains Solvent Accessible VOIDS of .       1540 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-50pc - ellipsoid plot