

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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-92-15h-71pc

Bond precision: O- C = 0.0001 Å Wavelength=0.71080

Cell: a=17.1180(11) b=17.1180(11) c=17.1180(11)
 alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	5016.0(10)	5016.0(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 H3.50 N0.50 O1.08 Zn0.33), 4(C1.24 H1.06 N0.09 O0.38 Zn0.1	1(C84 H48 N6 O13 Zn4), 1(C29.73 H25.48 N2.12 O9.2 Zn2.83)
Sum formula	C18.96 H12.25 N1.35 O3.70 Zn1.14	C113.71 H73.46 N8.12 O22.20 Zn6.83
Mr	392.65	2355.08
Dx, g cm-3	0.780	0.780
Z	6	1
Mu (mm-1)	0.843	0.842
F000	1195.4	1195.0
F000'	1197.78	
h, k, lmax	18, 18, 18	18, 19, 19
Nref	1400[778]	1400
Tmin, Tmax		0.678, 0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.678 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.80/1.00 Theta(max)= 23.233

R(reflections)= 0.1071(1112) wR2(reflections)= 0.3114(1400)

S = 1.312 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

PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of . 1531 Ang**3

Alert level B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575

Calculated sin(theta_max)/wavelength = 0.5550

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 0.7799 Check

PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C8A Check

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

Alert level C

RADNW01_ALERT_1_C The radiation wavelength lies outside the expected range

for the supplied radiation type. Expected range 0.71065-0.71075

Wavelength given = 0.71080

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: _refine_ls_abs_structure_Flack 0.368

From the CIF: _refine_ls_abs_structure_Flack_su 0.015

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

PLAT082_ALERT_2_C High R1 Value 0.11 Report

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.31 Report

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . ZN2A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C5A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C6A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C7A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C8A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . N9A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C11A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C12A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C17A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C16A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C15A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C14A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C13A Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . N9B Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . ZN2A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C5A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C6A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C7A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C8A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . N9A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C11A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C12A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C17A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C16A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C15A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C14A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C13A Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . N9B Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . ZN2A Check

PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C5A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C6A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C7A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C8A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	N9A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C11A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C12A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C17A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C16A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C15A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C14A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	C13A	Check
PLAT163_ALERT_4_C	Missing or Zero s.u. (esd) on z-coordinate for .	N9B	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	03A	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.6	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Zn2A	0.126	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Zn2B	0.149	Check

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and _chemical_formula_moiety. This is
 usually due to the moiety formula being in the wrong format.
 Atom count from _chemical_formula_sum: C113.71 H73.46 N8.12 O22.2 Zn
 Atom count from _chemical_formula_moiety: C113.73 H73.48 N8.12 O22.2 Zn

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: C113.71 H73.46 N8.12 O22.2 Zn6.8
 Atom count from the _atom_site data: C104.7276 H67.81858 N7.061434 O2

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 C113.71 H73.46 N8.12 O22.20 Zn6.83
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	113.72	104.74	8.98
H	73.47	67.82	5.64
N	8.12	7.06	1.06
O	22.20	22.20	0.00
Zn	6.83	3.50	3.33

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	15	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	17	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	3	Report
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	6.00	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	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
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3	Note
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	3	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 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
PLAT300_ALERT_4_G	Atom Site Occupancy of H7A	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
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		3	Note
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 !

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

15 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 74 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.

