

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-77pc-2

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

Cell: a=17.147(3) b=17.147(3) c=17.147(3)
 alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	5042(3)	5042(2)
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(C1.35 H1.16 N0.10 O0.42 Zn0.1	1(C84 H48 N6 O13 Zn4), 1(C32.49 H27.84 N2.32 O10.06 Zn3.09)
Sum formula	C19.42 H12.64 N1.39 O3.84 Zn1.18	C116.48 H75.83 N8.32 O23.06 Zn7.09
Mr	404.24	2424.29
Dx, g cm-3	0.799	0.799
Z	6	1
Mu (mm-1)	0.870	0.870
F000	1230.6	1230.0
F000'	1233.09	
h, k, lmax	15, 15, 15	15, 15, 15
Nref	800[454]	795
Tmin, Tmax		0.613, 0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.613 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.75/0.99 Theta(max)= 18.809

R(reflections)= 0.1310(716) wR2(reflections)= 0.3509(795)

S = 1.734 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 $\sin(\theta_{\max})/\lambda$ is less than 0.550
Calculated $\sin(\theta_{\max})/\lambda = 0.4536$
PLAT601_ALERT_2_A Structure Contains Solvent Accessible Voids of . 1550 Ang³

Alert level B

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm⁻³ 0.7988 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

STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: `_refine_ls_abs_structure_Flack` 0.740
From the CIF: `_refine_ls_abs_structure_Flack_su` 0.020
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 0.13 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.35 Report
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 6.88 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.19 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
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Zn2A	0.172 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Zn2B	0.199 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .	0.74 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: C116.48 H75.83 N8.32 O23.06 Z
 Atom count from _chemical_formula_moiety: C116.49 H75.84 N8.32 O23.06 Z

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: C116.48 H75.83 N8.32 O23.06 Zn7.
 Atom count from the _atom_site data: C107.4994 H69.66643 N7.163426 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 C116.48 H75.83 N8.32 O23.06 Zn7.09
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	116.49	107.51	8.98
H	75.84	69.67	6.16
N	8.32	7.16	1.16
O	23.06	23.06	0.00
Zn	7.09	3.76	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

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 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 !

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

14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 13 ALERT type 2 Indicator that the structure model may be wrong or deficient
 5 ALERT type 3 Indicator that the structure quality may be low
 72 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.

