

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-93-60h-63pc

Bond precision: C-C = 0.0006 Å Wavelength=0.70850

Cell: a=17.098(7) b=17.098(7) c=17.098(7)
 alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4999(6)	4998(6)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	7.56(C3.50 H2 Co0.33 O), C42 H12 O13 Zn4, 24(C1.75 H1.25), 0.64	C84 H48 N6 O13 Zn4, C26.67 H15.24 Co2.54 O8.25
Sum formula	C110.46 H63.12 Co2.52 N6 O21.20 Zn4	C110.67 H63.24 Co2.54 N6 O21.25 Zn4
Mr	2223.57	2228.11
Dx, g cm ⁻³	0.739	0.740
Z	1	1
Mu (mm ⁻¹)	0.706	0.715
F000	1125.5	1128.0
F000'	1127.99	
h, k, lmax	18, 18, 18	18, 18, 18
Nref	1395[775]	1380
Tmin, Tmax		0.613, 0.745
Tmin'		

Correction method= # Reported T Limits: Tmin=0.613 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.78/0.99 Theta(max)= 23.148

R(reflections)= 0.1313(1141) wR2(reflections)= 0.3832(1380)

S = 1.705 Npar= 55

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 . 1614 Ang**3

 Alert level B

THETM01_ALERT_3_B The value of $\sin(\theta_{\max})/\lambda$ is less than 0.575

Calculated $\sin(\theta_{\max})/\lambda = 0.5548$

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 0.7386 Check

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.38 Report

PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C15 Check

 Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: `_refine_ls_abs_structure_Flack` 0.340

From the CIF: `_refine_ls_abs_structure_Flack_su` 0.020

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 4.54 Check

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT082_ALERT_2_C High R1 Value 0.13 Report

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C12 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C13 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . N1 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C15 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C16 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C17 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C18 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C19 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C20 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C21 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C12 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C13 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . N1 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C15 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C16 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C17 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C18 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C19 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C20 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . C21 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C12 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C13 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . N1 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C15 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C16 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C17 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C18 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C19 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C20 Check

PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for . C21 Check

PLAT234_ALERT_4_C Large Hirshfeld Difference O4 --C30 . 0.22 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference Zn1 --O2 . 0.18 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference O2 --C10 . 0.17 Ang.

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 3.2 Note

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Co2 0.145 Check

● Alert level 6

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: C110.6699 H63.24 Co2.54 N6 O21.2
 Atom count from the _atom_site data: C110.46 H63.12 Co2.52 N6 O21.2 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: check formula stoichiometry or atom site occupancies.

From the CIF: _cell_formula_units_Z 1

From the CIF: _chemical_formula_sum C110.67 H63.24 Co2.54 N6 O21.25 Zn

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	110.67	110.46	0.21
H	63.24	63.12	0.12
Co	2.54	2.52	0.02
N	6.00	6.00	0.00
O	21.25	21.20	0.05
Zn	4.00	4.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	16	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
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
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.20	Report
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.70850	Ang.
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	2	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	3	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C12 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H20 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13 Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)	39%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	03	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C14 - C14_b .	1.50	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C14 ..N1 .	2.53	Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C14 ..N1	2.53	Ang.

PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	y, x, z =	20_555 Check
		..N1	2.53 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	1-x, 1-y, z =	3_665 Check
		..N1	2.53 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	1-y, 1-x, z =	19_665 Check
		..N1	3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	1-x, y, 2-z =	9_657 Check
		..N1	3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	1-y, x, 2-z =	4_657 Check
		..N1	3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	y, 1-x, 2-z =	2_567 Check
		..N1	3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	x, 1-y, 2-z =	6_567 Check
		..C15	3.18 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	1-y, 1-x, z =	19_665 Check
		..C15	3.18 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	y, x, z =	20_555 Check
		..C15	3.18 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	x, y, z =	1_555 Check
		..C15	3.18 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact	C14	1-x, 1-y, z =	3_665 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #			38 Check
	C12 -C11 -C12	19.665 1.555 3.665	21.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #			41 Check
	C12 -C11 -C12	20.555 1.555 1.555	21.26 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #			17 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) .			2.17 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms			! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints			223 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...			4 Note
PLAT984_ALERT_1_G The Zn-f' = 0.2839 Deviates from the B&C-Value			0.2932 Check

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

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 25 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
 63 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.

