

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-scan1-pos9-26pc

Bond precision: = 0.0000 Å

Wavelength=0.71075

Cell: a=17.033(8) b=17.033(8) c=17.033(8)
 alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4942(7)	4942(7)
Space group	P -4 3 m	P -4 3 m
Hall group	P -4 2 3	P -4 2 3
Moiety formula	C3.95 H2.26 Co0.04 N0.25 00.68 Zn0.17	1(C84 H48 N6 O13 Zn4), 1(C10.81 H6.18 Co1.03 O3.35)
Sum formula	C3.95 H2.26 Co0.04 N0.25 00.68 Zn0.17	C94.80 H54.18 Co1.03 N6 O16.35 Zn4
Mr	77.60	1860.97
Dx, g cm ⁻³	0.626	0.625
Z	24	1
Mu (mm ⁻¹)	0.594	0.594
F000	944.2	944.0
F000'	946.09	
h, k, lmax	11, 11, 11	11, 11, 11
Nref	327[193]	321
Tmin, Tmax		0.459, 0.745
Tmin'		

Correction method= # Reported T Limits: Tmin=0.459 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.66/0.98 Theta(max)= 13.653

R(reflections)= 0.1905(243) wR2(reflections)= 0.4302(321)

S = 1.880 Npar= 99

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 $\sin(\theta_{\max})/\lambda = 0.3321$

PLAT090_ALERT_3_A Poor Data / Parameter Ratio ($Z_{\max} > 18$) 1.95 Note

Alert level B

RINTA01_ALERT_3_B The value of R_{int} is greater than 0.18

R_{int} given 0.186

PLAT020_ALERT_3_B The Value of R_{int} is Greater Than 0.12 0.186 Report

PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm⁻³ 0.6258 Check

PLAT082_ALERT_2_B High R_1 Value 0.19 Report

PLAT084_ALERT_3_B High wR_2 Value (i.e. > 0.25) 0.43 Report

PLAT260_ALERT_2_B Large Average Ueq of Residue Including Zn1 0.343 Check

PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C14 Check

PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C34 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: $_{\text{refine}}\text{ls_abs_structure_Flack}$ 0.710

From the CIF: $_{\text{refine}}\text{ls_abs_structure_Flack_su}$ 0.040

PLAT029_ALERT_3_C $_{\text{diff}}\text{rn_measured_fraction_theta_full}$ value Low . 0.969 Why?

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

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . 01 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . ZN1 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . 02 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C10 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C11 Check

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 . C14 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

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C02 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . 03 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . 04 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C30 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C31 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C32 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C33 Check

PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for . C34 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . 01 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for . ZN1 Check

PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	02 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	C10 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	C11 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 .	C14 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
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	C02 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	03 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	04 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	C30 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	C31 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	C32 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	C33 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .	C34 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	01 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	ZN1 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	02 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	C10 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	C11 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 .	C14 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
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	C02 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	03 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	04 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	C30 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	C31 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	C32 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	C33 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .	C34 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ...	2.3 Note
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #	1 Note
C3.95 H2.26 Co0.04 N0.25 O0.68 Zn0.17	
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .	0.71 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: C94.8 H54.18 Co1.03 N6 O16.35 Zn
 Atom count from the _atom_site data: C74.76602 H48.11615 Co0.171986 N
 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 C94.80 H54.18 Co1.03 N6 O16.35 Zn4
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	94.81	74.77	20.04
H	54.18	48.12	6.06
Co	1.03	0.17	0.86
N	6.00	6.00	0.00
O	16.35	7.61	8.74
Zn	4.00	0.67	3.33

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
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 ...	24.00	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
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 Zn1 Constrained at	0.1667	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1 Constrained at	0.0417	Check
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 N1 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C11 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14 Constrained at	0.25	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 H12 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13 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
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 1	7.35	Check
PLAT607_ALERT_4_G	VOID Test Skipped Due to Severe Disorder		! Info
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	33	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	235	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 ...	2	Note

2 **ALERT level A** = Most likely a serious problem - resolve or explain

9 **ALERT level B** = A potentially serious problem, consider carefully

82 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

44 **ALERT level G** = General information/check it is not something unexpected

13 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data

12 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
104 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

