

# 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-pos3-59pc

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Bond precision:    = 0.0000 Å

Wavelength=0.71075

Cell:                    a=17.103(4)            b=17.103(4)            c=17.103(4)  
                          alpha=90            beta=90            gamma=90  
Temperature:            100 K

|                        | Calculated                               | Reported                                               |
|------------------------|------------------------------------------|--------------------------------------------------------|
| Volume                 | 5003(4)                                  | 5003(3)                                                |
| Space group            | P -4 3 m                                 | P -4 3 m                                               |
| Hall group             | P -4 2 3                                 | P -4 2 3                                               |
| Moiety formula         | C4.53 H2.59 Co0.10 N0.25<br>00.86 Zn0.17 | C84 H42 N6 O13 Zn4, 6(H),<br>C24.68 H14.1 Co2.35 O7.64 |
| Sum formula            | C4.53 H2.59 Co0.10 N0.25<br>00.86 Zn0.17 | C111.43 H Co2.61 N6 O21.49<br>Zn4                      |
| Mr                     | 90.94                                    | 2182.47                                                |
| Dx, g cm <sup>-3</sup> | 0.724                                    | 0.724                                                  |
| Z                      | 24                                       | 1                                                      |
| Mu (mm <sup>-1</sup> ) | 0.699                                    | 0.720                                                  |
| F000                   | 1105.0                                   | 1074.0                                                 |
| F000'                  | 1107.36                                  |                                                        |
| h, k, lmax             | 15, 15, 15                               | 15, 15, 15                                             |
| Nref                   | 786[ 446]                                | 786                                                    |
| Tmin, Tmax             |                                          | 0.524, 0.745                                           |
| Tmin'                  |                                          |                                                        |

Correction method= # Reported T Limits: Tmin=0.524 Tmax=0.745  
AbsCorr = MULTI-SCAN

Data completeness= 1.76/1.00            Theta(max)= 18.818

R(reflections)= 0.1609( 452)            wR2(reflections)= 0.3807( 786)

S = 1.344                                    Npar= 99

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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.

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### Alert level A

THETM01\_ALERT\_3\_A The value of  $\sin(\theta_{\max})/\lambda$  is less than 0.550  
Calculated  $\sin(\theta_{\max})/\lambda = 0.4538$

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### Alert level B

|                   |                                                          |        |              |
|-------------------|----------------------------------------------------------|--------|--------------|
| PLAT049_ALERT_1_B | Calculated Density Less Than 1.0 gcm <sup>-3</sup> ..... | 0.7244 | Check        |
| PLAT082_ALERT_2_B | High R1 Value .....                                      | 0.16   | Report       |
| PLAT084_ALERT_3_B | High wR2 Value (i.e. > 0.25) .....                       | 0.38   | Report       |
| PLAT090_ALERT_3_B | Poor Data / Parameter Ratio (Zmax > 18) .....            | 4.51   | Note         |
| 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 |

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### Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.148

STRVA01\_ALERT\_4\_C Flack test results are ambiguous.

From the CIF: `_refine_ls_abs_structure_Flack` 0.620

From the CIF: `_refine_ls_abs_structure_Flack_su` 0.030

|                   |                                                  |       |              |
|-------------------|--------------------------------------------------|-------|--------------|
| PLAT020_ALERT_3_C | The Value of Rint is Greater Than 0.12 .....     | 0.148 | Report       |
| 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 |
| PLAT068_ALERT_1_C | Reported F000 Differs from Calcd (or Missing)... |       | 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 |
| PLAT260_ALERT_2_C | Large Average Ueq of Residue Including Zn1       | 0.266 | Check |
| PLAT790_ALERT_4_C | Centre of Gravity not Within Unit Cell: Resd. #  | 1     | Note  |
|                   | C4.53 H2.59 Co0.10 N0.25 O0.86 Zn0.17            |       |       |
| PLAT907_ALERT_2_C | Flack x > 0.5, Structure Needs to be Inverted? . | 0.62  | 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: C111.43 H1 Co2.61 N6 O21.49 Z  
     Atom count from \_chemical\_formula\_moiety:C108.68 H62.1 Co2.35 N6 O20.6

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:C111.43 H1 Co2.61 N6 O21.49 Zn4  
     Atom count from the \_atom\_site data: C80.20201 H55.05600 Co0.392 N6 O

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 C111.43 H Co2.61 N6 O21.49 Zn4  
 TEST: Compare cell contents of formula and atom\_site data

| atom | Z*formula | cif sites | diff   |
|------|-----------|-----------|--------|
| C    | 111.43    | 80.20     | 31.23  |
| H    | 1.00      | 55.06     | -54.06 |
| Co   | 2.61      | 0.39      | 2.22   |
| N    | 6.00      | 6.00      | 0.00   |
| O    | 21.49     | 9.59      | 11.90  |
| 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        |
| 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 H 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      | 8.49   | 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         |

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1 **ALERT level A** = Most likely a serious problem - resolve or explain  
 7 **ALERT level B** = A potentially serious problem, consider carefully  
 84 **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

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

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

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**PLATON version of 07/08/2019; check.def file version of 30/07/2019**

