checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound_3

```
Bond precision:  C-C = 0.0132 A          Wavelength=0.71073

Cell:            a=7.0598(3)     b=20.8448(10)       c=7.4944(3)
                 alpha=90        beta=92.482(3)      gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	1101.84(8)	1101.84(8)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	C10 H9 N O5 Zn	?
Sum formula	C10 H9 N O5 Zn	C10 H11 N O5 Zn
Mr	288.57	290.57
Dx,g cm-3	1.740	1.752
Z	4	4
Mu (mm-1)	2.237	2.238
F000	584.0	592.0
F000’	585.41	
h,k,lmax	9,27,9	9,27,9
Nref	2529	2501
Tmin,Tmax	0.948,0.956	
Tmin’	0.874	

```
Correction method= Not given

Data completeness= 0.989          Theta(max)= 27.490

R(reflections)= 0.0856( 1534)     wR2(reflections)= 0.2137( 2501)

S = 1.158                 Npar= 154
```

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 C

```
DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
           _refine_diff_density_max given =      2.560
           Test value =      2.250
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
```

```
           The relevant atom site should be identified.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...         ?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      3.30
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density      2.56 eA-3
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       3.2 Ratio
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C9
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C7
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0132 Ang
```

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:C10 H11 N1 O5 Zn1
           Atom count from the _atom_site data:  C10 H9 N1 O5 Zn1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C10 H11 N O5 Zn
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         40.00     40.00    0.00
          H         44.00     36.00    8.00
          N          4.00      4.00    0.00
          O         20.00     20.00    0.00
          Zn         4.00      4.00    0.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .         3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....         ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      8.43
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......     P21/n
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....         ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....         ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....         ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature       293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature       293 K
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....         R
```

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

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   2 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*, 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.

PLATON version of 21/12/2011; check.def file version of 16/12/2011

Datablock compound_3 - ellipsoid plot