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_5

```
Bond precision:  C-C = 0.0105 A          Wavelength=0.71073

Cell:              a=7.331(5)      b=21.735(5)      c=7.213(5)
                   alpha=90        beta=90          gamma=90
Temperature:       293 K
```

	Calculated	Reported
Volume	1149.3(11)	1149.3(11)
Space group	P m n n	Pmnn
Hall group	-P 2n 2	?
Moiety formula	C9 H10 N2 O5 Zn	?
Sum formula	C9 H10 N2 O5 Zn	C9 H10 N2 O5 Zn
Mr	291.58	291.56
Dx,g cm-3	1.685	1.685
Z	4	4
Mu (mm-1)	2.148	2.148
F000	592.0	592.0
F000’	593.40	
h,k,lmax	9,28,9	9,28,9
Nref	1422	1407
Tmin,Tmax	0.440,0.424	
Tmin’	0.407	

```
Correction method= Not given

Data completeness= 0.989          Theta(max)= 27.490

R(reflections)= 0.0718( 879)      wR2(reflections)= 0.1113( 1407)

S = 1.102                 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 B

```
PLAT213_ALERT_2_B Atom N2             has ADP max/min Ratio .....        5.0 prola
PLAT220_ALERT_2_B Large Non-Solvent   N     Ueq(max)/Ueq(min) ...        4.5 Ratio
```

Alert level C

```
PLAT213_ALERT_2_C Atom C6              has ADP max/min Ratio .....       3.5 prola
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       3.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N1     --  C4B     ..      0.16 Ang.
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        N1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C6
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       3.2
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0105 Ang
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #         1
             C9 H10 N2 O5 Zn
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         2
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.      5.83
PLAT153_ALERT_1_G The su's on the Cell Axes   are Equal .........   0.00500 Ang.
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
PLAT301_ALERT_3_G Note: Main Residue  Disorder ..................        23 Perc.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C7A    ..  C7A     ..      2.19 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C7A    ..  C8A     ..      2.68 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........         1
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.14 Ratio
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....         S
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         1
```

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

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   5 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*, 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 15/02/2012; check.def file version of 10/02/2012

Datablock compound_5 - ellipsoid plot