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: shelxl

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Bond precision:  C-C = 0.0103 A          Wavelength=0.71073

Cell:           a=9.6100(19)      b=11.400(2)       c=11.750(2)
                alpha=93.51(3)    beta=103.50(3)    gamma=96.66(3)
Temperature:    173 K
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	Calculated	Reported
Volume	1238.0(4)	1238.0(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C66 H46 N6 Zn	C66 H46 N6 Zn
Sum formula	C66 H46 N6 Zn	C66 H46 N6 Zn
Mr	988.48	988.46
Dx,g cm-3	1.326	1.326
Z	1	1
Mu (mm-1)	0.546	0.546
F000	514.0	514.0
F000’	514.44	
h,k,lmax	11,13,13	11,13,13
Nref	4360	4239
Tmin,Tmax	0.854,0.897	0.858,0.899
Tmin’	0.854	

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Correction method= MULTI-SCAN

Data completeness= 0.972          Theta(max)= 25.000

R(reflections)= 0.0865( 2047)     wR2(reflections)= 0.2914( 4239)

S = 0.997                  Npar= 308
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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.

Alert level C

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RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.291
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....         48 %
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.972 Note
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.29 Report
PLAT165_ALERT_3_C Nr. of Status R Flagged Non-Hydrogen Atoms .....          9
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.4 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Zn1    --  N3      ..        7.8 su
PLAT234_ALERT_4_C Large Hirshfeld Difference C11    --  C16     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13    --  C14     ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C30    --  C31     ..       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31    --  C32     ..       0.21 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        Zn1 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C13 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C15 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C30 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C31 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C32 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0103 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C10    -   C23    ...       1.54 Ang.
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Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.17 Report
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........    0.03000 Degree
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          4
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  20 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   6 ALERT level G = General information/check it is not something unexpected

   2 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
   6 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 20/08/2014; check.def file version of 18/08/2014

Datablock shelxl - ellipsoid plot