# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0174_0m

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: mo_b0174_0m

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Bond precision: C-C = 0.0035 A Wavelength=0.71073

Cell: a=7.7381(7) b=11.9130(9) c=19.5044(19)
alpha=86.737(3) beta=89.057(3) gamma=88.737(3)
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1794.4(3) | 1794.4(3) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C30 H44 Cl2 Fe2 N2 O2 Si2 Zn2 | 0.5(C30 H44 Cl2 Fe2 N2 O2 Si2 Zn2) |
| Sum formula | C30 H44 Cl2 Fe2 N2 O2 Si2 Zn2 | C15 H22 Cl Fe N O Si Zn |
| Mr | 834.23 | 417.09 |
| Dx,g cm-3 | 1.544 | 1.544 |
| Z | 2 | 4 |
| Mu (mm-1) | 2.358 | 2.358 |
| F000 | 856.0 | 856.0 |
| F000’ | 859.59 | |
| h,k,lmax | 10,15,25 | 10,15,25 |
| Nref | 8664 | 8657 |
| Tmin,Tmax | 0.726,0.799 | 0.045,0.075 |
| Tmin’ | 0.712 | |

Correction method= # Reported T Limits: Tmin=0.045 Tmax=0.075
AbsCorr = ?

Data completeness= 0.999 Theta(max)= 28.000

R(reflections)= 0.0300( 6981) wR2(reflections)= 0.0610( 8657)

S = 1.021 Npar= 387

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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

PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used value .... Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min value ..... Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max value ..... Please Do !

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## Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for C21 -- C22 .. 11.5 s.u.

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## Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C7 -- C8 .. 5.7 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.025 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Report

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## Alert level G

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES ..... 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 4 Note

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
0 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.

**Validation response form**

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT183_mo_b0174_0m
;
PROBLEM: Missing _cell_measurement_reflns_used value ....     Please Do !
RESPONSE: ...
;
_vrf_PLAT184_mo_b0174_0m
;
PROBLEM: Missing _cell_measurement_theta_min value ......     Please Do !
RESPONSE: ...
;
_vrf_PLAT185_mo_b0174_0m
;
PROBLEM: Missing _cell_measurement_theta_max value ......     Please Do !
RESPONSE: ...
;
# end Validation Reply Form
```

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**PLATON version of 11/08/2016; check.def file version of 04/08/2016**

**Datablock mo_b0174_0m** - ellipsoid plot

