# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0093_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_b0093_0m

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Bond precision: C-C = 0.0025 A Wavelength=0.71073

Cell: a=7.6971(9) b=10.4780(9) c=24.508(3)
alpha=90 beta=90 gamma=90
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1976.6(4) | 1976.6(4) |
| Space group | P 21 21 21 | P 21 21 21 |
| Hall group | P 2ac 2ab | P 2ac 2ab |
| Moiety formula | C21 H27 Fe N O2 Si | C21 H27 Fe N O2 Si |
| Sum formula | C21 H27 Fe N O2 Si | C21 H27 Fe N O2 Si |
| Mr | 409.38 | 409.37 |
| Dx,g cm-3 | 1.376 | 1.376 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.838 | 0.838 |
| F000 | 864.0 | 864.0 |
| F000’ | 865.96 | |
| h,k,lmax | 10,14,33 | 10,14,33 |
| Nref | 5271[ 3007] | 5236 |
| Tmin,Tmax | | 0.390,0.433 |
| Tmin’ | | |

Correction method= # Reported T Limits: Tmin=0.390 Tmax=0.433
AbsCorr = MULTI-SCAN

Data completeness= 1.74/0.99 Theta(max)= 28.995

R(reflections)= 0.0201( 5152) wR2(reflections)= 0.0525( 5236)

S = 1.105 Npar= 239

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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**

```
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
PLAT213_ALERT_2_C Atom C7              has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C8              has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          2 Report
```

**Alert level G**

```
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          3 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          5 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
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 21/06/2015; check.def file version of 21/06/2015

**Datablock mo_b0093_0m** - ellipsoid plot