checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0610_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_b0610_0m

```
Bond precision:  C-C = 0.0073 A          Wavelength=0.71073

Cell:            a=13.173(4)     b=11.838(5)         c=13.877(5)
                 alpha=90        beta=97.130(7)      gamma=90
Temperature:     146 K
```

	Calculated	Reported
Volume	2147.3(14)	2147.3(13)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C23 H25 Fe N O2 Si	C23 H25 Fe N O2 Si
Sum formula	C23 H25 Fe N O2 Si	C23 H25 Fe N O2 Si
Mr	431.38	431.38
Dx,g cm-3	1.334	1.334
Z	4	4
Mu (mm-1)	0.776	0.776
F000	904.0	904.0
F000’	905.98	
h,k,lmax	16,15,17	16,15,17
Nref	4683	4644
Tmin,Tmax	0.646,0.788	0.617,1.000
Tmin’	0.609	

```
Correction method= # Reported T Limits: Tmin=0.617 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992          Theta(max)= 27.000

R(reflections)= 0.0654( 4110)     wR2(reflections)= 0.1343( 4644)

S = 1.180                 Npar= 355
```

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 A

PLAT213_ALERT_2_A Atom C17B has ADP max/min Ratio ..... 5.6 prolat

Alert level B

PLAT213_ALERT_2_B Atom C7 has ADP max/min Ratio ..... 4.3 prolat
PLAT213_ALERT_2_B Atom C16B has ADP max/min Ratio ..... 4.1 prolat

Alert level C

PLAT213_ALERT_2_C Atom C6 has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C8 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom C17A has ADP max/min Ratio ..... 3.5 prolat
PLAT213_ALERT_2_C Atom C18A has ADP max/min Ratio ..... 3.6 prolat
PLAT213_ALERT_2_C Atom C19A has ADP max/min Ratio ..... 3.7 prolat
PLAT213_ALERT_2_C Atom C14B has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C18B has ADP max/min Ratio ..... 3.9 prolat
PLAT213_ALERT_2_C Atom C19B has ADP max/min Ratio ..... 3.4 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.5 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00727 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 9.514 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.213 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min) 5 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 26 Report

Alert level G

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.63 mm
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.41 Why ?
PLAT230_ALERT_2_G Hirshfeld Test Diff for C19A -- C20A .. 9.8 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1).. 36 % Note
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C18B -C23B 0.44 Ang.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 8 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
20 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
2 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* 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_PLAT213_mo_b0610_0m
;
PROBLEM: Atom C17B            has ADP max/min Ratio .....        5.6 prolat
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 24/11/2016; check.def file version of 23/11/2016

Datablock mo_b0610_0m - ellipsoid plot