checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: mo_b0003_0m_a

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: **a=14.5175(5)** **b=13.6757(5)** **c=14.6276(6)**
alpha=90 **beta=116.753(1)** **gamma=90**
Temperature: **100 K**

	Calculated	Reported
Volume	2593.25(17)	2593.25(17)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C26 H33 Fe N O2 Si2	C26 H33 Fe N O2 Si2
Sum formula	C26 H33 Fe N O2 Si2	C26 H33 Fe N O2 Si2
Mr	503.56	503.56
Dx,g cm-3	1.290	1.290
Z	4	4
Mu (mm-1)	0.696	0.696
F000	1064.0	1064.0
F000'	1066.33	
h,k,lmax	18,17,18	18,17,18
Nref	5777	5760
Tmin,Tmax	0.933,0.952	0.695,0.746
Tmin'	0.933	

Correction method= # Reported T Limits: Tmin=0.695 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.997 **Theta(max)= 27.184**

R(reflections)= 0.0334(5355) **wR2(reflections)= 0.1033(5760)**

S = 1.113 **Npar= 302**

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 C21		has ADP max/min Ratio	4.2 prolat
PLAT220_ALERT_2_B Large Non-Solvent	C	Ueq(max)/Ueq(min) Range	7.7 Ratio
PLAT222_ALERT_3_B Large Non-Solvent	H	Uiso(max)/Uiso(min) ...	8.4 Ratio

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Alert level C

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PLAT213_ALERT_2_C Atom C9              has ADP max/min Ratio .....        3.5 prolat
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         C9 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        Si2 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   0 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 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*, 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 21/04/2015; check.def file version of 09/03/2015

Datablock mo_b0003_0m_a - ellipsoid plot