checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3103_twin1_hklf4

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: 3103_twin1_hklf4

```
Bond precision:  C-C = 0.0161 A          Wavelength=0.71073

Cell:            a=7.5429(5)     b=10.7933(6)        c=26.917(2)
                 alpha=90        beta=93.719(6)      gamma=90
Temperature:     173 K
```

	Calculated	Reported
Volume	2186.8(2)	2186.7(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C23 H28 Fe2 N O2 Si, Cl	C23 H28 Fe2 N O2 Si, Cl
Sum formula	C23 H28 Cl Fe2 N O2 Si	C23 H28 Cl Fe2 N O2 Si
Mr	525.70	525.70
Dx,g cm-3	1.597	1.597
Z	4	4
Mu (mm-1)	1.525	1.525
F000	1088.0	1088.0
F000’	1091.94	
h,k,lmax	9,13,34	9,13,34
Nref	4773	5183
Tmin,Tmax	0.700,0.796	0.888,1.000
Tmin’	0.581	

```
Correction method= # Reported T Limits: Tmin=0.888 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.086          Theta(max)= 26.999

R(reflections)= 0.0869( 4259)     wR2(reflections)= 0.2450( 5183)

S = 1.142                 Npar= 280
```

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

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01614 Ang.

Alert level C

PLAT213_ALERT_2_C Atom C6 has ADP max/min Ratio ..... 3.3 oblate
PLAT213_ALERT_2_C Atom C8 has ADP max/min Ratio ..... 3.1 prolat
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 6.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C9 -- C10 .. 0.17 Ang.
PLAT245_ALERT_2_C U(iso) H1A Smaller than U(eq) N1 by ... 0.014 AngSq
PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N1 - H1A .. 1.03 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 3.584 Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 1 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 32.32 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe2 -- C21 .. 7.4 s.u.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 6 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 2 Note
PLAT931_ALERT_5_G Found Twin Law ( )[1 0 4] Estimated BASF 0.24 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
8 **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
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

PLATON version of 26/02/2017; check.def file version of 21/02/2017

Datablock 3103_twin1_hklf4 - ellipsoid plot