

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3193_twin1_hklf4

Bond precision: C-C = 0.0128 Å

Wavelength=0.71073

Cell: a=10.4038(9) b=11.5162(11) c=16.0747(16)
 alpha=71.308(9) beta=81.097(8) gamma=89.850(7)
Temperature: 173 K

	Calculated	Reported
Volume	1800.1(3)	1800.1(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H26 Fe N Si, Cl	C16 H26 Fe N Si, Cl
Sum formula	C16 H26 Cl Fe N Si	C16 H26 Cl Fe N Si
Mr	351.77	351.77
Dx,g cm-3	1.298	1.298
Z	4	4
Mu (mm-1)	1.044	1.044
F000	744.0	744.0
F000'	746.43	
h,k,lmax	12,14,19	12,14,19
Nref	7072	8830
Tmin,Tmax	0.894,0.990	0.839,1.000
Tmin'	0.894	

Correction method= # Reported T Limits: Tmin=0.839 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.249

Theta(max)= 26.000

R(reflections)= 0.0621(5165)

wR2(reflections)= 0.1843(8830)

S = 0.990

Npar= 372

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 C25 has ADP max/min Ratio 5.4 prolat



Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for C24 -- C25 .. 8.6 su



Alert level C

PLAT213_ALERT_2_C Atom C7	has ADP max/min Ratio	3.3	prolat
PLAT213_ALERT_2_C Atom C8	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C Atom C26	has ADP max/min Ratio	3.4	prolat
PLAT220_ALERT_2_C Large Non-Solvent C	Ueq(max)/Ueq(min) Range	4.3	Ratio
PLAT220_ALERT_2_C Large Non-Solvent C	Ueq(max)/Ueq(min) Range	5.0	Ratio
PLAT222_ALERT_3_C Large Non-Solvent H	Uiso(max)/Uiso(min) ...	4.1	Ratio
PLAT222_ALERT_3_C Large Non-Solvent H	Uiso(max)/Uiso(min) ...	5.5	Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C22 -- C26 ..		5.4	su
PLAT234_ALERT_4_C Large Hirshfeld Difference C6 -- C7 ..		0.18	Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C8 -- C9 ..		0.18	Ang.
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for		C7	Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for		C8	Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for		C23	Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for		Fe1	Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for		Fe2	Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds		0.0128	Ang.



Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...	10	Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	2	Report
PLAT021_ALERT_4_G Ratio Unique / Expected Reflections too High ...	1.249	
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C16 H26 Fe N Si	2	Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C1	4	Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints	60	Note

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
 2 **ALERT level B** = A potentially serious problem, consider carefully
 16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 6 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 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
 5 ALERT type 4 Improvement, methodology, query or suggestion
 1 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.

