

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: 3202

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Bond precision:	C-C = 0.0035 A	Wavelength=0.71073	
Cell:	a=10.9706(5)	b=23.7261(9)	c=17.2222(7)
	alpha=90	beta=91.143(4)	gamma=90
Temperature:	173 K		
	Calculated	Reported	
Volume	4481.9(3)	4481.8(3)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	2(C42 H54 Fe2 N2 O3 Si4), C5 H11	2(C42 H54 Fe2 N2 O3 Si4), C5 H11	
Sum formula	C89 H119 Fe4 N4 O6 Si8	C89 H119 Fe4 N4 O6 Si8	
Mr	1789.00	1788.99	
Dx,g cm-3	1.326	1.326	
Z	2	2	
Mu (mm-1)	0.795	0.795	
F000	1890.0	1890.0	
F000'	1894.54		
h,k,lmax	14,32,23	14,31,23	
Nref	11980	10546	
Tmin,Tmax	0.853,0.984	0.971,1.000	
Tmin'	0.853		

Correction method= # Reported T Limits: Tmin=0.971 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.880      Theta(max)= 29.071

R(reflections)= 0.0434( 7880)      wR2(reflections)= 0.0944( 10546)

S = 1.038      Npar= 514

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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.

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### Alert level C

PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	3.2 Ratio
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of		C44 Check

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## ● Alert level G

PLAT300_ALERT_4_G	Atom Site Occupancy of *C43	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H43A	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H43B	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H43C	is Constrained at	0.500	Check
PLAT302_ALERT_4_G	Anion/Solvent Disorder .....	Percentage =	20	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle from 150 Deg for	O2	138.5	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle from 150 Deg for	O3	137.0	Degree
PLAT793_ALERT_4_G	The Model has Chirality at Si1	(Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	The Model has Chirality at Si2	(Centro SPGR)	S	Verify

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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  
2 **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  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
8 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.

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