

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

**Datablock: 3021**

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Bond precision:    C-C = 0.0086 Å

Wavelength=0.71073

Cell:                    a=13.2912(7)                    b=13.5363(7)                    c=30.9964(18)

                          alpha=90                    beta=96.859(5)                    gamma=90

Temperature:            150 K

	Calculated	Reported
Volume	5536.8(5)	5536.8(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C52 H69 Fe4 N4 O8 Si4, O	C52 H69 Fe4 N4 O8 Si4, O
Sum formula	C52 H69 Fe4 N4 O9 Si4	C52 H69 Fe4 N4 O9 Si4
Mr	1229.88	1229.87
Dx, g cm <sup>-3</sup>	1.475	1.475
Z	4	4
Mu (mm <sup>-1</sup> )	1.171	1.171
F000	2564.0	2564.0
F000'	2571.58	
h,k,lmax	17,17,40	17,17,40
Nref	13372	12846
Tmin,Tmax	0.857,0.932	0.942,1.000
Tmin'	0.849	

Correction method= MULTI-SCAN

Data completeness= 0.961

Theta(max)= 27.998

R(reflections)= 0.0655( 7040)

wR2(reflections)= 0.1667( 12846)

S = 1.014

Npar= 686

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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 B

Crystal system given = monoclinic

PLAT306\_ALERT\_2\_B Isolated Oxygen Atom (H-atoms Missing ?) .....

09 Check

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## Alert level C

PLAT220\_ALERT\_2\_C Large Non-Solvent    C

Ueq(max)/Ueq(min) Range

3.8 Ratio

PLAT222_ALERT_3_C	Large Non-Solvent	H	Uiso(max)/Uiso(min)	..	4.5	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C48	--	C78	..	5.2 su
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	.....			C42 Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	.....			C59 Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	.....			C60 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	.....			N8 Check
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....		0.0086	Ang.
PLAT355_ALERT_3_C	Long	O-H (X0.82,N0.98A)	O6	-	H6E	... 1.01 Ang.



#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			9	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records			2	Report
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle from 150 Deg for	01		139.9	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle from 150 Deg for	04		139.7	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	.....		6	Note
PLAT793_ALERT_4_G	The Model has Chirality at Si5	.....		S	Verify
PLAT793_ALERT_4_G	The Model has Chirality at Si6	.....		R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at Si7	.....		R	Verify
PLAT793_ALERT_4_G	The Model has Chirality at Si8	.....		S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....		5	Note

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  - 10 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
  - 6 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.

