

```
R(reflections)= 0.0302( 3057)      wR2(reflections)=
S = 1.053                        0.0707( 3652)
Npar= 217
```

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 C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report



Alert level G

PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1	(II)	.	2.14	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe2	(II)	.	2.12	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters			3	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		32	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			12	Info

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-

Datablock: MW253

Bond precision: C-C = 0.0078 A

Wavelength=0.71073

Cell: a=7.5042(5) b=13.5729(5) c=14.4725(6)

alpha=90

beta=90

gamma=90

Temperature: 150 K

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully
 3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 8 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 3 ALERT type 3 Indicator that the structure quality may be low
 2 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

Datablock: MW259

Bond precision: C-C = 0.0198 A Wavelength=0.71073

Cell: a=9.243(4) b=11.592(6) c=18.243(8)
 alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	1954.6(16)	1954.7(16)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C17 H25 Fe I O S Si	C17 H25 Fe I O S Si
Sum formula	C17 H25 Fe I O S Si	C17 H25 Fe I O S Si
Mr	488.27	488.27
Dx, g cm ⁻³	1.659	1.659
Z	4	4
Mu (mm ⁻¹)	2.518	2.518
F000	976.0	976.0
F000'	976.54	
h, k, lmax	11, 14, 23	11, 14, 23
Nref	4275 [2436]	4064
Tmin, Tmax	0.586, 0.818	0.508, 0.818
Tmin'	0.454	

Correction method= # Reported T Limits: Tmin=0.508 Tmax=0.818
 AbsCorr = MULTI-SCAN

Data completeness= 1.67/0.95 Theta(max)= 27.038

R(reflections)= 0.0605(2808) wR2(reflections)=
 0.1491(4064)
 S = 0.980 Npar= 205

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 C

PLAT213_ALERT_2_C	Atom C11	has ADP max/min Ratio	3.8	oblate
PLAT234_ALERT_4_C	Large Hirshfeld Difference C9	--C10	0.18	Ang.
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.2	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.01985	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	18	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.00Ang From I1	1.95	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.05Ang From I1	1.90	eA-3



Alert level G

PLAT431_ALERT_2_G	Short Inter HL..A Contact I1	..014	2.96	Ang.
	3/2-x,1-y,-1/2+z =		2_664	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (II)		2.13	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	58	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
7 **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
6 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
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-

Datablock: MW239

Bond precision: C-C = 0.0068 A

Wavelength=0.71073

Cell:	a=9.2687(9)	b=11.6233(9)	c=18.3737(18)
	alpha=90	beta=90	gamma=90

Temperature: 150 K

- ```
0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
0 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
```

2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 ALERT type 3 Indicator that the structure quality may be low  
1 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* 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.

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**PLATON version of 20/01/2022; check.def file version of 19/01/2022**









