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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**

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report

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● **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

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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  
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
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## Datablock: MW253

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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

	Calculated	Reported
Volume	1474.08(13)	1474.08(13)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C14 H17 Fe I O S	C14 H17 Fe I O S
Sum formula	C14 H17 Fe I O S	C14 H17 Fe I O S
Mr	416.09	416.08
Dx, g cm <sup>-3</sup>	1.875	1.875
Z	4	4
Mu (mm <sup>-1</sup> )	3.244	3.244
F000	816.0	816.0
F000'	816.20	
h, k, lmax	9, 17, 18	9, 17, 18
Nref	3384[ 1949]	3247
Tmin, Tmax	0.213, 0.321	0.229, 0.321
Tmin'	0.140	

Correction method= # Reported T Limits: Tmin=0.229 Tmax=0.321  
AbsCorr = MULTI-SCAN

Data completeness= 1.67/0.96                      Theta(max)= 27.486

R(reflections)= 0.0359( 3063)    wR2(reflections)=  
0.0920( 3247)  
S = 1.101    Npar= 125

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**Alert level C**

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	40 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.86Ang From O11	0.41 eA-3

**Alert level G**

PLAT019_ALERT_1_G _diffn_measured_fraction_theta_full/*_max < 1.0	0.997 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	5.88 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1 --C3	5.3 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (II)	2.12 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	5 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....	2.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	2 Info

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- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
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## 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 <sup>-3</sup>	1.659	1.659
Z	4	4
Mu (mm <sup>-1</sup> )	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





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  
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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**







