

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) fe1-ttmbncs

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: fe1-ttmbncs

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Bond precision:      C-C = 0.0030 Å      Wavelength=1.54184

Cell:                      a=8.5918 (4)                      b=9.4947 (3)                      c=11.7005 (3)  
                              alpha=80.490 (2)                      beta=85.194 (3)                      gamma=89.497 (3)  
Temperature:              298 K

	Calculated	Reported
Volume	938.05 (6)	938.05 (6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H30 Fe N20 S2 [+ solvent]	C32 H30 Fe N20 S2
Sum formula	C32 H30 Fe N20 S2 [+ solvent]	C32 H30 Fe N20 S2
Mr	814.73	814.73
Dx, g cm <sup>-3</sup>	1.442	1.442
Z	1	1
Mu (mm <sup>-1</sup> )	4.722	4.722
F000	420.0	420.0
F000'	420.62	
h, k, lmax	10, 11, 13	10, 11, 13
Nref	3348	3321
Tmin, Tmax		0.618, 0.641
Tmin'		

Correction method= # Reported T Limits: Tmin=0.618 Tmax=0.641

AbsCorr = SPHERE

Data completeness= 0.992

Theta(max)= 67.031

R(reflections)= 0.0383( 3006)

wR2(reflections)=  
0.1035( 3321)

S = 1.076

Npar= 250

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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.



#### Alert level C

PLAT242_ALERT_2_C Low	'MainMol' Ueq as Compared to Neighbors of	C16 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=	0.597	27 Report



#### Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	1 Info
PLAT230_ALERT_2_G Hirshfeld Test Diff for S1 --C16 .	7.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for N10 --C16 .	5.4 s.u.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H12 ..N2 .	2.64 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H15 ..S1 .	2.98 Ang.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure	39 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (II) .	1.98 Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still	82% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....	3.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	6 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  
2 **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  
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  
3 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

