

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

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Bond precision:    C-C = 0.0051 A                      Wavelength=0.71073

Cell:                      a=9.6020(7)              b=18.9796(14)              c=23.8123(18)  
                                    alpha=90                      beta=90                      gamma=90  
Temperature:              173 K

	Calculated	Reported
Volume	4339.6(6)	4339.6(6)
Space group	I b a m	I b a m
Hall group	-I 2 2c	-I 2 2c
Moiety formula	C50 H32 Fe N6 S2	?
Sum formula	C50 H32 Fe N6 S2	C50 H32 Fe N6 S2
Mr	836.79	836.78
Dx,g cm-3	1.281	1.281
Z	4	4
Mu (mm-1)	0.485	0.485
F000	1728.0	1728.0
F000'	1730.86	
h,k,lmax	12,24,30	12,24,30
Nref	2541	2537
Tmin,Tmax	0.850,0.925	0.830,0.930
Tmin'	0.832	

Correction method= # Reported T Limits: Tmin=0.830 Tmax=0.930  
AbsCorr = MULTI-SCAN

Data completeness= 0.998                      Theta(max)= 27.400

R(reflections)= 0.0597( 2125)              wR2(reflections)= 0.1786( 2537)

S = 0.907                                      Npar= 140

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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**

PLAT601\_ALERT\_2\_B Structure Contains Solvent Accessible VOIDS of . 117 Ang3

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**Alert level C**

PLAT250\_ALERT\_2\_C Large U3/U1 Ratio for Average U(i,j) Tensor ... 2.9 Note  
PLAT911\_ALERT\_3\_C Missing # FCF Refl Between THmin & STh/L= 0.600 2 Report  
PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check  
PLAT934\_ALERT\_3\_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ... 1 Check  
PLAT971\_ALERT\_2\_C Check Calcd Residual Density 1.26A From S1 1.59 eA-3

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**Alert level G**

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 2 Info  
PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 25.88 Why ?  
PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for N2 -- C13 .. 5.3 s.u.  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 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  
5 **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

1 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  
3 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 27/03/2017; check.def file version of 24/03/2017**

