

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 1

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Bond precision:	C-C = 0.0058 A	Wavelength=0.71073	
Cell:	a=8.6043(11)	b=16.1504(19)	c=19.470(2)
	alpha=90	beta=92.126(9)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	2703.8(5)	2703.7(6)	
Space group	P 21/n	P2(1)/n	
Hall group	-P 2yn	?	
Moiety formula	C44 H40 B2 Fe2 Mn N30, 2(H2 O)	?	
Sum formula	C44 H44 B2 Fe2 Mn N30 O2	C44 H44 B2 Fe2 Mn N30 O2	
Mr	1213.35	1213.35	
Dx,g cm-3	1.490	1.490	
Z	2	2	
Mu (mm-1)	0.828	0.828	
F000	1242.0	1242.0	
F000'	1244.31		
h,k,lmax	10,19,23	10,19,23	
Nref	4760	4754	
Tmin,Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.999      Theta(max)= 25.000

R(reflections)= 0.0417( 3547)      wR2(reflections)= 0.1165( 4754)

S = 1.079      Npar= 367

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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**

PLAT420\_ALERT\_2\_B D-H Without Acceptor      OlW      --H1WA      Please Check

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**Alert level C**

PLAT053\_ALERT\_1\_C Minimum Crystal Dimension Missing (or Error) ...      Please Check  
PLAT054\_ALERT\_1\_C Medium Crystal Dimension Missing (or Error) ...      Please Check  
PLAT055\_ALERT\_1\_C Maximum Crystal Dimension Missing (or Error) ...      Please Check

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**Alert level G**

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension      1 Info  
PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF      Please Do !  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms .....      2 Report  
PLAT093\_ALERT\_1\_G No s.u.'s on H-positions, Refinement Reported as      mixed Check  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fel      --C13      .      6.0 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Fel      --C15      .      5.1 s.u.  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels .....      2 Note  
PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL      2018 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  
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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
3 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 30/01/2018; check.def file version of 30/01/2018**

