

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ad2101

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: ad2101

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Bond precision:	C-C = 0.0039 A	Wavelength=0.71073	
Cell:	a=16.3327(6)	b=15.7996(6)	c=15.0588(6)
	alpha=90	beta=90	gamma=90
Temperature:	120 K		
	Calculated	Reported	
Volume	3885.9(3)	3885.9(3)	
Space group	P b c n	P b c n	
Hall group	-P 2n 2ab	-P 2n 2ab	
Moiety formula	C20 H24 Fe N6 O4, C24 H20 B	C20 H24 Fe N6 O4, C24 H20 B	
Sum formula	C44 H44 B Fe N6 O4	C44 H44 B Fe N6 O4	
Mr	787.51	787.51	
Dx, g cm <sup>-3</sup>	1.346	1.346	
Z	4	4	
Mu (mm <sup>-1</sup> )	0.440	0.440	
F000	1652.0	1652.0	
F000'	1653.96		
h,k,lmax	21,20,19	21,20,19	
Nref	4633	4610	
Tmin,Tmax	0.959,0.965	0.699,0.746	
Tmin'	0.854		

Correction method= # Reported T Limits: Tmin=0.699 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.995      Theta(max)= 27.874

R(reflections)= 0.0508( 2496)      wR2(reflections)= 0.1077( 4610)

S = 0.998      Npar= 259

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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**

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.124  
PLAT905\_ALERT\_3\_C Negative K value in the Analysis of Variance ... -3.347 Report  
PLAT905\_ALERT\_3\_C Negative K value in the Analysis of Variance ... -0.105 Report

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● **Alert level G**

PLAT020\_ALERT\_3\_G The Value of Rint is Greater Than 0.12 ..... 0.124 Report  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O2 ..C3 2.95 Ang.  
-1/2+x,3/2-y,1-z = 4\_466 Check  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Fel (III) . 3.11 Info  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 24 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 2 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  
3 **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  
2 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  
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 16/05/2021; check.def file version of 13/05/2021**

