

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: mm10-2

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Bond precision:    C-C = 0.0050 Å

Wavelength=0.71073

Cell:                    a=10.9164(6)            b=25.1685(13)            c=18.3340(11)  
                          alpha=90                beta=91.060(5)            gamma=90  
Temperature:            123 K

	Calculated	Reported
Volume	5036.4(5)	5036.4(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	?
Moiety formula	C21 H22 Fe O	C21 H22 Fe O
Sum formula	C21 H22 Fe O	C21 H22 Fe O
Mr	346.24	346.24
Dx, g cm <sup>-3</sup>	1.370	1.370
Z	12	12
Mu (mm <sup>-1</sup> )	0.900	0.900
F000	2184.0	2184.0
F000'	2188.80	
h,k,lmax	13,32,23	13,32,23
Nref	10983	10967
Tmin,Tmax	0.947,0.956	0.834,1.000
Tmin'	0.763	

Correction method= MULTI-SCAN

Data completeness= 0.999

Theta(max)= 27.000

R(reflections)= 0.0580( 6409)

wR2(reflections)= 0.1252( 10967)

S = 0.990

Npar= 631

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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 G

PLAT128_ALERT_4_G	Alternate Setting of Space-group P21/c	.....	P21/n
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	.....	12
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Fe1	(II)	2.08
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Fe1A	(II)	2.11
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Fe1B	(II)	2.08

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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  
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
0 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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### **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*, 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 16/02/2011; check.def file version of 16/02/2011**

