

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: klat222

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Bond precision:	C-C = 0.0071 Å	Wavelength=0.71073	
Cell:	a=10.215(6)	b=19.386(11)	c=15.891(9)
	alpha=90	beta=90.936(9)	gamma=90
Temperature:	120 K		
	Calculated	Reported	
Volume	3146(3)	3147(3)	
Space group	P 21/n	P2(1)/n	
Hall group	-P 2yn	?	
Moiety formula	C24 H40 B Fe I N6, 0.5(C10 H8)	C24 H40 B Fe I N6, 0.5(C10 H8)	
Sum formula	C29 H44 B Fe I N6	C29 H44 B Fe I N6	
Mr	670.26	670.26	
Dx,g cm-3	1.415	1.415	
Z	4	4	
Mu (mm-1)	1.488	1.488	
F000	1376.0	1376.0	
F000'	1375.79		
h,k,lmax	13,25,21	12,24,20	
Nref	7816	7209	
Tmin,Tmax	0.694,0.849	0.563,0.855	
Tmin'	0.514		

Correction method= MULTI-SCAN

Data completeness= 0.922      Theta(max)= 28.280

R(reflections)= 0.0578( 5825)      wR2(reflections)= 0.1591( 7209)

S = 1.078      Npar= 359

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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

PLAT232\_ALERT\_2\_B Hirshfeld Test Diff (M-X) I      -- Fe      ..      18.92 su

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### Alert level C

PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density ....      2.89

PLAT213_ALERT_2_C Atom C26	has ADP max/min Ratio .....	3.10 prola
PLAT213_ALERT_2_C Atom C27	has ADP max/min Ratio .....	3.60 prola
PLAT213_ALERT_2_C Atom C28	has ADP max/min Ratio .....	3.10 prola



#### Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.	10.45
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c .....	P21/n

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0 **ALERT level A** = In general: serious problem

1 **ALERT level B** = Potentially serious problem

4 **ALERT level C** = Check and explain

2 **ALERT level G** = General alerts; check

0 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

0 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

0 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 31/03/2010; check.def file version of 22/03/2010

