

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: klat442a

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Bond precision:    C-C = 0.0060 Å                      Wavelength=0.71073

Cell:                      a=30.827(8)              b=9.854(3)              c=19.364(5)  
                            alpha=90              beta=107.462(4)              gamma=90

Temperature:              120 K

	Calculated	Reported
Volume	5611(3)	5611(3)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C25 H43 B Fe N6 S	?
Sum formula	C25 H43 B Fe N6 S	C25 H43 B Fe N6 S
Mr	526.38	526.37
Dx, g cm <sup>-3</sup>	1.246	1.246
Z	8	8
Mu (mm <sup>-1</sup> )	0.636	0.636
F000	2256.0	2256.0
F000'	2260.22	
h,k,lmax	41,13,25	40,12,25
Nref	13978	12468
Tmin,Tmax	0.885,0.927	0.804,0.930
Tmin'	0.795	

Correction method= MULTI-SCAN

Data completeness= 0.892                      Theta(max)= 28.330

R(reflections)= 0.0712( 6559)              wR2(reflections)= 0.1431( 12468)

S = 1.003                      Npar= 645

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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

PLAT380\_ALERT\_4\_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety              C24

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- 0 ALERT level A = In general: serious problem
- 0 ALERT level B = Potentially serious problem
- 0 ALERT level C = Check and explain

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

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

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**

