checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: klat634

Bond precision: C-C = 0.0024 A   Wavelength=0.71073

Cell: a=22.341(7)   b=22.341(7)   c=22.341(7)
                   alpha=90   beta=90   gamma=90
Temperature: 120 K

                   Calculated   Reported
Volume   11151(6)   11151(6)
Space group   I -4 3 d   I-43d
Hall group   I -4bd 2c 3   ?
Moiety formula   C25 H43 B Fe N6   ?
Sum formula   C25 H43 B Fe N6   C25 H43 B Fe N6
Mr   494.31   494.31
Dx,g cm-3   1.178   1.178
Z   16   16
Mu (mm-1)   0.564   0.564
F000   4256.0   4256.0
F000'   4262.40
h,k,lmax   29,29,29   29,29,29
Nref   1243[2313]   2315
Tmin,Tmax   0.812,0.914   0.818,0.915
Tmin'   0.812

Correction method= MULTI-SCAN

Data completeness= 1.86/1.00   Theta(max)= 28.290

R(reflections)= 0.0334(2168)   wR2(reflections)= 0.0837(2315)

S = 1.078   Npar= 106

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.

🟡 **Alert level C**
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.37
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe   -- C9   ..   7.97 su

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🔘 **Alert level G**
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is

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             correct. If it is not, please give the correct count in the
             _publ_section_exptl_refinement section of the submitted CIF.
             From the CIF: _diffrn_reflns_theta_max        28.29
             From the CIF: _reflns_number_total            2315
             Count of symmetry unique reflns        1243
             Completeness (_total/calc)          186.24%
             TEST3: Check Friedels for noncentro structure
             Estimate of Friedel pairs measured      1072
             Fraction of Friedel pairs measured      0.862
             Are heavy atom types Z>Si present         yes
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.13 Ratio
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   0 ALERT level A = In general: serious problem
   0 ALERT level B = Potentially serious problem
   2 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
   2 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
   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.

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