checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: fl206_a

```
Bond precision:   C-C = 0.0114 A            Wavelength=0.71073

Cell:             a=21.131(4)      b=17.391(4)          c=21.069(4)
                  alpha=90         beta=107.00(3)       gamma=90
Temperature:      293 K

                  Calculated                 Reported
Volume            7404(3)                    7404(3)
Space group       C 2/c                      C 1 2/c 1
Hall group        -C 2yc                     -C 2yc
                  2(C63 H54 Fe2 N18),        C63 H54 Fe2 N18, 2(B0.4
Moiety formula    4(B0.40 F1.60), 4(B F4),   F0.8), 2(B F4), 2(B0.6
                  4(C0.50 H0.75 N0.5         F3.2), 2(C0.5 H0
Sum formula       C130 H114 B8 F32 Fe4 N39   C65 H57 B4 F16 Fe2 N19.50
Mr                3140.49                    1570.24
Dx,g cm-3         1.409                      1.409
Z                 2                          4
Mu (mm-1)         0.486                      0.486
F000              3198.0                     3198.0
F000'             3202.45
h,k,lmax          26,21,26                   26,21,26
Nref              7678                       6995
Tmin,Tmax         0.994,0.995
Tmin'             0.990


Correction method= Not given

Data completeness= 0.911          Theta(max)= 26.499

R(reflections)= 0.1035( 4686)     wR2(reflections)= 0.3220( 6995)

S = 1.096                  Npar= 630
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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.

🔴 Alert level A
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .   0.917 Note

Author Response: 'The MX1 beam line of the Australian Synchrtron is a single circle instrument, leaving gaps in the coverage of the reciprical space.'

🟡 Alert level C
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ....   0.32 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.47 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference N3B   -- C4B   ..   0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5A   -- C20A   ..   0.16 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.2 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.01136 Ang.

⚪ Alert level G
FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum: C65 H57 B4 F16 Fe2 N19.5
            Atom count from _chemical_formula_moiety:C64 H55.5 B4 F16 Fe2 N19
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   13 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   42 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   4 Report
PLAT012_ALERT_1_G No   _shelx_res_checksum found in CIF .... Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.50 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.13 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   69.22 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records   1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records   6 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)   293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe01   -- N1A   ..   5.2 s.u.
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of   B01A Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1B'   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1B   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2B'   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2B   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7A'   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1B   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8A'   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2B   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9A'   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3B   is Constrained at   0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of C5A'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4B       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4C       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6A'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5A       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1B'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6A       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2B'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7A       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3B'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8A       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9A       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1A       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4B       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4C       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9A'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6A       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1BA      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7A       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2BA      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9        is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1B'      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9A       is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2BB      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11B      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11C      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11D      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A      is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F009      is Constrained at        0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1        is Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F00X      is Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3        is Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F10       is Constrained at        0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B01B      is Constrained at        0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2        is Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C1AA    is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2AA    is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2AB    is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2AC    is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2AD    is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N01L    is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4      is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C0AA    is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4D     is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4E     is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4F     is Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F00H    is Constrained at      0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F00T    is Constrained at      0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F00Y    is Constrained at      0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B01C    is Constrained at      0.6 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..       46 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9)..      100 % Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.75) in Resd. #        4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   1.50) in Resd. #        5 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.80) in Resd. #        6 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.80) in Resd. #        7 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.80) in Resd. #        8 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.60) in Resd. #        9 Check
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C8B    -    C11B    ..    1.51 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F00A   ..  C0AA    ..    2.95 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F00Y   ..  C20A    ..    2.93 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       40 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      218 Note
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 128 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
 112 ALERT type 4 Improvement, methodology, query or suggestion
   2 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT084_fl206_a
;
PROBLEM: High wR2 Value (i.e. > 0.25) ...................     0.32 Report
RESPONSE: ...
;
_vrf_PLAT094_fl206_a
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....     2.47 Report
RESPONSE: ...
;
_vrf_PLAT234_fl206_a
;
PROBLEM: Large Hirshfeld Difference N3B    --  C4B     ..     0.23 Ang.
RESPONSE: ...
;
_vrf_PLAT250_fl206_a
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.2 Note
RESPONSE: ...
;
_vrf_PLAT341_fl206_a
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............  0.01136 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 27/03/2017; check.def file version of 24/03/2017

Datablock **fl206_a** - ellipsoid plot