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: I

Bond precision: C-C = 0.0065 A Wavelength=0.71073

Cell: a=13.837(3) b=13.855(3) c=20.684(4)
alpha=77.43(3) beta=77.58(3) gamma=86.73(3)
Temperature: 100 K

	Calculated	Reported
Volume	3779.5(15)	3779.5(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C60 H48 Fe2 N18 O3, 0.25(C4 H6 N2), 4(B F4), 1.5(C2 H3 N)	C60 H48 Fe2 N18 O3, 2(C2 H3 N), 4(B F4)
Sum formula	C64 H54 B4 F16 Fe2 N20 O3	C64 H54 B4 F16 Fe2 N20 O3
Mr	1610.22	1610.21
Dx,g cm-3	1.415	1.415
Z	2	2
Mu (mm-1)	0.481	0.481
F000	1636.0	1636.0
F000’	1638.28	
h,k,lmax	17,17,26	17,17,26
Nref	16519	14860
Tmin,Tmax	0.994,0.995	
Tmin’	0.990	

Correction method= Not given

Data completeness= 0.900 Theta(max)= 26.999

R(reflections)= 0.0691(11524) wR2(reflections)= 0.2111(14860)

S = 1.071 Npar= 1095

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 . 0.909 Note

Author Response: 'The MX2 beam line of the Australian Synchrtron is a single circle instrument, leaving gaps in the coverage of the reciprical space.'

Alert level B

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Fe02 -- N4B .. 16.3 s.u.

Author Response: 'Data sets corrected for absorption effects often show large DELU values for bonds involving the heaviest atom. The data was treated with SADABS absorption correction, which may be a cause of such test results around the heavy scattering Fe(II).'

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Fe02 -- N6C .. 11.8 s.u.

Author Response: 'Data sets corrected for absorption effects often show large DELU values for bonds involving the heaviest atom. The data was treated with SADABS absorption correction, which may be a cause of such test results around the heavy scattering Fe(II).'

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for N1B -- C1B .. 6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for N1B -- C3B .. 5.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for N2B -- C2B .. 5.7 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C16A Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C17B Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00647 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 16 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 7 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
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.12 Why ?
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem. c 92 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group C2/c Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report

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PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         10 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C7AA   --  C17B    ..        7.3 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C17B   --  C18B    ..        6.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe01   --  N1A     ..        7.6 s.u.
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Author Response: 'Data sets corrected for absorption effects often show large DELU values for bonds involving the heaviest atom. The data was treated with SADABS absorption correction, which may be a cause of such test results around the heavy scattering Fe(II).'

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PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe01   --  N1B     ..        6.5 s.u.
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Author Response: 'Data sets corrected for absorption effects often show large DELU values for bonds involving the heaviest atom. The data was treated with SADABS absorption correction, which may be a cause of such test results around the heavy scattering Fe(II).'

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PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe01   --  N3B     ..        9.2 s.u.
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Author Response: 'Data sets corrected for absorption effects often show large DELU values for bonds involving the heaviest atom. The data was treated with SADABS absorption correction, which may be a cause of such test results around the heavy scattering Fe(II).'

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PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       B02R Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       B02N Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       B02P Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       B02Q Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N5B     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N6B     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9C     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5B     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9C     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2AB    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N0AA    is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N4      is Constrained at       0.25 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C2      is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5      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 C2AA    is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2D     is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2E     is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2F     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 H2AE    is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N031    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C02S    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C02W    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N02Y    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C02X    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C02Z    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02D    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02E    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H02F    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3      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 C1AA    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1D     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1E     is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1F     is Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1)..          8 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..        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
PLAT432_ALERT_2_G Short Inter X...Y Contact  F00T   ..  C0AA    ..       2.94 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         56 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7 Note
             C2 H3 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
             C2 H3 N
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         33 Note
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  87 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  70 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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checkCIF publication errors

Alert level A

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PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

3 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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

Datablock I - ellipsoid plot