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 = 0.0095 A   Wavelength=0.71073

Cell: a=9.5210(19)   b=16.723(3)   c=23.621(5)
               alpha=95.29(3)   beta=100.29(3)   gamma=92.93(3)
Temperature: 100 K

	Calculated	Reported
Volume	3675.9(13)	3675.8(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C60 H48 Fe2 N18 S3), 2(B F3.50), 6(B F4), 4(C2 H3 N)	C60 H48 Fe2 N18 S3, 3(B F4), B F3.5, 2(C2 H3 N)
Sum formula	C128 H108 B8 F31 Fe4 N40 S6	C64 H54 B4 F15.50 Fe2 N20 S3
Mr	3297.79	1648.89
Dx,g cm-3	1.490	1.490
Z	1	2
Mu (mm-1)	0.575	0.575
F000	1675.0	1675.0
F000'	1677.95	
h,k,lmax	11,20,29	11,20,29
Nref	15022	13521
Tmin,Tmax	0.995,0.996	
Tmin'	0.991	

Correction method= Not given

Data completeness= 0.900   Theta(max)= 26.371

R(reflections)= 0.1086(8552)   wR2(reflections)= 0.3308(13521)

S = 1.138   Npar= 1047

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: 'MX2 of the Australian synchtrotron employs a one circle goniometer, collecting data by rotation around the spindle axis only and therefore may leave gaps in the coverage of the recprical space.'

🟠 Alert level B
PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor ....   4.1 Note
PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of .   111 Ang3

🟡 Alert level C
PLAT082_ALERT_2_C High R1 Value ....   0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ....   0.33 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C17A   -- C18A   ..   6.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2A   -- C2A   ..   0.16 Ang.
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of   F2AA Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   C02V Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of   C02M Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00952 Ang.

⚪ Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   19 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   27 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   6 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   0.20 Report
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
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   7 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records   5 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records   1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records   10 Report
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of   B02Q Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of   B0AA Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1AA   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5AA   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7AA   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1AB   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F0BA   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B2   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B2A   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F0AA   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4   is Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B9   is Constrained at   0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of F8       is Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F10      is Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F11      is Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F15      is Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of B9A      is Constrained at       0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..       78 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3)..      100 % Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5)..      100 % Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   4.50) in Resd. #        2 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   2.50) in Resd. #        3 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   2.50) in Resd. #        5 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F2AA   .. C4C      ..    2.90 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       34 Note
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 .............      193 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        1 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
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  44 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
  37 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.
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   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
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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