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 = 0.0042 A          Wavelength=0.71073

Cell:          a=8.877(2)       b=12.628(3)     c=13.810(4)
               alpha=74.68(2)   beta=74.48(2)   gamma=83.105(18)
Temperature:   173 K
```

	Calculated	Reported
Volume	1436.6(7)	1436.6(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C60 H80 Cl2 Fe N8	C60 H80 Cl2 Fe N8
Sum formula	C60 H80 Cl2 Fe N8	C60 H80 Cl2 Fe N8
Mr	1040.07	1040.07
Dx,g cm-3	1.202	1.202
Z	1	1
Mu (mm-1)	0.400	0.400
F000	556.0	556.0
F000’	556.79	
h,k,lmax	10,15,16	10,15,16
Nref	5213	5214
Tmin,Tmax	0.908,0.942	0.966,1.000
Tmin’	0.905	

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Correction method= # Reported T Limits: Tmin=0.966 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 25.249

R(reflections)= 0.0426( 3012)     wR2(reflections)= 0.0693( 5214)

S = 0.795                 Npar= 339
```

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

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GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      0.795
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C10    --  C12A    ..       0.16 Ang.
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C10 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2     ..  CL1     ..       2.92 Ang.
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          5 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C10    --  C11B    ..        5.7 su
PLAT300_ALERT_4_G Atom Site Occupancy of >C11A   is Constrained at      0.727 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C12A   is Constrained at      0.727 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C11B   is Constrained at      0.273 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C12B   is Constrained at      0.273 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C11A_a is Constrained at      0.727 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C12A_a is Constrained at      0.727 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C11B_a is Constrained at      0.273 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C12B_a is Constrained at      0.273 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          6 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....          4 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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Datablock: II

Bond precision: C-C = 0.0071 A Wavelength=0.71073

Cell: a=9.0391(11) b=12.7658(11) c=13.689(2)
       alpha=74.502(9) beta=74.481(12) gamma=84.343(9)
Temperature: 173 K

	Calculated	Reported
Volume	1466.0(3)	1466.0(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C60 H80 Br2 Fe N8	C60 H80 Br2 Fe N8
Sum formula	C60 H80 Br2 Fe N8	C60 H80 Br2 Fe N8
Mr	1128.97	1128.99
Dx,g cm-3	1.279	1.279
Z	1	1
Mu (mm-1)	1.663	1.663
F000	592.0	592.0
F000'	591.92	
h,k,lmax	10,15,16	10,15,16
Nref	5312	5312
Tmin,Tmax	0.724,0.847	0.456,0.496
Tmin'	0.710	

Correction method= # Reported T Limits: Tmin=0.456 Tmax=0.496
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.243

R(reflections)= 0.0461(3013) wR2(reflections)= 0.0805(5312)

S = 0.808 Npar= 350

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

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C10 -- C11B .. 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C10 -- C12A .. 0.19 Ang.
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C10 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C13 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0071 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of *C11A is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C11B is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C12A is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C12B is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C11A_a is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C11B_a is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C12A_a is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C12B_a is Constrained at 0.500 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 6 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 1 Note

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 2 Note

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6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: IIb

Bond precision: C-C = 0.0039 A Wavelength=0.71073

Cell: a=11.6710(8) b=12.4758(9) c=13.5759(10)
alpha=64.464(5) beta=81.515(6) gamma=88.982(6)
Temperature: 173 K

	Calculated	Reported
Volume	1761.8(2)	1761.8(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C60 H80 Br2 Fe N8, 2(C4 H10 O)	C60 H80 Br2 Fe N8, 2(C4 H10 O)
Sum formula	C68 H100 Br2 Fe N8 O2	C68 H100 Br2 Fe N8 O2
Mr	1277.21	1277.22
Dx,g cm-3	1.204	1.204
Z	1	1
Mu (mm-1)	1.394	1.394
F000	676.0	676.0
F000’	675.96	
h,k,lmax	14,14,16	14,14,16
Nref	6381	6374
Tmin,Tmax	0.503,0.498	0.557,0.672
Tmin’	0.493	

Correction method= # Reported T Limits: Tmin=0.557 Tmax=0.672
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.250

R(reflections)= 0.0307(5714) wR2(reflections)= 0.0773(6374)

S = 1.026 Npar= 378

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

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C10 Check
PLAT410_ALERT_2_C Short Intra H...H Contact H31B .. H33D .. 1.91 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H17 .. BR1 .. 3.02 Ang.

Alert level G

PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) C31 -- C32 .. 5.4 su
PLAT300_ALERT_4_G Atom Site Occupancy of *C33A is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C33B is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C34A is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C34B is Constrained at 0.500 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 40 Note

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4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
8 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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

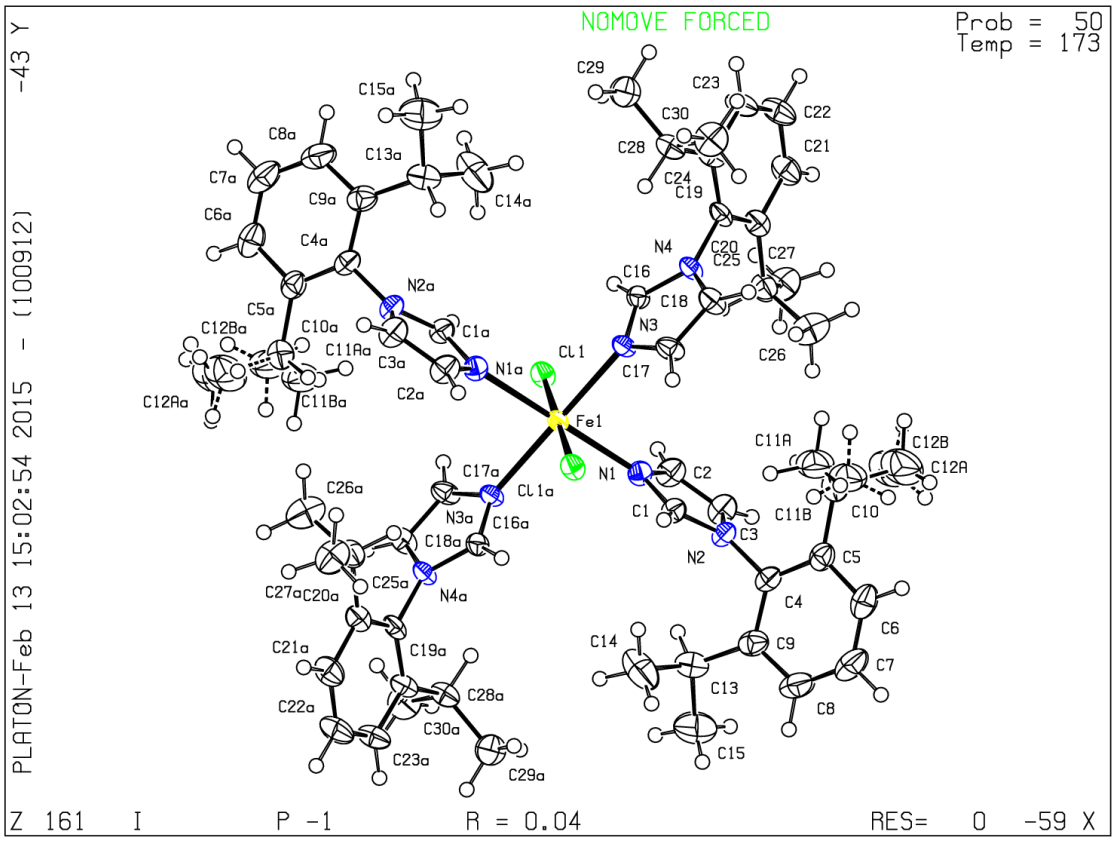
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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

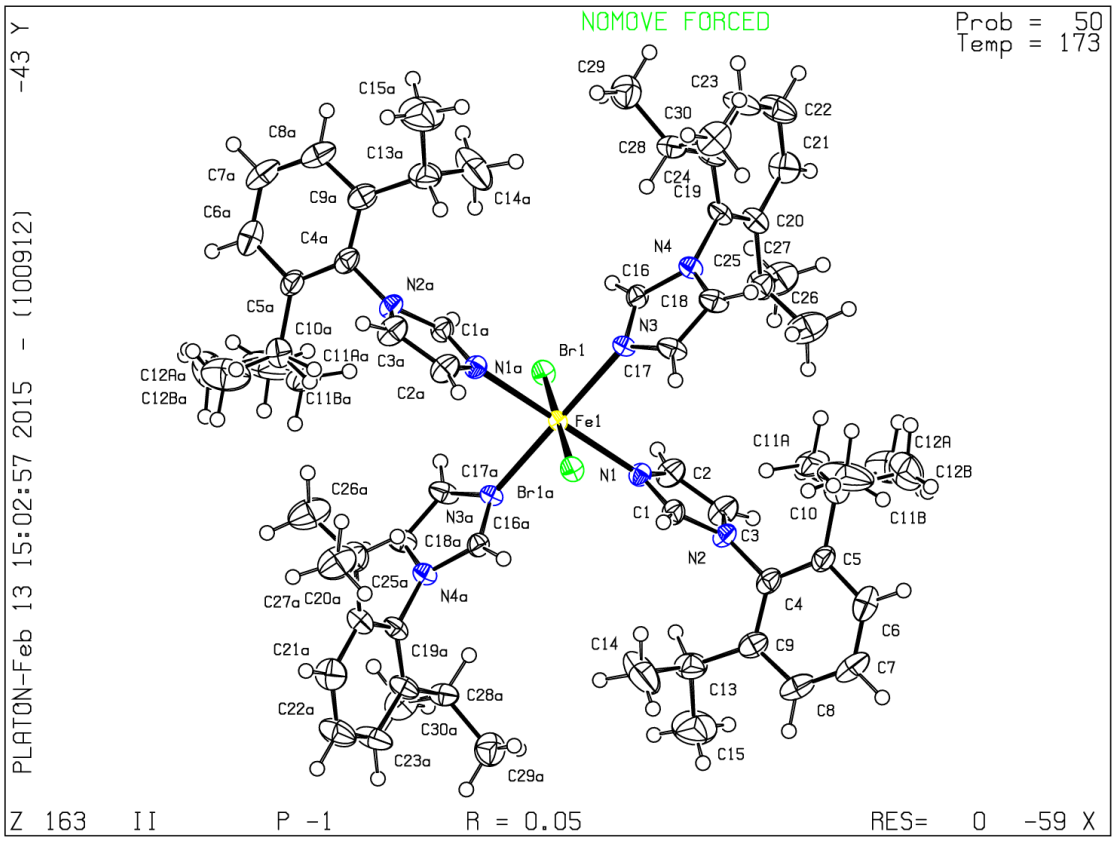
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 29/01/2015; check.def file version of 29/01/2015

Datablock I - ellipsoid plot



Datablock II - ellipsoid plot



Datablock IIb - ellipsoid plot