checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: 20130606a

Bond precision: C-C = 0.0154 A Wavelength=0.71073

Cell: a=10.5274(3) b=15.7581(6) c=23.8577(7)
alpha=88.861(3) beta=85.958(3) gamma=82.435(3)
Temperature: 293 K

	Calculated	Reported
Volume	3913.4(2)	3913.4(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H34 Ir N6 S2, F6 P	C40 H34 Ir N6 S2, F6 P
Sum formula	C40 H34 F6 Ir N6 P S2	C40 H34 F6 Ir N6 P S2
Mr	1000.04	1000.02
Dx,g cm-3	1.697	1.697
Z	4	4
Mu (mm-1)	3.627	3.627
F000	1976.0	1976.0
F000’	1972.53	
h,k,lmax	13,19,29	13,19,29
Nref	15983	15976
Tmin,Tmax		0.786,1.000
Tmin’		

Correction method= # Reported T Limits: Tmin=0.786 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 26.370

R(reflections)= 0.0616(7864) wR2(reflections)= 0.1041(15976)

S = 0.890 Npar= 1017

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

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low .... 49 %
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

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PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N3     --  C11     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N4     --  C24     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C7     --  C8      ..       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C8     --  C9      ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N10    --  C65     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N12    --  C80     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1     --  F1      ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1     --  F3      ..       0.25 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1     --  F4      ..       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1     --  F5      ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1     --  F6      ..       0.25 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         S1 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         C4 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         S4 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C48 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         N4 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        N10 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        N12 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0154 Ang.
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Alert level G

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PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........    0.00300 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of          P1 Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of          P2 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  27 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

   7 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
   2 ALERT type 3 Indicator that the structure quality may be low
  13 ALERT type 4 Improvement, methodology, query or suggestion
   0 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*, 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 21/04/2015; check.def file version of 09/03/2015

Datablock 20130606a - ellipsoid plot