

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a23061302a0229

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: a23061302a0229

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Bond precision:      C-C = 0.0077 Å      Wavelength=1.54184

Cell:                      a=8.3615 (3)                      b=10.6980 (5)                      c=19.2560 (7)  
                              alpha=76.136 (4)                      beta=84.487 (3)                      gamma=77.048 (3)  
Temperature:              150 K

	Calculated	Reported
Volume	1628.11 (12)	1628.11 (12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H26 F2 Ir N4, F6 P [+ solvent]	C32 H26 F2 Ir N4, 2 (F3 P0.5)
Sum formula	C32 H26 F8 Ir N4 P [+ solvent]	C32 H26 F8 Ir N4 P
Mr	841.76	841.74
Dx, g cm <sup>-3</sup>	1.717	1.717
Z	2	2
Mu (mm <sup>-1</sup> )	9.072	9.072
F000	820.0	820.0
F000'	813.56	
h, k, lmax	10, 13, 23	10, 13, 23
Nref	6502	6299
Tmin, Tmax	0.311, 0.404	0.534, 1.000
Tmin'	0.223	

Correction method= # Reported T Limits: Tmin=0.534 Tmax=1.000  
AbsCorr = MULTII-SCAN

Data completeness= 0.969

Theta(max)= 72.953

R(reflections)= 0.0365( 5831)

wR2(reflections)=  
0.0930( 6299)

S = 1.055

Npar= 418

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

PLAT414_ALERT_2_C	Short Intra D-H..H-X	H2	..H3A	.	1.90 Ang.
			x,y,z =	1_555	Check
PLAT414_ALERT_2_C	Short Intra D-H..H-X	H4A	..H17	.	1.93 Ang.
			x,y,z =	1_555	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N4	--H4B	.	Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		8	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.00Ang	From Ir1	1.99	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.13Ang	From Ir1	1.83	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.01Ang	From Ir1	1.72	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.81Ang	From Ir1	-2.11	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.93Ang	From Ir1	-1.97	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H3B			-0.42	eA-3



### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	4	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	4	Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P002	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P003	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	224	A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	8	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	4	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed	!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	194	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	1.8	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
10 **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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
11 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  
7 ALERT type 4 Improvement, methodology, query or suggestion  
1 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* 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.

