

# 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: 4cn

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Bond precision:    C-C = 0.0047 A

Wavelength=0.71073

Cell:                a=11.8797(4)                b=12.1298(4)                c=12.8946(4)  
                      alpha=88.936(2)        beta=86.581(2)        gamma=68.125(3)  
Temperature:        110 K

	Calculated	Reported
Volume	1721.22(10)	1721.22(10)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C32 H16 F4 I Ir N4 O2, 2(C H2 Cl2)	C32 H16 F4 I Ir N4 O2, 2(C H2 Cl2)
Sum formula	C34 H20 Cl4 F4 I Ir N4 O2	C34 H20 Cl4 F4 I Ir N4 O2
Mr	1053.46	1053.44
Dx,g cm-3	2.033	2.033
Z	2	2
Mu (mm-1)	5.147	5.147
F000	1004.0	1004.0
F000'	1001.83	
h,k,lmax	16,16,17	16,15,17
Nref	9377	7983
Tmin,Tmax	0.034,0.157	0.340,1.000
Tmin'	0.014	

Correction method= # Reported T Limits: Tmin=0.340 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.851

Theta(max)= 29.250

R(reflections)= 0.0236( 7055)

wR2(reflections)= 0.0558( 7983)

S = 1.012

Npar= 463

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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	Non-Solvent Resd 1	N	Ueq(max)/Ueq(min) Range	4.0	Ratio
PLAT243_ALERT_4_C	High	'Solvent'	Ueq as Compared to Neighbors of	C33	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	C34	Check
PLAT350_ALERT_3_C	Short	C-H (X0.96,N1.08A)	C34 - H34B ..	0.84	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #			1	Note
	C32 H16 F4 I Ir N4 O2				



#### Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size ....	0.76 mm
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	2 Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder ..... Percentage =	17 Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	128 Check
	CL4' -C34 -CL4 1.555 1.555 1.555	29.70 Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2 Note
	C H2 Cl2	
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 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  
7 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 ALERT type 3 Indicator that the structure quality may be low  
9 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.

