

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: 4m

Bond precision: C-C = 0.0071 A

Wavelength=0.71073

Cell: a=8.5721(2) b=10.9433(3) c=16.9964(6)
 alpha=95.019(2) beta=97.165(2) gamma=91.412(2)
Temperature: 110 K

| | Calculated | Reported |
|----------------|---------------------------------------|---------------------------------------|
| Volume | 1574.85(8) | 1574.85(8) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | ? |
| Moiety formula | C32 H19 F4 I Ir N3 O2, 0.5(C6 H14) | C32 H19 F4 I Ir N3 O2, 0.5(C6 H14) |
| Sum formula | C35 H26 F4 I Ir N3 O2 | C35 H26 F4 I Ir N3 O2 |
| Mr | 915.71 | 915.69 |
| Dx,g cm-3 | 1.931 | 1.931 |
| Z | 2 | 2 |
| Mu (mm-1) | 5.280 | 5.280 |
| F000 | 878.0 | 878.0 |
| F000' | 874.64 | |
| h,k,lmax | 11,15,23 | 11,14,22 |
| Nref | 8532 | 7249 |
| Tmin,Tmax | 0.031,0.121 | 0.468,1.000 |
| Tmin' | 0.014 | |

Correction method= # Reported T Limits: Tmin=0.468 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.850

Theta(max)= 29.200

R(reflections)= 0.0317(6292)

wR2(reflections)= 0.0723(7249)

S = 1.030

Npar= 409

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

| | | | | |
|-------------------|---|-----------------------------|-----|--------|
| PLAT213_ALERT_2_C | Atom C23 | has ADP max/min Ratio | 3.2 | prolat |
| PLAT220_ALERT_2_C | Non-Solvent Resd 1 | C Ueq(max)/Ueq(min) Range | 3.1 | Ratio |
| PLAT790_ALERT_4_C | Centre of Gravity not Within Unit Cell: Resd. # | | 1 | Note |
| | C32 H19 F4 I Ir N3 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 | 0.75 mm |
| PLAT154_ALERT_1_G | The s.u.'s on the Cell Angles are Equal ..(Note) | 0.002 Degree |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Ir -- I .. | 6.5 s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Ir -- C13 .. | 6.9 s.u. |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact C9 .. C9 .. | 3.18 Ang. |
| PLAT790_ALERT_4_G | Centre of Gravity not Within Unit Cell: Resd. # | 2 Note |
| | C6 H14 | |
| 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
- 3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 8 **ALERT level G** = General information/check it is not something unexpected

- 1 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
- 0 ALERT type 3 Indicator that the structure quality may be low
- 4 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.

