# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:    C-C = 0.0099 A              Wavelength=0.71069

Cell:              a=30.7102(6)      b=18.9149(4)        c=15.7234(2)
                   alpha=90          beta=90.301(1)      gamma=90
Temperature:       173 K

|  | Calculated | Reported |
|---|---|---|
| Volume | 9133.3(3) | 9133.3(3) |
| Space group | C 2/c | C 2/c |
| Hall group | -C 2yc | -C 2yc |
| Moiety formula | 8(C25 H27 Cl Fe Ir N), 2(C (H2 O), 2 (C H2 Cl2), 8 H2 Cl2), H2 O | (C25 H27 Cl Fe Ir N) |
| Sum formula | C202 H222 Cl12 Fe8 Ir8 N8 O | C202 H222 Cl12 Fe8 Ir8 N8 O |
| Mr | 5187.84 | 5187.66 |
| Dx,g cm-3 | 1.886 | 1.886 |
| Z | 2 | 2 |
| Mu (mm-1) | 6.646 | 6.646 |
| F000 | 5052.0 | 5052.0 |
| F000' | 5040.22 | |
| h,k,lmax | 36,22,18 | 36,22,18 |
| Nref | 8362 | 8342 |
| Tmin,Tmax | 0.420,0.819 | 0.386,0.568 |
| Tmin' | 0.176 | |

Correction method= # Reported T Limits: Tmin=0.386 Tmax=0.568
AbsCorr = MULTI-SCAN

Data completeness= 0.998              Theta(max)= 25.345

R(reflections)= 0.0303( 6736)                      wR2(reflections)= 0.0811( 8342)

S = 1.029                    Npar= 552

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.

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### 🟠 Alert level B
```
PLAT213_ALERT_2_B Atom C122              has ADP max/min Ratio .....      4.3 prolat
PLAT220_ALERT_2_B NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range      6.2 Ratio
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O1W      --H1W      .   Please Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).      18 Note
             0  2  0,   1  1  0,   2  0  0,   2  2  0,   3  1  0,   4  0  0,
            -3  1  1,  -2  2  1,  -1  1  1,   0  2  1,   1  1  1,   2  2  1,
             3  1  1,  -2  0  2,  -1  1  2,   0  0  2,   1  1  2,   2  0  2,
```

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### 🟡 Alert level C
```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ    Please Check
            Calc: 8(C25 H27 Cl Fe Ir N), 2(C H2 Cl2), H2 O
            Rep.: (H2 O), 2 (C H2 Cl2), 8 (C25 H27 Cl Fe Ir N)
PLAT213_ALERT_2_C Atom C112              has ADP max/min Ratio .....      3.8 prolat
PLAT213_ALERT_2_C Atom C121              has ADP max/min Ratio .....      3.5 prolat
PLAT213_ALERT_2_C Atom C123              has ADP max/min Ratio .....      3.4 prolat
PLAT213_ALERT_2_C Atom C125              has ADP max/min Ratio .....      3.3 prolat
PLAT222_ALERT_3_C NonSolvent Resd 1   H   Uiso(max)/Uiso(min) Range      6.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C111     --C112     .    0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C112     --C113     .    0.19 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C112 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     Ir1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of     Fe1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C120 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    1)      2.4 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl1M    0.180 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00986 Ang.
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on        Ir1     1.15 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H12D      .    -0.35 eA-3
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### ⚪ Alert level G
```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       2 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT   Unusually Large   65.61 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H1M1        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1M2        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1W         Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1W         Constrained at     0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)    100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)    0.75 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for     C101 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range in Main Residue for     C201 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       2 Note
            H1M1     H1M2
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (II)     .     2.10 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (II)     .     2.09 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600        2 Note
```

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PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....      2 Note
                4  0  0,    2  0  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     3.6 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged    Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........    2.29 Note
                Predicted wR2: Based on SigI**2  3.53 or SHELX Weight  8.15
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      1 Info
```

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  21 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  11 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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# checkCIF publication errors

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### Alert level A
```
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
              Abstract of paper in English.
```

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### Alert level G
```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

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```
   2 ALERT level A = Data missing that is essential or data in wrong format
   1 ALERT level G = General alerts. Data that may be required is missing
```

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**Publication of your CIF**

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

**Validation response form**

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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**PLATON version of 13/12/2023; check.def file version of 13/12/2023**

NOMOVE FORCED

Prob = 50
Temp = 173

74 Y

PLATON-Jan 8 12:39:14 2024 — (131223)

Z 75    shelx            C 2/c         R = 0.03        RES= 0-110 X