# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) gm34b_0m_sq

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: gm34b_0m_sq

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Bond precision:   C-C = 0.0274 A          Wavelength=0.71073

Cell:             a=16.295(8)     b=12.504(5)           c=21.712(9)
                  alpha=90        beta=103.013(16)      gamma=90
Temperature:      296 K
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| | Calculated | Reported |
|---|---|---|
| Volume | 4310(3) | 4310(3) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C46 H34 F2 Ir N4, F6 P [+ solvent] | ? |
| Sum formula | C46 H34 F8 Ir N4 P [+ solvent] | C46 H34 F8 Ir N4 P |
| Mr | 1017.96 | 1017.94 |
| Dx,g cm-3 | 1.569 | 1.569 |
| Z | 4 | 4 |
| Mu (mm-1) | 3.207 | 3.206 |
| F000 | 2008.0 | 2008.0 |
| F000' | 2003.70 | |
| h,k,lmax | 19,14,25 | 19,14,25 |
| Nref | 7588 | 7473 |
| Tmin,Tmax | 0.908,0.938 | 0.454,0.745 |
| Tmin' | 0.382 | |

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Correction method= # Reported T Limits: Tmin=0.454 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.985           Theta(max)= 25.000
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R(reflections)= 0.0905( 4739)

wR2(reflections)= 0.2727( 7473)

S = 1.094 Npar= 543

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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.

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**Alert level B**

PLAT234_ALERT_4_B Large Hirshfeld Difference C27 --C28 . 0.26 Ang.

**Author Response: This is probably due to the bad crystal quality and the unefficient absorption correction (rather usual in heavy atom compound data)**

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02743 Ang.

**Author Response: This is probably due to the bad crystal quality and the unefficient absorption correction (rather usual in heavy atom compound data)**

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**Alert level C**

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.163
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.163 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.27 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for C15 --C38 . 5.1 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ir1 --N4 . 0.17 Ang.

**Author Response: This is probably due to the bad crystal quality and the unefficient absorption correction (rather usual in heavy atom compound data)**

PLAT234_ALERT_4_C Large Hirshfeld Difference N1 --C15 . 0.16 Ang.

**Author Response: This is probably due to the bad crystal quality and the unefficient absorption correction (rather usual in heavy atom compound data)**

PLAT234_ALERT_4_C Large Hirshfeld Difference N2 --C1 . 0.16 Ang.

**Author Response: This is probably due to the bad crystal quality and the unefficient absorption correction (rather usual in heavy atom compound data)**

PLAT234_ALERT_4_C Large Hirshfeld Difference C13 --C14 . 0.20 Ang.

**Author Response: This is probably due to the bad crystal quality and the unefficient absorption correction (rather usual in heavy atom compound data)**

PLAT234_ALERT_4_C Large Hirshfeld Difference C42 --C45 . 0.20 Ang.

**Author Response: This is probably due to the bad crystal quality and the unefficient absorption correction (rather usual in heavy atom compound data)**

PLAT234_ALERT_4_C Large Hirshfeld Difference P1 --F4 . 0.22 Ang.

**Author Response: This is probably due to the bad crystal quality and the unefficient absorption correction (rather usual in heavy atom compound data)**

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C19 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C27 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C43 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C44 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.4 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        P1      0.153 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C25      -C29      .       1.37 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C29      - C30      .       1.55 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      9.948 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.470 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          7 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595        109 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.20Ang From Ir1             1.65 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H19       .      -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H26       .      -0.36 eA-3
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**Alert level G**

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          1 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      11.75 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         P1 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         88 A**3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             F6 P
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         6 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
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PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         5 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  26 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 ALERT type 2 Indicator that the structure model may be wrong or deficient
  10 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   2 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* 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.

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**PLATON version of 28/11/2022; check.def file version of 28/11/2022**

**Datablock gm34b_0m_sq** - ellipsoid plot