checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 14037a

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: 14037a

Bond precision:  C-C = 0.0220 A  Wavelength=0.71073

Cell:  
\[ a = 10.0115(16) \quad b = 20.330(3) \quad c = 28.620(5) \]
\[ \alpha = 105.9143(17) \quad \beta = 94.6438(17) \quad \gamma = 90.319(2) \]
Temperature:  100 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>5581.1(16)</td>
</tr>
<tr>
<td>Space group</td>
<td>P -1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 1</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C2 H2 B22 Cl22 In0.13, 6(C6 H5 Br)</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C79.24 H67.37 B88 Br11.87</td>
</tr>
<tr>
<td>Mr</td>
<td>6957.80</td>
</tr>
<tr>
<td>Dx, g cm^-3</td>
<td>2.070</td>
</tr>
<tr>
<td>Z</td>
<td>1</td>
</tr>
<tr>
<td>Mu (mm^-1)</td>
<td>4.031</td>
</tr>
<tr>
<td>F000</td>
<td>3286.4</td>
</tr>
<tr>
<td>F000'</td>
<td>3290.77</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>12,25,35</td>
</tr>
<tr>
<td>Nref</td>
<td>22186</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.244,0.311</td>
</tr>
<tr>
<td>Tmin'</td>
<td>0.192</td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.295 Tmax=0.388 
AbsCorr = MULTI-SCAN

Data completeness= 1.332  Theta(max)= 26.095

R(reflections)= 0.0874(22942)  wr2(reflections)= 0.2560(29544)

S = 1.007  Npar= 1265
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 A

- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ................. In1 Check
- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ................. In2 Check
- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ................. In3 Check
- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ................. >In4 Check
- **PLAT307_ALERT_2_A** Isolated Metal Atom (Unusual !) ................. <In4’ Check
- **PLAT308_ALERT_2_A** Single Bonded Metal Atom (Unusual !) ............ <In5 Check

### Alert level B

- **PLAT342_ALERT_3_B** Low Bond Precision on C-C Bonds ............... 0.0220 Ang.

### Alert level C

- **RFACR01_ALERT_3_C** The value of the weighted R factor is > 0.25
  - Weighted R factor given: 0.256
  - _diff_rn_measured_fraction_theta_full Low_ ............... 0.978 Note
  - High wr2 Value (i.e. > 0.25) .............................. 0.26 Report
  - Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.2 Note
  - Large Average Phenyl C-C Dist. C1E - C6E ............... 1.42 Ang.
  - Small Average Phenyl C-C Dist. CIF - C6F ............... 1.37 Ang.
  - Long C-H (X0.96,N1.08A) C1I - H1I ........ 1.12 Ang.
  - Long C-H (X0.96,N1.08A) C1G - H1G ........ 1.12 Ang.
  - Long C-H (X0.96,N1.08A) C1H - H1H ........ 1.12 Ang.
  - Long C-H (X0.96,N1.08A) C1J - H1J ........ 1.12 Ang.
  - Large K value in the Analysis of Variance .......... 6.803 Check
  - Large K value in the Analysis of Variance .......... 2.056 Check
  - Missing # of FCF Reflection(s) Below Th(Min) ..... 5 Report
  - Missing # FCF Refl Between THmin & STh/L= 0.600 ...... 728 Report

### Alert level G

- **PLAT002_ALERT_2_G** Number of Distance or Angle Restraints on AtSite .............. 14 Note
- **PLAT003_ALERT_2_G** Number of Uiso or Uij Restained non-H Atoms .......... 136 Report
- **PLAT21_ALERT_4_G** Ratio Unique / Expected Reflections too High ........ 1.332
- **PLAT42_ALERT_1_G** Calc. and Reported MoietyFormula Strings Differ Please Check
- **PLAT45_ALERT_1_G** Calculated and Reported Z Differ by .............. 0.50 Ratio
- **PLAT68_ALERT_1_G** Reported F000 Differences from Calcd (or Missing)... Please Check
- **PLAT83_ALERT_2_G** SHELXL Second Parameter in WGHT Unusually Large. 164.00 Why ?
- **PLAT175_ALERT_4_G** The CIF-Embedded .res File Contains SAME Records 1 Report
- **PLAT301_ALERT_3_G** Main Residue Disorder ................ Percentage = 0 Note
- **PLAT302_ALERT_4_G** Anion/Solvent Disorder ................. Percentage = 16 Note
- **PLAT304_ALERT_4_G** Non-Integer Number of Atoms ( 48.13) in Resd. # 1 Check
- **PLAT304_ALERT_4_G** Non-Integer Number of Atoms ( 11.24) in Resd. # 10 Check
- **PLAT304_ALERT_4_G** Non-Integer Number of Atoms ( 0.56) in Resd. # 14 Check
- **PLAT304_ALERT_4_G** Non-Integer Number of Atoms ( 0.38) in Resd. # 15 Check
- **PLAT343_ALERT_2_G** Unusual sp? Angle Range in Main Residue for C11 Check
- **PLAT343_ALERT_2_G** Unusual sp? Angle Range in Main Residue for C1G Check
- **PLAT343_ALERT_2_G** Unusual sp? Angle Range in Main Residue for C1H Check
- **PLAT343_ALERT_2_G** Unusual sp? Angle Range in Main Residue for C1J Check
- **PLAT434_ALERT_2_G** Short Inter HL..HL Contact Br1E ...... C16H .... 3.49 Ang.
- **PLAT434_ALERT_2_G** Short Inter HL..HL Contact C1AG ...... C13G .... 3.25 Ang.
- **PLAT434_ALERT_2_G** Short Inter HL..HL Contact C11H ...... C18H .... 3.34 Ang.
- **PLAT434_ALERT_2_G** Short Inter HL..HL Contact C11I ...... C12G .... 3.24 Ang.
<table>
<thead>
<tr>
<th>ALERT code</th>
<th>Description</th>
<th>Value</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT434_ALERT_2_G</td>
<td>Short Inter HL..HL Contact C11J .. C15G ..</td>
<td>3.38 Ang.</td>
<td></td>
</tr>
<tr>
<td>PLAT434_ALERT_2_G</td>
<td>Short Inter HL..HL Contact C13I .. C14H ..</td>
<td>3.23 Ang.</td>
<td></td>
</tr>
<tr>
<td>PLAT434_ALERT_2_G</td>
<td>Short Inter HL..HL Contact C14I .. C17J ..</td>
<td>3.37 Ang.</td>
<td></td>
</tr>
<tr>
<td>PLAT434_ALERT_2_G</td>
<td>Short Inter HL..HL Contact C15J .. C16I ..</td>
<td>3.25 Ang.</td>
<td></td>
</tr>
<tr>
<td>PLAT720_ALERT_4_G</td>
<td>Number of Unusual/Non-Standard Labels ..............................................</td>
<td>13 Note</td>
<td></td>
</tr>
<tr>
<td>PLAT780_ALERT_1_G</td>
<td>Coordinates do not Form a Properly Connected Set ................................</td>
<td>Please Do !</td>
<td></td>
</tr>
<tr>
<td>PLAT794_ALERT_5_G</td>
<td>Tentative Bond Valency for In3 (I) ......</td>
<td>0.46 Note</td>
<td></td>
</tr>
<tr>
<td>PLAT860_ALERT_3_G</td>
<td>Number of Least-Squares Restraints ..................................................</td>
<td>658 Note</td>
<td></td>
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<tr>
<td>PLAT870_ALERT_4_G</td>
<td>ALERTS Related to Twinning Effects Suppressed .....................................</td>
<td></td>
<td>Info</td>
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<tr>
<td>PLAT912_ALERT_4_G</td>
<td>Missing # of FCF Reflections Above Sth/L= 0.600 ..................................</td>
<td>1517 Note</td>
<td></td>
</tr>
<tr>
<td>PLAT931_ALERT_5_G</td>
<td>Found Twin Law ( [ 2 1 0] Estimated BASF .........................................</td>
<td>0.39 Check</td>
<td></td>
</tr>
<tr>
<td>PLAT994_ALERT_5_G</td>
<td>Found Twin Law ( 0 8 -3) [ ] Estimated BASF .......................................</td>
<td>0.37 Check</td>
<td></td>
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<tr>
<td>PLAT954_ALERT_1_G</td>
<td>Reported (CIF) and Actual (FCF) Kmax Differ by . ................................</td>
<td>1 Units</td>
<td></td>
</tr>
<tr>
<td>PLAT957_ALERT_1_G</td>
<td>Calculated (ThMax) and Actual (FCF) Kmax Differ . ................................</td>
<td>2 Units</td>
<td></td>
</tr>
</tbody>
</table>

### ALERT level A
- Most likely a serious problem - resolve or explain

### ALERT level B
- A potentially serious problem, consider carefully

### ALERT level C
- Check. Ensure it is not caused by an omission or oversight

### ALERT level G
- General information/check it is not something unexpected

### ALERT type 1
- CIF construction/syntax error, inconsistent or missing data

### ALERT type 2
- Indicator that the structure model may be wrong or deficient

### ALERT type 3
- Indicator that the structure quality may be low

### ALERT type 4
- Improvement, methodology, query or suggestion

### 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*, 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 21/06/2015; check.def file version of 21/06/2015**