checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.  CIF dictionary  Interpreting this report

Datablock: b

Bond precision:  C-C = 0.0082 Å  Wavelength=0.71073 Å

Cell:
  a=7.6102(13)  b=17.572(3)  c=12.245(2)
  alpha=90  beta=96.947(2)  gamma=90

Temperature: 296 K

Volume  Calculated  Reported
        1625.5(5)  1625.5(5)
Space group  P 21/c  P2(1)/c
Hall group  -P 2ybc  ?
Moiety formula  C20 H15 Cl Fe N2  ?
Sum formula  C20 H15 Cl Fe N2  C20 H15 Cl Fe N2
Mr  374.64  374.64
Dx, g cm\(^{-3}\)  1.531  1.531
Z  4  4
Mu (mm\(^{-1}\))  1.094  1.094
F000  768.0  768.0
F000’  770.16  ?

h,k,lmax  9,21,14  9,21,14
Nref  3025  3019
Tmin,Tmax  0.709,0.786  0.701,0.795
Tmin’  0.675  ?

Correction method= MULTI-SCAN

Data completeness= 0.998  Theta(max)= 25.500
R(reflections)= 0.0557( 2689)  wr2(reflections)= 0.1866( 3019)
S = 1.054  Npar= 217

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

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Alert message</th>
<th>Alert level</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT094_ALERT_2_C</td>
<td>Ratio of Maximum / Minimum Residual Density</td>
<td>C</td>
<td>3.93</td>
</tr>
<tr>
<td>PLAT241_ALERT_2_C</td>
<td>Check High Ueq as Compared to Neighbors for C8</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT242_ALERT_2_C</td>
<td>Check Low Ueq as Compared to Neighbors for Fe1</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT341_ALERT_3_C</td>
<td>Low Bond Precision on C-C Bonds</td>
<td>C</td>
<td>0.0082 Å</td>
</tr>
</tbody>
</table>
Alert level G

PLAT005_ALERT_5_G  No _iucr_refine_instructions_details  in the CIF

PLAT083_ALERT_2_G  SHELXL Second Parameter in WGHT Unusually Large.  5.12

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

0  ALERT type 1  CIF construction/syntax error, inconsistent or missing data
4  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
0  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, 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.

PLATON version of 05/11/2012; check.def file version of 05/11/2012