checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 13018

No syntax errors found.  CIF dictionary  Interpreting this report

Datablock: 13018

Bond precision:  C-C = 0.0053 Å  Wavelength=0.7107 Å

Cell:  
a=9.5563(4)  b=9.6307(4)  c=12.6223(5)

alpha=83.241(2)  beta=74.191(2)  gamma=76.385(3)

Temperature:  100 K

Calculated  Reported

Volume  1084.55(8)  1084.55(8)

Space group  P -1  P -1

Hall group  -P 1  -P 1

Moiety formula  C50 H36 F3 N5 O7 Ru  C50 H36 F3 N5 O7 Ru

Sum formula  C50 H36 F3 N5 O7 Ru  C50 H36 F3 N5 O7 Ru

Mr  976.91  976.91

Dx, g cm\(^{-3}\)  1.496  1.496

Z  1  1

Mu (mm\(^{-1}\))  0.435  0.435

F000  498.0  498.0

F000’  496.98

h,k,lmax  12,12,16  12,12,16

Nref  5392  5377

Tmin,Tmax  0.805,0.937  0.812,0.938

Tmin’  0.805

Correction method= MULTI-SCAN

Data completeness= 0.997  Theta(max)= 28.295

R(reflections)= 0.0691( 5330)  wR2(reflections)= 0.1928( 5377)

S = 1.084  Npar= 350

The following ALERTS were generated. Each ALERT has the format

```plaintext
  test-name_ALERT_alert-type_alert-level
```

Click on the hyperlinks for more details of the test.

**Alert level B**

Crystal system given = triclinic

PLAT230_ALERT_2_B  Hirshfeld Test Diff for  C11  --  C12  ..  7.5 su
### Alert level C

<table>
<thead>
<tr>
<th>Alert ID</th>
<th>Alert Type</th>
<th>Message Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT213_ALERT_2_C</td>
<td>Alert level C</td>
<td>Atom Ru1 has ADP max/min Ratio ...</td>
<td>3.1 prola</td>
</tr>
<tr>
<td>PLAT241_ALERT_2_C</td>
<td>Alert level C</td>
<td>Check High Ueq as Compared to Neighbors for Ru1</td>
<td></td>
</tr>
<tr>
<td>PLAT906_ALERT_3_C</td>
<td>Alert level C</td>
<td>Large K value in the Analysis of Variance ...</td>
<td>8.644</td>
</tr>
<tr>
<td>PLAT906_ALERT_3_C</td>
<td>Alert level C</td>
<td>Large K value in the Analysis of Variance ...</td>
<td>2.041</td>
</tr>
<tr>
<td>PLAT918_ALERT_3_C</td>
<td>Alert level C</td>
<td>Reflection(s) # with I(obs) much smaller I(calc)</td>
<td>1</td>
</tr>
<tr>
<td>PLAT976_ALERT_2_C</td>
<td>Alert level C</td>
<td>Negative Residual Density at 0.88Å from O1</td>
<td>-0.41 eÅ^{-3}</td>
</tr>
</tbody>
</table>

### Alert level G

<table>
<thead>
<tr>
<th>Alert ID</th>
<th>Alert Type</th>
<th>Message Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT002_ALERT_2_G</td>
<td>Alert level G</td>
<td>Number of Distance or Angle Restraints on AtSite</td>
<td>4</td>
</tr>
<tr>
<td>PLAT003_ALERT_2_G</td>
<td>Alert level G</td>
<td>Number of Uiso or Uij Restrained Atom Sites</td>
<td>26</td>
</tr>
<tr>
<td>PLAT232_ALERT_2_G</td>
<td>Alert level G</td>
<td>Hirshfeld Test Diff (M-X) Ru1 -- O4</td>
<td>20.7 su</td>
</tr>
<tr>
<td>PLAT232_ALERT_2_G</td>
<td>Alert level G</td>
<td>Hirshfeld Test Diff (M-X) Ru1 -- N3</td>
<td>32.3 su</td>
</tr>
<tr>
<td>PLAT242_ALERT_2_G</td>
<td>Alert level G</td>
<td>Check Low Ueq as Compared to Neighbors for N3</td>
<td></td>
</tr>
<tr>
<td>PLAT242_ALERT_2_G</td>
<td>Alert level G</td>
<td>Check Low Ueq as Compared to Neighbors for C25</td>
<td></td>
</tr>
<tr>
<td>PLAT242_ALERT_2_G</td>
<td>Alert level G</td>
<td>Check Low Ueq as Compared to Neighbors for C26</td>
<td></td>
</tr>
<tr>
<td>PLAT301_ALERT_3_G</td>
<td>Alert level G</td>
<td>Note: Main Residue Disorder</td>
<td>17 Perc.</td>
</tr>
<tr>
<td>PLAT811_ALERT_5_G</td>
<td>Alert level G</td>
<td>No ADDSYM Analysis: Too Many Excluded Atoms</td>
<td>!</td>
</tr>
<tr>
<td>PLAT960_ALERT_3_G</td>
<td>Alert level G</td>
<td>Note: Number of Least-Squares Restraints</td>
<td>22</td>
</tr>
<tr>
<td>PLAT912_ALERT_4_G</td>
<td>Alert level G</td>
<td>Missing # of FCF Reflections Above STh/L= 0.600</td>
<td>16</td>
</tr>
</tbody>
</table>

### Alert level A

- 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 level B

- 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 05/11/2012; check.def file version of 05/11/2012**