checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a

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: a**

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0106 Å</th>
<th>Wavelength=0.71073</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td>a=17.2026(6)</td>
<td>b=14.8535(5)</td>
</tr>
<tr>
<td></td>
<td>alpha=90</td>
<td>beta=107.334(1)</td>
</tr>
<tr>
<td>Temperature:</td>
<td>173 K</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Calculated</td>
<td>Reported</td>
</tr>
<tr>
<td>Volume</td>
<td>4289.1(2)</td>
<td>4289.1(2)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21/n</td>
<td>P 1 21/n 1</td>
</tr>
<tr>
<td>Hall group</td>
<td>-P 2yn</td>
<td>-P 2yn</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C33 H63 N15 P2 Rh2 U</td>
<td>C33 H63 N15 P2 Rh2 U</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C33 H63 N15 P2 Rh2 U</td>
<td>C33 H63 N15 P2 Rh2 U</td>
</tr>
<tr>
<td>Mr</td>
<td>1175.78</td>
<td>1175.77</td>
</tr>
<tr>
<td>Dx,g cm⁻³</td>
<td>1.821</td>
<td>1.821</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Mu (mm⁻¹)</td>
<td>4.646</td>
<td>4.645</td>
</tr>
<tr>
<td>F000</td>
<td>2312.0</td>
<td>2312.0</td>
</tr>
<tr>
<td>F000'</td>
<td>2265.87</td>
<td></td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>20,17,21</td>
<td>20,17,21</td>
</tr>
<tr>
<td>Nref</td>
<td>7848</td>
<td>7834</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.552,0.628</td>
<td>0.359,0.751</td>
</tr>
<tr>
<td>Tmin'</td>
<td>0.541</td>
<td></td>
</tr>
</tbody>
</table>

Correction method= # Reported T Limits: Tmin=0.359 Tmax=0.751
AbsCorr = NONE

Data completeness= 0.998 Theta(max)= 25.343

R(reflections)= 0.0310( 7050) wR2(reflections)= 0.0794( 7834)
S = 1.039 Npar= 487
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 level C</th>
<th>Description</th>
<th>Alert Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT057_ALERT_3_C</td>
<td>Correction for Absorption Required</td>
<td>RT(exp) ... 1.14 Do !</td>
</tr>
<tr>
<td>PLAT241_ALERT_2_C</td>
<td>High 'MainMol' Ueq as Compared to Neighbors of</td>
<td>N10 Check</td>
</tr>
<tr>
<td>PLAT241_ALERT_2_C</td>
<td>High 'MainMol' Ueq as Compared to Neighbors of</td>
<td>C21 Check</td>
</tr>
<tr>
<td>PLAT241_ALERT_2_C</td>
<td>High 'MainMol' Ueq as Compared to Neighbors of</td>
<td>C24 Check</td>
</tr>
<tr>
<td>PLAT241_ALERT_2_C</td>
<td>High 'MainMol' Ueq as Compared to Neighbors of</td>
<td>C29 Check</td>
</tr>
<tr>
<td>PLAT241_ALERT_2_C</td>
<td>High 'MainMol' Ueq as Compared to Neighbors of</td>
<td>C32 Check</td>
</tr>
<tr>
<td>PLAT242_ALERT_2_C</td>
<td>Low 'MainMol' Ueq as Compared to Neighbors of</td>
<td>U1 Check</td>
</tr>
<tr>
<td>PLAT242_ALERT_2_C</td>
<td>Low 'MainMol' Ueq as Compared to Neighbors of</td>
<td>Rh1 Check</td>
</tr>
<tr>
<td>PLAT342_ALERT_3_C</td>
<td>Low Bond Precision on C-C Bonds</td>
<td>0.01058 Ang.</td>
</tr>
<tr>
<td>PLAT360_ALERT_2_C</td>
<td>Short C(sp3)-C(sp3) Bond</td>
<td>C28 - C29 . 1.43 Ang.</td>
</tr>
<tr>
<td>PLAT360_ALERT_2_C</td>
<td>Short C(sp3)-C(sp3) Bond</td>
<td>C32 - C33 . 1.43 Ang.</td>
</tr>
<tr>
<td>PLAT911_ALERT_3_C</td>
<td>Missing FCF Refl Between Tmin &amp; STh/L= 0.600</td>
<td>9 Report</td>
</tr>
<tr>
<td>PLAT977_ALERT_2_C</td>
<td>Check Negative Difference Density on H20B</td>
<td>-0.32 eA-3</td>
</tr>
<tr>
<td>PLAT977_ALERT_2_C</td>
<td>Check Negative Difference Density on H32A</td>
<td>-0.36 eA-3</td>
</tr>
</tbody>
</table>

**Alert level G**

<table>
<thead>
<tr>
<th>ALERT level G</th>
<th>Description</th>
<th>Alert Level</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT003_ALERT_2_G</td>
<td>Number of Ulso or Uij Restrained non-H Atoms ...</td>
<td>20 Report</td>
</tr>
<tr>
<td>PLAT012_ALERT_1_G</td>
<td>No _shelx_res_checksum Found in CIF ...</td>
<td>Please Check</td>
</tr>
<tr>
<td>PLAT178_ALERT_4_G</td>
<td>The CIF-Embedded .res File Contains SIMU Records</td>
<td>13.72 Why ?</td>
</tr>
<tr>
<td>PLAT232_ALERT_2_G</td>
<td>Hirshfeld Test Diff (M-X) U1 --N4 . 8.5 s.u.</td>
<td>5 Report</td>
</tr>
<tr>
<td>PLAT232_ALERT_2_G</td>
<td>Hirshfeld Test Diff (M-X) U1 --N7 . 9.5 s.u.</td>
<td></td>
</tr>
<tr>
<td>PLAT232_ALERT_2_G</td>
<td>Hirshfeld Test Diff (M-X) Rh1 --N4 . 5.5 s.u.</td>
<td></td>
</tr>
<tr>
<td>PLAT794_ALERT_5_G</td>
<td>Tentative Bond Valency for U1 (IV) . 3.88 Info</td>
<td></td>
</tr>
<tr>
<td>PLAT860_ALERT_3_G</td>
<td>Number of Least-Squares Restraints ...</td>
<td>96 Note</td>
</tr>
<tr>
<td>PLAT912_ALERT_4_G</td>
<td>Missing # of FCF Reflections Above STh/L= 0.600</td>
<td>6 Note</td>
</tr>
<tr>
<td>PLAT913_ALERT_3_G</td>
<td>Missing # of Very Strong Reflections in FCF ...</td>
<td>2 Note</td>
</tr>
<tr>
<td>PLAT978_ALERT_2_G</td>
<td>Number C-C Bonds with Positive Residual Density.</td>
<td>0 Info</td>
</tr>
</tbody>
</table>

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
15 ALERT level C = Check. Ensure it is not caused by an omission or oversight
12 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
5 ALERT type 3 Indicator that the structure quality may be low
2 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* 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 18/12/2021; check.def file version of 18/12/2021**