### checkCIF/PLATON report

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

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.  

### Datablock: DiolAmbRietveld

<table>
<thead>
<tr>
<th>Bond precision:</th>
<th>C-C = 0.0019 Å</th>
<th>Wavelength=1.54056</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell:</td>
<td>a=11.9118(6)</td>
<td>b=11.9118(6)</td>
</tr>
<tr>
<td></td>
<td>c=10.9590(7)</td>
<td>alpha=90</td>
</tr>
<tr>
<td></td>
<td>beta=90</td>
<td>gamma=120</td>
</tr>
<tr>
<td>Temperature:</td>
<td>294 K</td>
<td></td>
</tr>
</tbody>
</table>

| Volume          | 1346.66(19)    | 1346.66(13)       |
| Space group     | P 6 3/m c m    | P 6 3/m c m      |
| Hall group      | -P 6c 2        | -P 6c 2          |
| Moiety formula  | C10 H16 O2     | C10 H16 O2       |
| Sum formula     | C10 H16 O2     | C10 H16 O2       |
| Mr              | 168.23         | 168.23            |
| Dx, g cm^{-3}   | 1.245          | 1.245             |
| Z               | 6              | 6                 |
| Mu (mm^{-1})    | 0.676          | 0.000             |
| F000            | 552.0          | 0.0               |
| F000’           | 553.62         |                   |
| h, k, l max     |                |                   |
| Nref            |                |                   |
| Tmin, Tmax      |                |                   |
| Tmin’           |                |                   |

Correction method= Not given

Data completeness=  

Theta(max)=

R(reflections)=  

wR2(reflections)=

S = Npar=

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**

**ATOM007_ALERT_1_A**  
_atom_site_aniso_label is missing  
Unique label identifying the atom site.

**PLAT029_ALERT_3_A**  
_diffrn_measured_fraction_theta_full value Low .  0.000 Why?

**PLAT183_ALERT_1_A**  
Missing _cell_measurement_reflns_used Value ....  Please Do!

**PLAT880_ALERT_1_A**  
N0 datum for _diffrn_reflns_number ..............  Please Do!

**PLAT881_ALERT_1_A**  
No Datum for _diffrn_reflns_av_R_equivalents ...  Please Do!

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**Alert level B**

**PLAT201_ALERT_2_B**  
Isotropic non-H Atoms in Main Residue(s) .......  6 Report

01  C1  C2  C3  C4  C5

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**Alert level C**

**PLAT162_ALERT_4_C**  
Missing or Zero s.u. (esd) on y-coordinate for .  C2 Check

**PLAT163_ALERT_4_C**  
Missing or Zero s.u. (esd) on z-coordinate for .  C2 Check

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**Alert level G**

**PLAT005_ALERT_5_G**  
No Embedded Refinement Details Found in the CIF  Please Do!

**PLAT152_ALERT_1_G**  
The Supplied and Calc. Volume s.u. Differ by ...  6 Units

**PLAT300_ALERT_4_G**  
Atom Site Occupancy of H1 Constrained at 0.5 Check

**PLAT882_ALERT_5_G**  
No Parseable SHELXL Style Weighting Scheme Found Please Check

**PLAT883_ALERT_1_G**  
No Info/Value for _atom_sites_solution_primary .  Please Do!

**PLAT980_ALERT_1_G**  
No Anomalous Scattering Factors Found in CIF ... Please Check

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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 17/03/2019; check.def file version of 04/03/2019**