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.  
[CIF dictionary]  [Interpreting this report]

Datablock: R28

Bond precision:  C-C = 0.0036 Å  Wavelength=0.7107Å

Cell:  
a=10.9779(7)  b=5.7869(5)  c=12.1402(10)  
alpha=90  beta=92.349(4)  gamma=90  
Temperature:  100 K

<table>
<thead>
<tr>
<th>Calculated</th>
<th>Reported</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>770.60(10)</td>
</tr>
<tr>
<td>Space group</td>
<td>P 21</td>
</tr>
<tr>
<td>Hall group</td>
<td>P 2yb</td>
</tr>
<tr>
<td>Moiety formula</td>
<td>C14 H19 N O5 S</td>
</tr>
<tr>
<td>Sum formula</td>
<td>C14 H19 N O5 S</td>
</tr>
<tr>
<td>Mr</td>
<td>313.37</td>
</tr>
<tr>
<td>Dx, g cm-3</td>
<td>1.351</td>
</tr>
<tr>
<td>Z</td>
<td>2</td>
</tr>
<tr>
<td>Mu (mm-1)</td>
<td>0.230</td>
</tr>
<tr>
<td>F000</td>
<td>332.0</td>
</tr>
<tr>
<td>F000’</td>
<td>332.42</td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>13,7,15</td>
</tr>
<tr>
<td>Nref</td>
<td>3179[1752]</td>
</tr>
<tr>
<td>Tmin,Tmax</td>
<td>0.962,0.982</td>
</tr>
<tr>
<td>Tmin’</td>
<td>0.921</td>
</tr>
</tbody>
</table>

Correction method= MULTI-SCAN

Data completeness= 1.80/0.99  Theta(max)= 26.441

R(reflections)= 0.0325(2970)  wR2(reflections)= 0.0695(3156)

S = 1.014  Npar= Npar = 196

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

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.6 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 5.3 Ratio

Alert level G

PLAT791_ALERT_4_G The Model has Chirality at C1 ............... R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............... 2 Note

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
2 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
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: R35

Bond precision: C-C = 0.0062 A Wavelength=0.71070

Cell: a=5.7297(3) b=16.2240(9) c=17.5243(9)
    alpha=90 beta=90 gamma=90
Temperature: 100 K

Calculated                              Reported
Volume       1629.04(15)                  1629.04(15)
Space group  P 21 21 21                  P 21 21 21
Hall group   P 2ac 2ab                    P 2ac 2ab
Moiety formula C14 H18 N4 O5 S          C14 H18 N4 O5 S1
Sum formula  C14 H18 N4 O5 S             C14 H18 N4 O5 S
Mr           354.39                       354.38
Dx,g cm-3    1.445                        1.445
Z             4                            4
Mu (mm-1)    0.232                        0.232
F000         744.0                        744.0
F000’        744.85
h,k,lmax     7,20,21                      7,20,21
Nref         3362[1963]                   3347
Tmin,Tmax    0.989,0.991                  0.808,0.970
Tmin’        0.939

Correction method= MULTI-SCAN

Data completeness= 1.71/1.00            Theta(max)= 26.462
R(reflections) = 0.0465 (2496) \hspace{1cm} \text{wr}^2(\text{reflections}) = 0.1098 (3347)

S = 0.854 \hspace{1cm} \text{Npar} = 223

The following ALERTS were generated. Each ALERT has the format
\text{test-name_ALERT_alert-type_alert-level}.
Click on the hyperlinks for more details of the test.

\begin{itemize}
  \item \textbf{Alert level C}
  \begin{itemize}
    \item \text{PLAT340_ALERT_3_C} \hspace{1cm} \text{Low Bond Precision on C-C Bonds ...............} \hspace{1cm} 0.0062 \text{ Ang.}
  \end{itemize}

  \item \textbf{Alert level G}
  \begin{itemize}
    \item \text{PLAT791_ALERT_4_G} \hspace{1cm} \text{The Model has Chirality at C1 .............} \hspace{1cm} R \hspace{1cm} \text{Verify}
    \item \text{PLAT860_ALERT_3_G} \hspace{1cm} \text{Number of Least-Squares Restraints .............} \hspace{1cm} 4 \hspace{1cm} \text{Note}
  \end{itemize}

\end{itemize}

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
1 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
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

checkCIF publication errors

\begin{itemize}
  \item \textbf{Alert level A}
  \begin{itemize}
    \item \text{PUBL006_ALERT_1_A} \_publ_requested_journal is missing
      \begin{itemize}
        \item e.g. 'Acta Crystallographica Section C'
      \end{itemize}
    \item \text{PUBL008_ALERT_1_A} \_publ_section_title is missing. Title of paper.
    \item \text{PUBL009_ALERT_1_A} \_publ_author_name is missing. List of author(s) name(s).
    \item \text{PUBL010_ALERT_1_A} \_publ_author_address is missing. Author(s) address(es).
    \item \text{PUBL012_ALERT_1_A} \_publ_section_abstract is missing.
      \begin{itemize}
        \item Abstract of paper in English.
      \end{itemize}
  \end{itemize}

  \item \textbf{Alert level G}
  \begin{itemize}
    \item \text{PUBL017_ALERT_1_G} The \_publ_section_references section is missing or empty.
  \end{itemize}

\end{itemize}

5 ALERT level A = Data missing that is essential or data in wrong format
1 ALERT level G = General alerts. Data that may be required is missing
Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

# start Validation Reply Form
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via[the web]. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic[submission] or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 05/02/2014; check.def file version of 05/02/2014