checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 13137a_sq

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: 13137a_sq

Bond precision:  C-C = 0.0059 Å  Wavelength=0.7107 Å

Cell:  
a=17.0675(10)  b=8.6294(5)  c=27.5407(17)  
alpha=90  beta=106.231(2)  gamma=90

Temperature:  100 K

Calculated  Reported

Volume  3894.6(4)  3894.6(4)
Space group  \text{P 21/n}  \text{P 21/n}
Hall group  \text{-P 2yn}  \text{-P 2yn}
Moiety formula  \text{C35 H30 Cu N10 O3, F6 Sb, F H}  \text{C35 H30 Cu N10 O3, F6 Sb, F H}
Sum formula  \text{C35 H31 Cu F7 N10 O3 Sb}  \text{C35 H31 Cu F7 N10 O3 Sb}
Mr  958.01  957.99
Dx, g cm\(^{-3}\)  1.634  1.634
Z  4  4
Mu (mm\(^{-1}\))  1.322  1.322
\text{F000}  1912.0  1912.0
\text{F000'}  1911.86  1911.86
h, k, l max  22, 11, 36  22, 11, 36
Nref  9709  9696
Tmin, Tmax  0.690, 0.809  0.594, 0.816
Tmin'  0.553

Correction method= # Reported T Limits: Tmin=0.594 Tmax=0.816
AbsCorr = MULTI-SCAN

Data completeness= 0.999  Theta(max) = 28.319

R(reflections)= 0.0616( 8173)  wR2(reflections)= 0.1605( 9696)

S = 0.993  Npar= 526
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.

### Alert level C

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT244_ALERT_4_C</td>
<td>Low ‘Solvent’ Ueq as Compared to Neighbors of Sb1 Check</td>
<td></td>
</tr>
<tr>
<td>PLAT431_ALERT_2_C</td>
<td>Short Inter HL..A Contact F1E .. N1B .. 2.90 Ang.</td>
<td></td>
</tr>
<tr>
<td>PLAT480_ALERT_4_C</td>
<td>Long H...A H-Bond Reported H10C .. N1D .. 2.68 Ang.</td>
<td></td>
</tr>
<tr>
<td>PLAT906_ALERT_3_C</td>
<td>Large K value in the Analysis of Variance ...... 3.974 Check</td>
<td></td>
</tr>
<tr>
<td>PLAT911_ALERT_3_C</td>
<td>Missing # FCF Refl Between THmin &amp; STh/L= 0.600 9 Report</td>
<td></td>
</tr>
</tbody>
</table>

### Alert level G

<table>
<thead>
<tr>
<th>ALERT</th>
<th>Description</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT002_ALERT_2_G</td>
<td>Number of Distance or Angle Restraints on AtSite 2 Note</td>
<td></td>
</tr>
<tr>
<td>PLAT003_ALERT_2_G</td>
<td>Number of Uiso or Uij Restrained non-H Atoms ... 7 Report</td>
<td></td>
</tr>
<tr>
<td>PLAT083_ALERT_2_G</td>
<td>SHEXL Second Parameter in WGHT Unusually Large. 21.00 Why ?</td>
<td></td>
</tr>
<tr>
<td>PLAT233_ALERT_4_G</td>
<td>Hirshfeld (M-X Solvent) Sb1 -- F4 .. 8.5 su</td>
<td></td>
</tr>
<tr>
<td>PLAT233_ALERT_4_G</td>
<td>Hirshfeld (M-X Solvent) Sb1 -- F6 .. 10.5 su</td>
<td></td>
</tr>
<tr>
<td>PLAT605_ALERT_4_G</td>
<td>Structure Contains Solvent Accessible VOIDS of . 156 A**3</td>
<td></td>
</tr>
<tr>
<td>PLAT720_ALERT_4_G</td>
<td>Number of Unusual/Non-Standard Labels .......... 6 Note</td>
<td></td>
</tr>
<tr>
<td>PLAT860_ALERT_3_G</td>
<td>Number of Least-Squares Restraints ............. 76 Note</td>
<td></td>
</tr>
<tr>
<td>PLAT869_ALERT_4_G</td>
<td>ALERTS Related to the use of SQUEEZE Suppressed ! Info</td>
<td></td>
</tr>
<tr>
<td>PLAT912_ALERT_4_G</td>
<td>Missing # of FCF Reflections Above STh/L= 0.600 5 Note</td>
<td></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
5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
10 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
3 ALERT type 3 Indicator that the structure quality may be low
8 ALERT type 4 Improvement, methodology, query or suggestion
0 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 21/06/2015; check.def file version of 21/06/2015**