checkCIF/PLATON report

Structure factors have been supplied for datablock(s) t

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: t

Bond precision: C-C = 0.0200 Å Wavelength=0.71073

Cell: a=4.65600 b=23.27500 c=23.28100
alpha=108.4000 beta=91.13000 gamma=91.1000
Temperature: 293 K

Calculated Reported
Volume 2392.617 2393
Space group P -1 ?
Hall group -P 1 ?
Moiety formula C16 H11 N O2 ?
Sum formula C16 H11 N O2 C24 H0.50 N24 O24
Mr 249.26 1008.98
Dx,g cm-3 1.384 1.401
Z 8 2
Mu (mm-1) 0.092 0.128
F000 1040.0 1009.0
F000’ 1040.48
h,k,lmax 6,30,30 6,30,30
Nref 11077 10872
Tmin,Tmax
Tmin’

Correction method= Not given

Data completeness= 0.981 Theta(max)= 27.620

R(reflections)= 0.1036( 2176) wR2(reflections)= 0.4083( 10872)

S = 0.857 Npar= 305

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

**SYM001_ALERT_1_A** _symmetry_cell_setting is missing_

The cell setting should be one of the following:
* triclinic
* monoclinic
* orthorhombic
* tetragonal
* rhombohedral
* trigonal
* hexagonal
* cubic

The following tests will not be performed.
SYMMS_01, SYMMS_02

**EXPT005_ALERT_1_A** _exptl_crystal_description is missing_

Crystal habit description.
The following tests will not be performed.
CrysR_01

**DIFF003_ALERT_1_A** _diffrn_measurement_device_type is missing_

Diffractometer make and type. Replaces _diffrn_measurement_type.

**ATOM007_ALERT_1_A** _atom_site_aniso_label is missing_

Unique label identifying the atom site.

**PLAT026_ALERT_3_A** Ratio Observed / Unique Reflections (too) Low .. 20 %
**PLAT051_ALERT_1_A** Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by 28.04 %
**PLAT122_ALERT_1_A** No _symmetry_space_group_name_H-M Given ......... Please Do !
**PLAT183_ALERT_1_A** Missing _cell_measurement_reflns_used value .... Please Do !
**PLAT184_ALERT_1_A** Missing _cell_measurement_theta_min value .... Please Do !
**PLAT185_ALERT_1_A** Missing _cell_measurement_theta_max value .... Please Do !
**PLAT201_ALERT_2_A** Isotropic non-H Atoms in Main Residue(s) ........ 76 Report
**PLAT902_ALERT_1_A** No (Interpretable) Reflections found in FCF .... Please Check

Alert level B

**PLAT043_ALERT_1_B** Calculated and Reported Mol. Weight Differ by .. 2.99 Check
**PLAT084_ALERT_3_B** High wR2 Value (i.e. > 0.25) .................. 0.41 Report
**PLAT097_ALERT_2_B** Large Reported Max. (Positive) Residual Density 0.81 eA-3
**PLAT110_ALERT_2_B** ADDSYM Detects Potential Lattice Translation ... ? Check
**PLAT112_ALERT_2_B** ADDSYM Detects New (Pseudo) Symm. Elem. A 100 %Fit
**PLAT112_ALERT_2_B** ADDSYM Detects New (Pseudo) Symm. Elem. d 100 %Fit
**PLAT113_ALERT_2_B** ADDSYM Suggests Possible Pseudo/New Space Group P21/c Check

Note: (Pseudo) Lattice Translation Implemented
**PLAT241_ALERT_2_B** High ‘MainMol’ Ueq as Compared to Neighbors of 05 Check
**PLAT340_ALERT_3_B** Low Bond Precision on C-C Bonds .............. 0.01998 Ang.

Alert level C

**DIFMN02_ALERT_2_C** The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -0.655
Test value = -0.600

**DIFMN03_ALERT_1_C** The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

**DIFMX02_ALERT_1_C** The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

**RINTA01_ALERT_3_C** The value of Rint is greater than 0.12
Rint given 0.161
**PLAT20_ALERT_3_C** The value of Rint is greater than 0.12 ........ 0.161 Report
**PLAT041_ALERT_1_C** Calc. and Reported SumFormula Strings Differ Please Check
**PLAT052_ALERT_1_C** Info on Absorption Correction Method Not Given Please Do !
**PLAT053_ALERT_1_C** Minimum Crystal Dimension Missing (or Error) ... Please Check
**PLAT054_ALERT_1_C** Medium Crystal Dimension Missing (or Error) ... Please Check
**PLAT055_ALERT_1_C** Maximum Crystal Dimension Missing (or Error) ... Please Check
**PLAT068_ALERT_1_C** Reported F000 Differs from Calcd (or Missing)... Please Check
<table>
<thead>
<tr>
<th>Alert</th>
<th>Description</th>
<th>Level</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>PLAT098_ALERT_2_C</td>
<td>Large Reported Min. (Negative) Residual Density</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT141_ALERT_4_C</td>
<td>s.u. on a - Axis Small or Missing</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT142_ALERT_4_C</td>
<td>s.u. on b - Axis Small or Missing</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT143_ALERT_4_C</td>
<td>s.u. on c - Axis Small or Missing</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT144_ALERT_4_C</td>
<td>s.u. on alpha Small or Missing</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT145_ALERT_4_C</td>
<td>s.u. on beta Small or Missing</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT146_ALERT_4_C</td>
<td>s.u. on gamma Small or Missing</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT151_ALERT_1_C</td>
<td>No s.u. (esd) Given on Volume</td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>PLAT241_ALERT_2_C</td>
<td>High ‘MainMol’ Ueq as Compared to Neighbors of O8</td>
<td>C</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT242_ALERT_2_C</td>
<td>Low ‘MainMol’ Ueq as Compared to Neighbors of N3</td>
<td>C</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT242_ALERT_2_C</td>
<td>Low ‘MainMol’ Ueq as Compared to Neighbors of C25</td>
<td>C</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT242_ALERT_2_C</td>
<td>Low ‘MainMol’ Ueq as Compared to Neighbors of N4</td>
<td>C</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT242_ALERT_2_C</td>
<td>Low ‘MainMol’ Ueq as Compared to Neighbors of C8</td>
<td>C</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT790_ALERT_4_C</td>
<td>Centre of Gravity not Within Unit Cell: Resd. # 1</td>
<td>C</td>
<td>Note</td>
</tr>
</tbody>
</table>

**Alert level G**

<table>
<thead>
<tr>
<th>Alert</th>
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<th>Level</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>FORMU01_ALERT_2_G</td>
<td>There is a discrepancy between the atom counts in the _chemical_formula_sum and the formula from the _atom_site* data.</td>
<td>G</td>
<td></td>
</tr>
<tr>
<td>PLAT005_ALERT_5_G</td>
<td>No Embedded Refinement Details found in the CIF</td>
<td>G</td>
<td>Please Do !</td>
</tr>
<tr>
<td>PLAT045_ALERT_1_G</td>
<td>Calculated and Reported Z Differ by a Factor 4.00</td>
<td>G</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT072_ALERT_2_G</td>
<td>SHELXL First Parameter in WGHT Unusually Large 0.16</td>
<td>G</td>
<td>Report</td>
</tr>
<tr>
<td>PLAT093_ALERT_1_G</td>
<td>No s.u.’s on H-positions, Refinement Reported as mixed</td>
<td>G</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT104_ALERT_1_G</td>
<td>The Reported Crystal System is Inconsistent with P-1</td>
<td>G</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT154_ALERT_1_G</td>
<td>The s.u.’s on the Cell Angles are Equal ..(Note) 0. Degree</td>
<td>G</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT199_ALERT_1_G</td>
<td>Reported _cell_measurement_temperature ..... (K) 293</td>
<td>G</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT200_ALERT_1_G</td>
<td>Reported _diffrn_ambient_temperature ..... (K) 293</td>
<td>G</td>
<td>Check</td>
</tr>
<tr>
<td>PLAT790_ALERT_4_G</td>
<td>Centre of Gravity not Within Unit Cell: Resd. # 2</td>
<td>C</td>
<td>Note</td>
</tr>
<tr>
<td>PLAT790_ALERT_4_G</td>
<td>Centre of Gravity not Within Unit Cell: Resd. # 3</td>
<td>C</td>
<td>Note</td>
</tr>
<tr>
<td>PLAT790_ALERT_4_G</td>
<td>Centre of Gravity not Within Unit Cell: Resd. # 4</td>
<td>C</td>
<td>Note</td>
</tr>
<tr>
<td>PLAT899_ALERT_4_G</td>
<td>SHELXL97 is Deprecated and Succeeded by SHELXL 2014</td>
<td>C</td>
<td>Note</td>
</tr>
</tbody>
</table>

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

26 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 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
11 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 11/08/2016; check.def file version of 04/08/2016