

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1530

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: 1530

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|                 |                     |                                |
|-----------------|---------------------|--------------------------------|
| Bond precision: | C-C = 0.0086 Å      | Wavelength=0.71073             |
| Cell:           | a=9.6006(6)         | b=14.2054(8)      c=13.3890(8) |
|                 | alpha=90            | beta=91.537(6)      gamma=90   |
| Temperature:    | 173 K               |                                |
|                 | Calculated          | Reported                       |
| Volume          | 1825.34(19)         | 1825.34(19)                    |
| Space group     | P 21                | P 21                           |
| Hall group      | P 2yb               | P 2yb                          |
| Moiety formula  | C17 H22 N Si, Cl O4 | C22 H24 N Si, C H4 O, Cl       |
| Sum formula     | C17 H22 Cl N O4 Si  | C17 H22 Cl N O4 Si             |
| Mr              | 367.90              | 367.90                         |
| Dx,g cm-3       | 1.339               | 1.339                          |
| Z               | 4                   | 4                              |
| Mu (mm-1)       | 0.295               | 0.295                          |
| F000            | 776.0               | 776.0                          |
| F000'           | 777.24              |                                |
| h,k,lmax        | 11,17,16            | 11,17,16                       |
| Nref            | 7181[ 3744]         | 7177                           |
| Tmin,Tmax       | 0.943,0.971         | 0.943,0.971                    |
| Tmin'           | 0.943               |                                |

Correction method= # Reported T Limits: Tmin=0.943 Tmax=0.971  
AbsCorr = MULTI-SCAN

Data completeness= 1.92/1.00      Theta(max)= 26.000

R(reflections)= 0.0596( 5069)      wR2(reflections)= 0.1745( 7177)

S = 1.000      Npar= 435

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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.

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### Alert level B

PLAT934\_ALERT\_3\_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 2 Check

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### Alert level C

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C28 -- C29 .. 6.0 s.u.  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0086 Ang.  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 2.241 Check  
PLAT978\_ALERT\_2\_C Number C-C Bonds with Positive Residual Density. 0 Info

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### Alert level G

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C17 H22 Cl1 N1 O4 Si1  
Atom count from \_chemical\_formula\_moiety:C23 H28 Cl1 N1 O1 Si1  
PLAT005\_ALERT\_5\_G No Embedded Refinement Details found in the CIF Please Do !  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 Report  
PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report  
PLAT244\_ALERT\_4\_G Low 'Solvent' Ueq as Compared to Neighbors of Cl1 Check  
PLAT244\_ALERT\_4\_G Low 'Solvent' Ueq as Compared to Neighbors of Cl2 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O2 .. C15 .. 3.02 Ang.  
PLAT791\_ALERT\_4\_G The Model has Chirality at C14 (Chiral SPGR) S Verify  
PLAT791\_ALERT\_4\_G The Model has Chirality at C31 (Chiral SPGR) S Verify  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
4 **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

3 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  
4 ALERT type 3 Indicator that the structure quality may be low  
4 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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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.

