checkCIF/PLATON report

Structure factors have been supplied for datablock(s) si358a_r171214_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: si358a_r171214_sq

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Bond precision:   C-C = 0.0017 A              Wavelength=0.71073

Cell:          a=11.4093(11)      b=15.6821(15)      c=19.5623(19)
               alpha=84.802(1)    beta=75.911(1)   gamma=71.975(1)
Temperature:   173 K

                 Calculated                 Reported
Volume           3227.8(5)                  3227.8(5)
Space group      P -1                       P -1
Hall group       -P 1                       -P 1
Moiety formula   C38 H98 Si14 [+ solvent]   ?
Sum formula      C38 H98 Si14 [+ solvent]   C38 H98 O0 Si14
Mr               948.42                     948.42
Dx,g cm-3        0.976                      0.976
Z                2                          2
Mu (mm-1)        0.300                      0.300
F000             1044.0                     1044.0
F000'            1046.40
h,k,lmax         14,20,25                   14,20,25
Nref             14828                      14622
Tmin,Tmax        0.965,0.970                0.956,0.971
Tmin'            0.956

Correction method= # Reported T Limits: Tmin=0.956 Tmax=0.971
AbsCorr = EMPIRICAL

Data completeness= 0.986        Theta(max)= 27.500

R(reflections)= 0.0266( 13006)    wR2(reflections)= 0.0759( 14622)

S = 1.039                    Npar= 500
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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.

Alert level C

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PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si1      --Si5       .        6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si4      --Si6       .        5.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si5      --C9        .        5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si8      --C15       .        5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si9      --C18       .        5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Si11     --C29       .        6.2 s.u.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        49 Report
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Alert level G

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CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
          symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C38 H98 O0 Si14
          TEST: Compare cell contents of formula and atom_site data

          atom     Z*formula  cif sites diff
          C           76.00     76.00    0.00
          H          196.00    196.00    0.00
          O            2.00      0.00    2.00
          Si          28.00     28.00    0.00
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.001 Degree
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       ! Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       155 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        12 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...        37 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         1 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   7 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

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 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.

PLATON version of 13/12/2017; check.def file version of 12/12/2017