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: I

Bond precision: C-C = 0.0087 A Wavelength=0.71073

Cell: a=13.799(7) b=14.548(8) c=16.957(9)
alpha=88.869(8) beta=80.964(7) gamma=64.328(6)
Temperature: 296 K

	Calculated	Reported
Volume	3026(3)	3026(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	6(C19 H31 N3 O4 Si), O	3(C19 H31.33 N3 O4.17 Si), 0.5(H2 O)
Sum formula	C114 H186 N18 O25 Si6	C19 H31.33 N3 O4.17 Si
Mr	2377.35	396.56
Dx,g cm-3	1.305	1.306
Z	1	6
Mu (mm-1)	0.147	0.147
F000	1280.0	1282.0
F000’	1281.01	
h,k,lmax	16,17,20	16,17,20
Nref	10811	10577
Tmin,Tmax	0.974,0.985	0.664,0.745
Tmin’	0.971	

Correction method= MULTI-SCAN

Data completeness= 0.978 Theta(max)= 25.120

R(reflections)= 0.0723(3741) wR2(reflections)= 0.1805(10577)

S = 0.915 Npar= 740

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 B

```
           Crystal system given = triclinic
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections too Low ....         35 %
```

Alert level C

```
SHFSU01_ALERT_2_C  The absolute value of parameter shift to su ratio > 0.05
           Absolute value of the parameter shift to su ratio given   0.090
           Additional refinement cycles may be required.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.979
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT080_ALERT_2_C Maximum Shift/Error ............................       0.09
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C53 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C54 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C56 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         N7 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0087 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N5     -   H42    ...     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N8     -   H73    ...     Please Check
```

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:   C19 H31.33 N3 O4.17 Si1
           Atom count from _chemical_formula_moiety:C57 H94.99 N9 O13.01 Si3
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C19 H31.33 N3 O4.17 Si1
           Atom count from the _atom_site data:  C19 H31 N3 O4.166666 Si1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    6
          From the CIF: _chemical_formula_sum  C19 H31.33 N3 O4.17 Si
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        114.00    114.00    0.00
          H        187.98    186.00    1.98
          N         18.00     18.00    0.00
          O         25.02     25.00    0.02
          Si         6.00      6.00    0.00
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          6 Why ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ............       0.17 Ratio
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =        100 Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O13 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  12 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

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
```

```
  10 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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checkCIF publication errors

Alert level A

```
PUBL003_ALERT_1_A  The contact author’s name is missing,
            _publ_contact_author_name.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
            _publ_contact_author_phone are all missing.
            At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. ’Acta Crystallographica Section C’
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
```

```
   5 ALERT level A = Data missing that is essential or data in wrong format
   0 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_PUBL003_GLOBAL
;
PROBLEM: The contact author’s name is missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
```

```
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
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: ...
;
# 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 18/09/2013; check.def file version of 12/09/2013

Datablock I - ellipsoid plot