checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_200721b_0m_a

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: cu_200721b_0m_a

```
Bond precision:   C-C = 0.0033 A          Wavelength=1.54178

Cell:             a=9.7784(5)     b=13.5406(6)     c=20.4628(10)
                  alpha=90        beta=90          gamma=90
Temperature:      273 K

                 Calculated                Reported
Volume           2709.4(2)                 2709.4(2)
Space group      P 21 21 21                P2(1)2(1)2(
Hall group       P 2ac 2ab                 ?
Moiety formula   C28 H36 O5 Si             ?
Sum formula      C28 H36 O5 Si             C28 H36 O5 Si
Mr               480.66                    480.66
Dx,g cm-3        1.178                     1.178
Z                4                         4
Mu (mm-1)        1.038                     1.038
F000             1032.0                    1032.0
F000'            1035.91
h,k,lmax         10,15,22                  10,15,22
Nref             3888[ 2225]               3877
Tmin,Tmax        0.883,0.901               0.528,0.752
Tmin'            0.813

Correction method= # Reported T Limits: Tmin=0.528 Tmax=0.752
AbsCorr = NONE

Data completeness= 1.74/1.00        Theta(max)= 58.920

R(reflections)= 0.0299( 3796)                wR2(reflections)=
                                             0.0822( 3877)
S = 1.043                 Npar= 312
```

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

PLAT902_ALERT_1_A No (Interpretable) Reflections Found in FCF .... Please Check

Alert level B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5555
PLAT035_ALERT_1_B _chemical_absolute_configuration Info Not Given Please Do !
PLAT230_ALERT_2_B Hirshfeld Test Diff for Si1 --C25 . 7.4 s.u.

Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard
identifier.
uncolor
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for Si1 --C23 . 5.2 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for Si1 --C27 . 6.0 s.u.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 Check

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 273 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 273 Check
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O1 . 132.3 Degree
PLAT791_ALERT_4_G Model has Chirality at C4 (Sohnke SpGr) R Verify
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL/ 2018 Note

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
2 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_THETM01_cu_200721b_0m_a
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.575
RESPONSE: ...
;
_vrf_CRYSC01_cu_200721b_0m_a
;
PROBLEM: The word below has not been recognised as a standard
RESPONSE: ...
;
_vrf_PLAT902_cu_200721b_0m_a
;
PROBLEM: No (Interpretable) Reflections Found in FCF ....     Please Check
RESPONSE: ...
;
_vrf_PLAT035_cu_200721b_0m_a
;
PROBLEM: _chemical_absolute_configuration Info  Not Given     Please Do !
RESPONSE: ...
;
_vrf_PLAT230_cu_200721b_0m_a
```

```
;
PROBLEM: Hirshfeld Test Diff for    Si1      --C25      .        7.4 s.u.
RESPONSE: ...
;
_vrf_PLAT220_cu_200721b_0m_a
;
PROBLEM: NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
RESPONSE: ...
;
_vrf_PLAT242_cu_200721b_0m_a
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of         C6 Check
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock cu_200721b_0m_a - ellipsoid plot