checkCIF/PLATON report

Structure factors have been supplied for datablock(s) txx017

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: txx017

```
Bond precision:   C-C = 0.0027 A          Wavelength=0.71073

Cell:             a=23.2043(14)    b=14.7092(9)        c=18.2065(18)
                  alpha=90         beta=128.410(1)     gamma=90
Temperature:      173 K

                 Calculated                Reported
Volume           4869.3(6)                 4869.3(6)
Space group      C 2/c                     C 2/c
Hall group       -C 2yc                    -C 2yc
Moiety formula   C53 H76 N5 Sc             C44 H64 N4 Sc, C9 H12 N
Sum formula      C53 H76 N5 Sc             C53 H76 N5 Sc
Mr               828.15                    828.14
Dx,g cm-3        1.130                     1.130
Z                4                         4
Mu (mm-1)        0.190                     0.190
F000             1800.0                    1800.0
F000'            1801.53
h,k,lmax         30,19,23                  30,19,23
Nref             5607                      5597
Tmin,Tmax        0.911,0.942               0.915,1.000
Tmin'            0.899

Correction method= # Reported T Limits: Tmin=0.915 Tmax=1.000
AbsCorr = NUMERICAL

Data completeness= 0.998           Theta(max)= 27.524

R(reflections)= 0.0442( 5056)                wR2(reflections)=
                                             0.1164( 5597)
S = 1.055                  Npar= 277
```

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.32 Report
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.1 Ratio
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.302 Check

Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.29 Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a Note
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Sc --N1S .	8.1 s.u.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	9 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	6 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	15 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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

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 06/07/2023; check.def file version of 30/06/2023

Datablock txx017 - ellipsoid plot