checkCIF/PLATON report

Structure factors have been supplied for datablock(s) txx019

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: txx019

```
Bond precision:    C-C = 0.0032 A              Wavelength=1.54178

Cell:           a=10.7544(2)       b=10.7984(2)        c=18.6252(4)
                alpha=82.296(1)    beta=81.306(1)      gamma=60.879(1)
Temperature:    173 K

                Calculated                    Reported
Volume          1863.24(7)                    1863.24(7)
Space group     P -1                          P -1
Hall group      -P 1                          -P 1
Moiety formula  C39 H58 N3 O Sc               C39 H58 N3 O Sc
Sum formula     C39 H58 N3 O Sc               C39 H58 N3 O Sc
Mr              629.84                        629.84
Dx,g cm-3       1.123                         1.123
Z               2                             2
Mu (mm-1)       1.918                         1.918
F000            684.0                         684.0
F000'           686.23
h,k,lmax        12,13,22                      12,13,22
Nref            6816                          6791
Tmin,Tmax       0.756,0.832                   0.578,0.780
Tmin'           0.504

Correction method= # Reported T Limits: Tmin=0.578 Tmax=0.780
AbsCorr = NUMERICAL

Data completeness= 0.996          Theta(max)= 68.276

R(reflections)= 0.0433( 6209)                 wR2(reflections)=
                                              0.1198( 6791)
S = 1.053                  Npar= 407
```

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
```
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range      5.0 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    Sc Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C20 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600     25 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H3SB      .   -0.31 eA-3
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Alert level G
```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.001 Degree
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for    C1S Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for    C3S Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for    C6S Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........     10 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........    3.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      7 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
   5 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
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   2 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

NOMOVE FORCED

Prob = 50
Temp = 173

66 Y

PLATON-Sep 23 4:50:39 2023 - (607231)

Z 130   txx019   P -1   R = 0.04   RES= 0-160 X