checkCIF/PLATON report

Structure factors have been supplied for datablock(s) txx025

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: txx025

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Bond precision:   C-C = 0.0050 A           Wavelength=1.54178

Cell:              a=19.6196(6)      b=17.7629(5)      c=22.6924(6)
                   alpha=90          beta=90           gamma=90
Temperature:       173 K

                 Calculated                  Reported
Volume           7908.3(4)                   7908.3(4)
Space group      A b a 2                     A b a 2
Hall group       A 2 -2ac                    A 2 -2ac
Moiety formula   C91 H88 N5 Sc [+ solvent]   C82 H76 N4 Sc, C9 H12 N
Sum formula      C91 H88 N5 Sc [+ solvent]   C91 H88 N5 Sc
Mr               1296.62                     1296.62
Dx,g cm-3        1.089                       1.089
Z                4                           4
Mu (mm-1)        1.143                       1.143
F000             2760.0                      2760.0
F000'            2768.05
h,k,lmax         25,22,28                    24,22,28
Nref             8594[ 4411]                 7739
Tmin,Tmax        0.760,0.839                 0.695,0.912
Tmin'            0.575

Correction method= # Reported T Limits: Tmin=0.695 Tmax=0.912
AbsCorr = NUMERICAL

Data completeness= 1.75/0.90        Theta(max)= 79.301

R(reflections)= 0.0451( 6950)                wR2(reflections)=
                                             0.1150( 7739)
S = 1.031                Npar= 507
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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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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         12 Report
                0 18  0,  13  6  0,  16  2  0,  16  4  0,  16  5  3,   0 12  6,
                2 12  6,   9 12  6,   4 11  9,   6 13  9,   0 12 10,   5  9 15,
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C91 H88 N5 Sc
             Rep.: C82 H76 N4 Sc, C9 H12 N
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Sc       --N1S      .        6.1 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        25% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        227 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         12 Note
             H1SA    H1SB    H3SA    H4SA    H5SA    H6SA    H8SA    H8SB
             H8SC    H9SA    H9SB    H9SC
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        147 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         65 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 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
   2 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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
   6 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 29/11/2023; check.def file version of 14/09/2023

Datablock txx025 - ellipsoid plot