checkCIF/PLATON report

Structure factors have been supplied for datablock(s) txx015

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: txx015

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Bond precision:   C-C = 0.0030 A           Wavelength=0.71073

Cell:           a=12.7599(6)       b=16.3242(8)      c=17.1387(8)
                alpha=69.953(1)    beta=84.307(1)    gamma=74.610(1)
Temperature:    173 K

                Calculated                 Reported
Volume          3233.2(3)                  3233.2(3)
Space group     P -1                       P -1
Hall group      -P 1                       -P 1
Moiety formula  C67 H92 N5 Sc [+ solvent]  C49 H68 N3 Sc, 2(C9 H12 N)
Sum formula     C67 H92 N5 Sc [+ solvent]  C67 H92 N5 Sc
Mr              1012.42                    1012.41
Dx,g cm-3       1.040                      1.040
Z               2                          2
Mu (mm-1)       0.154                      0.154
F000            1100.0                     1100.0
F000'           1100.83
h,k,lmax        15,19,20                   15,19,20
Nref            11876                      11856
Tmin,Tmax       0.936,0.964                0.914,0.992
Tmin'           0.933

Correction method= # Reported T Limits: Tmin=0.914 Tmax=0.992
AbsCorr = NUMERICAL

Data completeness= 0.998           Theta(max)= 25.367

R(reflections)= 0.0472( 10165)                wR2(reflections)=
                                              0.1149( 11856)
S = 1.027                  Npar= 734
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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

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 5 Note

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 38 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 4 Report
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 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C61 --C62X . 13.1 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C61 --C68X . 12.7 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C61 --C69X . 12.1 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C61 --C62Y . 12.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C61 --C68Y . 12.3 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C61 --C69Y . 12.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sc --N1S . 6.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Sc --N2S . 5.3 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 25% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H13 ..H36A . 2.08 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H13 ..H32C . 2.09 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H15 ..H39A . 2.08 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H15 ..H39C . 2.06 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H45 ..H68C . 2.13 Ang.
x,y,z = 1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ..... ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 12 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C61 --C68Y 1.71 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 176 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 8 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 12 Info

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

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

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 17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
  8 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
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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 txx015 - ellipsoid plot