checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1a

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: 1a

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Bond precision:   C-C = 0.0055 A          Wavelength=1.54178

Cell:             a=9.8336(3)     b=26.7597(8)        c=18.6548(5)
                  alpha=90        beta=93.756(1)      gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           4898.4(2)                 4898.4(2)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C50 H64 O14, 0.6(H2 O)    C50 H64 O14, 0.6(H2 O)
Sum formula      C50 H65.20 O14.60         C50 H65.20 O14.60
Mr               899.82                    899.82
Dx,g cm-3        1.220                     1.220
Z                4                         4
Mu (mm-1)        0.733                     0.733
F000             1928.0                    1928.0
F000'            1934.29
h,k,lmax         11,31,22                  11,31,22
Nref             8695                      8636
Tmin,Tmax        0.876,0.896               0.408,0.753
Tmin'            0.876

Correction method= # Reported T Limits: Tmin=0.408 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.993           Theta(max)= 66.802

R(reflections)= 0.0981( 5657)                wR2(reflections)=
                                             0.3492( 8636)
S = 1.325                Npar= 745
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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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PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.35 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.4 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C014     --C016     .        5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C019     --C01D     .        5.1 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00W     --C01M     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00Y     --C01B     .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O00Y     --C01O     .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C01B     --C01E     .       0.22 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C019 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01B Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01K Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C01M Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00R Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       O00Y Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C012 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O1      0.143 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O017      0.133 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00553 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C01B     - C01E     .       1.36 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C01N     - C01O     .       1.40 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      7.331 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.596         59 Report
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         39 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         47 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          5 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          5 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          8 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0300 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O4       --C01M     .        7.6 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C10      --C012     .        5.7 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O017       Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H          Constrained at        0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7         Constrained at        0.6 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         27% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )       1.80 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C01K     - C01M     .       1.52 Ang.
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O2       .      109.9 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O3       .      148.1 Degree
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PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O3A      .      138.1 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O00Y     .      108.9 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O12A     .       84.8 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O00{     .      109.7 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O4       .       92.7 Degree
PLAT410_ALERT_2_G Short Intra H...H Contact  H00G     ..H01J     .       1.74 Ang.
                                                     x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H00S     ..H01N     .       2.06 Ang.
                                                     x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H00S     ..H01O     .       2.05 Ang.
                                                     x,y,z  =      1_555 Check
PLAT415_ALERT_2_G Short Inter D-H..H-X       H        ..H01Y     .       2.07 Ang.
                                          x,1/2-y,-1/2+z  =      4_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O017     ..C8       .       2.98 Ang.
                                             1-x,1-y,1-z  =      3_666 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....        121 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....      ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............   614 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....     1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File     5 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........   4.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.     1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by     6 Check
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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
23 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
42 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
34 ALERT type 2 Indicator that the structure model may be wrong or deficient
14 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
3 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 1a - ellipsoid plot