checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

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Bond precision:    C-C = 0.0046 A              Wavelength=1.54178

Cell:            a=10.1835(7)        b=12.9146(9)        c=16.3030(11)
                 alpha=81.259(2)    beta=87.322(2)    gamma=68.522(2)
Temperature:     140 K

                 Calculated                  Reported
Volume           1972.0(2)                   1971.9(2)
Space group      P -1                        P -1
Hall group       -P 1                        -P 1
                 2(C20 H36 Ca4 N4 O22),
Moiety formula                               ?
                 12(H2 O), 3(O)
Sum formula      C40 H96 Ca8 N8 O59          C40 H96 Ca8 N8 O59
Mr               1953.89                     1953.88
Dx,g cm-3        1.645                       1.645
Z                1                           1
Mu (mm-1)        5.749                       5.695
F000             1024.0                      1024.0
F000'            1030.75
h,k,lmax         11,14,18                    11,14,18
Nref             6287                        6121
Tmin,Tmax        0.530,0.711                 0.482,0.726
Tmin'            0.405

Correction method= # Reported T Limits: Tmin=0.482 Tmax=0.726
AbsCorr = MULTI-SCAN

Data completeness= 0.974            Theta(max)= 62.490


R(reflections)= 0.0531( 5693)                      wR2(reflections)=
                                                   0.1440( 6121)
S = 1.074                    Npar= 546
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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 B
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PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......      O01C Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......      O01M Check
PLAT417_ALERT_2_B Short Inter D-H..H-D       H00B     ..H00R     .      1.86 Ang.
                                             1-x,1-y,1-z  =      2_666 Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O00T     --H00R     .   Please Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O006     ..O01C     .      2.82 Ang.
                                             1-x,1-y,1-z  =      2_666 Check
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🟡 Alert level C
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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as multi-scan
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
            Calculated sin(theta_max)/wavelength =    0.5753
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .     0.973 Why?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.91 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density      1.78 eA-3
PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem       I          89 %Fit
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range       4.9 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       5.6 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Ca04 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including     O01M       0.147 Check
PLAT411_ALERT_2_C Short Inter H...H Contact  H01F     ..H01F     .      2.08 Ang.
                                             2-x,2-y,2-z  =      2_777 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4   Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     2.048 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.575        167 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....       34 Note
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.89Ang From O01E          1.70 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.86Ang From O00Z    .     0.68 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.58Ang From O01M    .     0.66 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.48Ang From O01M    .    -0.58 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.52Ang From O01C    .    -0.48 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.74Ang From O00M    .    -0.45 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.75Ang From O00V    .    -0.42 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.62Ang From O00T    .    -0.41 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.66Ang From O01E    .    -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H00E       .    -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H00T       .    -0.32 eA-3
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⚪ Alert level G
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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        24 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      5.06 Why ?
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PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.002 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        105 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.10 Ratio
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Ca01      --Ca01      ..       4.03 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Ca02      --Ca04      ..       4.43 Ang.
PLAT774_ALERT_1_G Check   X-Y Bond in CIF: Ca03      --Ca04      ..       4.06 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      37.17 Deg.
           O009 -C01F -CA01     1_555   1_555   1_555 ......    #  400 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        90% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         18 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged   Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..      125.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
PLAT982_ALERT_1_G The  C-f'=    0.0192 Deviates from  IT-value =       0.0181 Check
PLAT982_ALERT_1_G The Ca-f'=    0.3660 Deviates from  IT-value =       0.3641 Check
PLAT982_ALERT_1_G The  N-f'=    0.0330 Deviates from  IT-value =       0.0311 Check
PLAT982_ALERT_1_G The  O-f'=    0.0517 Deviates from  IT-value =       0.0492 Check
PLAT983_ALERT_1_G The Ca-f"=    1.2937 Deviates from  IT-Value =       1.2855 Check
PLAT983_ALERT_1_G The  O-f"=    0.0336 Deviates from  IT-Value =       0.0322 Check
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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   5 **ALERT level B** = A potentially serious problem, consider carefully
  27 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  22 **ALERT level G** = General information/check it is not something unexpected

  13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  27 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
   4 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 28/11/2022; check.def file version of 28/11/2022

Datablock 1 - ellipsoid plot

NOMOVE FORCED

Prob =   50
Temp = 140

-52 Y

PLATON-Mar 29 11:28:39 2023 - (281122)

Z 20   1   P -1   R = 0.05   RES= 0 -16 X