checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 14944sadabs

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: 14944sadabs

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Bond precision:   C-C = 0.0019 A          Wavelength=0.71073

Cell:           a=7.2022(5)       b=8.4003(5)      c=15.0621(10)
                alpha=99.969(4)   beta=94.673(4)   gamma=111.188(2)
Temperature:    100 K

                 Calculated                Reported
Volume           826.48(10)                826.48(9)
Space group      P -1                      P -1
Hall group       -P 1                      -P 1
Moiety formula   C21 H19 N O4              C21 H19 N O4
Sum formula      C21 H19 N O4              C21 H19 N O4
Mr               349.37                    349.37
Dx,g cm-3        1.404                     1.404
Z                2                         2
Mu (mm-1)        0.098                     0.098
F000             368.0                     368.0
F000'            368.18
h,k,lmax         10,12,21                  10,12,21
Nref             5070                      5061
Tmin,Tmax        0.987,0.998               0.985,0.998
Tmin'            0.977

Correction method= # Reported T Limits: Tmin=0.985 Tmax=0.998
AbsCorr = GAUSSIAN

Data completeness= 0.998           Theta(max)= 30.555

R(reflections)= 0.0483( 3946)                wR2(reflections)=
                                             0.1418( 5061)
S = 1.027                 Npar= 261
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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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PLAT213_ALERT_2_C Atom N1              has ADP max/min Ratio .....       3.2 prolat
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        N1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C9 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.3 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         2 Report
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        11 Note
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used    0.0400 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    N1       --C11'     .      25.6 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        8% Note
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O1'      .     105.5 Degree
PLAT410_ALERT_2_G Short Intra H...H Contact  H7'      ..H11B     .      2.06 Ang.
                                                    x,y,z  =     1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         2 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        29 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         6 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        19 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
  16 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   5 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 28/11/2022; check.def file version of 28/11/2022

Datablock 14944sadabs - ellipsoid plot