checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_3498_sq

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: exp_3498_sq

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Bond precision:   C-C = 0.0041 A          Wavelength=1.54184

Cell:           a=14.4553(6)       b=15.1300(6)      c=21.0270(7)
                alpha=92.220(3)    beta=94.235(3)    gamma=98.658(4)
Temperature:    100 K

                Calculated                 Reported
Volume          4528.2(3)                  4528.2(3)
Space group     P -1                       P -1
Hall group      -P 1                       -P 1
Moiety formula  C50 H41 B N2 O2 [+ solvent] C50 H41 B N2 O2
Sum formula     C50 H41 B N2 O2 [+ solvent] C50 H41 B N2 O2
Mr              712.66                     712.66
Dx,g cm-3       1.045                      1.045
Z               4                          4
Mu (mm-1)       0.487                      0.487
F000            1504.0                     1504.0
F000'           1508.08
h,k,lmax                                   17,18,25
Nref                                       15982
Tmin,Tmax       0.907,0.976                0.621,1.000
Tmin'           0.907

Correction method= # Reported T Limits: Tmin=0.621 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness=                 Theta(max)= 66.600

R(reflections)= 0.0622( 11576)                wR2(reflections)=
                                              0.1684( 15982)
S = 1.029                  Npar= 1005
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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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DIFMN02_ALERT_2_C  The minimum difference density is < -0.1*ZMAX*0.75
           _refine_diff_density_min given =     -0.704
           Test value =     -0.600
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT098_ALERT_2_C Large Reported Min.  (Negative) Residual Density      -0.70 eA-3
PLAT213_ALERT_2_C Atom C84             has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.4 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.1 Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.5 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0041 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.442 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595          9 Report
             -16  8  6,   8  5  7, -16  7  7,  -7 -9 12,   1  4 15,   1  4 16,
              -1  5 16,   4  2 18,  -3 -7 23,
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         13 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3 Note
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          6 Report
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         78 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
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         65% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
               0  0  1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          3 Note
              -1  5 16,   8  5  7,  -7 -9 12,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          7 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
  10 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
   4 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 14/11/2023; check.def file version of 14/09/2023

Datablock exp_3498_sq - ellipsoid plot