checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_3473_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_3473_sq

```
Bond precision:   C-C = 0.0061 A          Wavelength=1.54184

Cell:           a=11.6677(12)      b=12.7694(11)     c=14.5328(8)
                alpha=103.399(7)   beta=109.908(8)   gamma=94.935(7)
Temperature:    100 K

                 Calculated                 Reported
Volume           1948.0(3)                  1948.0(3)
Space group      P -1                       P -1
Hall group       -P 1                       -P 1
Moiety formula   C49 H39 B N2 [+ solvent]   C49 H39 B N2
Sum formula      C49 H39 B N2 [+ solvent]   C49 H39 B N2
Mr               666.63                     666.63
Dx,g cm-3        1.137                      1.137
Z                2                          2
Mu (mm-1)        0.495                      0.495
F000             704.0                      704.0
F000'            705.81
h,k,lmax                                    13,15,17
Nref                                        6887
Tmin,Tmax        0.976,0.976                0.762,1.000
Tmin'            0.976

Correction method= # Reported T Limits: Tmin=0.762 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness=                 Theta(max)= 66.600

R(reflections)= 0.0815( 4447)                wR2(reflections)=
                                             0.2447( 6887)
S = 1.047                  Npar= 475
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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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DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
          The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.04 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       0.54 eA-3
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00615 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.599 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595          7 Report
               9  7  0,   9  8  0,   1 -1  1,   8  9  1,  -7  0  7, -13  3  7,
               6 -6 12,
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Alert level G

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PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.13 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H26A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26C       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28B       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28C       Constrained at        0.5 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        248 A**3
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              H26A -C26  -H26A    1_555   1_555   1_555 ......     #   89 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              H28A -C28  -H28A    1_555   1_555   1_555 ......     #  108 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...       0.00 Deg.
              H28B -C28  -H28B    1_555   1_555   1_555 ......     #  117 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #          6 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          2 Check
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        53% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.7 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 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
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  18 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
  13 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_3473_sq - ellipsoid plot