checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_3517_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_3517_sq

```
Bond precision:   C-C = 0.0059 A          Wavelength=1.54184

Cell:              a=13.211(2)     b=20.856(2)          c=15.732(3)
                   alpha=90        beta=114.86(2)       gamma=90
Temperature:       100 K

                 Calculated                  Reported
Volume           3933.0(12)                  3932.9(11)
Space group      P 21/c                      P 1 21/c 1
Hall group       -P 2ybc                     -P 2ybc
Moiety formula   C49 H39 B N2 O2 [+ solvent] C49 H39 B N2 O2
Sum formula      C49 H39 B N2 O2 [+ solvent] C49 H39 B N2 O2
Mr               698.63                      698.63
Dx,g cm-3        1.180                       1.180
Z                4                           4
Mu (mm-1)        0.552                       0.552
F000             1472.0                      1472.0
F000'            1476.01
h,k,lmax                                     15,24,18
Nref                                         6939
Tmin,Tmax        0.967,0.973                 0.338,1.000
Tmin'            0.946

Correction method= # Reported T Limits: Tmin=0.338 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness=                  Theta(max)= 66.597

R(reflections)= 0.0543( 3043)                wR2(reflections)=
                                             0.1331( 6939)
S = 0.779                  Npar= 498
```

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

PLAT420_ALERT_2_B D-H Bond Without Acceptor O1 --H1 . Please Check

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 0.779
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.132
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 44% Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00595 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.140 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 3 Report
7 8 5, 5 13 5, 6 12 6,

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
H1
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.132 Report
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/c P21/n Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 124 A**3
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT931_ALERT_5_G CIFcalcFCF Twin Law (0 0 1) Est.d BASF 0.11 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
5 13 5, 6 12 6, 7 8 5,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

0 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
7 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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 29/11/2023; check.def file version of 14/09/2023

Datablock exp_3517_sq - ellipsoid plot