checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_3736_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_3736_sq

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Bond precision:   C-C = 0.0085 A           Wavelength=1.54184

Cell:           a=11.9190(12)      b=12.5825(11)     c=14.8081(16)
                alpha=104.186(8)   beta=110.328(9)   gamma=96.071(8)
Temperature:    100 K

                 Calculated                 Reported
Volume           1974.0(4)                  1974.0(4)
Space group      P -1                       P -1
Hall group       -P 1                       -P 1
Moiety formula   C49 H39 B N2 O [+ solvent] C49 H39 B N2 O
Sum formula      C49 H39 B N2 O [+ solvent] C49 H39 B N2 O
Mr               682.63                     682.63
Dx,g cm-3        1.148                      1.148
Z                2                          2
Mu (mm-1)        0.519                      0.519
F000             720.0                      720.0
F000'            721.91
h,k,lmax         14,14,17                   14,14,17
Nref             6973                       6960
Tmin,Tmax        0.969,0.974                0.593,1.000
Tmin'            0.949

Correction method= # Reported T Limits: Tmin=0.593 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 66.599

R(reflections)= 0.0818( 3802)                    wR2(reflections)=
                                                 0.2274( 6960)
S = 1.027                  Npar= 485
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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

PLAT420_ALERT_2_B D-H Bond Without Acceptor O004 --H004 . Please Check

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Alert level C

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -0.663
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 -0.66 eA-3
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00851 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 14.023 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.509 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 13 Report
2 0 0, 0 1 0, -6-12 2, 2-14 4, -1-10 4, -7 -5 4,
-3 6 5, 2 8 9, -4 10 9, -5 9 11, -1 -4 12, -10 -8 13,
-6 7 13,

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 1 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
H004
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 259 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 92 Note
O004 H004 N005 N006 C007 C008 C009 C00A
C00B C00C C00D C00E H00E C00F C00G H00G
C00H C00I C00J C00K C00L C00M C00N H00N
C00O H00O C00P C00Q H00Q C00R H00R C00S
H00S C00T C00U C00V C00W H00W C00X H00X
C00Y H00A H00B H00C C00Z C010 H010 C011
C012 H012 C013 C014 C015 C016 H016 C017
H01A H01B H01C C018 H018 C019 H01D H01E
H01F C01A H01G C01B H01H C01C H01I C01D
H01J C01E H01K C01F H01L C01G H01M C01H
H01N H01O H01P C01I H01Q H01R H01S C01J
H01T H01U H01V B01K
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 6 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 41% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
-4 10 9, -6 7 13, 0 1 0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 1.60 Note
Predicted wR2: Based on SigI**2 14.17 or SHELX Weight 23.05
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  6 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
  2 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 06/01/2024; check.def file version of 05/01/2024

Datablock exp_3736_sq - ellipsoid plot