checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_2024031102_0m

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: cu_2024031102_0m

Bond precision: C-C = 0.0133 A Wavelength=1.54178

Cell: a=10.0277(2) b=10.9571(3) c=26.1879(7)
alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	2877.38(12)	2877.38(12)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C29 H26 Br N3 O2 [+ solvent]	C29 H26 Br N3 O2
Sum formula	C29 H26 Br N3 O2 [+ solvent]	C29 H26 Br N3 O2
Mr	528.43	528.44
Dx,g cm-3	1.220	1.220
Z	4	4
Mu (mm-1)	2.162	2.162
F000	1088.0	1088.0
F000'	1087.99	
h,k,lmax	12,13,31	12,13,31
Nref	5262[2994]	5247
Tmin,Tmax	0.802,0.933	0.539,0.753
Tmin'	0.467	

Correction method= # Reported T Limits: Tmin=0.539 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.75/1.00 Theta(max)= 68.329

R(reflections)= 0.0734(5172)

wR2(reflections)= 0.1795(5247)

S = 1.105 Npar= 318

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 C19             has ADP max/min Ratio .....        3.6 oblate
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C8       --C9       .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11      --C12      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C26      --C27      .       0.18 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01331 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         3 Report
                  0  2  0,   0  5  1,   0  0  4,
PLAT977_ALERT_2_C Check Negative Difference Density on H28       .     -0.40 eA-3
PLAT987_ALERT_1_C The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         1 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.140 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      17.55 Why ?
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par     0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar     0.0200 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        299 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         6 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed         ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         2 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
                  0  0  4,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.48 Note
              Predicted wR2: Based on SigI**2  4.01 or SHELX Weight 16.77
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
   9 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
   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
  10 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 cu_2024031102_0m - ellipsoid plot