checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_0315_n3_nh3_br_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_0315_n3_nh3_br_0m

```
Bond precision:   C-C = 0.0064 A          Wavelength=1.54178

Cell:             a=20.9596(12)     b=20.9596(12)     c=20.9596(12)
                  alpha=90          beta=90           gamma=90
Temperature:      300 K
```

	Calculated	Reported
Volume	9207.7(16)	9207.7(16)
Space group	I 2 3	I 2 3
Hall group	I 2 2 3	I 2 2 3
Moiety formula	2(C21 H12 N O6), 2(C21 H15 N O6), 2(C H Br3), 3(H O), 6(H4 N)	2(C21 H12 N O6), 2(C21 H15 N O6), 6(H4 N), 1.5(H2 O2), 2(C H Br
Sum formula	C86 H83 Br6 N10 O27	C86 H83 Br6 N10 O27
Mr	2168.02	2168.08
Dx,g cm-3	1.564	1.564
Z	4	4
Mu (mm-1)	3.846	3.846
F000	4380.0	4380.0
F000'	4375.98	
h,k,lmax		24,24,25
Nref		2828
Tmin,Tmax	0.502,0.562	0.668,0.753
Tmin'	0.441	

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Correction method= # Reported T Limits: Tmin=0.668 Tmax=0.753
AbsCorr = NONE

Data completeness=                 Theta(max)= 68.281
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R(reflections)= 0.0677(2624)

wR2(reflections)= 0.1932(2828)

S = 1.157 Npar= 194

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

```
STRVA01_ALERT_4_C          Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.500
          From the CIF: _refine_ls_abs_structure_Flack_su   24.000
PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ...      3.000 Sigma
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C21 H12 N O6), 2(C21 H15 N O6), 2(C H Br3), 3(H O), 6(H4 N
             Rep.: 2(C21 H12 N O6), 2(C21 H15 N O6), 6(H4 N), 1.5(H2 O2), 2(C H
PLAT057_ALERT_3_C Correction for Absorption Required   RT(exp) ...       1.12 Do !
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       7.93 Note
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          2 Check
             Br1     C5
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.7 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.9 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O00M      0.183 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00643 Ang.
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          4 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      11.03 Check
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.60Ang From O00M    .      -0.49 eA-3
PLAT987_ALERT_1_C The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          2 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          5 Report
             H003  H00M  H00A  H00C  H00D
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.500 Note
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.14 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H00M       Constrained at        0.5 Check
PLAT344_ALERT_2_G Unusual           Angle Range in Solvent/Ion for         C5 Check
PLAT417_ALERT_2_G Short Inter D-H..H-D       H00D     ..H00M     .       1.93 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  Br1      ..C00J     .       3.35 Ang.
                                                     x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         36 Note
             O001    O002    O003    H003    O004    N005    N006    H00A
             H00C    H00D    H00H    C007    C008    C009    C00A    C00B
             H00B    C00C    N00D    C00E    H00E    C00F    H00F    C00G
             H00G    C00H    C00I    H00I    C00J    H00J    C00K    H00K
             C00L    H00L    O00M    H00M
PLAT722_ALERT_1_G Angle   Calc       85.00, Rep       86.10 Dev...       1.10 Degree
             H00C    -N006    -H00H       1_555  1_555  1_555     #    9 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C21 H15 N O6
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          1 Note
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```
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                0  1  1,   0  0  2,
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.41 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 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
  14 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 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
   7 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_STRVA01_cu_0315_n3_nh3_br_0m
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_PLAT031_cu_0315_n3_nh3_br_0m
;
PROBLEM: Refined Extinction Parameter Within Range of ...      3.000 Sigma
RESPONSE: ...
;
_vrf_PLAT042_cu_0315_n3_nh3_br_0m
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT057_cu_0315_n3_nh3_br_0m
;
PROBLEM: Correction for Absorption Required   RT(exp) ...       1.12 Do !
RESPONSE: ...
;
_vrf_PLAT090_cu_0315_n3_nh3_br_0m
;
PROBLEM: Poor Data / Parameter Ratio (Zmax > 18) ........       7.93 Note
RESPONSE: ...
;
_vrf_PLAT202_cu_0315_n3_nh3_br_0m
;
PROBLEM: Isotropic non-H Atoms in Anion/Solvent .........          2 Check
RESPONSE: ...
;
_vrf_PLAT250_cu_0315_n3_nh3_br_0m
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.7 Note
RESPONSE: ...
```

```
;
_vrf_PLAT260_cu_0315_n3_nh3_br_0m
;
PROBLEM: Large Average Ueq of Residue Including      O00M      0.183 Check
RESPONSE: ...
;
_vrf_PLAT341_cu_0315_n3_nh3_br_0m
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.00643 Ang.
RESPONSE: ...
;
_vrf_PLAT918_cu_0315_n3_nh3_br_0m
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .          4 Check
RESPONSE: ...
;
_vrf_PLAT939_cu_0315_n3_nh3_br_0m
;
PROBLEM: Large Value of Not (SHELXL) Weight Optimized S .      11.03 Check
RESPONSE: ...
;
_vrf_PLAT976_cu_0315_n3_nh3_br_0m
;
PROBLEM: Check Calcd Resid. Dens.  0.60Ang From O00M    .      -0.49 eA-3
RESPONSE: ...
;
_vrf_PLAT987_cu_0315_n3_nh3_br_0m
;
PROBLEM: The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
RESPONSE: ...
;
# end Validation Reply Form
```

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 cu_0315_n3_nh3_br_0m - ellipsoid plot