checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: dppbianganancn

```
Bond precision:  C-C = 0.0131 A          Wavelength=0.71073

Cell:           a=13.7559(16)    b=18.926(2)         c=24.235(3)
                alpha=90         beta=104.957(4)     gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          6095.7(12)                6095.5(13)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C58 H88 Ga N6 Na O4, C6 H6?
Sum formula     C64 H94 Ga N6 Na O4       C64 H94 Ga N6 Na O4
Mr              1104.16                   1104.16
Dx,g cm-3       1.203                     1.203
Z               4                         4
Mu (mm-1)       0.509                     0.509
F000            2376.0                    2376.0
F000'           2377.75
h,k,lmax        16,22,28                  16,22,28
Nref            10741                     10442
Tmin,Tmax       0.880,0.975               0.281,0.745
Tmin'           0.841

Correction method= # Reported T Limits: Tmin=0.281 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.972          Theta(max)= 24.998

R(reflections)= 0.1491( 6751)     wR2(reflections)= 0.3468( 10442)

S = 1.055                 Npar= 724
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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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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.132
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........      0.132 Report
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.972 Why?
PLAT082_ALERT_2_C High R1 Value ..................................       0.15 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.35 Report
PLAT213_ALERT_2_C Atom C1              has ADP max/min Ratio .....        3.2 oblate
PLAT213_ALERT_2_C Atom C3              has ADP max/min Ratio .....        4.0 oblate
PLAT213_ALERT_2_C Atom C5              has ADP max/min Ratio .....        3.3 oblate
PLAT213_ALERT_2_C Atom C7              has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C13             has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C54             has ADP max/min Ratio .....        3.3 oblate
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        4.8 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        5.0 Ratio
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01306 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         39 Ang**3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         12 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         17 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.14 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     101.49 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          6 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         14 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  2          7.49 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  3          4.51 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         18 Note
PLAT722_ALERT_1_G Angle   Calc      121.00, Rep      119.70 Dev...       1.30 Degree
              C6S'    -C1S'    -H1SB       1.555  1.555  1.555     #  353 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        116 Note
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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
  15 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
   8 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 03/05/2019; check.def file version of 29/04/2019

Datablock dppbianganancn - ellipsoid plot