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: nagabian1m

Bond precision: C-C = 0.0051 A   Wavelength=0.71073

Cell: a=13.7910(5)   b=36.8339(13)   c=15.0725(5)
               alpha=90   beta=93.043(1)   gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	7645.7(5)	7645.7(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C62 H84 Ga N6, C12 H30 Na O6, 0.51(C4 H10 O2), 0.49(C4 H10 O)	?
Sum formula	C78 H124 Ga N6 Na O7.51	C78 H124 Ga N6 Na O7.51
Mr	1358.70	1358.69
Dx,g cm-3	1.180	1.180
Z	4	4
Mu (mm-1)	0.421	0.421
F000	2944.3	2944.0
F000'	2946.34	
h,k,lmax	18,48,19	18,48,19
Nref	18454	18399
Tmin,Tmax	0.862,0.887	0.794,0.901
Tmin'	0.862	

Correction method= # Reported T Limits: Tmin=0.794 Tmax=0.901
AbsCorr = MULTI-SCAN

Data completeness= 0.997   Theta(max)= 27.999

R(reflections)= 0.0709(12900)   wR2(reflections)= 0.1990(18399)

S = 1.074   Npar= 1130

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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PLAT220_ALERT_2_C NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range        3.2 Ratio
PLAT221_ALERT_2_C Solv./Anion  Resd 3  C   Ueq(max)/Ueq(min) Range         6.0 Ratio
PLAT221_ALERT_2_C Solv./Anion  Resd 6  C   Ueq(max)/Ueq(min) Range         4.6 Ratio
PLAT223_ALERT_4_C Solv./Anion  Resd 3  H   Ueq(max)/Ueq(min) Range         7.4 Ratio
PLAT223_ALERT_4_C Solv./Anion  Resd 6  H   Ueq(max)/Ueq(min) Range         5.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C39      --C44      .         5.5 s.u.
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of      C53 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Na1Q    0.101 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O7Q    0.193 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O7W    0.180 Check
PLAT410_ALERT_2_C Short Intra H...H Contact  H39A     ..H45A     .      1.90 Ang.
                                                 x,y,z  =      1_555 Check
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       52 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       57 Report
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......  Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...  Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     7.01 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       20 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O7S        Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O8S        Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13S       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14S       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15S       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16S       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13C       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14A       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14B       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15B       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15C       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16C       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16D       Constrained at     0.51 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7Q        Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13Q       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14Q       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15Q       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16Q       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13D       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13G       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14C       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14D       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14E       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15D       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15E       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16E       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16F       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16G       Constrained at    0.295 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7W        Constrained at    0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13W       Constrained at    0.195 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C14W         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15W         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16W         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13E         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13F         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14F         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14G         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14H         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15F         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15G         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16H         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16I         Constrained at      0.195 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16J         Constrained at      0.195 Check
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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )       27.49 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )       21.51 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  4  )        8.16 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5  )        4.43 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  6  )        2.92 Check
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O7S             107.9 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O8S             109.0 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O7Q             109.3 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O7W             106.7 Degree
PLAT411_ALERT_2_G Short Inter H...H Contact  H6SB    ..H46A    .          2.02 Ang.
                                                x,y,z  =      1_555 Check
PLAT411_ALERT_2_G Short Inter H...H Contact  H7SB    ..H46A    .          1.96 Ang.
                                                x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H1SB    ..H53B    .          2.07 Ang.
                                           1-x,1-y,1-z  =      3_666 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        46 Note
PLAT722_ALERT_1_G Angle   Calc       110.00, Rep      111.40 Dev...        1.40 Degree
          C14W    -C13W    -H13F        1.555  1.555  1.555    #  635 Check
PLAT722_ALERT_1_G Angle   Calc       108.00, Rep      109.50 Dev...        1.50 Degree
          H14F    -C14W    -H14G        1.555  1.555  1.555    #  639 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       387 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        47 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
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  76 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  20 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
  61 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 22/12/2019; check.def file version of 13/12/2019

Datablock nagabian1m - ellipsoid plot

NOMOVE FORCED

Prob = 50
Temp = 100

42 Y

PLATON-Mar 12 09:39:52 2020 - (70316)

Z -41   nagabian1mP 21/c   R = 0.07   RES=   0 -104 X