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: 250421_zn_wb4ga

```
Bond precision:   C-C = 0.0067 A           Wavelength=1.34139

Cell:           a=13.440(4)       b=14.183(5)       c=14.856(7)
                alpha=90.51(5)    beta=100.64(4)    gamma=116.401(19)
Temperature:    170 K
```

	Calculated	Reported
Volume	2479.5(18)	2479.7(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C74 H112 Ga4 N8, 4(C7 H8)	C74 H112 Ga4 N8, 4(C7 H8)
Sum formula	C102 H144 Ga4 N8	C102 H144 Ga4 N8
Mr	1761.13	1761.12
Dx,g cm-3	1.179	1.179
Z	1	1
Mu (mm-1)	1.046	1.077
F000	936.0	936.0
F000'	929.76	
h,k,lmax	16,17,17	16,17,17
Nref	9160	9043
Tmin,Tmax	0.962,0.968	0.653,0.751
Tmin'	0.948	

```
Correction method= # Reported T Limits: Tmin=0.653 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 0.987            Theta(max)= 54.148

R(reflections)= 0.0663( 6301)                    wR2(reflections)=
                                                 0.1835( 9043)
S = 1.110                  Npar= 650
```

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

PLAT051_ALERT_1_C Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 2.88 %
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.76 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C38 --C39 . 0.17 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C21 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C24 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 3) 2.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 5) 2.5 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00675 Ang.

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 32 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 28 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 32 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 3 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0200 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0400 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 2% Note
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
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2) 12.27 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 3) 13.11 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 4) 2.73 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 5) 1.89 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C51 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H13A ..H51F . 1.93 Ang.

```
                                                  x,-1+y,z  =      1_545 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H13B     ..H51F     .       1.54 Ang.
                                                  x,-1+y,z  =      1_545 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H13C     ..H51F     .       2.10 Ang.
                                                  x,-1+y,z  =      1_545 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C13      ..C51A     .       2.82 Ang.
                                                  x,-1+y,z  =      1_545 Check
PLAT722_ALERT_1_G Angle   Calc      122.00, Rep      120.90 Dev...       1.10 Degree
              C40A    -C41A    -H41A       1_555  1_555  1_555     #  254 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        476 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         24 Note
              -15 12  6, -14 12  7, -11 15  5, -11 16  3, -11 16  4,  -8 17  1,
               -7  2  1,  -7 17  1,  -6  1  0,  -6 17  0,  -6 17  1,  -5 16  2,
               -1-14  4,  -1  1  0,   0  0  1,   0  1  0,   0  1  2,   1  0  0,
                2-16  1,   2 -1  1,   2  4  3,   9-11  1,  10-10 11,  13-10  6,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.9 Low
```

---

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

3 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
24 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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

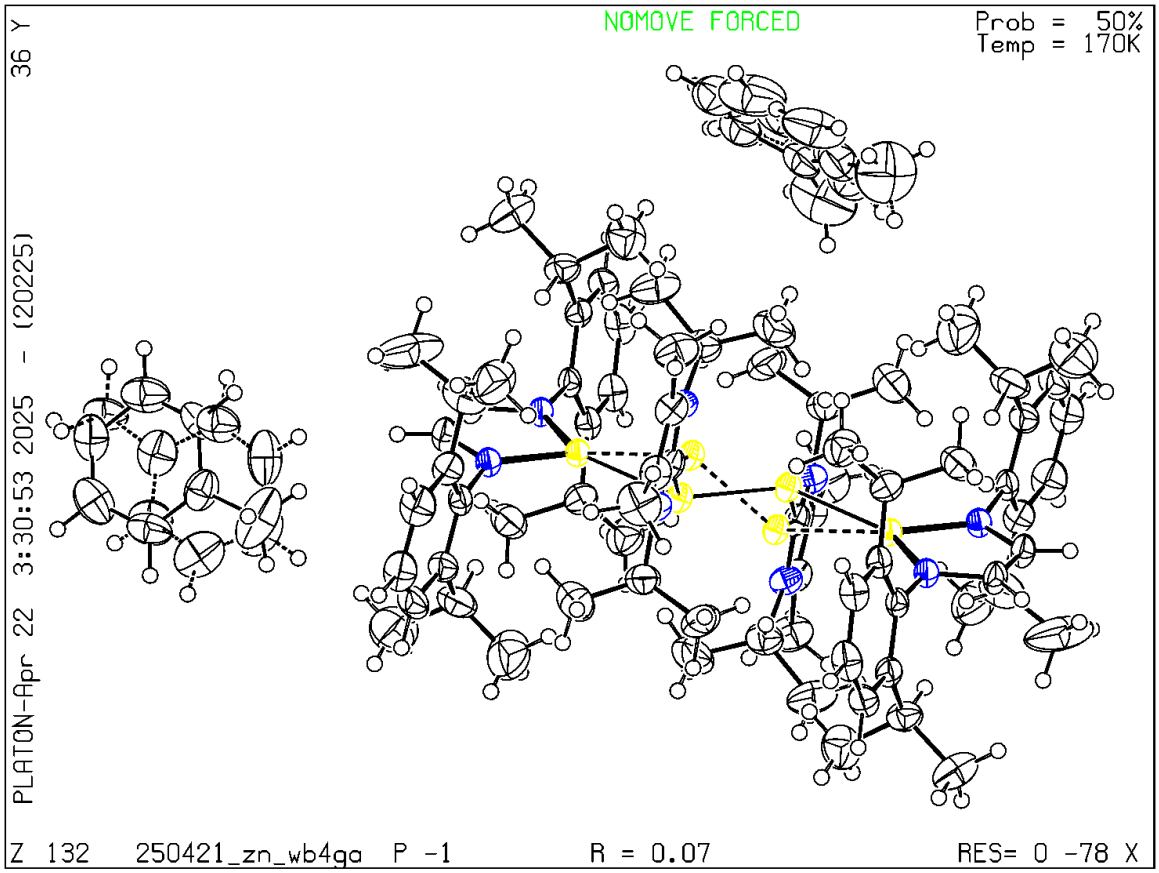
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 02/02/2025; check.def file version of 02/02/2025

Datablock 250421_zn_wb4ga - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_230330_wd_zsx0330_lanse_2

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: mo_230330_wd_zsx0330_lanse_2

```
Bond precision:   C-C = 0.0099 A          Wavelength=0.71073

Cell:             a=13.6465(7)     b=19.1173(10)        c=14.6407(8)
                  alpha=90         beta=100.627(2)      gamma=90
Temperature:      170 K

                 Calculated                Reported
Volume           3754.0(3)                 3754.0(3)
Space group      P 21/n                    P 1 21/n 1
Hall group       -P 2yn                    -P 2yn
Moiety formula   C74 H115.25 Ga4 N8        C74 H115.247 Ga4 N8
Sum formula      C74 H115.25 Ga4 N8        C74 H115.26 Ga4 N8
Mr               1395.87                   1395.88
Dx,g cm-3        1.235                     1.235
Z                2                         2
Mu (mm-1)        1.464                     1.464
F000             1478.5                    1479.0
F000'            1480.58
h,k,lmax         17,24,19                  17,24,19
Nref             8636                      8623
Tmin,Tmax        0.763,0.942               0.646,0.746
Tmin'            0.728

Correction method= # Reported T Limits: Tmin=0.646 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 27.517

R(reflections)= 0.0853( 5412)                wR2(reflections)=
                                             0.1943( 8623)
S = 1.072                  Npar= 427
```

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

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.143
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .....      0.143 Report
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT234_ALERT_4_C Large Hirshfeld Difference C21      --C22      .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21      --C22A     .       0.21 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C30 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0099 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     16.535 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.909 Check
```

Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C74 H115.2599 Ga4 N8
           Atom count from _chemical_formula_moiety:C74 H115.2469 Ga4 N8
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C74 H115.2599 Ga4 N8
           Atom count from the _atom_site data:  C74 H115.2460 Ga4 N8
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          5 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          5 Report
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      14.78 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         7% Note
PLAT303_ALERT_2_G Full Occupancy Atom H35       with # Connections       1.12 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1  )     201.25 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C16      - C21      .       1.52 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         44 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         11 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

---

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
  8 ALERT type 2 Indicator that the structure model may be wrong or deficient
  9 ALERT type 3 Indicator that the structure quality may be low
  7 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
```

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

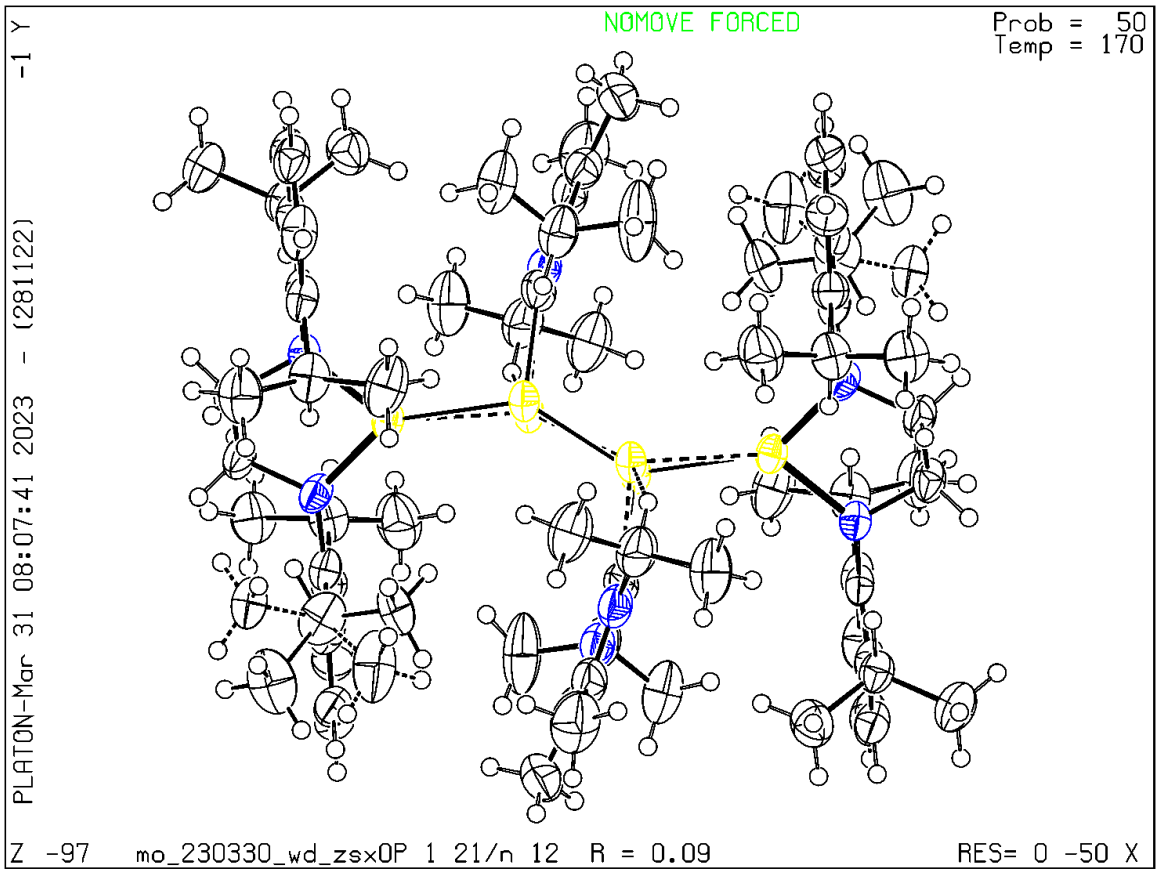
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 28/11/2022; check.def file version of 28/11/2022

Datablock mo_230330_wd_zsx0330_lanse_2 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_220527_wb0524_tolh_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: mo_220527_wb0524_tolh_0m

```
Bond precision:   C-C = 0.0033 A          Wavelength=0.71073

Cell:             a=12.6105(4)      b=15.4880(5)      c=18.2307(5)
                  alpha=90          beta=90           gamma=90
Temperature:      170 K

                 Calculated                Reported
Volume           3560.66(19)               3560.66(19)
Space group      P 21 21 21                P 21 21 21
Hall group       P 2ac 2ab                 P 2ac 2ab
Moiety formula   C37 H57 Ga N4             C37 H57 Ga N4
Sum formula      C37 H57 Ga N4             C37 H57 Ga N4
Mr               627.59                    627.58
Dx,g cm-3        1.171                     1.171
Z                4                         4
Mu (mm-1)        0.802                     0.802
F000             1352.0                    1352.0
F000'            1353.21
h,k,lmax         16,19,23                  16,19,23
Nref             7865[ 4373]               7852
Tmin,Tmax        0.721,0.786               0.628,0.746
Tmin'            0.674

Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.80/1.00        Theta(max)= 27.107

R(reflections)= 0.0222( 7451)                wR2(reflections)=
                                             0.0534( 7852)
S = 1.034                 Npar= 396
```

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

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C12 Check
PLAT410_ALERT_2_C Short Intra H...H Contact H24 ..H30 . 1.98 Ang.
x,y,z = 1_555 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report

Alert level G

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 5 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 11 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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

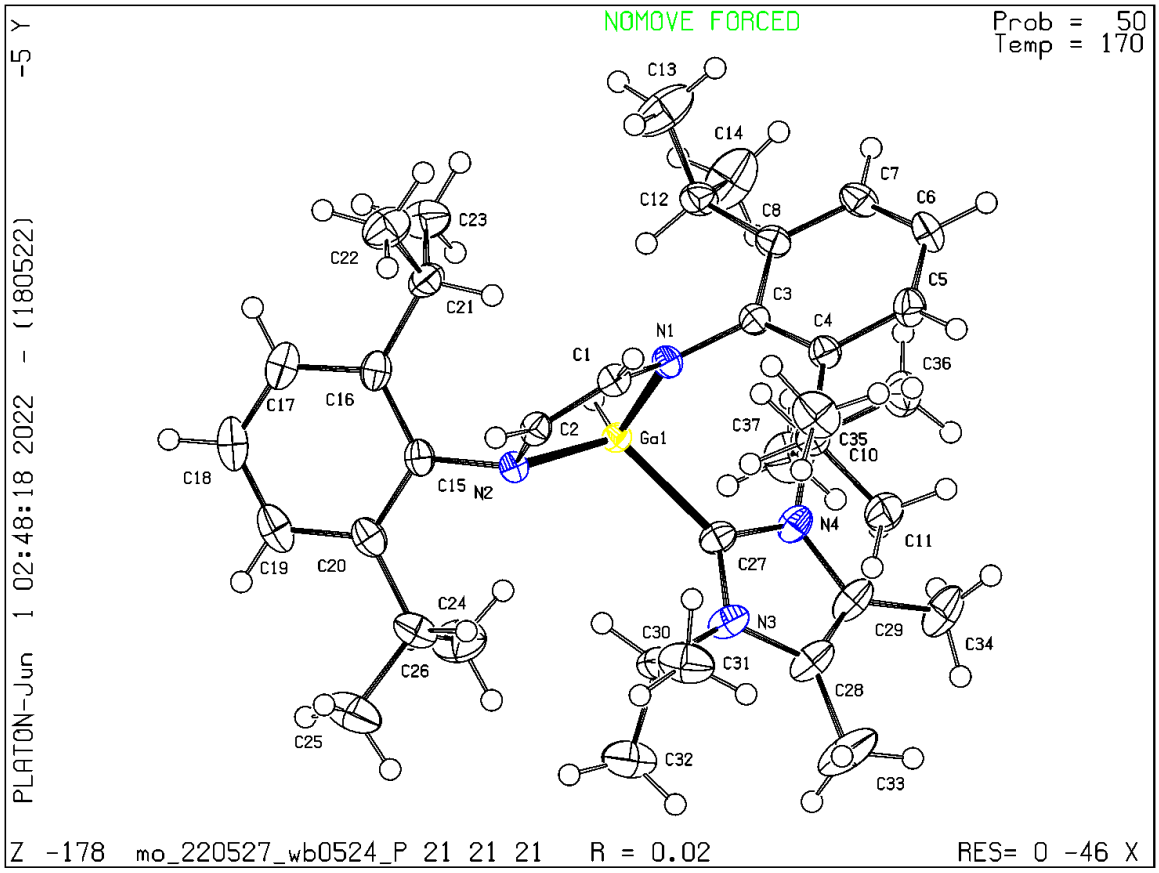
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 18/05/2022; check.def file version of 17/05/2022

Datablock mo_220527_wb0524_tolh_0m - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_221117_wb1117_bhgaz_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: mo_221117_wb1117_bhgaz_0m

```
Bond precision:   C-C = 0.0040 A          Wavelength=0.71073

Cell:             a=13.0363(6)     b=18.9681(8)         c=15.1215(6)
                  alpha=90         beta=102.014(2)      gamma=90
Temperature:      170 K

                 Calculated                Reported
Volume           3657.3(3)                 3657.3(3)
Space group      P 21/n                    P 1 21/n 1
Hall group       -P 2yn                    -P 2yn
Moiety formula   C37 H58 Ga N4             C37 H58 Ga N4
Sum formula      C37 H58 Ga N4             C37 H58 Ga N4
Mr               628.59                    628.59
Dx,g cm-3        1.142                     1.142
Z                4                         4
Mu (mm-1)        0.781                     0.781
F000             1356.0                    1356.0
F000'            1357.21
h,k,lmax         16,24,19                  16,24,19
Nref             8135                      8105
Tmin,Tmax        0.785,0.859               0.669,0.746
Tmin'            0.753

Correction method= # Reported T Limits: Tmin=0.669 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.996           Theta(max)= 27.180

R(reflections)= 0.0443( 6716)                wR2(reflections)=
                                             0.1282( 8105)
S = 1.032                 Npar= 393
```

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.54 Report
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C21 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3 Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.63Ang From C27	1.63 eA-3

Alert level G

PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	25 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	9 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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

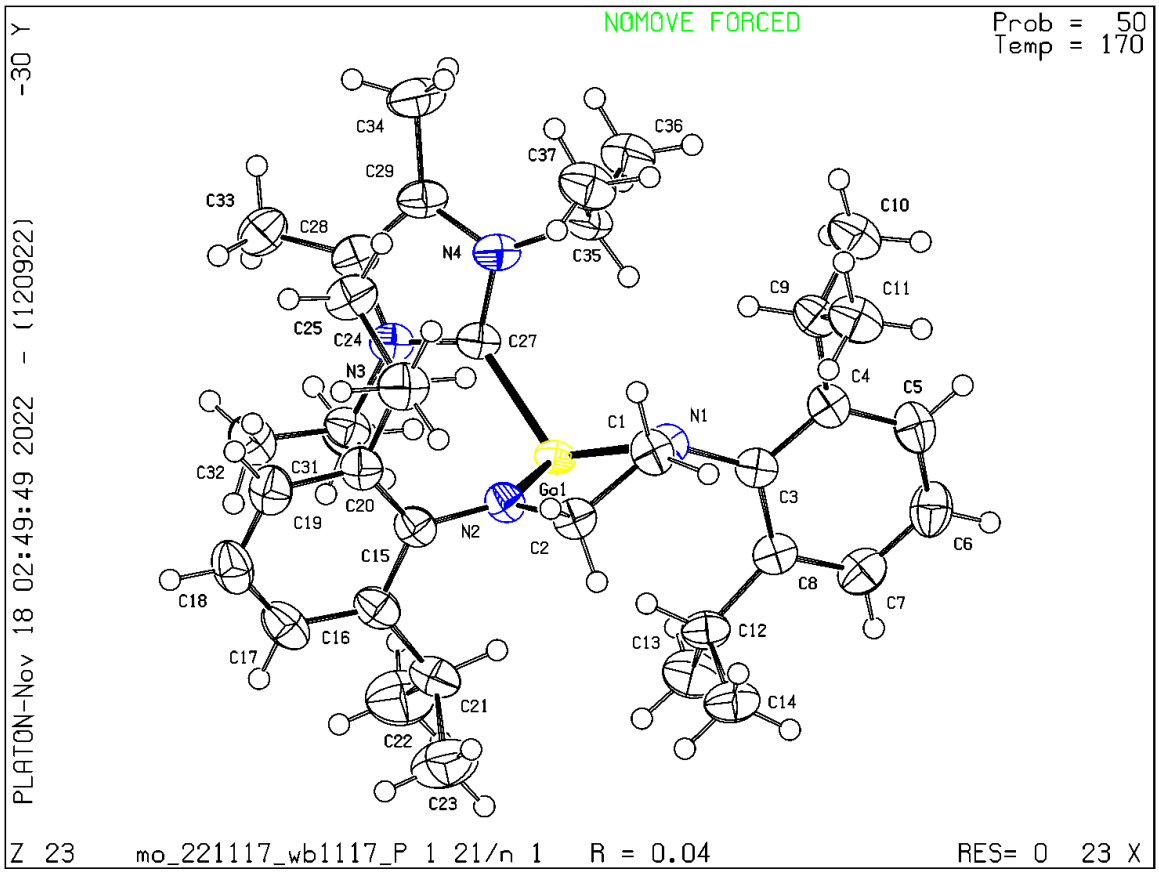
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 12/09/2022; check.def file version of 09/08/2022

Datablock mo_221117_wb1117_bhgaz_0m - ellipsoid plot



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: 241119_zn1118_wb4gai2

Bond precision: C-C = 0.0064 A Wavelength=1.34139

Cell: a=13.166(3) b=14.419(3) c=44.430(19)
alpha=91.50(3) beta=94.888(12) gamma=95.940(12)
Temperature: 170 K

	Calculated	Reported
Volume	8354(4)	8354(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C74 H112 Ga4 I2 N8, C7 H8	C74 H112 Ga4 I2 N8, C7 H8
Sum formula	C81 H120 Ga4 I2 N8	C81 H120 Ga4 I2 N8
Mr	1738.54	1738.52
Dx,g cm-3	1.382	1.382
Z	4	4
Mu (mm-1)	5.182	5.183
F000	3568.0	3568.0
F000'	3542.40	
h,k,lmax	17,18,58	17,18,57
Nref	38987	38231
Tmin,Tmax	0.830,0.856	0.680,0.752
Tmin'	0.772	

Correction method= # Reported T Limits: Tmin=0.680 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.981 Theta(max)= 61.190

R(reflections)= 0.0505(28262) wR2(reflections)= 0.1270(38231)

S = 1.054 Npar= 1817

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

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.35 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.4 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        5.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2  H   Uiso(max)/Uiso(min) Range        4.8 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C5       --C147     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C67      --C147     .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C77      --C141     .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C155     --C161     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C157     --C159     .       0.18 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C63 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C119 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C159 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C141 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C155 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    4)        2.9 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       C77     0.143 Check
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C155     - C161     .       1.36 Ang.
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         16 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         21 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         12 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3 Note
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C47      --C67      .        5.4 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C73      --C143     .        7.0 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C141     --C151     .        7.6 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         7% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H21      ..H79C     .       2.13 Ang.
                                                      x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3 Note
              H1AA    H1AB    H1AC
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
              C7 H8
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
```

```
              C7 H8
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        211 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        200 Note
                -3  6  7,  -2  3 11,   1 -3  2,   0  0  2,   2  0  2,   2 -2 14,
                 2 -1 11,  -4  1  1,   2 -4  4,  -1  0  1,  -1  1  8,   0 -1  1,
                 1  4  7,   2  1 11,  -2 -1  1, -17  3  0,  -3  1  6,   4  2  2,
                 4 -1  1,   2 -2 10,  -1 -4 11,  -2 -4 14,  -2  1 13,  -3  0 13,
                -3  0 17,   6 -2  8,   2  2  6,  -2  3  3,   0  0 24,   0  0 14,
                -5  0  3,   1 -6  3,   2 -3  9,   1  3 12,  -3  1 18,   0 -5  7,
                -4  5 11,  -5 -1 12,  -6  3  3,   3 -3  4,  -3  1 12,   4  4  0,
                -4  1 17,   2  6  2,   4  3  3,   1  4  1,  -1 -1  8,   1 -7  2,
                -3 -4  5,   6  0  6,
```

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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  12 ALERT type 2 Indicator that the structure model may be wrong or deficient
  13 ALERT type 3 Indicator that the structure quality may be low
  18 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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

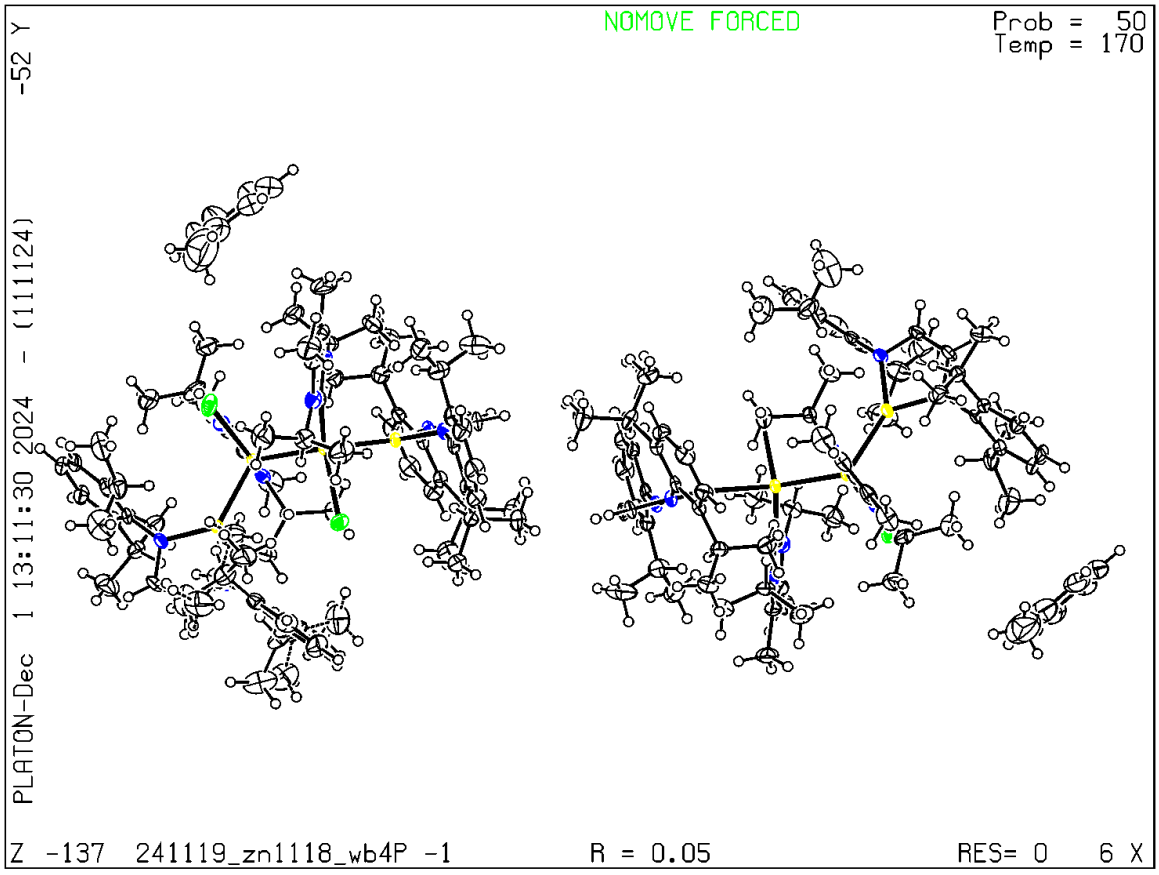
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 11/11/2024; check.def file version of 11/11/2024

Datablock 241119_zn1118_wb4gai2 - ellipsoid plot



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: 241119_zn_1118_wb4gass

```
Bond precision:   C-C = 0.0063 A          Wavelength=1.34139

Cell:             a=22.905(4)     b=13.390(2)          c=28.905(5)
                  alpha=90        beta=105.023(6)      gamma=90
Temperature:      170 K
```

	Calculated	Reported
Volume	8562(2)	8562(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C86 H122 Ga4 N8 S2	C86 H122 Ga4 N8 S2
Sum formula	C86 H122 Ga4 N8 S2	C86 H122 Ga4 N8 S2
Mr	1610.92	1610.91
Dx,g cm-3	1.250	1.250
Z	4	4
Mu (mm-1)	1.476	1.476
F000	3400.0	3400.0
F000'	3376.56	
h,k,lmax	29,17,37	29,17,37
Nref	10014	9880
Tmin,Tmax	0.899,0.943	0.650,0.728
Tmin'	0.889	

```
Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.728
AbsCorr = MULTI-SCAN

Data completeness= 0.987           Theta(max)= 61.204

R(reflections)= 0.0528( 8024)                    wR2(reflections)=
                                                 0.1660( 9880)
S = 1.122                  Npar= 465
```

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

```
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.4 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00634 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H2       ..H2       .       2.11 Ang.
                                              1-x,1-y,1-z  =      5_666 Check
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
               not performed for this radiation type.
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      15.56 Why ?
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         35 Note
             -18  6  5, -16  4  1, -15  3  2, -13  1 14,  -7  1  3,  -6  2  2,
              -5  7  3,  -4  4 13,  -3  7  6,  -2  2  1,  -2  4  9,  -2  4 11,
              -2  6  6,  -2  6  7,  -2 10  5,  -1  3  6,  -1  5  5,  -1  5 11,
              -1  7  2,  -1  9  4,   0  0  2,   0 12  3,   2  4  2,   3  1 12,
               3  3  0,   3  5  0,   3  9  7,   3 11  0,   6  4  5,   6  4  7,
               7  5  0,   9  7  0,   9  9 10,  11  3 10,  13  1  0,
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **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
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

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

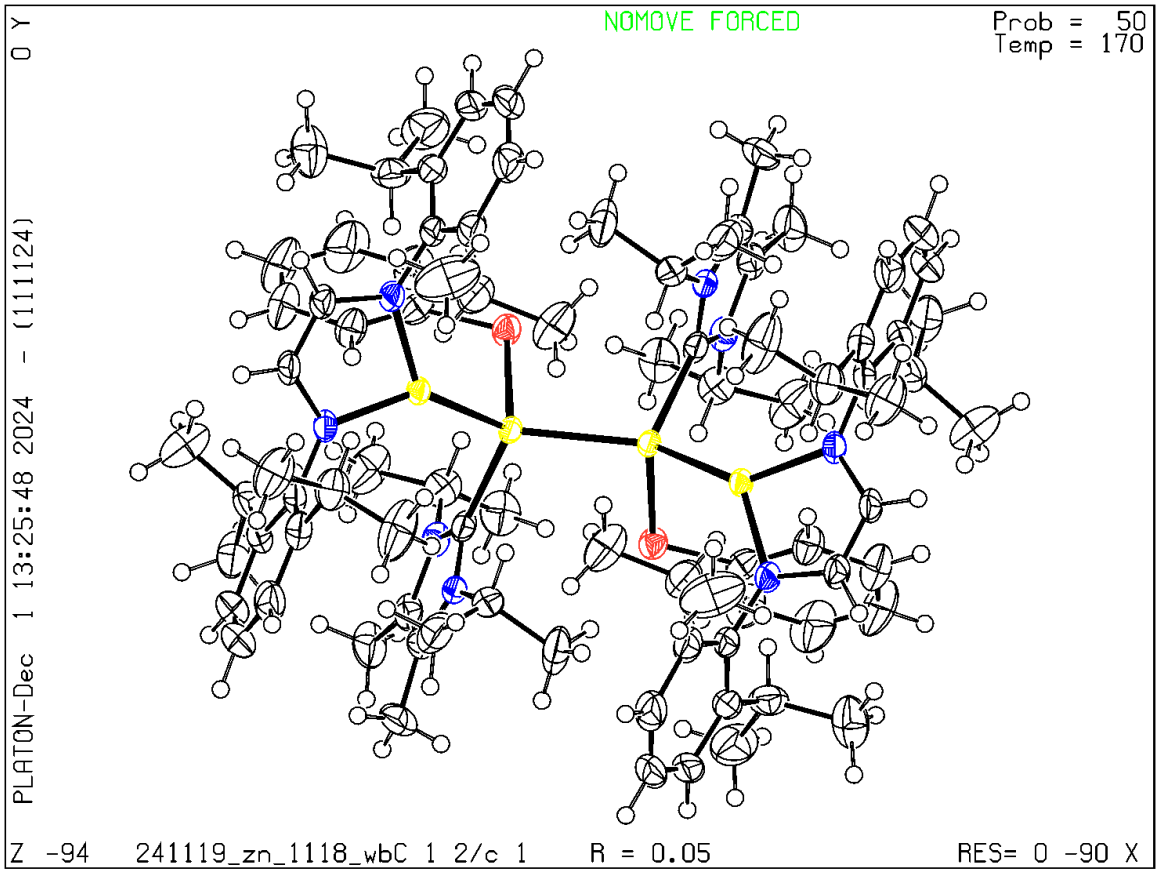
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 11/11/2024; check.def file version of 11/11/2024

Datablock 241119_zn_1118_wb4gass - ellipsoid plot



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: 241120_zn1118_wb4gaph3ps

Bond precision: C-C = 0.0078 A Wavelength=1.34139

Cell: a=13.2381(10) b=14.6550(11) c=21.4397(16)
alpha=93.237(3) beta=99.157(3) gamma=99.405(3)
Temperature: 170 K

	Calculated	Reported
Volume	4036.6(5)	4036.6(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C74 H112 Ga4 N8 S, 0.5(C6 H14)	2(C37 H56 Ga2 N4 S0.5), 0.5(C6 H14)
Sum formula	C77 H119 Ga4 N8 S	C77 H119 Ga4 N8 S
Mr	1467.74	1467.73
Dx,g cm-3	1.208	1.208
Z	2	2
Mu (mm-1)	1.377	1.377
F000	1554.0	1554.0
F000'	1541.46	
h,k,lmax	17,19,27	17,19,27
Nref	18612	18364
Tmin,Tmax	0.906,0.946	0.668,0.752
Tmin'	0.896	

Correction method= # Reported T Limits: Tmin=0.668 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 60.771

R(reflections)= 0.0758(12286) wR2(reflections)= 0.1782(18364)

S = 1.059 Npar= 1107

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

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C74 H112 Ga4 N8 S, 0.5(C6 H14)
             Rep.: 2(C37 H56 Ga2 N4 S0.5), 0.5(C6 H14)
PLAT213_ALERT_2_C Atom Ga4A            has ADP max/min Ratio .....        3.7 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        4.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2  H   Uiso(max)/Uiso(min) Range        5.0 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C24 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C46 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C49 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C58 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd    3)        2.8 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       C75      0.267 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00776 Ang.
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
              not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         64 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         60 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      10.80 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.003 Degree
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         70 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          4 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     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
```

```
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used     0.0400 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............       0.5 Check
              S1      S2      C75     C76     C77     C78     C79     C80
              H75A    H75B    H75C    H76A    H76B    H77A    H77B    H78A
              H78B    H79A    H79B    H80A    H80B    H80C
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        31% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    2)        31% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)       100% Note
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H25B     ..H75A     .       1.66 Ang.
                                               -1+x,-1+y,z  =      1_445 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H50A     ..H75B     .       2.13 Ang.
                                                2-x,2-y,-z  =      2_775 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H51A     ..H75B     .       2.04 Ang.
                                                2-x,2-y,-z  =      2_775 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H51C     ..H75B     .       1.48 Ang.
                                                2-x,2-y,-z  =      2_775 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C25      ..C75      .       3.12 Ang.
                                               -1+x,-1+y,z  =      1_445 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C51      ..C75      .       2.94 Ang.
                                                2-x,2-y,-z  =      2_775 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        20 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers         1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       903 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File       100 Note
             -10  0  2,  -9 -1  2,  -6 -3  6,  -6 -2  4,  -6  2  6,  -6  5  5,
              -5 -5  5,  -5 -4  6,  -5  2  0,  -4 -1  6,  -3 -3  1,  -3  3  3,
              -2 -4  2,  -2  4  2,  -2  4  3,  -2  4  4,  -1 -8  2,  -1 -3  1,
              -1  0  1,  -1  0  2,  -1  2  4,  -1  2  6,   0 -2  1,   0  0  1,
               0  1  3,   0  3  4,   1 -5  1,   1 -3  7,   1  0  0,   1  0  4,
               1  3  0,   1  3  3,   1  3  5,   1  4  2,   2 -3  1,   2  0  3,
               2  1  0,   2  1  2,   2  3  1,   2  4  2,   3 -4  1,   3  1  0,
               3  2  2,   4 -2  6,   4  0  2,   5 -2  2,   5  1  4,   5  4  3,
               7 -4  7,   7  1  4,
```

---

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
 64 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 22 ALERT type 2 Indicator that the structure model may be wrong or deficient
 45 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
```

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

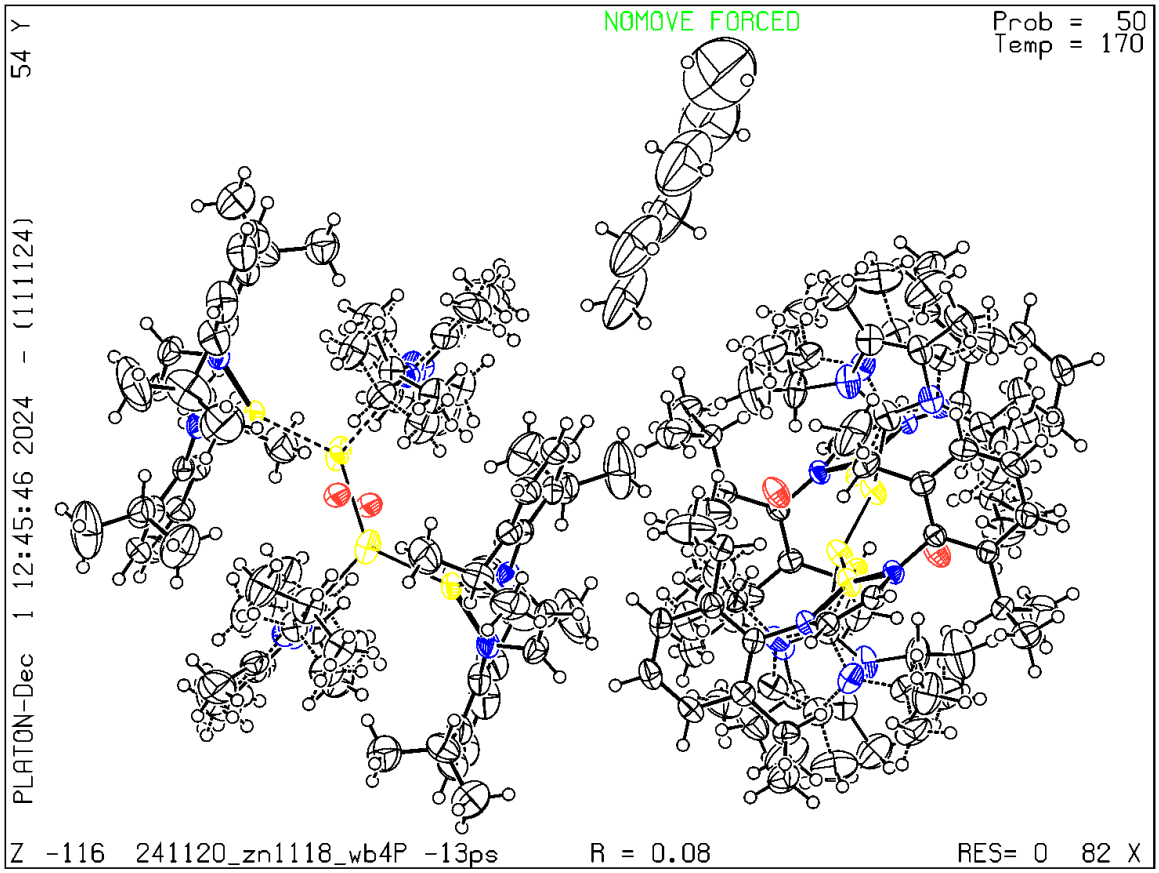
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 11/11/2024; check.def file version of 11/11/2024

Datablock 241120_zn1118_wb4gaph3ps - ellipsoid plot



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: 241015_cwh_wb4gaph2co

Bond precision: C-C = 0.0065 A Wavelength=1.34139

Cell: a=23.9327(14) b=16.5933(10) c=23.8819(14)
alpha=90 beta=109.544(2) gamma=90

Temperature: 170 K

	Calculated	Reported
Volume	8937.6(9)	8937.6(9)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C87 H122 Ga4 N8 O), C4 H10 O	C87 H122 Ga4 N8 O, 0.5(C4 H10 O)
Sum formula	C178 H254 Ga8 N16 O3	C89 H127 Ga4 N8 O1.50
Mr	3223.75	1611.86
Dx,g cm-3	1.198	1.198
Z	2	4
Mu (mm-1)	1.140	1.140
F000	3412.0	3412.0
F000'	3386.59	
h,k,lmax	31,21,31	31,21,30
Nref	20618	20477
Tmin,Tmax	0.896,0.955	0.680,0.752
Tmin'	0.862	

Correction method= # Reported T Limits: Tmin=0.680 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 60.772

R(reflections)= 0.0671(15665) wR2(reflections)= 0.1862(20477)

S = 1.046 Npar= 1001

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

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: 2(C87 H122 Ga4 N8 O), C4 H10 O
             Rep.: C87 H122 Ga4 N8 O, 0.5(C4 H10 O)
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.0 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C17      --C18      .        6.3 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C30 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C82 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O3      0.133 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00651 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C38      - C45      .       1.53 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H56C     ..H57A     .       1.80 Ang.
                                                    x,y,z  =      1_555 Check
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
              not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          8 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms           9 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      18.21 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par     0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0020 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
             O3      C1A     C1B     C1C     C1D     H1AA    H1AB    H1AC
             H1BA    H1BB    H1CA    H1CB    H1DA    H1DB    H1DC
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         7% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    2)       7.50 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C33 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C34 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C57 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C58 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H68      ..H75F     .       2.05 Ang.
                                                    x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         10 Note
             H1AA    H1AB    H1AC    H1BA    H1BB    H1CA    H1CB    H1DA
             H1DB    H1DC
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      42.80 Deg.
             O1   -C38  -GA3A    1_555   1_555   1_555 ......     #  247 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         15 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
```

```
             C4 H10 O
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         47 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          50 Note
                1  0  0,   2  0  2,  -1  1  1,   2  1  1,   0  1  1,   1  2  3,
               -2  1  1,  -1  3  1,   1  1  1,   3  1  2,   2 18 15,  -2  0  4,
                2  1  2,  -2  2  1,   3  2  7,   2  0  4,  -3  1  1,   1  3  1,
               -2  1  3,  -4  1  3,  -5  0 30,   4  1  1,   0  4 12,   1  1  3,
                3  1  0,   2  2  1,   5  2  3,  -3  1  5,  -2  1  5,   0  5  1,
               -9  1  4,  -7  6  6,   3  4  1,  -1  7  8,   3  7  2,   3  1  1,
               -4  0  4,   6  3  3,  -4  5  3,   7  6  3,   0  1  3,   4  4  9,
                3  0 28,   0  2  3,   5  5  1,  -1  1  5,  -8  7  4,  -4  8  5,
               -6  6  5,   3  5  4,
```

---

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
29 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
17 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

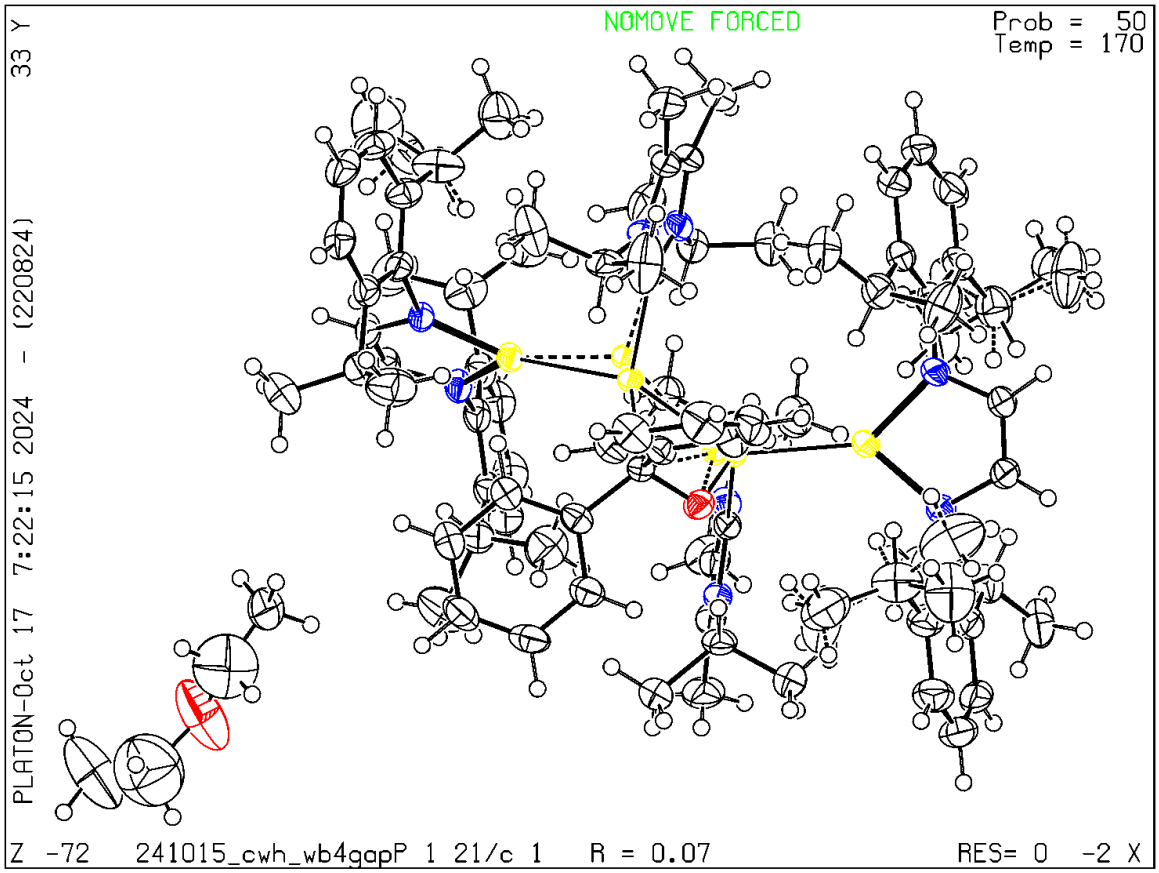
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 22/08/2024; check.def file version of 21/08/2024

Datablock 241015_cwh_wb4gaph2co - ellipsoid plot