checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4b, 4c, 4d, 5

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: 4b

Bond precision: C-C = 0.0087 A Wavelength=0.71073

Cell: a=13.499(5) b=21.049(8) c=19.661(7)
alpha=90 beta=100.305(5) gamma=90
Temperature: 153 K

	Calculated	Reported
Volume	5496(4)	5496(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C54 H88 Ga N6 Na O3	?
Sum formula	C54 H88 Ga N6 Na O3	C54 H92 Ga N6 Na O3
Mr	962.01	966.04
Dx,g cm-3	1.163	1.167
Z	4	4
Mu (mm-1)	0.554	0.554
F000	2080.0	2096.0
F000'	2081.61	
h,k,lmax	16,25,23	16,25,23
Nref	9927	9806
Tmin,Tmax	0.895,0.905	0.141,0.745
Tmin'	0.895	

Correction method= # Reported T Limits: Tmin=0.141 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.988 Theta(max)= 25.229

R(reflections)= 0.0794(8055) wR2(reflections)= 0.2123(9806)

S = 1.164 Npar= 610

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

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..      4.03 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT220_ALERT_2_C NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range       5.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       4.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C44      --C45      .      0.20 Ang.
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C43 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C50 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of         O1 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for ..........       C45 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for ..........      C46A Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00874 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H31      ..H34      .      1.91 Ang.
                                                     x,y,z  =     1_555 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       121 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.06A   From C45A           0.66 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H44A            -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H47B            -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H52A            -0.33 eA-3
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Alert level G

```
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:C54 H92 Ga1 N6 Na1 O3
           Atom count from the _atom_site data:  C54 H88 Ga1 N6 Na1 O3
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C54 H92 Ga N6 Na O3
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        216.00    216.00    0.00
          H        368.00    352.00   16.00
          Ga         4.00      4.00    0.00
          N         24.00     24.00    0.00
          Na         4.00      4.00    0.00
          O         12.00     12.00    0.00
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     26.67 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C45        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C45A       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C46        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C46A       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         3% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C43      - C44      .       1.51 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C45      --C46A            1.85 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C46      --C45A            1.71 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        222 Check
             C46  -C45  -C46A    1.555   1.555   1.555             26.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        228 Check
             C45  -C46  -C45A    1.555   1.555   1.555             35.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        279 Check
             C46A -C45A -C46     1.555   1.555   1.555             29.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        285 Check
             C45A -C46A -C45     1.555   1.555   1.555             32.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        316 Check
             C46A -O1   -C46     1.555   1.555   1.555             33.30 Deg.
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        68% Note
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PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 6 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 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
18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
21 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 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
13 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: 4c

Bond precision: C-C = 0.0090 A Wavelength=0.71073

Cell: a=20.165(5) b=15.683(3) c=22.026(5)
alpha=90 beta=109.960(3) gamma=90
Temperature: 153 K

	Calculated	Reported
Volume	6547(3)	6547(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C66 H108 Ga N6 Na O3	?
Sum formula	C66 H108 Ga N6 Na O3	C66 H108 Ga N6 Na O3
Mr	1126.30	1126.29
Dx,g cm-3	1.143	1.143
Z	4	4
Mu (mm-1)	0.474	0.474
F000	2448.0	2448.0
F000’	2449.73	
h,k,lmax	23,18,25	23,18,25
Nref	11209	11048
Tmin,Tmax	0.892,0.910	0.257,0.745
Tmin’	0.847	

Correction method= # Reported T Limits: Tmin=0.257 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.986 Theta(max)= 24.761

R(reflections)= 0.0645(6076) wR2(reflections)= 0.1525(11048)

S = 1.066 Npar= 706

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 B

```
PLAT220_ALERT_2_B NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range        6.5 Ratio
PLAT410_ALERT_2_B Short Intra H...H Contact  H36      ..H42      .       1.88 Ang.
                                                    x,y,z  =      1_555 Check
```

Alert level C

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5893
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        6.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C36      --C37      .        5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C38      --C39      .       0.16 Ang.
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C51 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C53 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C57 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C60 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C61 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C63 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C65 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of         O3 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C14 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C23 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C36 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C42 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        C52 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C59 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00898 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C61      - C62      .       1.37 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.495 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.589        158 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.00 Why ?
PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder           ! Report
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         43 Note
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          2 Check
```

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   0 ALERT level A = Most likely a serious problem - resolve or explain
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  24 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

   0 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
   6 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: 4d

Bond precision: C-C = 0.0082 A Wavelength=0.71073

Cell: a=20.293(12) b=13.197(8) c=26.694(16)
       alpha=90 beta=98.225(8) gamma=90
Temperature: 153 K

	Calculated	Reported
Volume	7075(7)	7076(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C70 H116 Ga K N6 O4	?
Sum formula	C70 H116 Ga K N6 O4	C70 H116 Ga K N6 O4
Mr	1214.52	1214.50
Dx,g cm-3	1.140	1.140
Z	4	4
Mu (mm-1)	0.496	0.496
F000	2640.0	2640.0
F000'	2642.49	
h,k,lmax	24,15,31	24,15,31
Nref	12657	12467
Tmin,Tmax	0.888,0.910	0.413,0.745
Tmin'	0.883	

Correction method= # Reported T Limits: Tmin=0.413 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.985 Theta(max)= 25.140

R(reflections)= 0.0597(7992) wR2(reflections)= 0.1903(12467)

S = 1.126 Npar= 749

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 B

PLAT230_ALERT_2_B Hirshfeld Test Diff for O3 --C66 . 7.2 s.u.
PLAT410_ALERT_2_B Short Intra H...H Contact H31 ..H37 . 1.85 Ang.
x,y,z = 1_555 Check

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 4.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C60 --C61 . 5.6 s.u.

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PLAT230_ALERT_2_C Hirshfeld Test Diff for    C69      --C70      .        5.3 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O2       --C62      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C61      --C62      .       0.21 Ang.
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of         O2 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C47 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C55 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C58 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C62 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C63 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C65 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C66 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C69 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C70 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of         K1 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of         O3 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of         O4 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C11 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C23 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C57 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C64 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C68 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00819 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C55      - C56      .       1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C57      - C58      .       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C60      - C61      .       1.36 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C64      - C65      .       1.39 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C67      - C69      .       1.36 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H39B     ..H69A     .       2.05 Ang.
                                       1-x,-1/2+y,3/2-z  =      2_646 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -2.268 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.598        189 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
```

Alert level G

```
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        273 Check
             K1   -C53  -H53B    1.555   1.555   1.555             28.50 Deg.
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        32% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          9 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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  34 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
  31 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: 5

Bond precision: C-C = 0.0085 A Wavelength=0.71073

Cell:	a=13.577(2)	b=13.777(2)	c=18.806(3)
	alpha=83.432(2)	beta=89.491(2)	gamma=89.466(2)
Temperature:	123 K		

	Calculated	Reported
Volume	3494.3(9)	3494.3(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C61 H89 Ga N4 Na O2 [+ solvent]	?
Sum formula	C61 H89 Ga N4 Na O2 [+ solvent]	C68 H98 Ga N4 Na O2
Mr	1003.07	1096.21
Dx,g cm-3	0.953	1.042
Z	2	2
Mu (mm-1)	0.436	0.441
F000	1082.0	1184.0
F000’	1082.82	
h,k,lmax	16,16,22	16,16,22
Nref	12323	11929
Tmin,Tmax	0.896,0.916	0.439,0.745
Tmin’	0.896	

Correction method= # Reported T Limits: Tmin=0.439 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.968 Theta(max)= 25.005

R(reflections)= 0.0662(8830) wR2(reflections)= 0.1658(11929)

S = 1.170 Npar= 631

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 B

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range 7.9 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for C54 --C55 . 7.4 s.u.
PLAT241_ALERT_2_B High MainMol Ueq as Compared to Neighbors of C56 Check
PLAT241_ALERT_2_B High MainMol Ueq as Compared to Neighbors of C58 Check
PLAT241_ALERT_2_B High MainMol Ueq as Compared to Neighbors of C61 Check
PLAT242_ALERT_2_B Low MainMol Ueq as Compared to Neighbors of O2 Check
PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note

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Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.968 Why?
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O2 --C61 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14 --C16 . 0.18 Ang.

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PLAT234_ALERT_4_C Large Hirshfeld Difference C55      --C56      .       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C56      --C57      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C59      --C60      .       0.21 Ang.
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of        C55 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        Na1 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of         O1 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C11 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C14 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C23 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C26 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C36 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C39 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C48 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C51 Check
PLAT242_ALERT_2_C Low    MainMol Ueq as Compared to Neighbors of        C57 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Ga1      0.104 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00854 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C54      - C55      .       1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C55      - C56      .       1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C59      - C60      .       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C60      - C61      .       1.42 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595        392 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          2 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H61A            -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H61B            -0.36 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
```

Alert level G

```
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:C68 H98 Ga1 N4 Na1 O2
           Atom count from the _atom_site data:  C61 H89 Ga1 N4 Na1 O2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C68 H98 Ga N4 Na O2
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        136.00    122.00   14.00
           H        196.00    178.00   18.00
           Ga         2.00      2.00    0.00
           N          8.00      8.00    0.00
           Na         2.00      2.00    0.00
           O          4.00      4.00    0.00
PLAT013_ALERT_1_G N.O.K.   _shelx_hkl_checksum Found in CIF ......     Please Check
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         -2 Units
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        49% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          9 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          1 Check
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  7 ALERT level B = A potentially serious problem, consider carefully
 31 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

  8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 28 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
  8 ALERT type 4 Improvement, methodology, query or suggestion
  2 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

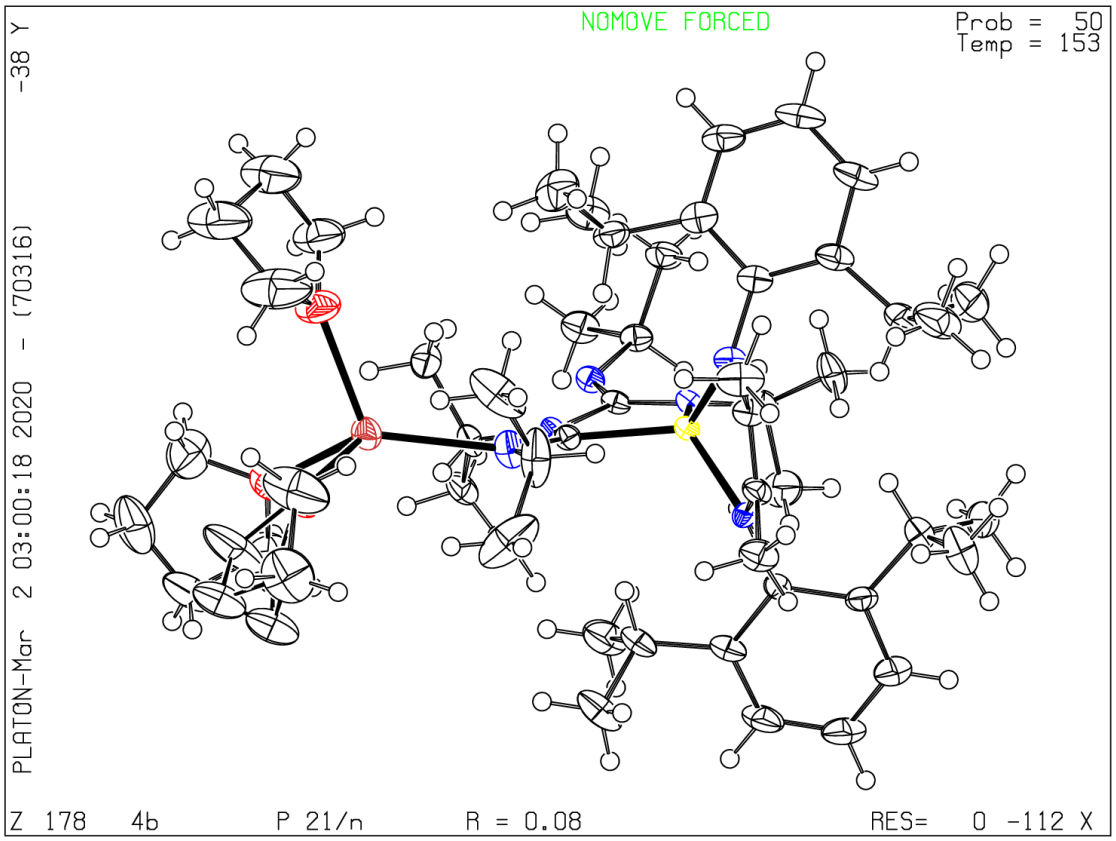
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

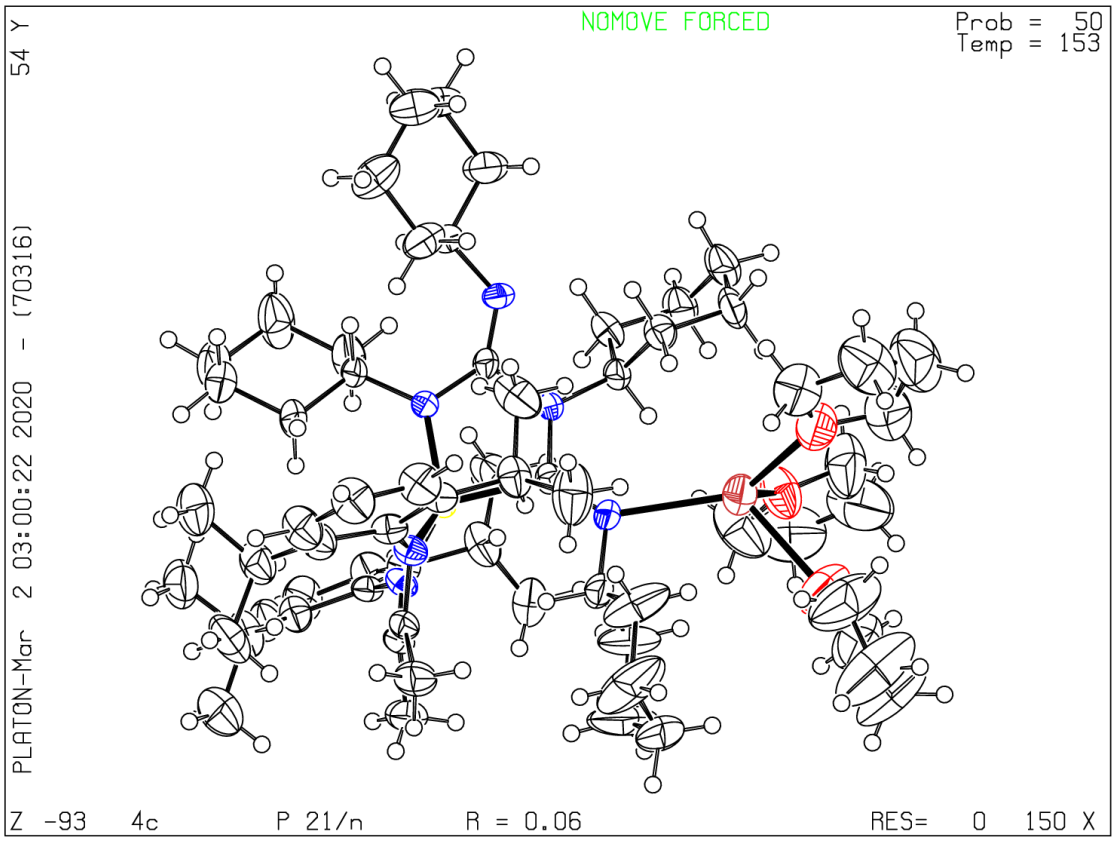
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/12/2019; check.def file version of 13/12/2019

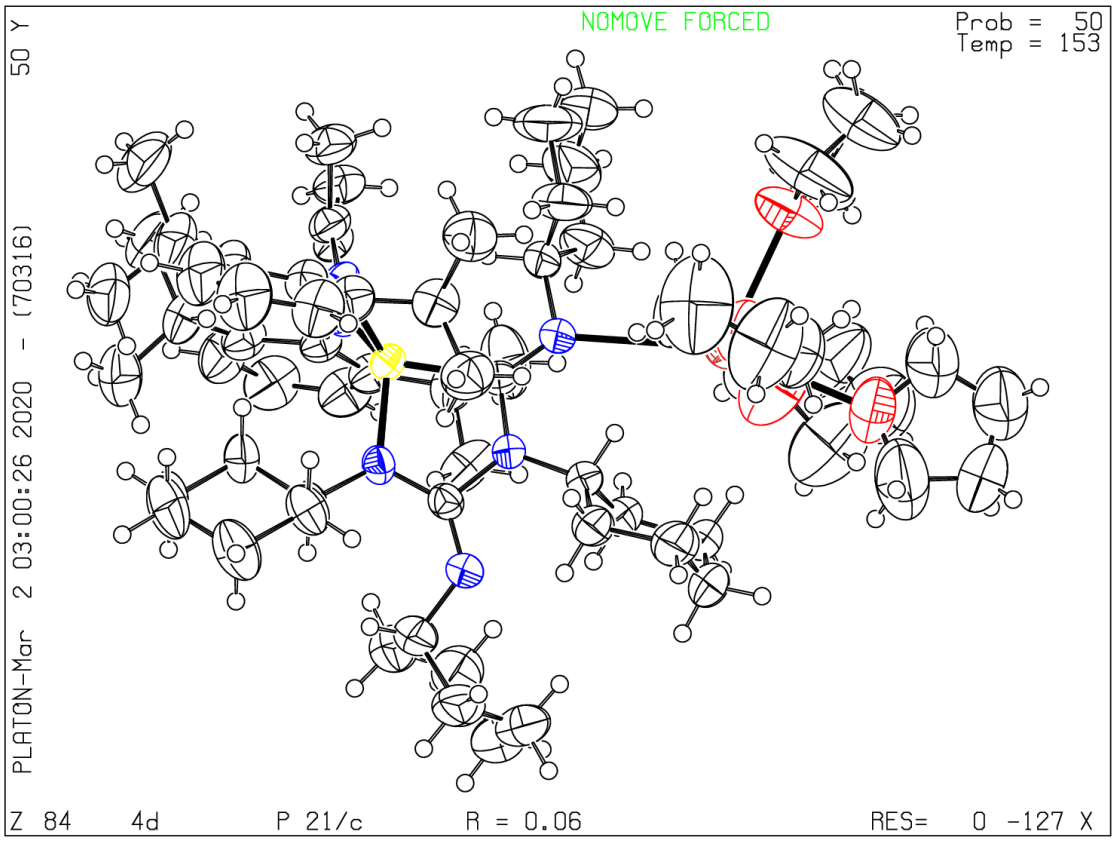
Datablock 4b - ellipsoid plot



Datablock 4c - ellipsoid plot



Datablock 4d - ellipsoid plot



Datablock 5 - ellipsoid plot