checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mw_163_2m, mw_163_3m, mw_163_4_tw4, mw_172_2fsam

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: mw_163_3m

```
Bond precision:   C-C = 0.0023 A          Wavelength=1.54178

Cell:             a=20.0030(6)    b=19.8324(6)          c=17.6419(6)
                  alpha=90        beta=115.0312(14)     gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           6341.3(4)                 6341.3(4)
Space group      C 2/c                     C 2/c
Hall group       -C 2yc                    -C 2yc
Moiety formula   C33 H47 Ga N2 O2          ?
Sum formula      C33 H47 Ga N2 O2          C33 H47 Ga N2 O2
Mr               573.45                    573.44
Dx,g cm-3        1.201                     1.201
Z                8                         8
Mu (mm-1)        1.406                     1.406
F000             2448.0                    2448.0
F000'            2443.29
h,k,lmax         25,25,22                  25,25,22
Nref             6929                      6890
Tmin,Tmax        0.744,0.902               0.570,0.750
Tmin'            0.677

Correction method= # Reported T Limits: Tmin=0.570 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.994           Theta(max)= 80.051

R(reflections)= 0.0297( 5743)                wR2(reflections)=
                                             0.0766( 6890)
S = 1.026                  Npar= 376
```

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

```
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         34 Ang**3
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       6.08 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         8% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C33 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H5C      ..H25D     .       2.13 Ang.
                                                    x,y,z  =      1_555 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        18 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         40 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         14 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 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
   6 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: mw_163_2m

```
Bond precision:   C-C = 0.0073 A          Wavelength=0.71073

Cell:             a=22.8793(14)     b=17.9690(11)     c=19.4578(12)
                  alpha=90          beta=90           gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	7999.5(8)	7999.5(9)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C37 H53 Ga N2 O4, C6 H6	?
Sum formula	C43 H59 Ga N2 O4	C43 H59 Ga N2 O4
Mr	737.64	737.64
Dx,g cm-3	1.225	1.225
Z	8	8
Mu (mm-1)	0.730	0.730
F000	3152.0	3152.0
F000'	3154.85	
h,k,lmax	35,27,29	35,27,29
Nref	30669[15724]	30570
Tmin,Tmax	0.810,0.869	0.670,0.750
Tmin'	0.763	

Correction method= # Reported T Limits: Tmin=0.670 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 1.94/1.00 Theta(max)= 33.217

R(reflections)= 0.0487(23517) wR2(reflections)= 0.1290(30570)

S = 1.059 Npar= 1128

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

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 3 Check

Author Response: Formation of ice, background scattering by mounting material

---

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.398
From the CIF: _refine_ls_abs_structure_Flack_su 0.012
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.16 Report
PLAT213_ALERT_2_C Atom C8_1 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C34'_1 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C13'_2 has ADP max/min Ratio ..... 3.6 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.9 Ratio

```
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        5.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2  H   Uiso(max)/Uiso(min) Range        5.9 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O1_1     --C31'_1   .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11_1    --C15'_1   .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C7_2     --C12_2    .       0.21 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C8_1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C4_4 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.4 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.2 Note
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C1_3     --C6_3     .       1.37 Ang.
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C1_4     --C6_4     .       1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0073 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          8 Report
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         50 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          6 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       6.60 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         11 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          4 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C7_2     --C12'_2   .        5.4 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        30% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  2  )         7% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       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  3  )       8.63 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5  )       3.37 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H10_1    ..H17F_1   .       2.10 Ang.
                                                      x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H13B_1   ..H36F_1   .       1.78 Ang.
                                                      x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H28B_1   ..H35E_1   .       1.67 Ang.
                                                      x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H4B_2    ..H14C_2   .       2.04 Ang.
                                                      x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H8_2     ..H13F_2   .       2.06 Ang.
                                                      x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H13B_2   ..H34C_2   .       2.05 Ang.
                                                      x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H17B_2   ..H17E_1   .       1.99 Ang.
                                                   1-x,1-y,1/2+z  =      2_665 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H35B_2   ..H2_3     .       2.11 Ang.
                                                      x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........        272 Note
PLAT792_ALERT_1_G Model has Chirality at C31_1       (Polar  SPGR)         S Verify
PLAT792_ALERT_1_G Model has Chirality at C32_1       (Polar  SPGR)         R Verify
PLAT792_ALERT_1_G Model has Chirality at C31_2       (Polar  SPGR)         S Verify
PLAT792_ALERT_1_G Model has Chirality at C32_2       (Polar  SPGR)         R Verify
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       691 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         34 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         4 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         6 Info
```

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

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

Datablock: mw_172_2fsam

```
Bond precision:   C-C = 0.0019 A          Wavelength=1.54178

Cell:             a=12.9494(6)     b=20.0900(9)        c=13.6605(6)
                  alpha=90         beta=97.216(2)      gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           3525.7(3)                 3525.7(3)
Space group      P 21/n                    P 21/n
Hall group       -P 2yn                    -P 2yn
Moiety formula   C41 H47 Al N2 O2          ?
Sum formula      C41 H47 Al N2 O2          C41 H47 Al N2 O2
Mr               626.79                    626.78
Dx,g cm-3        1.181                     1.181
Z                4                         4
Mu (mm-1)        0.782                     0.782
F000             1344.0                    1344.0
F000'            1348.25
h,k,lmax         16,25,17                  16,25,17
Nref             7748                      7713
Tmin,Tmax        0.898,0.915               0.660,0.750
Tmin'            0.817

Correction method= # Reported T Limits: Tmin=0.660 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.995          Theta(max)= 80.605

R(reflections)= 0.0358( 6532)                wR2(reflections)=
                                             0.0963( 7713)
S = 1.029                 Npar= 425
```

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

```
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           crimson
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.9 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.2 Ratio
```

Alert level G

```
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Al1      --O1       .        6.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Al1      --O2       .        6.5 s.u.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      44.79 Deg.
             O1   -C30  -AL1     1_555   1_555   1_555 ......     #   71 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      44.66 Deg.
             O2   -C31  -AL1     1_555   1_555   1_555 ......     #   77 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.96 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         35 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         15 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
   8 ALERT level G = General information/check it is not something unexpected

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

Datablock: mw_163_4_tw4

```
Bond precision:   C-C = 0.0028 A          Wavelength=0.71073

Cell:             a=10.685(5)     b=20.803(10)          c=17.129(8)
                  alpha=90        beta=107.264(13)      gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	3636(3)	3636(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C41 H47 Ga N2 O2	?
Sum formula	C41 H47 Ga N2 O2	C41 H47 Ga N2 O2
Mr	669.53	669.52
Dx,g cm-3	1.223	1.223
Z	4	4
Mu (mm-1)	0.793	0.793
F000	1416.0	1416.0
F000'	1417.33	
h,k,lmax	16,32,26	16,32,26
Nref	14067	13884
Tmin,Tmax	0.744,0.871	0.660,0.750
Tmin'	0.729	

Correction method= # Reported T Limits: Tmin=0.660 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 33.320

R(reflections)= 0.0443(9964) wR2(reflections)= 0.1349(13884)

S = 1.048 Npar= 425

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

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 6 Check

Author Response: Background scattering caused by icing of the crystal.

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 6.004 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 18 Report

---

Alert level G

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 164 Note

```
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.0 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         13 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          8 Check
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   2 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

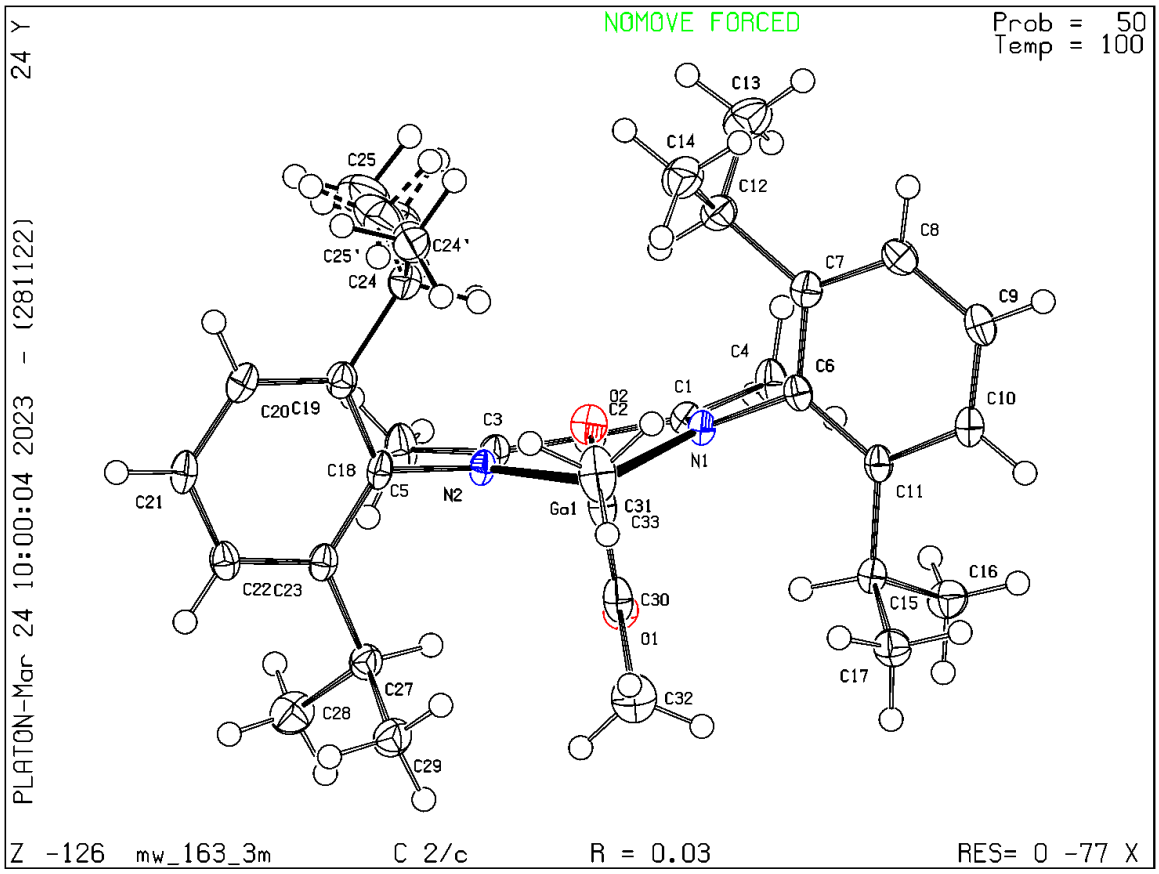
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

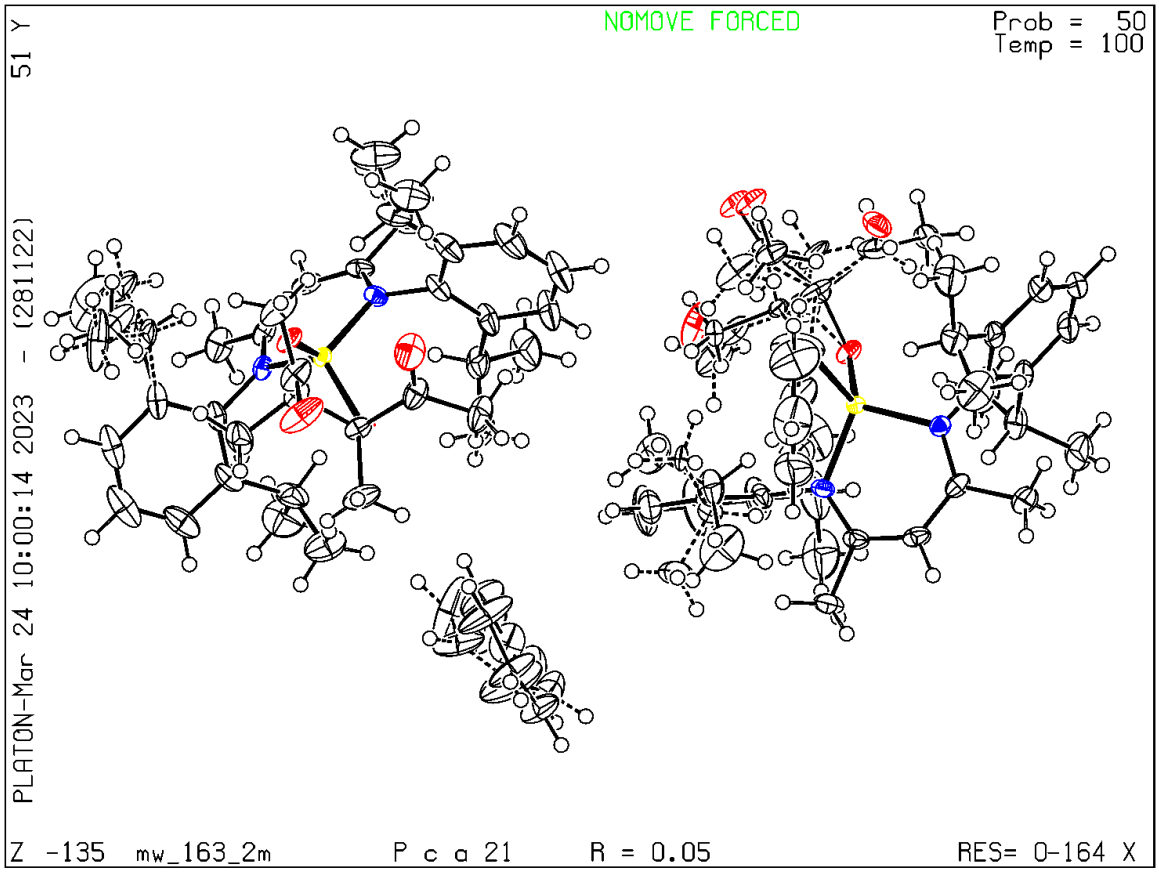
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

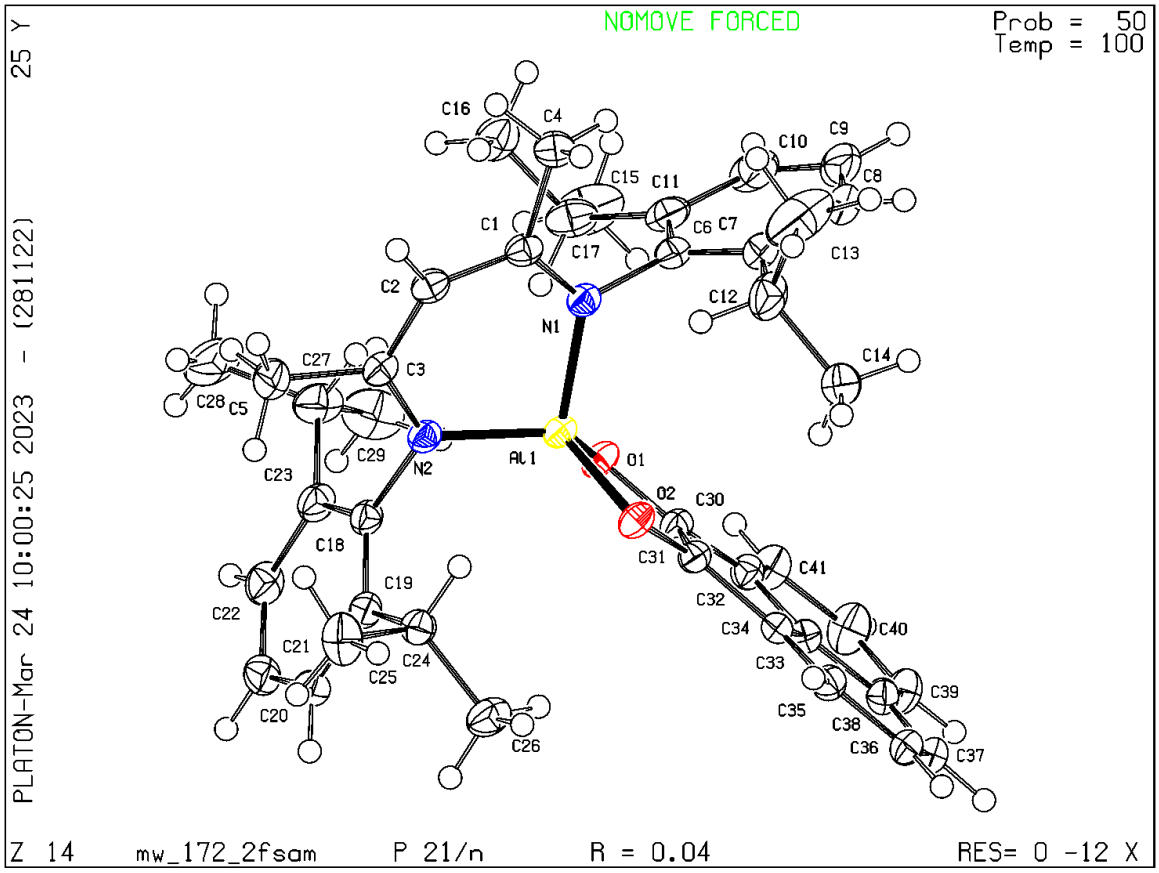
Datablock mw_163_3m - ellipsoid plot



Datablock mw_163_2m - ellipsoid plot



Datablock mw_172_2fsam - ellipsoid plot



Datablock mw_163_4_tw4 - ellipsoid plot