# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mw_165_11_methfam_sq, mw_1751filfil_gelbm, mw_175_2m, mw_176_1am_sq

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_165_11_methfam_sq

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Bond precision:   C-C = 0.0021 A          Wavelength=1.54178

Cell:             a=13.2394(4)    b=17.9680(6)         c=16.9249(5)
                  alpha=90        beta=92.4650(13)     gamma=90
Temperature:      100 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 4022.5(2) | 4022.5(2) |
| Space group | P 21/n | P 21/n |
| Hall group | -P 2yn | -P 2yn |
| Moiety formula | C82 H94 In2 N4 O4 [+ solvent] | ? |
| Sum formula | C82 H94 In2 N4 O4 [+ solvent] | C87 H104 In2 N4 O5 |
| Mr | 1429.25 | 1515.38 |
| Dx,g cm-3 | 1.180 | 1.251 |
| Z | 2 | 2 |
| Mu (mm-1) | 4.939 | 4.977 |
| F000 | 1488.0 | 1584.0 |
| F000' | 1491.90 | |
| h,k,lmax | 16,22,21 | 16,22,21 |
| Nref | 8813 | 8784 |
| Tmin,Tmax | 0.467,0.668 | 0.620,0.750 |
| Tmin' | 0.345 | |

```
Correction method= # Reported T Limits: Tmin=0.620 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.997           Theta(max)= 80.384
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R(reflections)= 0.0198( 7808)  wR2(reflections)= 0.0504( 8784)

S = 1.029  Npar= 425

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The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

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**Alert level G**

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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:C87 H104 In2 N4 O5
           Atom count from the _atom_site data:  C82 H94 In2 N4 O4
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  C87 H104 In2 N4 O5
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        174.00    164.00   10.00
           H        208.00    188.00   20.00
           In         4.00      4.00    0.00
           N          8.00      8.00    0.00
           O         10.00      8.00    2.00
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       0.76 %
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          5 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         29 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         15 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
  0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 12 **ALERT level G** = General information/check it is not something unexpected

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

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# Datablock: mw_176_1am_sq

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Bond precision:  C-C = 0.0041 A  Wavelength=0.71073

| | | | |
|---|---|---|---|
| Cell: | a=12.4414(12) | b=14.0266(13) | c=14.6235(13) |
| | alpha=61.987(4) | beta=74.874(5) | gamma=85.540(5) |
| Temperature: | 100 K | | |

| | Calculated | Reported |
|---|---|---|
| Volume | 2171.9(4) | 2171.9(4) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C82 H94 N4 O4 Tl2 [+ solvent] | ? |
| Sum formula | C82 H94 N4 O4 Tl2 [+ solvent] | C94 H122 N4 O4 Tl2 |
| Mr | 1608.37 | 1780.69 |
| Dx,g cm-3 | 1.230 | 1.361 |
| Z | 1 | 1 |
| Mu (mm-1) | 3.748 | 3.755 |
| F000 | 808.0 | 908.0 |
| F000' | 802.69 | |
| h,k,lmax | 16,18,19 | 16,18,19 |
| Nref | 10898 | 10869 |
| Tmin,Tmax | 0.730,0.880 | 0.570,0.750 |
| Tmin' | 0.460 | |

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

Data completeness= 0.997 Theta(max)= 28.399

R(reflections)= 0.0236( 9224) wR2(reflections)= 0.0574( 10869)

S = 1.037 Npar= 460

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The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

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**Alert level C**

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.135 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 8 Report

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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:C94 H122 N4 O4 Tl2

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            Atom count from the _atom_site data:  C82 H94 N4 O4 Tl2
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    1
            From the CIF: _chemical_formula_sum  C94 H122 N4 O4 Tl2
            TEST: Compare cell contents of formula and atom_site data

            atom    Z*formula  cif sites diff
            C         94.00     82.00   12.00
            H        122.00     94.00   28.00
            N          4.00      4.00    0.00
            O          4.00      4.00    0.00
            Tl         2.00      2.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6 Note
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         7% Note
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT793_ALERT_4_G Model has Chirality at C30         (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C31         (Centro 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 .............         25 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         22 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          6 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          8 Info
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   3 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
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   8 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check

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# Datablock: mw_1751filfil_gelbm

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Bond precision:  C-C = 0.0029 A  Wavelength=0.71073

Cell:  a=22.055(11)  b=17.741(9)  c=22.328(12)
       alpha=90  beta=118.486(8)  gamma=90
Temperature:  100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 7679(7) | 7679(7) |
| Space group | P 21/n | P 21/n |
| Hall group | -P 2yn | -P 2yn |
| Moiety formula | C43 H51 Al N2 O2 | ? |
| Sum formula | C43 H51 Al N2 O2 | C43 H51 Al N2 O2 |
| Mr | 654.84 | 654.83 |
| Dx,g cm-3 | 1.133 | 1.133 |
| Z | 8 | 8 |
| Mu (mm-1) | 0.090 | 0.090 |
| F000 | 2816.0 | 2816.0 |
| F000' | 2817.48 | |
| h,k,lmax | 29,24,30 | 29,23,29 |
| Nref | 19943 | 19336 |
| Tmin,Tmax | 0.978,0.994 | 0.640,0.750 |
| Tmin' | 0.962 | |

Correction method= # Reported T Limits: Tmin=0.640 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.970 Theta(max)= 28.758

R(reflections)= 0.0477( 12637) wR2(reflections)= 0.1258( 19336)

S = 1.017 Npar= 885

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The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

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**Alert level C**

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report

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**Alert level G**

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 198 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Al1_1 (III) . 3.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1_2 (III) . 3.05 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= 0.600 586 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 8 Info

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2 ALERT type 5 Informative message, check

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# Datablock: mw_175_2m

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Bond precision: C-C = 0.0024 A Wavelength=1.54178

Cell: a=12.7707(9) b=18.3465(8) c=20.262(3)
alpha=100.364(5) beta=92.789(7) gamma=108.952(4)
Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 4387.4(8) | 4387.4(7) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | 2(C43 H51 Ga N2 O2), 2.5(C6 H6) | ? |
| Sum formula | C101 H117 Ga2 N4 O4 | C50.50 H58.50 Ga N2 O2 |
| Mr | 1590.43 | 795.21 |
| Dx,g cm-3 | 1.204 | 1.204 |
| Z | 2 | 4 |
| Mu (mm-1) | 1.160 | 1.160 |
| F000 | 1690.0 | 1690.0 |
| F000' | 1688.85 | |
| h,k,lmax | 16,23,25 | 16,23,25 |
| Nref | 19283 | 19089 |
| Tmin,Tmax | 0.850,0.943 | 0.650,0.750 |
| Tmin' | 0.836 | |

Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.750
AbsCorr = MULTI-SCAN

Data completeness= 0.990 Theta(max)= 80.731

R(reflections)= 0.0301( 16240) wR2(reflections)= 0.0768( 19089)

S = 1.043 Npar= 1133

The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

## Alert level C

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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.040 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          8 Report
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## Alert level G

```
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        25% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        257 Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        168 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        188 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         15 Info
```

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

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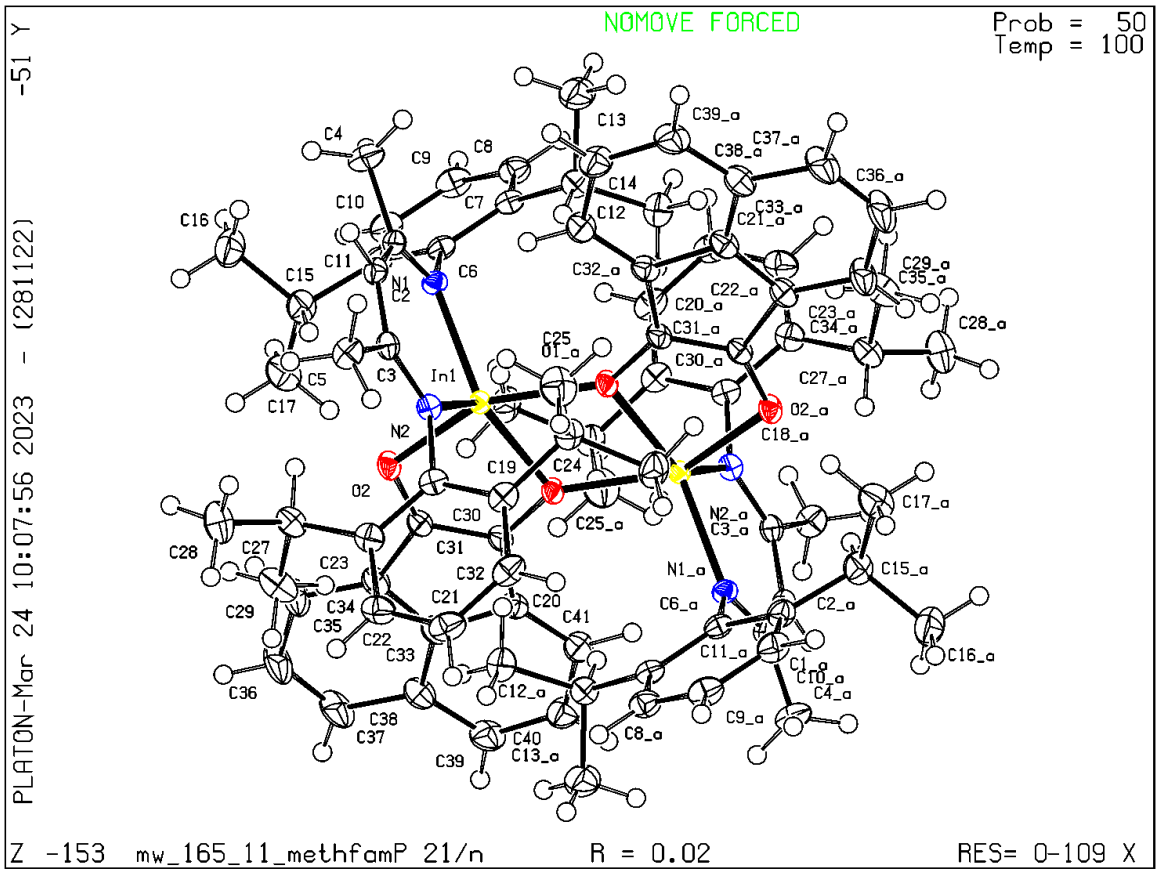
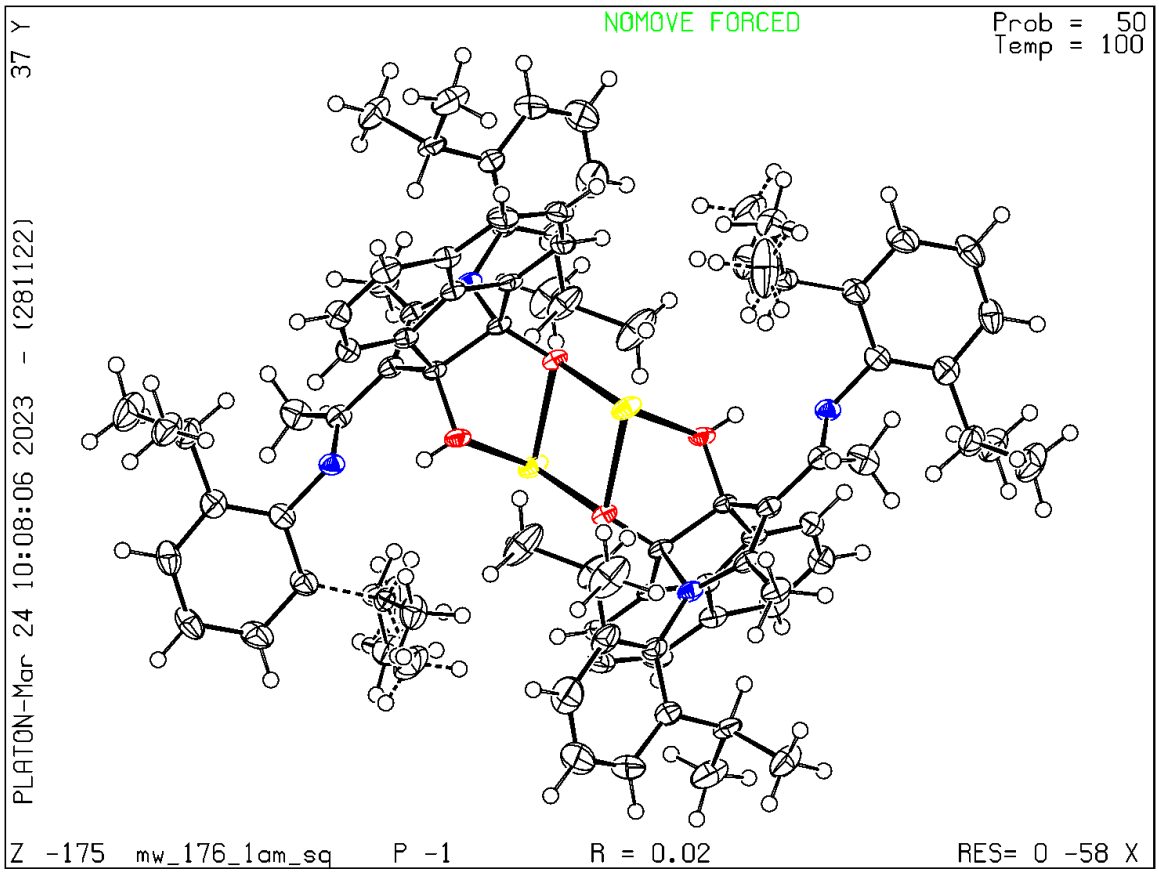
**PLATON version of 28/11/2022; check.def file version of 28/11/2022**

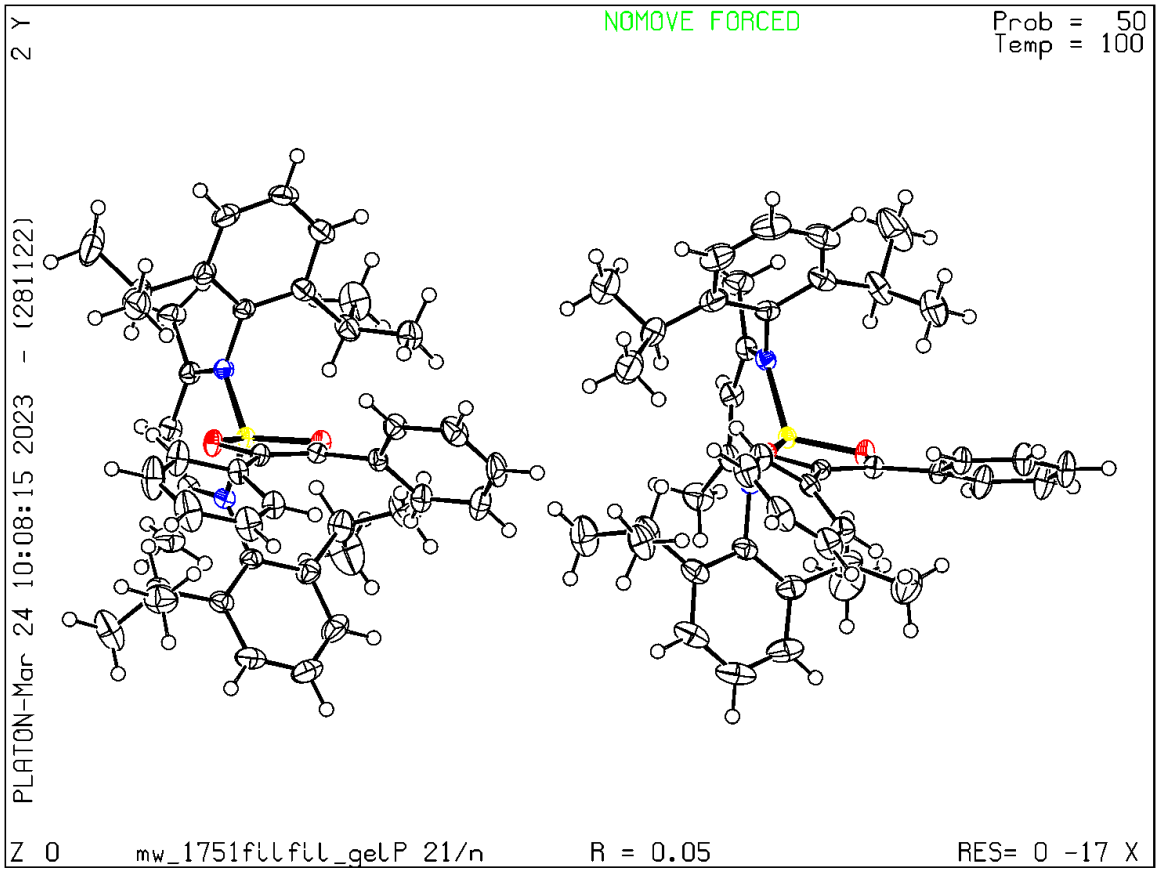
**Datablock mw_165_11_methfam_sq** - ellipsoid plot



**Datablock mw_176_1am_sq** - ellipsoid plot



**Datablock mw_1751filfil_gelbm** - ellipsoid plot



**Datablock mw_175_2m** - ellipsoid plot