checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1.BF4, 1.NO3, 1.OTf, 2.NO3, 3.NO3, L3

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: L3

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

Cell:           a=8.9160(7)       b=11.0941(10)     c=12.5663(10)
                alpha=94.783(3)   beta=103.724(3)   gamma=107.064(3)
Temperature:    110 K

                 Calculated                  Reported
Volume           1138.58(17)                 1138.58(17)
Space group      P -1                        P -1
Hall group       -P 1                        -P 1
Moiety formula   C30 H28 N2                  C30 H28 N2
Sum formula      C30 H28 N2                  C30 H28 N2
Mr               416.54                      416.54
Dx,g cm-3        1.215                       1.215
Z                2                           2
Mu (mm-1)        0.071                       0.071
F000             444.0                       444.0
F000'            444.15
h,k,lmax         10,13,15                    10,13,15
Nref             4329                        4323
Tmin,Tmax        0.983,0.986                 0.467,0.746
Tmin'            0.972

Correction method= # Reported T Limits: Tmin=0.467 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.999            Theta(max)= 25.680

R(reflections)= 0.0609( 2826)                    wR2(reflections)=
                                                 0.1406( 4323)
S = 1.002                  Npar= 293
```

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   0.140
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     15.363 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.403 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          7 Note
```

Alert level G

```
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.140 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.003 Degree
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          4 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 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
   7 ALERT level G = General information/check it is not something unexpected

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

Datablock: 1.BF4

```
Bond precision:   C-C = 0.0053 A          Wavelength=0.71073

Cell:             a=17.4954(15)     b=23.7716(18)     c=26.188(2)
                  alpha=90          beta=90           gamma=90
Temperature:      110 K
```

	Calculated	Reported
Volume	10891.4(15)	10891.2(15)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C62 H50 Cu N2 P2, B F4, C H2 Cl2	C62 H50 Cu N2 P2, B F4, C H2 Cl2
Sum formula	C63 H52 B Cl2 Cu F4 N2 P2	C63 H52 B Cl2 Cu F4 N2 P2
Mr	1120.27	1120.25
Dx,g cm-3	1.366	1.366
Z	8	8
Mu (mm-1)	0.614	0.614
F000	4624.0	4624.0
F000'	4632.26	
h,k,lmax	21,29,32	21,29,31
Nref	10412	10365
Tmin,Tmax	0.863,0.884	0.523,0.745
Tmin'	0.782	

Correction method= # Reported T Limits: Tmin=0.523 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 25.740

R(reflections)= 0.0581(7306) wR2(reflections)= 0.1617(10365)

S = 1.048 Npar= 676

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 0.172
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
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 6.208 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 16 Report

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Alert level G

PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.172 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 12.76 Why ?
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of B1 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C19 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C26 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F2 ..C63 . 2.96 Ang.

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                                                    x,y,z  =      1_555 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
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         26 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
PLAT954_ALERT_1_G Reported (CIF) and Actual (FCF) Kmax Differ by .          1 Units
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 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
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **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
6 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: 1.OTf

Bond precision: C-C = 0.0095 A Wavelength=0.71073

Cell: a=15.2564(10) b=16.0253(11) c=23.0757(15)
alpha=90.355(3) beta=93.137(3) gamma=98.235(3)
Temperature: 296 K

	Calculated	Reported
Volume	5574.6(6)	5574.6(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C62 H50 Cu N2 P2, C F3 O3 S	C62 H50 Cu N2 P2, C F3 O3 S
Sum formula	C63 H50 Cu F3 N2 O3 P2 S	C63 H50 Cu F3 N2 O3 P2 S
Mr	1097.60	1097.59
Dx,g cm-3	1.308	1.308
Z	4	4
Mu (mm-1)	0.544	0.544
F000	2272.0	2272.0
F000'	2275.49	
h,k,lmax	18,19,27	18,19,27
Nref	20430	20386
Tmin,Tmax	0.878,0.897	0.620,0.745
Tmin'	0.849	

Correction method= # Reported T Limits: Tmin=0.620 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.350

R(reflections)= 0.0788(12657) wR2(reflections)= 0.2374(20386)

S = 1.047 Npar= 1267

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 A

PLAT214_ALERT_2_A Atom C125 (Anion/Solvent) ADP max/min Ratio 8.0 prolat

Author Response: The high variation in ADP max/min ratio is caused by dynamic disorder or due to thermal motion. We have tried to resolve this disorder, but atom continues to have high ADP max/min ratio.

PLAT214_ALERT_2_A Atom C126 (Anion/Solvent) ADP max/min Ratio 8.0 prolat

Author Response: The high variation in ADP max/min ratio is caused by dynamic disorder or due to thermal motion. We have tried to resolve this disorder, but atom continues to have high ADP max/min ratio.

PLAT234_ALERT_4_A Large Hirshfeld Difference S2 --O4 . 0.40 Ang.

Author Response: Several atoms presented dynamic disorder or thermal motion that was impossible to solve. Therefore, they are still not ideally shaped. However, this does not indicate an incorrect atom-type assignment. Correct atom identies were also established by other chemical means.

PLAT234_ALERT_4_A Large Hirshfeld Difference F5 --C126 . 0.53 Ang.

Author Response: Several atoms presented dynamic disorder or thermal motion that was impossible to solve. Therefore, they are still not ideally shaped. However, this does not indicate an incorrect atom-type assignment. Correct atom identies were also established by other chemical means.

Alert level B

PLAT214_ALERT_2_B Atom O4 (Anion/Solvent) ADP max/min Ratio 5.1 prolat

Author Response: The high variation in ADP max/min ratio is caused by dynamic disorder or due to thermal motion. We have tried to resolve this disorder, but atom continues to have high ADP max/min ratio.

```
PLAT231_ALERT_4_B Hirshfeld Test (Solvent)   F3       --C125     .       30.3 s.u.
```

Author Response: Several atoms presented dynamic disorder or thermal motion that was impossible to solve. Therefore, they are still not ideally shaped. However, this does not indicate an incorrect atom-type assignment. Correct atom identies were also established by other chemical means.

```
PLAT231_ALERT_4_B Hirshfeld Test (Solvent)   S2       --C126     .       18.8 s.u.
```

Author Response: Several atoms presented dynamic disorder or thermal motion that was impossible to solve. Therefore, they are still not ideally shaped. However, this does not indicate an incorrect atom-type assignment. Correct atom identies were also established by other chemical means.

```
PLAT231_ALERT_4_B Hirshfeld Test (Solvent)   F4       --C126     .       19.2 s.u.
```

Author Response: Several atoms presented dynamic disorder or thermal motion that was impossible to solve. Therefore, they are still not ideally shaped. However, this does not indicate an incorrect atom-type assignment. Correct atom identies were also established by other chemical means.

```
PLAT260_ALERT_2_B Large Average Ueq of Residue Including        S1      0.441 Check
```

Author Response: The large average Ueq is due to thermal motion or dynamic disorder.

```
PLAT260_ALERT_2_B Large Average Ueq of Residue Including        S2      0.466 Check
```

Author Response: The large average Ueq is due to thermal motion or dynamic disorder.

```
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         20 Note
```

Author Response: The unit-cell is reasonably large causing reflections to be effected by the beamstop.

Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
            Rint given   0.150
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........      0.150 Report
PLAT214_ALERT_2_C Atom O3        (Anion/Solvent) ADP max/min Ratio        4.7 prolat
```

Author Response: The high variation in ADP max/min ratio is caused by dynamic disorder or due to thermal motion. We have tried to resolve this disorder, but atom continues to have high ADP max/min ratio.

```
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        4.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference S2       --O5       .       0.21 Ang.
```

Author Response: Several atoms presented dynamic disorder or thermal motion that was impossible to solve. Therefore, they are still not ideally shaped. However, this does not indicate an incorrect atom-type assignment. Correct atom identies were also established by other chemical means.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C31 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        C59 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C97 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C98 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C109 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C115 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C95 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C113 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C125 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of       C126 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         S1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         S2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        3.1 Note
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C27      --C32      .       1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00952 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         63 Ang**3
PLAT733_ALERT_1_C Torsion Calc   -24.61(1), Rep      -24.60 ......       5.00 s.u.-R
             F6  -C126-S2  -O6    1_555  1_555  1_555  1_555      #  244 Check
PLAT733_ALERT_1_C Torsion Calc  -156.46(1), Rep     -156.46 ......       5.00 s.u.-R
             F5  -C126-S2  -O4    1_555  1_555  1_555  1_555      #  249 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     10.583 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.376 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         25 Report
```

Alert level G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.003 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   F1       --C125     .        5.8 s.u.
```

Author Response: Several atoms presented dynamic disorder or thermal motion that was impossible to solve. Therefore, they are still not ideally shaped. However, this does not indicate an incorrect atom-type assignment. Correct atom identies were also established by other chemical means.

```
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   F2       --C125     .        5.8 s.u.
```

Author Response: Several atoms presented dynamic disorder or thermal motion that was impossible to solve. Therefore, they are still not ideally shaped. However, this does not indicate an incorrect atom-type assignment. Correct atom identies were also established by other chemical means.

```
PLAT344_ALERT_2_G Unusual           Angle Range in Solvent/Ion for       C126 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C19 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C26 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C81 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C88 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         12 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

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

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  26 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
   1 ALERT type 5 Informative message, check
```

Datablock: 1.NO3

```
Bond precision:   C-C = 0.0076 A           Wavelength=0.71073

Cell:             a=16.7053(12)     b=14.7608(11)      c=22.8229(17)
                  alpha=90          beta=95.361(2)     gamma=90
Temperature:      296 K
```

	Calculated	Reported
Volume	5603.1(7)	5603.1(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C62 H50 Cu N2 P2, C H Cl3, N O3	C62 H50 Cu N2 P2, C H Cl3, N O3
Sum formula	C63 H51 Cl3 Cu N3 O3 P2	C63 H51 Cl3 Cu N3 O3 P2
Mr	1129.91	1129.89
Dx,g cm-3	1.339	1.339
Z	4	4
Mu (mm-1)	0.639	0.639
F000	2336.0	2336.0
F000'	2340.59	
h,k,lmax	21,18,28	21,18,28
Nref	12005	11970
Tmin,Tmax	0.819,0.914	0.497,0.745
Tmin'	0.774	

Correction method= # Reported T Limits: Tmin=0.497 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 26.815

R(reflections)= 0.0728(6960) wR2(reflections)= 0.2296(11970)

S = 1.093 Npar= 679

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

Author Response: The unit-cell is reasonably large causing reflections to be effected by the beamstop.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.160
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 ..... 0.160 Report
PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ... 2.800 Sigma
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.09 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.8 Ratio

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C37 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        C59 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C23 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C63 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         N3 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl1      0.134 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O1      0.141 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C45      --C50      .       1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C20      -C25      .       1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00759 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      8.578 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        2 Report
```

Alert level G

```
PLAT480_ALERT_4_G Long H...A H-Bond Reported H40      ..O2       .       2.65 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H50      ..CL3      .       2.91 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H40      ..O2       .       2.65 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H50      ..CL3      .       2.91 Ang.
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        21 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         4 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
```

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

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

Datablock: 2.NO3

```
Bond precision:   C-C = 0.0069 A          Wavelength=0.71073

Cell:               a=17.979(3)      b=24.990(4)      c=27.167(4)
                    alpha=90         beta=90          gamma=90
Temperature:        110 K
```

	Calculated	Reported
Volume	12206(3)	12206(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C66 H58 Cu N2 P2, C H Cl3, N O3	C66 H58 Cu N2 P2, C H Cl3, N O3
Sum formula	C67 H59 Cl3 Cu N3 O3 P2	C67 H59 Cl3 Cu N3 O3 P2
Mr	1186.01	1186.00
Dx,g cm-3	1.291	1.291
Z	8	8
Mu (mm-1)	0.590	0.590
F000	4928.0	4928.0
F000'	4937.25	
h,k,lmax	21,30,33	21,30,33
Nref	11687	11645
Tmin,Tmax	0.844,0.889	0.593,0.745
Tmin'	0.838	

Correction method= # Reported T Limits: Tmin=0.593 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.772

R(reflections)= 0.0638(7888) wR2(reflections)= 0.1818(11645)

S = 1.056 Npar= 716

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 4.0 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C25 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C67 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N3 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl1 0.150 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1 0.175 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0069 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C28 - C29 . 1.42 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C28 - C30 . 1.34 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H28 ..H29C . 1.88 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H28 ..H30C . 1.81 Ang.
x,y,z = 1_555 Check
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 38 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 9.097 Check

```
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         10 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          6 Report
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      14.31 Why ?
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for        C28 Check
PLAT480_ALERT_4_G Long H...A H-Bond Reported H67      ..N3       .       2.68 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H67      ..N3       .       2.68 Ang.
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         27 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  16 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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: 3.NO3

```
Bond precision:   C-C = 0.0125 A           Wavelength=0.71073

Cell:             a=13.2253(4)     b=13.2253(4)     c=40.3250(19)
                  alpha=90         beta=90          gamma=90
Temperature:      296 K
```

	Calculated	Reported
Volume	7053.2(5)	7053.2(5)
Space group	P 41	P 41
Hall group	P 4w	P 4w
Moiety formula	C66 H58 Cu N2 P2, 3(C H Cl3), N O3	C66 H58 Cu N2 P2, 3(C H Cl3), N O3
Sum formula	C69 H61 Cl9 Cu N3 O3 P2	C69 H61 Cl9 Cu N3 O3 P2
Mr	1424.75	1424.73
Dx,g cm-3	1.342	1.342
Z	4	4
Mu (mm-1)	0.742	0.742
F000	2928.0	2928.0
F000'	2936.23	
h,k,lmax	16,16,49	15,15,49
Nref	13483[6845]	10328
Tmin,Tmax	0.837,0.888	0.585,0.745
Tmin'	0.825	

Correction method= # Reported T Limits: Tmin=0.585 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.51/0.77 Theta(max)= 25.749

R(reflections)= 0.0611(8353) wR2(reflections)= 0.1700(10328)

S = 0.997 Npar= 774

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.975 Why?
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C40 --C41 . 0.19 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C33 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C45 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C64 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C66 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C43 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C61 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C67 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C68 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C69 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N3 Check

```
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl1      0.193 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl4      0.250 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl7      0.254 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O1      0.190 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C43      --C48      .       1.36 Ang.
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C61      --C66      .       1.36 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01251 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .        48 Ang**3
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #         1 Note
              C66 H58 Cu N2 P2
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       155 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage        56 %
```

Alert level G

```
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         2         89 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem        21         89 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem        21         89 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem         2         89 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New  Space Group     P41212 Check
              Check Model Parameter Symmmetry for Reflection Data Support
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         1 Report
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        21 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        12 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.2 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
```

```
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   6 ALERT type 3 Indicator that the structure quality may be low
   9 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

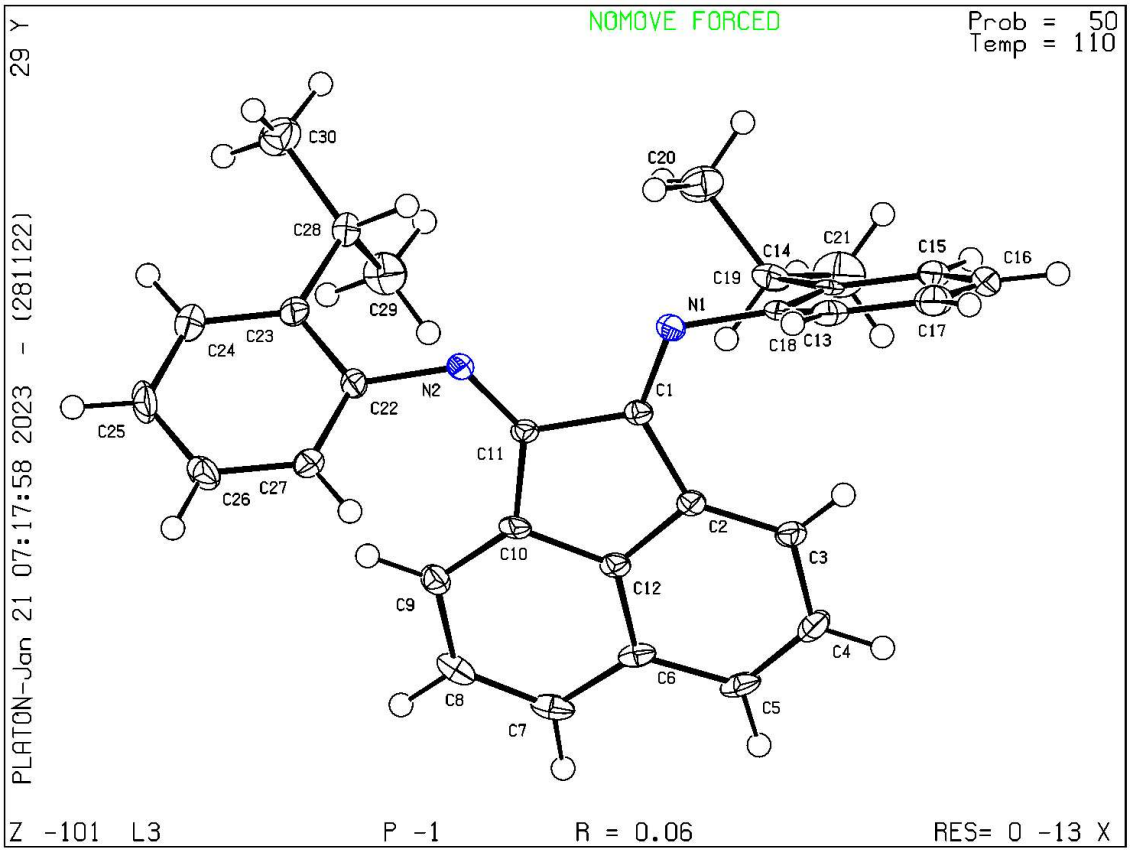
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

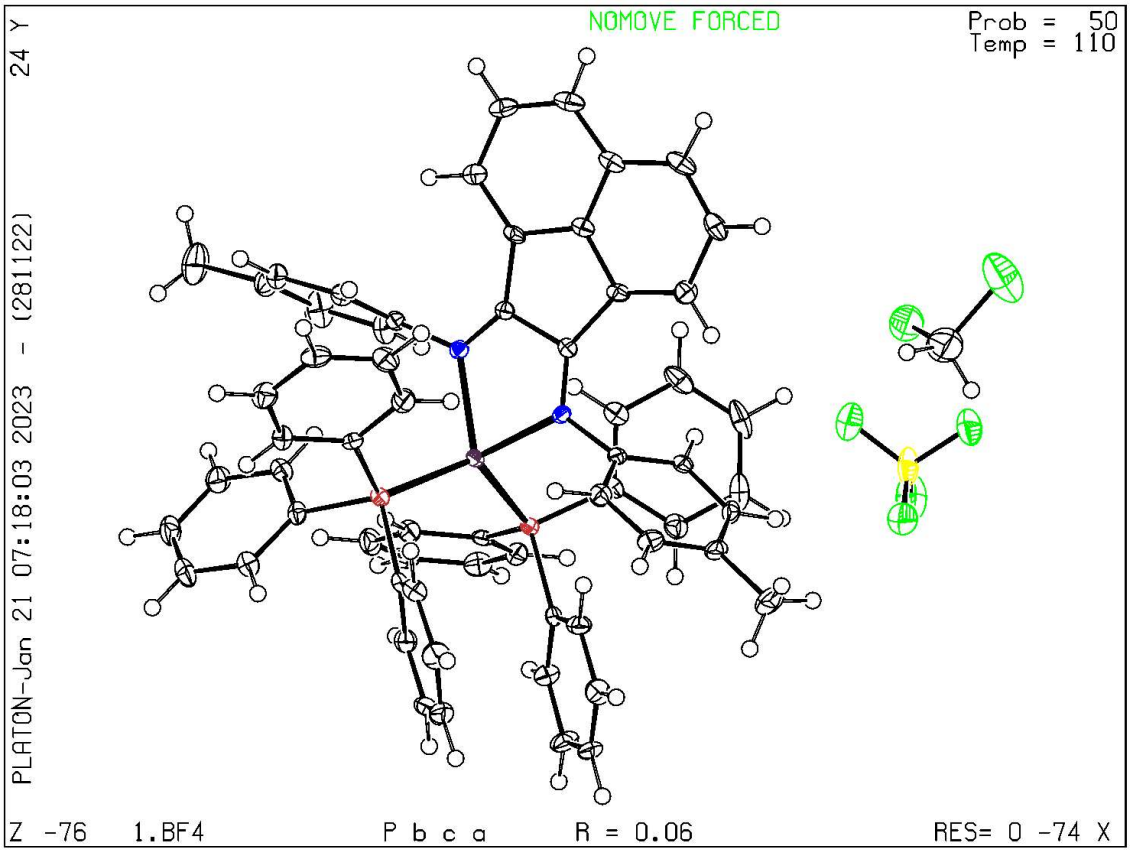
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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

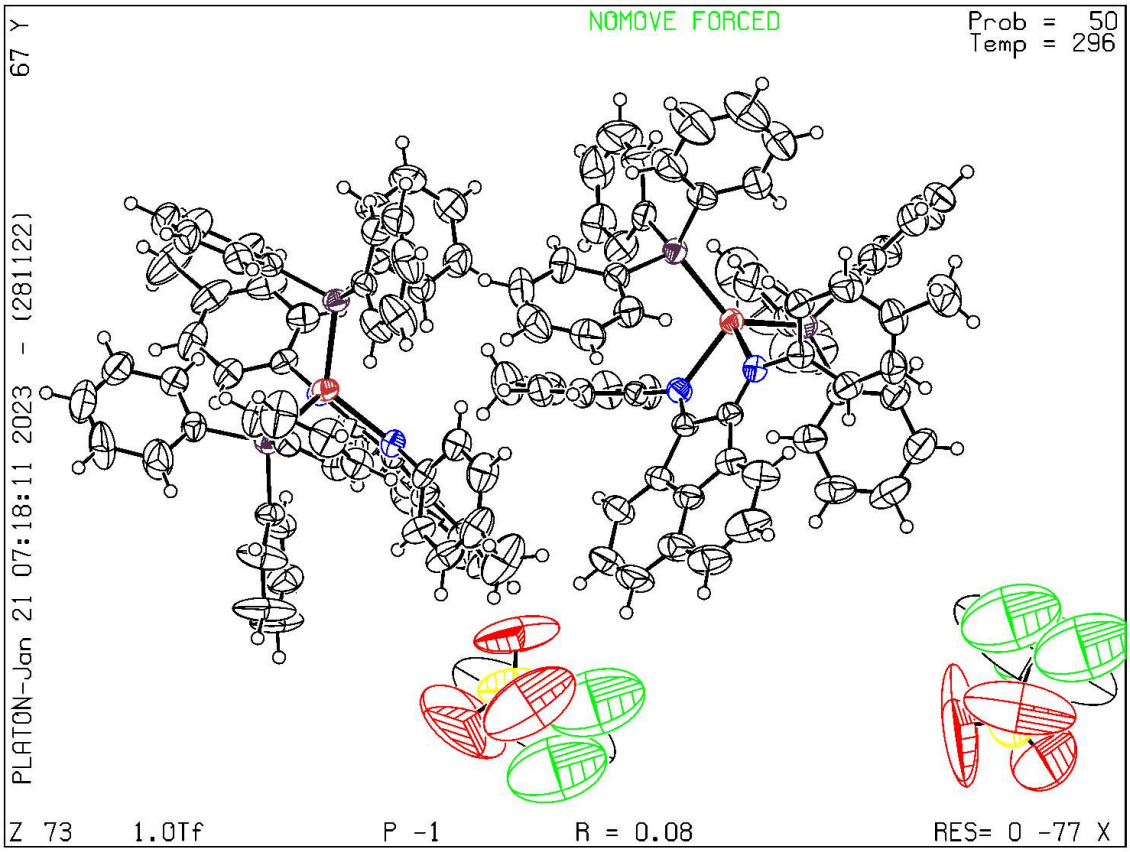
Datablock L3 - ellipsoid plot



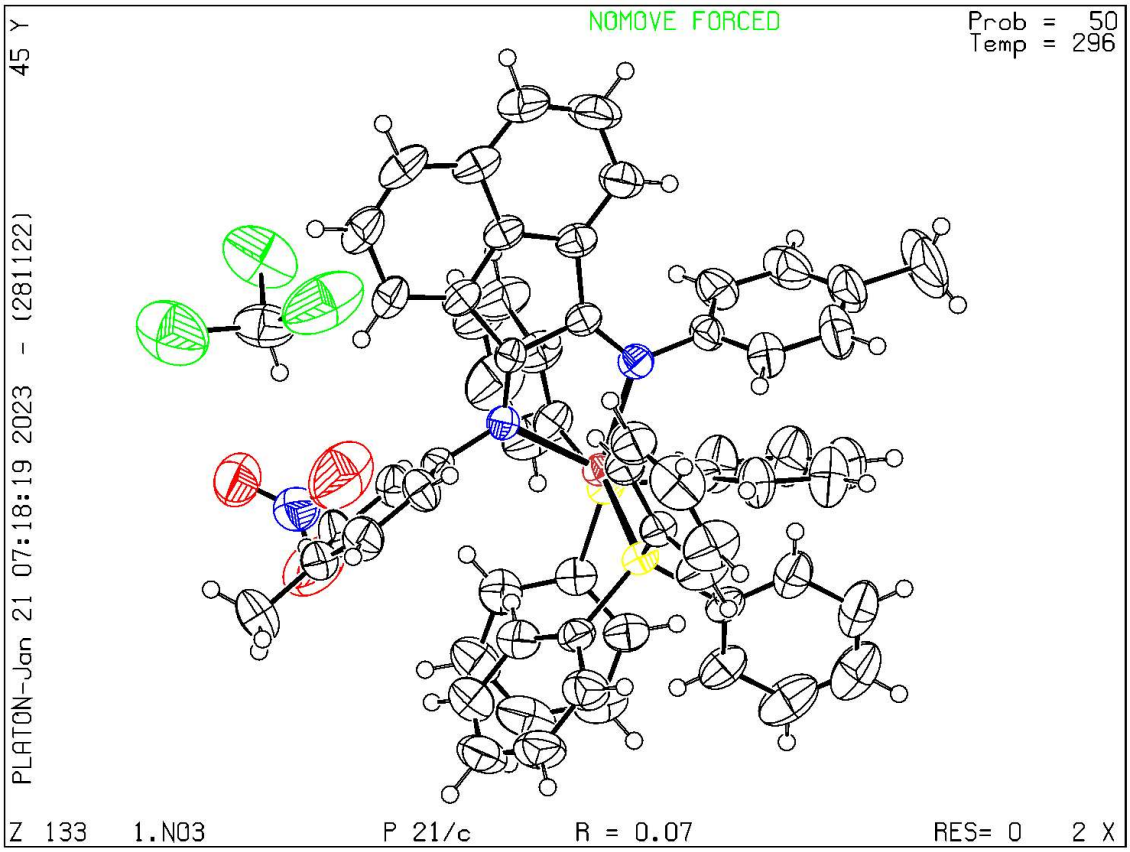
Datablock 1.BF4 - ellipsoid plot



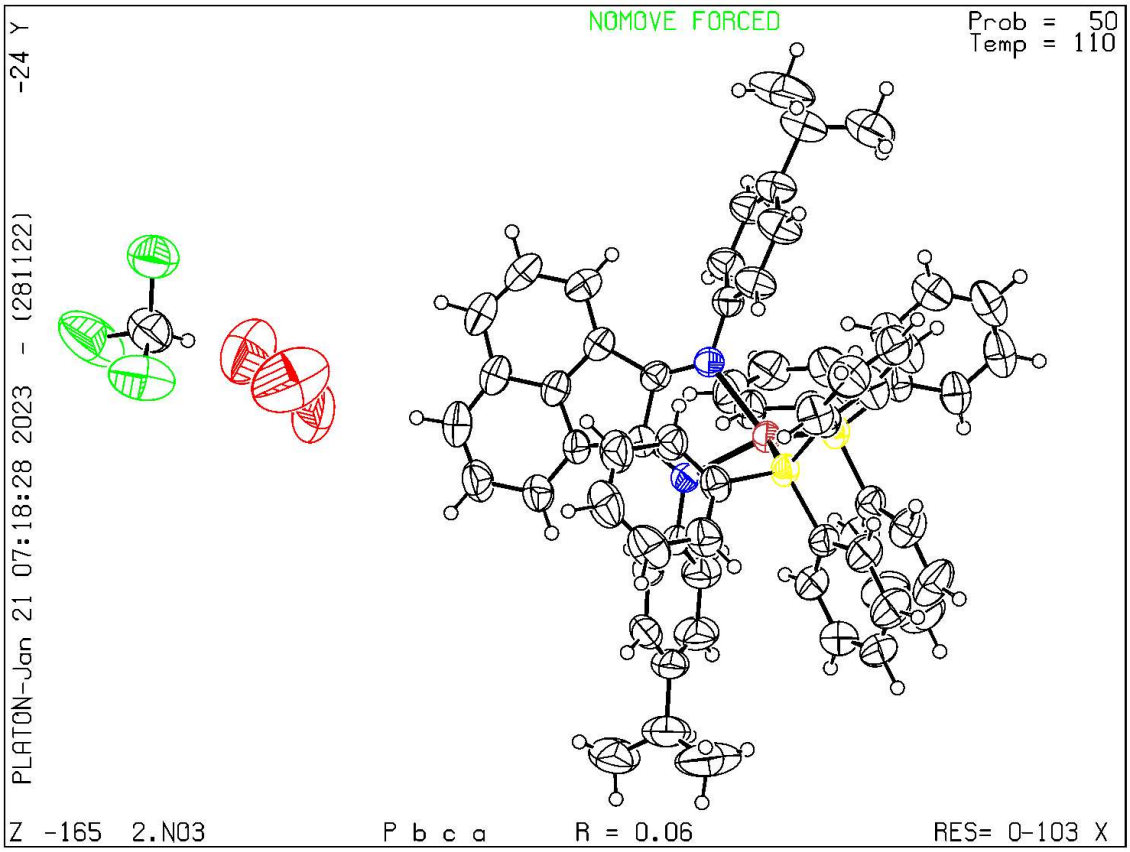
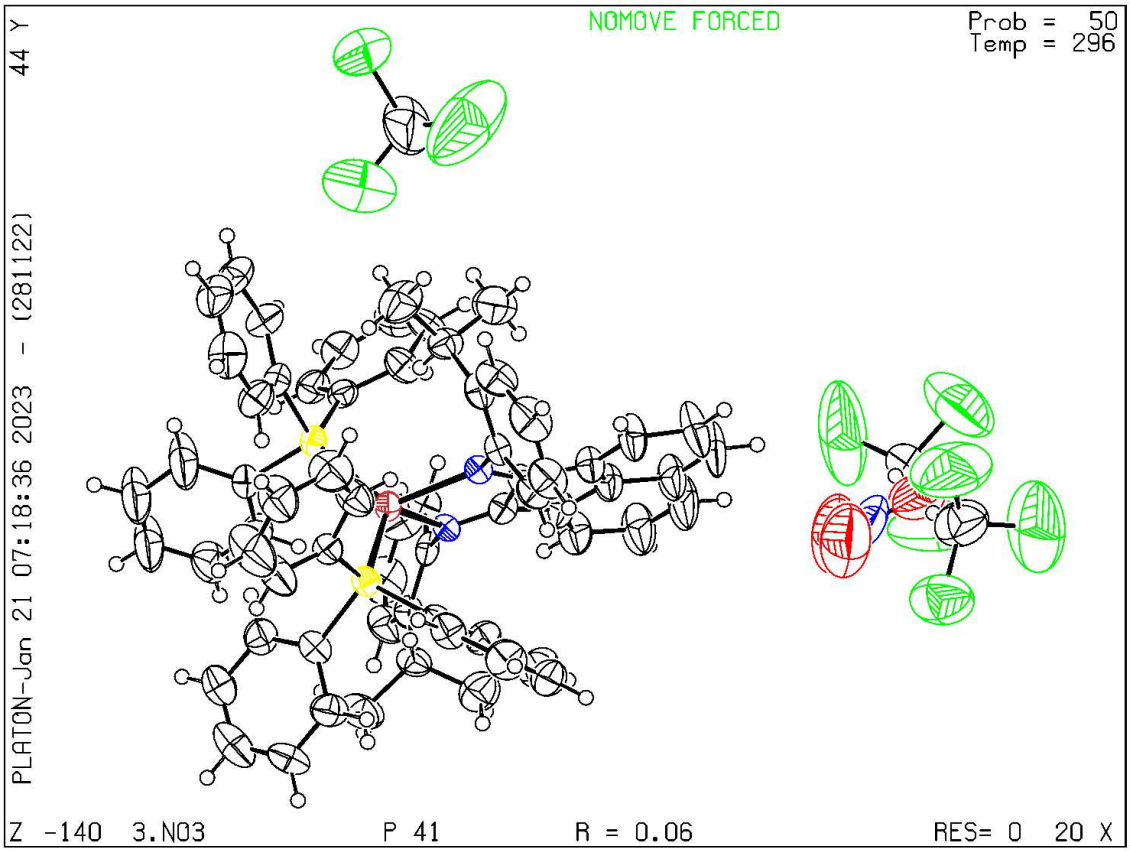
Datablock 1.OTf - ellipsoid plot



Datablock 1.NO3 - ellipsoid plot



Datablock 2.NO3 - ellipsoid plot



Datablock 3.NO3 - ellipsoid plot