checkCIF/PLATON (standard)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: LDiPPH2OTf2

```
Bond precision:        C-C = 0.0091 A                  Wavelength=0.71073
Cell:        a=15.6001(11)     b=24.6198(11)     c=9.9798(4)
             alpha=90          beta=103.562(4)   gamma=90
Temperature: 120 K
                    Calculated                          Reported
Volume              3726.1(4)                           3726.1(4)
Space group         C 2/c                               C2/c
Hall group          -C 2yc                              -C 2yc
Moiety formula      C31 H42 N4, 2(C F3 O3 S)            C31 H42 N4, 2(C F3 O3 S)
Sum formula         C33 H42 F6 N4 O6 S2                 C33 H42 F6 N4 O6 S2
Mr                  768.85                              768.83
Dx,g cm-3           1.371                               1.371
Z                   4                                   4
Mu (mm-1)           0.220                               0.220
F000                1608.0                              1608.0
F000'               1609.96
h,k,lmax            18,29,11                            18,29,11
Nref                3301                                3291
Tmin,Tmax           0.979,0.983                         0.961,0.981
Tmin'               0.961
Correction method= MULTI-SCAN
Data completeness= 0.997          Theta(max)= 25.030
R(reflections)= 0.1011( 2654)         wR2(reflections)= 0.2101( 3291)
S = 1.216               Npar= 241
```

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

RFACG01_ALERT_3_C The value of the R factor is > 0.10
R factor given 0.101
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S1
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C17
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0091 Ang
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond C1 - C2 ... 1.39 Ang.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond C2 - C3 ... 1.39 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 43.73
PLAT301_ALERT_3_G Note: Main Residue Disorder ..... 17 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 12
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 6

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **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
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: Lmes

```
Bond precision:        C-C = 0.0017 A                  Wavelength=0.69110
Cell:        a=8.030(3)        b=9.795(3)        c=28.373(10)
             alpha=90          beta=97.544(3)    gamma=90
Temperature: 120 K
                     Calculated                          Reported
Volume               2212.3(13)                          2212.3(13)
Space group          P 21/c                              P21/c
Hall group           -P 2ybc                             -P 2ybc
Moiety formula       C25 H28 N4                          C25 H28 N4
Sum formula          C25 H28 N4                          C25 H28 N4
Mr                   384.51                              384.51
Dx,g cm-3            1.155                               1.154
Z                    4                                   4
Mu (mm-1)            0.065                               0.069
F000                 824.0                               824.0
F000'                824.89
h,k,lmax             11,14,40                            11,14,39
Nref                 6994                                6380
Tmin,Tmax                                                0.989,0.995
Tmin'                0.961
Correction method= MULTI-SCAN
Data completeness= 0.912           Theta(max)= 29.950
R(reflections)= 0.0539( 5380)         wR2(reflections)= 0.1601( 6380)
S = 1.035               Npar= 268
```

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low 0.913

Alert level C

REFLT03_ALERT_3_C Reflection count < 95% complete
From the CIF: _diffrn_reflns_theta_max 29.95
From the CIF: _diffrn_reflns_theta_full 29.95
From the CIF: _reflns_number_total 6380
TEST2: Reflns within _diffrn_reflns_theta_max
Count of symmetry unique reflns 6994
Completeness (_total/calc) 91.22%

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT343_ALERT_2_G Check sp? Angle Range in Main Residue for .. C10
PLAT343_ALERT_2_G Check sp? Angle Range in Main Residue for .. C14
PLAT984_ALERT_1_G The H-f'= 0.000 Deviates from the B&C-Value 0.006

1 **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
4 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: LDiPPTe2

```
Bond precision:        C-C = 0.0082 A                  Wavelength=0.71073
Cell:        a=12.1082(10)     b=16.4200(13)     c=18.3694(15)
             alpha=90          beta=99.721(2)    gamma=90
Temperature: 120 K
                     Calculated                          Reported
Volume               3599.7(5)                           3599.7(5)
Space group          P 21/c                              P21/c
Hall group           -P 2ybc                             -P 2ybc
Moiety formula       C31 H40 N4 Te2, C6 H6               C31 H40 N4 Te2, C6 D6
```

Sum formula	C37 H46 N4 Te2	C37 H40 D6 N4 Te2
Mr	801.98	808.01
Dx,g cm-3	1.480	1.491
Z	4	4
Mu (mm-1)	1.650	1.650
F000	1600.0	1600.0
F000'	1596.18	
h,k,lmax	16,21,24	15,21,23
Nref	8698	8380
Tmin,Tmax	0.794,0.984	0.802,0.984
Tmin'	0.794	

Correction method= MULTI-SCAN

Data completeness= 0.963 Theta(max)= 28.020

R(reflections)= 0.0508(6807) wR2(reflections)= 0.1143(8380)

S = 1.104 Npar= 396

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

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.963
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 3.8
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0082 Ang

---

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:C37 H40 D6 N4 Te2
Atom count from the _atom_site data: C37 H46 N4 Te2
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 4
From the CIF: _chemical_formula_sum C37 H40 D6 N4 Te2
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	148.00	148.00	0.00
H	160.00	184.00	-24.00
D	24.00	0.00	24.00
N	16.00	16.00	0.00
Te	8.00	8.00	0.00

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT017_ALERT_1_G Check Consistency of Scattering Type H for D32
PLAT017_ALERT_1_G Check Consistency of Scattering Type H for D33
PLAT017_ALERT_1_G Check Consistency of Scattering Type H for D34
PLAT017_ALERT_1_G Check Consistency of Scattering Type H for D35
PLAT017_ALERT_1_G Check Consistency of Scattering Type H for D36
PLAT017_ALERT_1_G Check Consistency of Scattering Type H for D37
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 20.24
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6

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4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

10 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
2 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: complex1

Bond precision: C-C = 0.0035 A Wavelength=0.68930

Cell: a=9.2015(18) b=18.932(4) c=19.892(4)
alpha=90 beta=90 gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	3465.2(12)	3465.2(12)

Space group	P 21 21 21	P212121
Hall group	P 2ac 2ab	?
Moiety formula	C33 H46 N4 Pd, C4 H8 O	?
Sum formula	C37 H54 N4 O Pd	C148 H216 N16 O4 Pd4
Mr	677.24	2708.97
Dx,g cm-3	1.298	0.000
Z	4	1
Mu (mm-1)	0.518	0.000
F000	1432.0	0.0
F000'	1428.13	
h,k,lmax	13,27,29	13,26,28
Nref	6406[11601]	10304
Tmin,Tmax		
Tmin'	0.794	

Correction method= Not given

Data completeness= 1.61/0.89 Theta(max)= 30.510

R(reflections)= 0.0309(9778) wR2(reflections)= 0.0711(10304)

S = 1.019 Npar= 411

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

PLAT234_ALERT_4_C Large Hirshfeld Difference C35B -- C36B .. 0.16 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.9

Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
correct. If it is not, please give the correct count in the
_publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 30.51
From the CIF: _reflns_number_total 10304
Count of symmetry unique reflns 6406
Completeness (_total/calc) 160.85%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 3898
Fraction of Friedel pairs measured 0.608
Are heavy atom types Z>Si present yes
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 9
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 4.00 Ratio
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C34B
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C36B
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C34A
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C36A
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..... 80 Perc.
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 101
N2 -C3 -PD1 -C32 94.20 1.50 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 102
N3 -C3 -PD1 -C32 -85.70 1.50 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 111
N4 -C1 -PD1 -C33 -29.00 3.00 1.555 1.555 1.555 1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 112
N1 -C1 -PD1 -C33 143.00 3.00 1.555 1.555 1.555 1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 205
C34A -O1 -C34B 1.555 1.555 1.555 10.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 210
C37A -O1 -C37B 1.555 1.555 1.555 13.20 Deg.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 10
PLAT984_ALERT_1_G The Pd-f'= -0.999 Deviates from the B&C-Value -1.052
PLAT985_ALERT_1_G The Pd-f"= 1.007 Deviates from the B&C-Value 0.957

---

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

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

Datablock: complex2

```
Bond precision:        C-C = 0.0073 A                Wavelength=0.71073
Cell:        a=9.1685(1)       b=18.9619(2)      c=19.9278(2)
             alpha=90          beta=90           gamma=90
Temperature: 120 K
                    Calculated                          Reported
Volume              3464.49(6)                          3464.49(6)
Space group         P 21 21 21                          P212121
Hall group          P 2ac 2ab                           ?
Moiety formula      C33 H46 N4 Pt, C4 H8 O              C33 H46 N4 Pt, (C4 H8 O)
Sum formula         C37 H54 N4 O Pt                     C37 H54 N4 O Pt
Mr                  765.92                              765.93
Dx,g cm-3           1.468                               1.468
Z                   4                                   4
Mu (mm-1)           4.084                               4.084
F000                1560.0                              1560.0
F000'               1553.79
h,k,lmax            11,24,25                            11,24,25
Nref                4442[ 7946]                         7809
Tmin,Tmax           0.907,0.922                         0.686,0.923
Tmin'               0.665
Correction method= MULTI-SCAN
Data completeness= 1.76/0.98       Theta(max)= 27.490
R(reflections)= 0.0306( 7346)         wR2(reflections)= 0.0628( 7809)
S = 1.130               Npar= 399
```

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

STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: _refine_ls_abs_structure_Flack 0.915
From the CIF: _refine_ls_abs_structure_Flack_su 0.007
PLAT033_ALERT_4_C Flack x Parameter Value Deviates from Zero 0.915
PLAT223_ALERT_4_C Large Solvent/Anion H Ueq(max)/Ueq(min) ... 3.4 Ratio
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C47
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C45
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C46
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C45 - C47 ... 1.40 Ang.

Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
correct. If it is not, please give the correct count in the
_publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 27.49
From the CIF: _reflns_number_total 7809
Count of symmetry unique reflns 4442
Completeness (_total/calc) 175.80%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 3367
Fraction of Friedel pairs measured 0.758
Are heavy atom types Z>Si present yes
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ ?

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

1 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
1 ALERT type 5 Informative message, check

Datablock: complex3

```
Bond precision:        C-C = 0.0096 A                Wavelength=0.71073
Cell:        a=13.6258(4)      b=24.9908(7)      c=25.1385(4)
             alpha=90          beta=90           gamma=90
```

Temperature: 153 K

	Calculated	Reported
Volume	8560.2(4)	8560.2(4)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	?
Moiety formula	C39 H52 Ir N4, F6 P, C4 H8 O	C39 H52 Ir N4, P F6, C4 H8 O
Sum formula	C43 H60 F6 Ir N4 O P	C43 H60 F6 Ir N4 O P
Mr	986.14	986.12
Dx,g cm-3	1.530	1.530
Z	8	8
Mu (mm-1)	3.221	3.221
F000	4000.0	4000.0
F000'	3991.14	
h,k,lmax	16,30,31	16,30,31
Nref	8416	8381
Tmin,Tmax	0.497,0.773	0.435,0.445
Tmin'	0.487	

Correction method= CYLINDER

Data completeness= 0.996 Theta(max)= 26.000

R(reflections)= 0.0459(6086) wR2(reflections)= 0.1155(8381)

S = 1.046 Npar= 530

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 Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.3 Ratio
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of P1
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0096 Ang

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 12
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 57
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 17.54
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max datum .... ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min datum .... ?
PLAT301_ALERT_3_G Note: Main Residue Disorder ..... 5 Perc.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 142
C29A -C30 -C29B 1.555 1.555 1.555 27.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 147
C31A -C30 -C31B 1.555 1.555 1.555 35.20 Deg.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 387

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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
3 **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

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

Datablock: complex4

Bond precision: C-C = 0.0097 A Wavelength=0.69110

Cell: a=12.6116(13) b=14.5499(15) c=16.8485(17)
alpha=90 beta=90 gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	3091.7(5)	3091.7(5)
Space group	P 21 21 21	P212121
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C31 H40 Br2 N4 Ni	C31 H40 Br2 N4 Ni
Sum formula	C31 H40 Br2 N4 Ni	C31 H40 Br2 N4 Ni
Mr	687.16	687.20

Dx,g cm-3	1.476	1.476
Z	4	4
Mu (mm-1)	3.013	3.238
F000	1408.0	1408.0
F000'	1408.15	
h,k,lmax	13,15,18	13,15,18
Nref	2430[4279]	4280
Tmin,Tmax		0.782,0.968
Tmin'	0.487	

Correction method= MULTI-SCAN

Data completeness= 1.76/1.00 Theta(max)= 22.310

R(reflections)= 0.0401(3839) wR2(reflections)= 0.1016(4280)

S = 1.070 Npar= 351

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5493

Alert level C

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.3 Ratio
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0097 Ang

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Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
correct. If it is not, please give the correct count in the
_publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 22.31
From the CIF: _reflns_number_total 4280
Count of symmetry unique reflns 2430
Completeness (_total/calc) 176.13%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 1850
Fraction of Friedel pairs measured 0.761
Are heavy atom types Z>Si present yes
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT984_ALERT_1_G The Br-f'= -0.290 Deviates from the B&C-Value -0.195
PLAT984_ALERT_1_G The Ni-f'= 0.339 Deviates from the B&C-Value 0.343
PLAT985_ALERT_1_G The Br-f"= 2.460 Deviates from the B&C-Value 2.358

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2 **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

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

Datablock: complex5

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

Cell: a=10.4866(3) b=17.4528(4) c=19.3943(6)
alpha=90 beta=104.482(1) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	3436.77(17)	3436.77(16)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C33 H40 N4 Ni O2, C4 H8 O	C33 H40 N4 Ni O2, C4 H8 O
Sum formula	C37 H48 N4 Ni O3	C37 H48 N4 Ni O3
Mr	655.48	655.50
Dx,g cm-3	1.267	1.267
Z	4	4
Mu (mm-1)	0.605	0.605
F000	1400.0	1400.0

```
F000'                 1401.81
h,k,lmax              13,22,25                          13,22,25
Nref                  7913                              7853
Tmin,Tmax             0.930,0.953                       0.849,0.953
Tmin'                 0.844
Correction method= MULTI-SCAN
Data completeness= 0.992          Theta(max)= 27.510
R(reflections)= 0.0482( 5640)         wR2(reflections)= 0.1070( 7853)
S = 1.037               Npar= 414
```

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 G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c P21/n
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 -- C32 .. 8.0 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 -- C33 .. 6.8 su

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

0 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
1 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

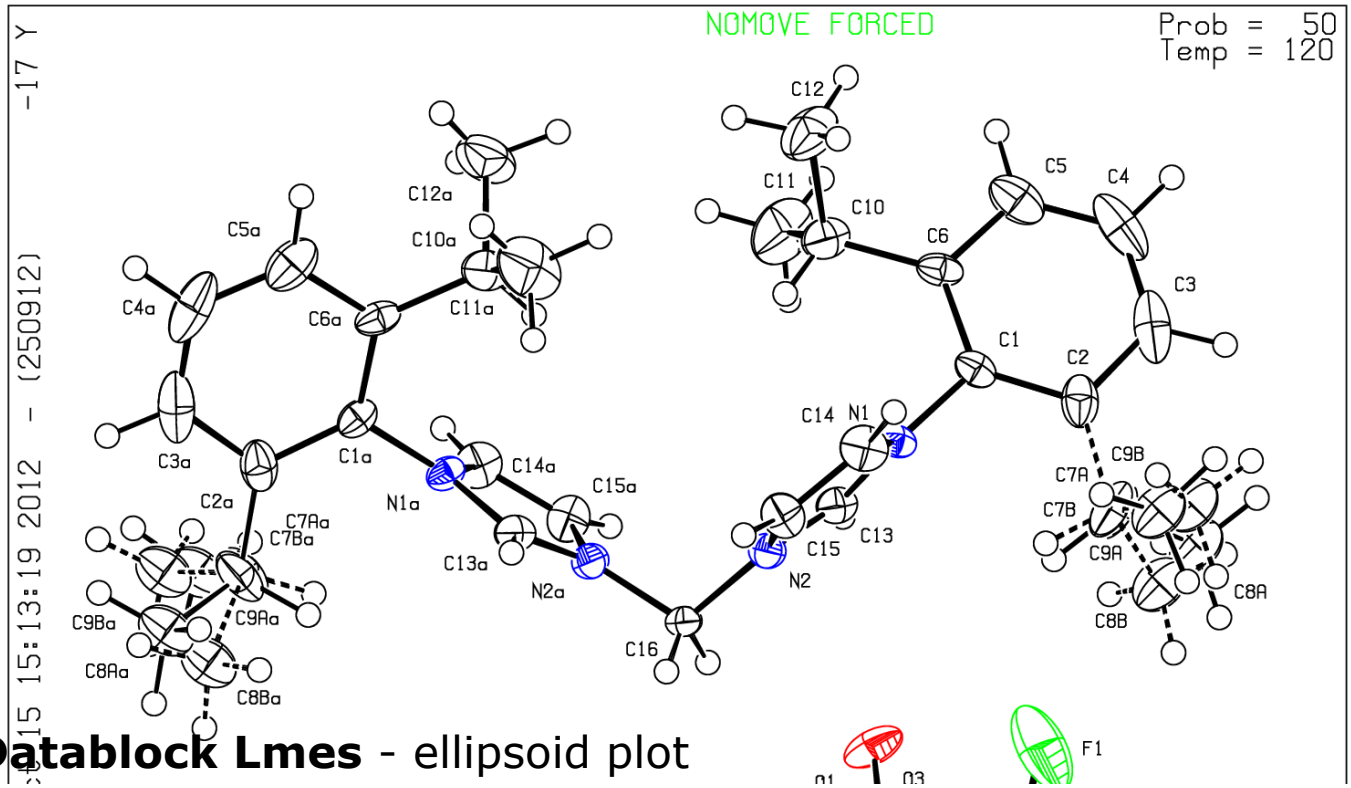
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

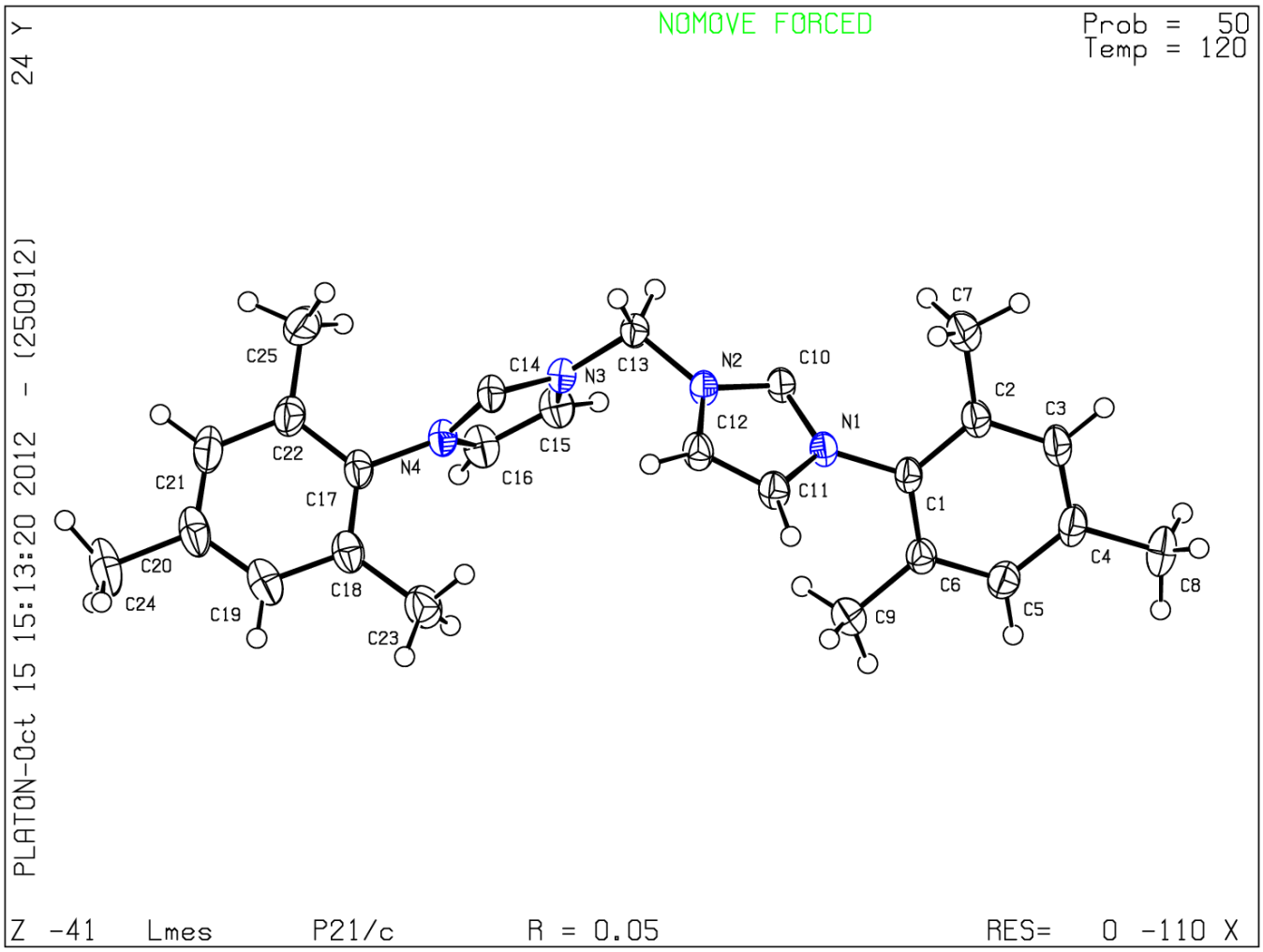
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 25/09/2012; check.def file version of 20/09/2012

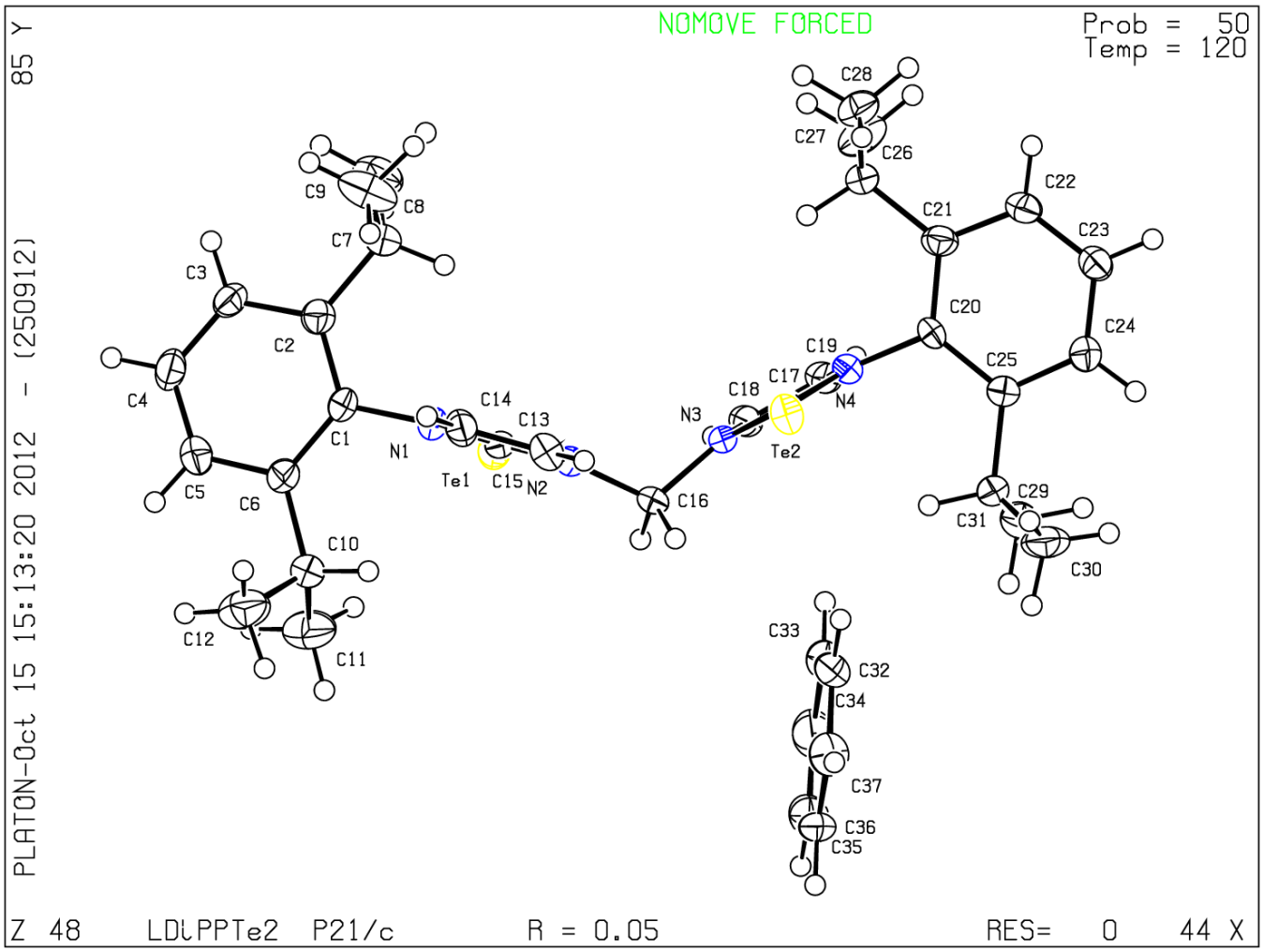
Datablock LDiPPH2OTf2 - ellipsoid plot



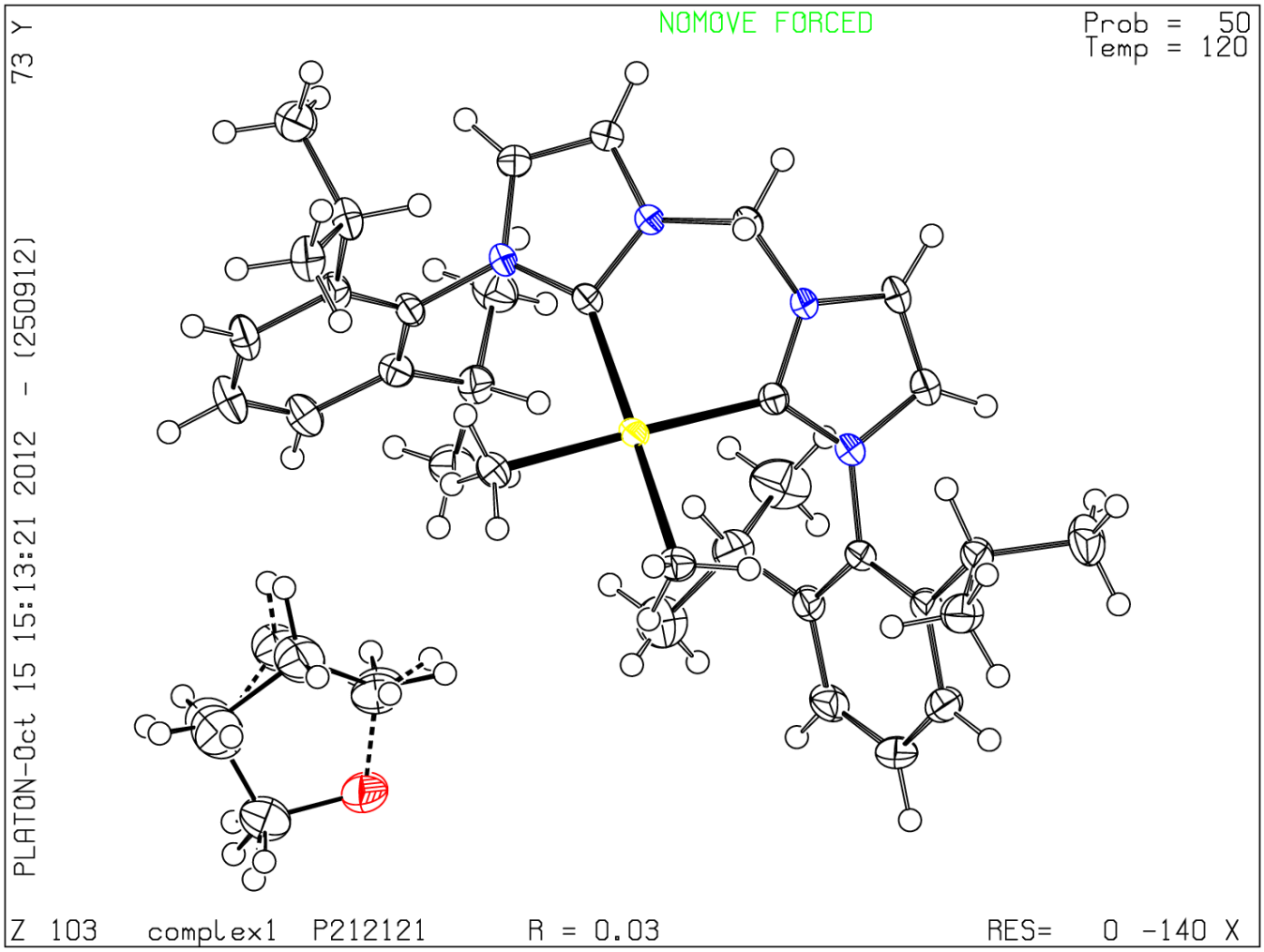
Datablock Lmes - ellipsoid plot



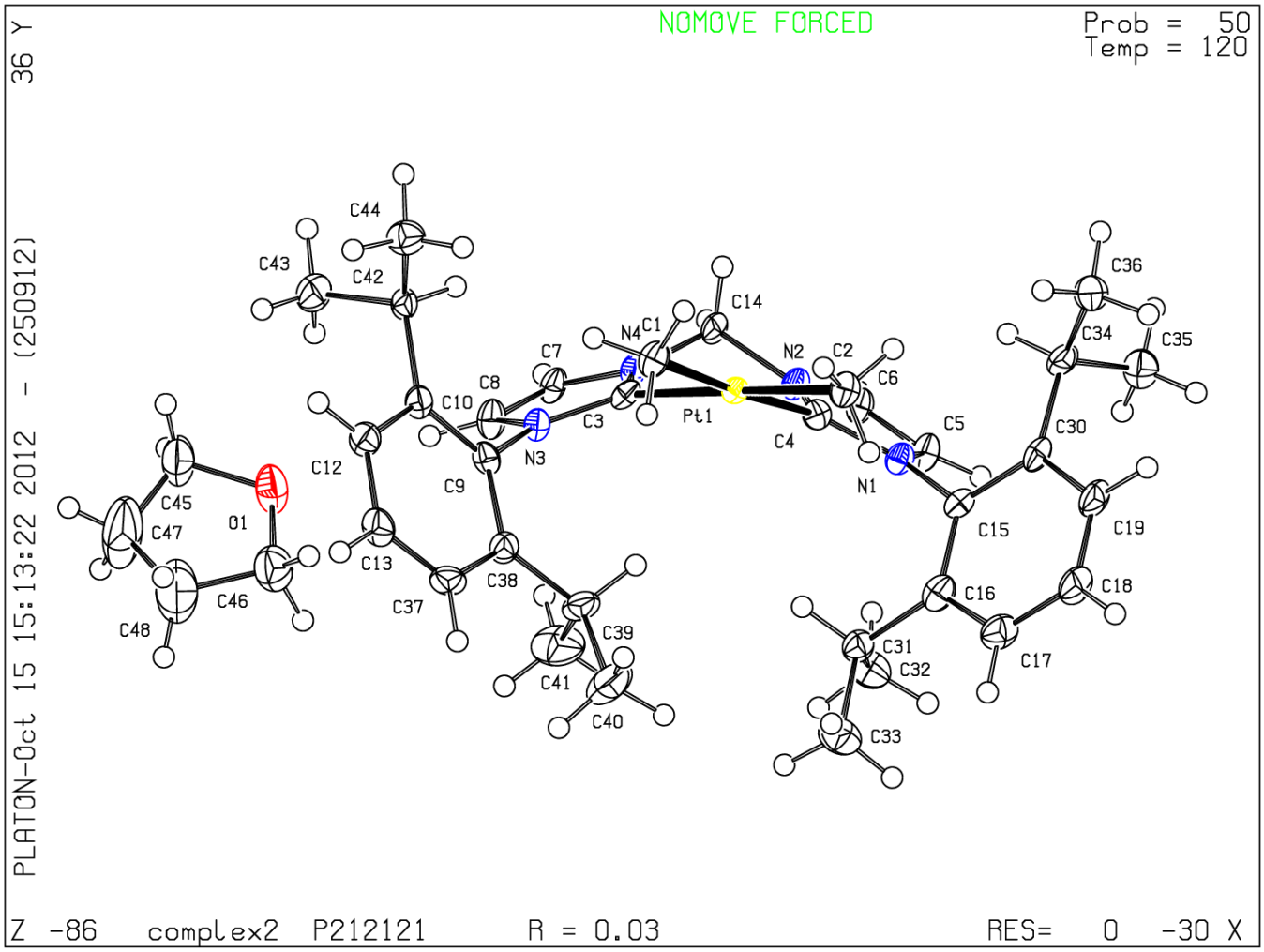
Datablock LDiPPTe2 - ellipsoid plot



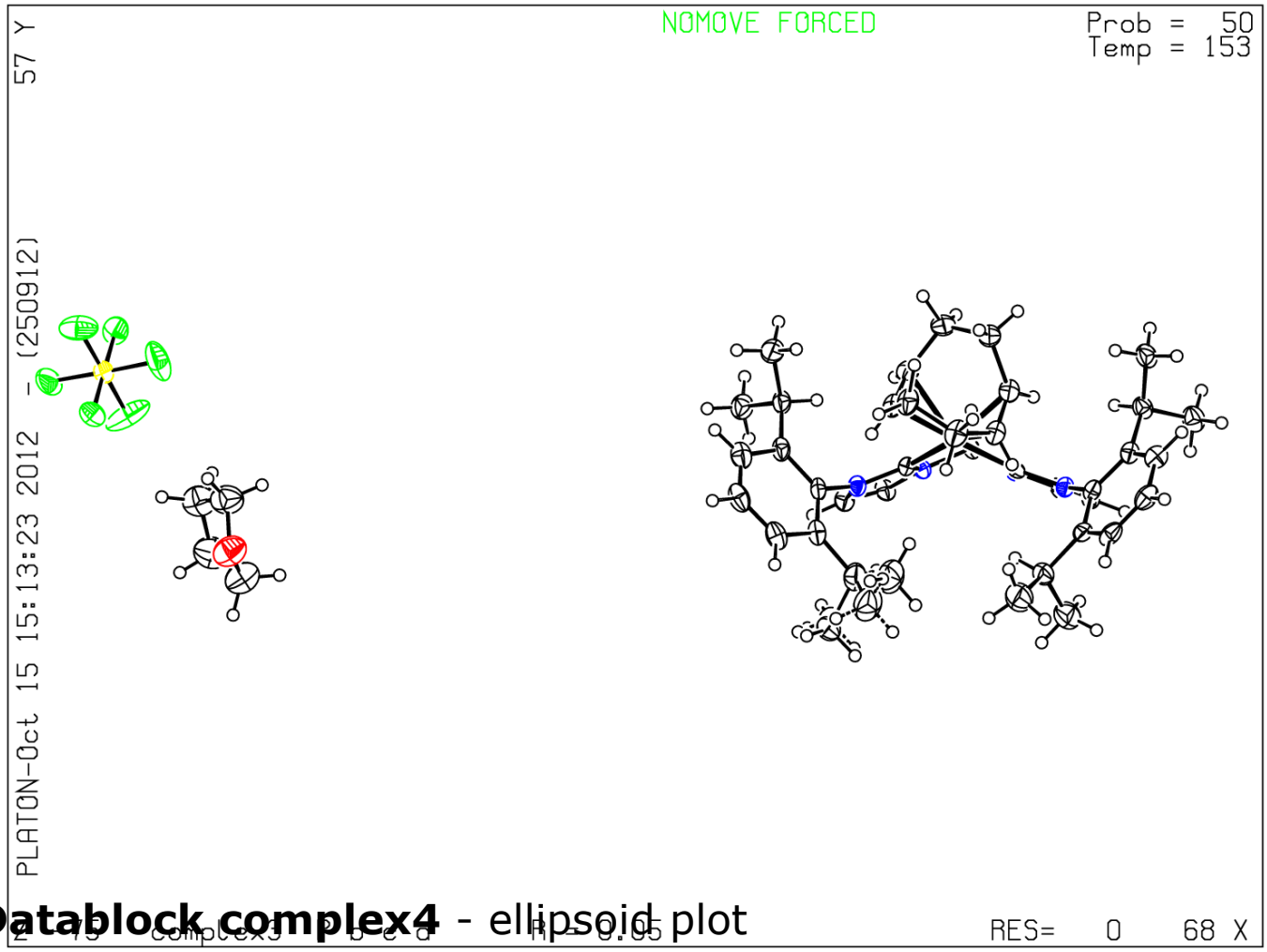
Datablock complex1 - ellipsoid plot



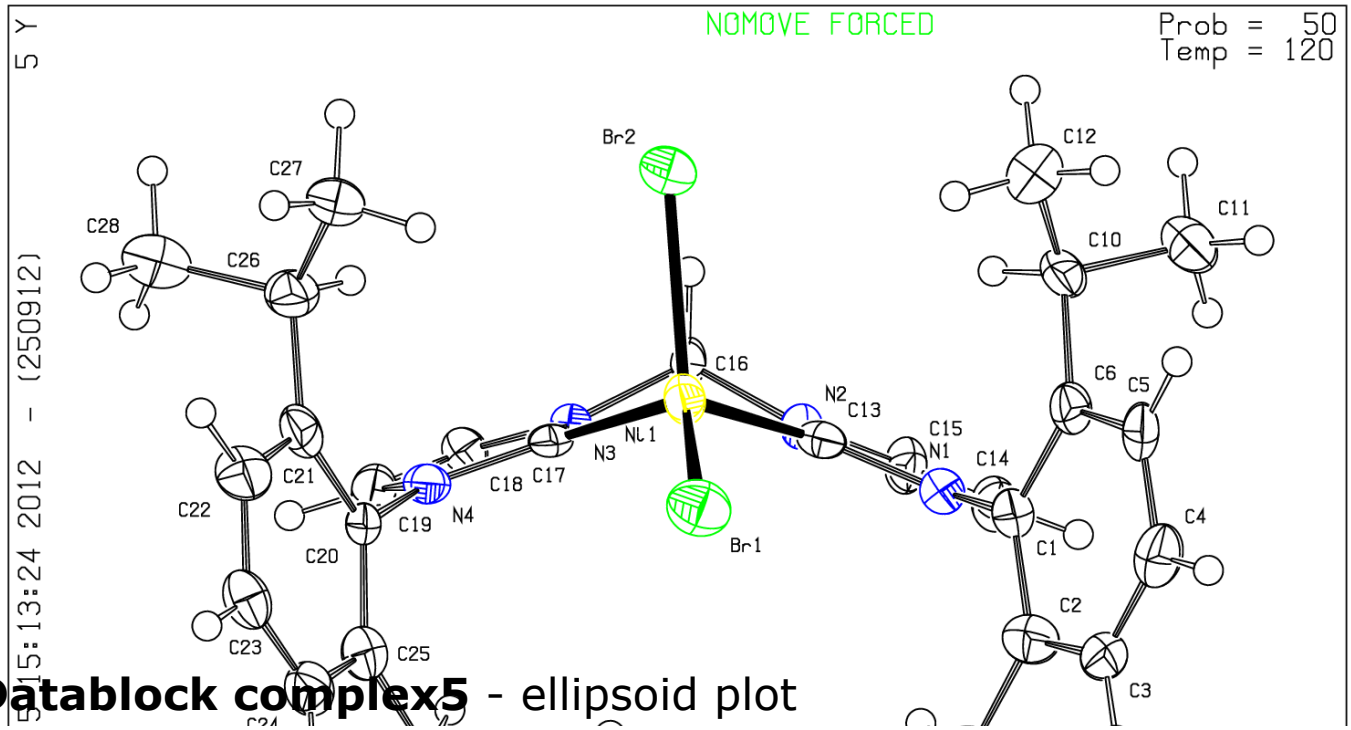
Datablock complex2 - ellipsoid plot



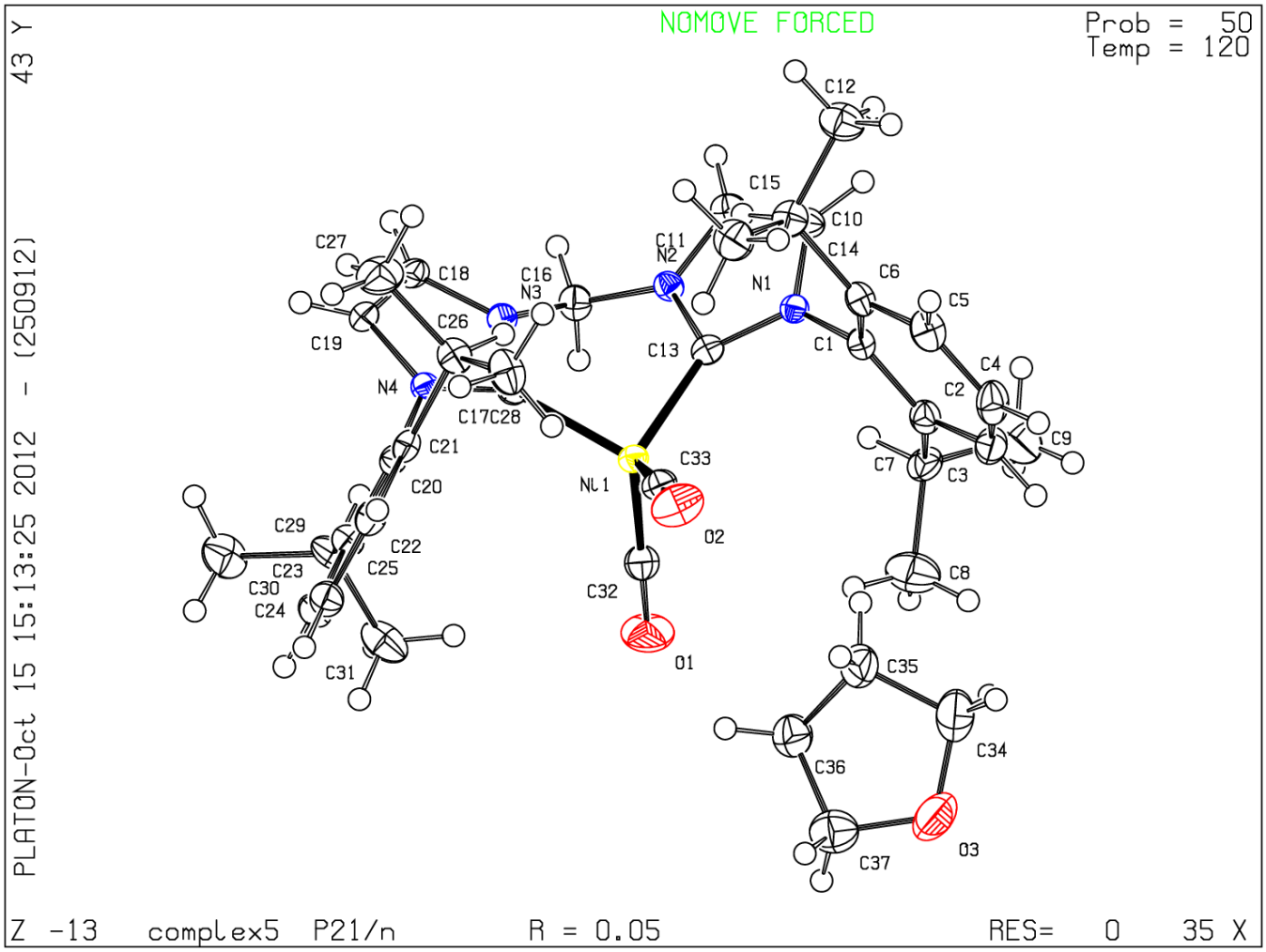
Datablock complex3 - ellipsoid plot



Datablock complex4 - ellipsoid plot



Datablock complex5 - ellipsoid plot



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