checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1, 2, 3, 4

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: 1

```
Bond precision:  C-C = 0.0108 A          Wavelength=0.71073

Cell:          a=11.1262(9)      b=14.6920(14)    c=14.7874(14)
               alpha=70.037(9)   beta=85.302(8)   gamma=81.302(7)
Temperature:   150 K
```

	Calculated	Reported
Volume	2244.7(4)	2244.7(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C35 H51 B2 Ce N14, C7 H8	C35 H51 B2 Ce N14, C7 H8
Sum formula	C42 H59 B2 Ce N14	C42 H59 B2 Ce N14
Mr	921.77	921.77
Dx,g cm-3	1.364	1.364
Z	2	2
Mu (mm-1)	1.061	1.061
F000	954.0	954.0
F000’	953.70	
h,k,lmax	13,17,17	13,17,17
Nref	8234	8201
Tmin,Tmax	0.834,0.905	0.806,1.000
Tmin’	0.834	

```
Correction method= # Reported T Limits: Tmin=0.806 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.996          Theta(max)= 25.350

R(reflections)= 0.0642( 6502)     wR2(reflections)= 0.1414( 8201)

S = 1.037                 Npar= 547
```

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 Th(Min) ... 16 Report

Author Response: Reduction of beam stop mask did not yield significant improvement. Most of those missing strong reflections appeared to be very strong and were treated as overflows.

PLAT971_ALERT_2_B Check Calcd Residual Density 1.05A From Ce1 3.46 eA-3

Author Response: The residual density could not be modelled as any chemically sensible species. Since the peak is in the proximity of a strong absorber, this could be due to imperfections in the absorption corrections.

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.15 Report
PLAT213_ALERT_2_C Atom N4 has ADP max/min Ratio ..... 3.8 oblate
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C37 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C36 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.8 Note
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist. C36 -C41 1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0108 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 62 Ang3
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 3.820 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 18 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 2 Note
PLAT971_ALERT_2_C Check Calcd Residual Density 1.02A From Ce1 2.26 eA-3

Author Response: The residual density could not be modelled as any chemically sensible species. Since the peak is in the proximity of a strong absorber, this could be due to imperfections in the absorption corrections.

PLAT975_ALERT_2_C Check Calcd Residual Density 0.85A From N6 0.78 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density 0.80A From N14 0.68 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 7 Report
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C42 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 51 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
14 **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

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

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

Datablock: 2

Bond precision: C-C = 0.0066 A Wavelength=0.71073

Cell: a=14.2034(4) b=20.6250(7) c=17.1106(6)
       alpha=90 beta=95.066(3) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	4992.9(3)	4992.9(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C40 H52 B2 Ce N14, 2(C4 H8 O)	C40 H52 B2 Ce N14, 2(C4 H8 O)
Sum formula	C48 H68 B2 Ce N14 O2	C48 H68 B2 Ce N14 O2
Mr	1034.90	1034.90
Dx,g cm-3	1.377	1.377
Z	4	4
Mu (mm-1)	0.965	0.965
F000	2152.0	2152.0
F000’	2151.54	
h,k,lmax	17,24,20	17,24,20
Nref	9143	9125
Tmin,Tmax	0.894,0.912	0.951,1.000
Tmin’	0.894	

Correction method= # Reported T Limits: Tmin=0.951 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.998 Theta(max)= 25.350

R(reflections)= 0.0523(7004) wR2(reflections)= 0.1163(9125)

S = 1.035 Npar= 708

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 Th(Min) ... 17 Report

Author Response: Reduction of beam stop mask did not yield significant improvement. Most of those missing strong reflections appeared to be very strong and were treated as overflows.

Alert level C

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PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H14C   ..  H46C    ..       2.12 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.852 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          2 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT971_ALERT_2_C Check Calcd Residual Density  1.09A From     Ce1       1.74 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  1.11A From     Ce1      -1.59 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.93A From     Ce1      -1.53 eA-3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         20 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          8 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =        100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   8.09) in Resd. #          2 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   7.05) in Resd. #          3 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   4.91) in Resd. #          4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   5.95) in Resd. #          5 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        158 Note
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  10 ALERT level G = General information/check it is not something unexpected

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

Datablock: 3

```
Bond precision:  C-C = 0.0081 A          Wavelength=1.54184

Cell:          a=10.0579(4)      b=13.3606(6)     c=13.6905(7)
               alpha=87.438(4)   beta=73.681(4)   gamma=71.869(4)
Temperature:   100 K
```

	Calculated	Reported
Volume	1676.10(14)	1676.10(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C50 H74 B4 Ce2 N20 O2	C50 H74 B4 Ce2 N20 O2, 2(C4 H8 O)
Sum formula	C50 H74 B4 Ce2 N20 O2	C62 H90 B4 Ce2 N20 O4
Mr	1310.77	1447.64
Dx,g cm-3	1.299	1.291
Z	1	1
Mu (mm-1)	10.750	10.730
F000	666.0	662.0
F000’	664.08	
h,k,lmax	12,16,16	12,16,16
Nref	6139	5891
Tmin,Tmax	0.088,0.172	0.197,1.000
Tmin’	0.013	

Correction method= # Reported T Limits: Tmin=0.197 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.960 Theta(max)= 68.251

R(reflections)= 0.0448(5342) wR2(reflections)= 0.1153(5891)

S = 1.040 Npar= 368

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

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10

From the CIF: _cell_formula_units_Z 1
From the CIF: _chemical_formula_weight 1447.64
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	50.00	600.55
H	1.01	74.00	74.59
B	10.81	4.00	43.24
Ce	140.12	2.00	280.24
N	14.01	20.00	280.14
O	16.00	2.00	32.00

Calculated formula weight 1310.76

PLAT046_ALERT_1_A Reported Z, MW and D(calc) are Inconsistent 1.434

Alert level B

DENSD01_ALERT_1_B The ratio of the submitted crystal density and that calculated from the formula is outside the range 0.95 <> 1.05

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            Crystal density given    =      1.291
            Calculated crystal density =      1.434
```

Alert level C

```
ABSMU01_ALERT_1_C  The ratio of given/expected absorption coefficient lies
               outside the range 0.99 <> 1.01
            Calculated value of mu =    10.851
            Value of mu given      =    10.730
CHEMW01_ALERT_1_C  The ratio of given/expected molecular weight as calculated
            from the _chemical_formula_sum lies outside
            the range 0.99 <> 1.01
            Calculated formula weight =  1503.0045
            Formula weight given      =  1447.6400
CHEMW01_ALERT_1_C  The difference between the given and expected weight for
            compound is greater 1 mass unit. Check that all hydrogen
            atoms have been taken into account.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.961 Note
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0081 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600        239 Report
```

Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C62 H90 B4 Ce2 N20 O4
            Atom count from _chemical_formula_moiety:C58 H90 B4 Ce2 N20 O4
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:C62 H90 B4 Ce2 N20 O4
            Atom count from the _atom_site data:  C50 H74 B4 Ce2 N20 O2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    1
           From the CIF: _chemical_formula_sum  C62 H90 B4 Ce2 N20 O4
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         62.00     50.00   12.00
           H         90.00     74.00   16.00
           B          4.00      4.00    0.00
           Ce         2.00      2.00    0.00
           N         20.00     20.00    0.00
           O          4.00      2.00    2.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         39 Report
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........    0.00400 Degree
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C9 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       357 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         10 Note
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```
  11 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
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   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: 4

Bond precision: C-C = 0.0106 A Wavelength=0.71073

Cell: a=11.2609(3) b=12.5209(3) c=16.7464(4)
       alpha=105.035(2) beta=96.314(2) gamma=112.313(3)
Temperature: 150 K

	Calculated	Reported
Volume	2051.38(11)	2051.38(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H44 B2 Ce N15, C7 H8	C30 H44 B2 Ce N15, C7 H8
Sum formula	C37 H52 B2 Ce N15	C37 H52 B2 Ce N15
Mr	868.68	868.67
Dx,g cm-3	1.406	1.406
Z	2	2
Mu (mm-1)	1.157	1.157
F000	894.0	894.0
F000’	893.68	
h,k,lmax	13,15,20	13,15,20
Nref	7512	28373
Tmin,Tmax	0.754,0.861	0.687,1.000
Tmin’	0.724	

Correction method= # Reported T Limits: Tmin=0.687 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 3.777 Theta(max)= 25.346

R(reflections)= 0.0515(22381) wR2(reflections)= 0.1518(28373)

S = 1.097 Npar= 510

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 Th(Min) ... 14 Report

Alert level C

```
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0106 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.530 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          6 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much smaller I(calc) .          2 Check
```

Alert level G

```
PLAT021_ALERT_4_G Ratio Unique / Expected Reflections too High ...      3.777
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C10 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C37 Check
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
```

```
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```

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

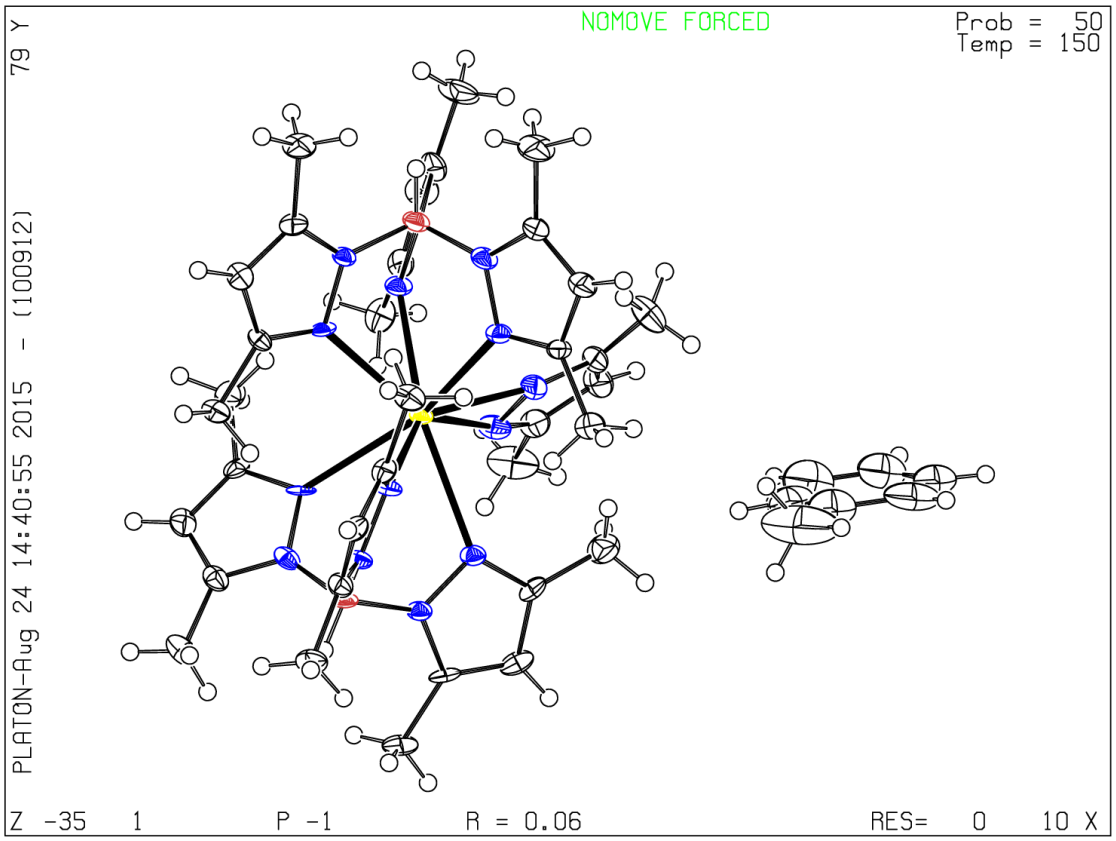
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

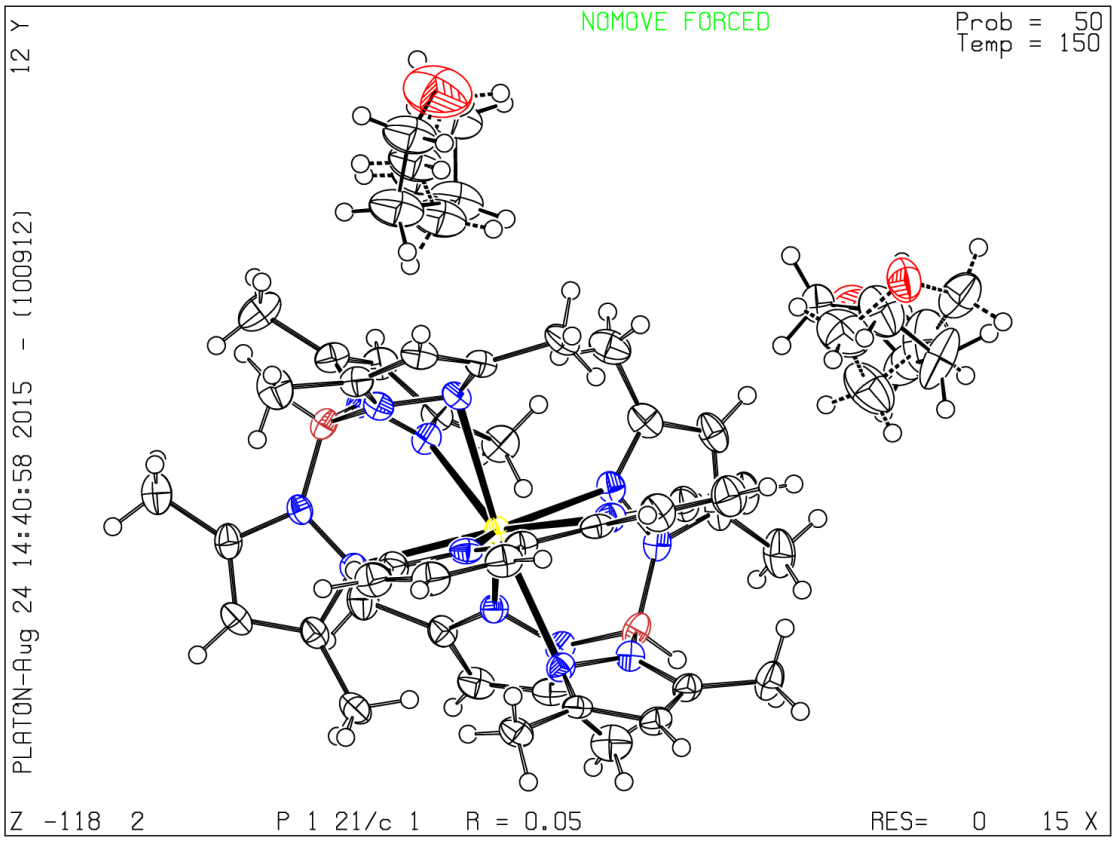
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 21/06/2015; check.def file version of 21/06/2015

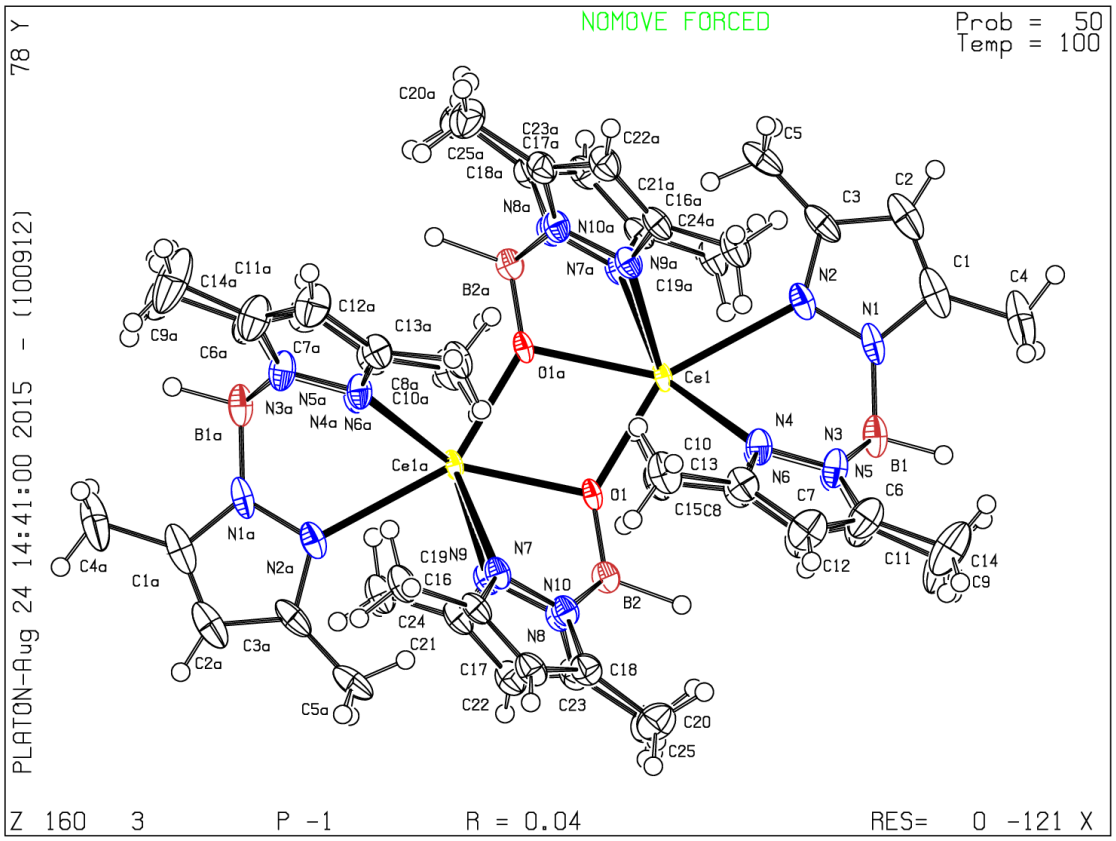
Datablock 1 - ellipsoid plot



Datablock 2 - ellipsoid plot



Datablock 3 - ellipsoid plot



Datablock 4 - ellipsoid plot