checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: Ligand_1a

Bond precision: C-C = 0.0021 A Wavelength=0.71073

Cell: **a=12.3641(12)** **b=16.3858(16)** **c=15.4945(15)**
alpha=90 **beta=90** **gamma=90**
Temperature: **173 K**

	Calculated	Reported
Volume	3139.1(5)	3139.1(5)
Space group	P c c n	Pccn
Hall group	-P 2ab 2ac	-P2ab2ac
Moiety formula	C17 H25 N O	C17 H25 N O
Sum formula	C17 H25 N O	C17 H25 N O
Mr	259.38	259.38
Dx,g cm-3	1.098	1.098
Z	8	8
Mu (mm-1)	0.067	0.067
F000	1136.0	1136.0
F000’	1136.42	
h,k,lmax	15,20,19	15,20,19
Nref	3336	3338
Tmin,Tmax	0.968,0.987	0.826,0.984
Tmin’	0.964	

Correction method= MULTI-SCAN

Data completeness= 1.001 **Theta(max)= 26.730**

R(reflections)= 0.0428(2431) **wR2(reflections)= 0.1201(3338)**

S = 1.032 **Npar= 182**

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

ABSTM02_ALERT_3_C The ratio of expected to reported Tmax/Tmin(RR’) is < 0.90
Tmin and Tmax reported: 0.826 0.984
Tmin(prime) and Tmax expected: 0.964 0.987
RR(prime) = 0.859
Please check that your absorption correction is appropriate.

Alert level G
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.54 mm

0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
1 **ALERT level C** = Check and explain
1 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: Ligand_1b

Bond precision: C-C = 0.0020 A Wavelength=0.71073

Cell: a=10.0068(6) b=9.8961(6) c=12.7933(8)
alpha=90 beta=99.138(1) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	1250.82(13)	1250.82(13)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	-P2yn
Moiety formula	C14 H19 N O	C14 H19 N O
Sum formula	C14 H19 N O	C14 H19 N O
Mr	217.30	217.30
Dx,g cm-3	1.154	1.154
Z	4	4
Mu (mm-1)	0.072	0.072
F000	472.0	472.0
F000’	472.18	
h,k,lmax	12,12,16	12,12,16
Nref	2762	2762
Tmin,Tmax	0.981,0.990	0.938,0.991
Tmin’	0.981	

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 27.100

R(reflections)= 0.0462(2330) wR2(reflections)= 0.1349(2762)

S = 1.047 Npar= 153

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

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.27 mm
PLAT128_ALERT_4_G Non-standard setting of Space-group P21/c P21/n

0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
0 **ALERT level C** = Check and explain
2 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: Ligand_1c

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=6.7423(4) b=13.9706(8) c=18.0631(10)
alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	1701.44(17)	1701.44(17)
Space group	P 21 21 21	P2(1)2(1)2(
Hall group	P 2ac 2ab	P2ac2ab
Moiety formula	C18 H27 N O	C18 H27 N O
Sum formula	C18 H27 N O	C18 H27 N O
Mr	273.41	273.41
Dx,g cm-3	1.067	1.067
Z	4	4
Mu (mm-1)	0.065	0.065
F000	600.0	600.0
F000’	600.22	
h,k,lmax	8,18,23	8,18,23
Nref	2228[3866]	2224
Tmin,Tmax	0.985,0.991	0.928,0.992
Tmin’	0.973	

Correction method= MULTI-SCAN

Data completeness= 1.00/0.58 Theta(max)= 27.400

R(reflections)= 0.0407(2022) wR2(reflections)= 0.1172(2224)

S = 1.031 Npar= 191

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) ...       3.58 Ratio
PLAT222_ALERT_3_C Large Non-Solvent    H     Ueq(max)/Ueq(min) ...       3.45 Ratio
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C13
```

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           27.40
          From the CIF: _reflns_number_total               2224
          Count of symmetry unique reflns         2228
          Completeness (_total/calc)             99.82%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured          0
          Fraction of Friedel pairs measured     0.000
          Are heavy atom types Z>Si present          no
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....       0.42 mm
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0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
3 **ALERT level C** = Check and explain
2 **ALERT level G** = General alerts; check

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

Datablock: Ligand_1d

Bond precision: C-C = 0.0020 A Wavelength=0.71073

Cell: a=18.8762(17) b=8.0097(7) c=19.0037(17)
alpha=90 beta=107.543(1) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	2739.6(4)	2739.6(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C2yc
Moiety formula	C15 H21 N O	C15 H21 N O
Sum formula	C15 H21 N O	C15 H21 N O
Mr	231.33	231.33
Dx,g cm-3	1.122	1.122
Z	8	8
Mu (mm-1)	0.069	0.069
F000	1008.0	1008.0
F000’	1008.38	
h,k,lmax	24,10,24	24,10,24
Nref	3152	3153
Tmin,Tmax	0.972,0.989	0.917,0.992
Tmin’	0.971	

Correction method= MULTI-SCAN

Data completeness= 1.000 **Theta(max)= 27.480**

R(reflections)= 0.0465(2517) **wR2(reflections)= 0.1402(3153)**

S = 1.053 **Npar= 163**

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
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.43 mm

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0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
0 **ALERT level C** = Check and explain
1 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
0 ALERT type 5 Informative message, check

Datablock: Complex_2a

Bond precision: C-C = 0.0031 A **Wavelength=0.71073**

Cell:	**a=9.4060(8)**	**b=10.7931(9)**	**c=11.9959(10)**
	alpha=69.040(1)	**beta=73.616(1)**	**gamma=67.016(1)**
Temperature:	**173 K**		

	Calculated	**Reported**
Volume	**1032.50(15)**	**1032.50(15)**
Space group	**P -1**	**P-1**
Hall group	**-P 1**	**-P1**
Moiety formula	**C42 H64 Li2 N2 O4**	**C42 H64 Li2 N2 O4**
Sum formula	**C42 H64 Li2 N2 O4**	**C42 H64 Li2 N2 O4**
Mr	**674.83**	**674.83**
Dx,g cm-3	**1.085**	**1.085**
Z	**1**	**1**
Mu (mm-1)	**0.067**	**0.067**
F000	**368.0**	**368.0**
F000’	**368.14**	
h,k,lmax	**11,13,14**	**11,13,14**
Nref	**4063**	**4040**
Tmin,Tmax	**0.984,0.992**	**0.914,0.992**
Tmin’	**0.976**	

Correction method= MULTI-SCAN

Data completeness= 0.994 **Theta(max)= 26.030**

R(reflections)= 0.0464(2908) **wR2(reflections)= 0.1274(4040)**

S = 1.035 **Npar= 232**

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

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.36 mm
PLAT154_ALERT_1_G The su’s on the Cell Angles are Equal (x 10000) 100 Deg.

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0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
0 **ALERT level C** = Check and explain
2 **ALERT level G** = General alerts; check

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
0 ALERT type 5 Informative message, check

Datablock: Complex_2b

Bond precision: C-C = 0.0024 A Wavelength=0.71073

Cell: a=8.0148(5) b=15.0628(9) c=14.5918(9)
alpha=90 beta=103.855(1) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	1710.35(18)	1710.35(18)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	-P2ybc
Moiety formula	C36 H52 Li2 N2 O4	C36 H52 Li2 N2 O4
Sum formula	C36 H52 Li2 N2 O4	C36 H52 Li2 N2 O4
Mr	590.68	590.68
Dx,g cm-3	1.147	1.147
Z	2	2
Mu (mm-1)	0.073	0.073
F000	640.0	640.0
F000’	640.25	
h,k,lmax	10,19,18	10,19,18
Nref	3925	3919
Tmin,Tmax	0.984,0.992	0.896,0.992
Tmin’	0.972	

Correction method= MULTI-SCAN

Data completeness= 0.998 **Theta(max)= 27.480**

R(reflections)= 0.0495(2722) **wR2(reflections)= 0.1409(3919)**

S = 1.025 **Npar= 204**

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
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.39 mm

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0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
0 **ALERT level C** = Check and explain
1 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
0 ALERT type 5 Informative message, check

Datablock: Complex_2c

Bond precision: C-C = 0.0023 A Wavelength=0.71073

Cell: a=20.843(5) b=10.495(2) c=21.365(5)
alpha=90 beta=112.886(2) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	4305.6(17)	4305.7(17)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	-P2yn
Moiety formula	C44 H68 Li2 N2 O4	C44 H68 Li2 N2 O4
Sum formula	C44 H68 Li2 N2 O4	C44 H68 Li2 N2 O4
Mr	702.88	702.88
Dx,g cm-3	1.084	1.084
Z	4	4
Mu (mm-1)	0.067	0.067
F000	1536.0	1536.0
F000’	1536.59	
h,k,lmax	27,13,27	27,13,27
Nref	9877	9865
Tmin,Tmax	0.985,0.989	0.927,0.992
Tmin’	0.970	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.480

R(reflections)= 0.0453(7855) wR2(reflections)= 0.1285(9865)

S = 1.030 Npar= 483

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) ... 3.66 Ratio
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.49 Ratio
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C21
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C16
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C38

Alert level G

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.46 mm
PLAT128_ALERT_4_G Non-standard setting of Space-group P21/c P21/n

0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
5 **ALERT level C** = Check and explain
2 **ALERT level G** = General alerts; check

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

Datablock: Complex_4b

Bond precision: C-C = 0.0032 A Wavelength=0.71073

Cell: **a=13.7530(9) b=18.3062(13) c=24.0904(17)**
alpha=90 beta=90 gamma=90
Temperature: **173 K**

	Calculated	Reported
Volume	6065.1(7)	6065.1(7)
Space group	P 21 21 21	P2(1)2(1)2(
Hall group	P 2ac 2ab	P2ac2ab
Moiety formula	C56 H72 Li4 N4 O4, C7 H8	C56 H72 Li4 N4 O4, C7 H8
Sum formula	C63 H80 Li4 N4 O4	C63 H80 Li4 N4 O4
Mr	985.07	985.07
Dx,g cm-3	1.079	1.079
Z	4	4
Mu (mm-1)	0.065	0.065
F000	2120.0	2120.0
F000’	2120.77	
h,k,lmax	17,23,31	17,23,31
Nref	7606[13898]	7604
Tmin,Tmax	0.969,0.985	0.915,0.984
Tmin’	0.969	

Correction method= MULTI-SCAN

Data completeness= 1.00/0.55 Theta(max)= 27.480

R(reflections)= 0.0386(6488) wR2(reflections)= 0.1077(7604)

S = 1.039 Npar= 762

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

```
PLAT214_ALERT_2_C Atom C14S    (Anion/Solvent) ADP max/min Ratio         4.50 prola
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...      3.05 Ratio
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.09
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.63
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C2S
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C9S
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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          27.48
          From the CIF: _reflns_number_total              7604
          Count of symmetry unique reflns         7606
          Completeness (_total/calc)             99.97%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured         0
          Fraction of Friedel pairs measured     0.000
          Are heavy atom types Z>Si present          no
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        42
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....      0.48 mm
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................     50.00 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         6
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0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
6 **ALERT level C** = Check and explain
5 **ALERT level G** = General alerts; check

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

Datablock: Complex_4c

Bond precision: C-C = 0.0042 A Wavelength=0.71073

Cell:	**a=14.3398(14)**	**b=27.504(3)**	**c=19.8735(19)**
	alpha=90	**beta=107.487(1)**	**gamma=90**
Temperature:	**173 K**		

	Calculated	Reported
Volume	7475.9(13)	7475.9(13)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	-P2yn
Moiety formula	C72 H104 Li4 N4 O4	C72 H104 Li4 N4 O4
Sum formula	C72 H104 Li4 N4 O4	C72 H104 Li4 N4 O4
Mr	1117.36	1117.35
Dx,g cm-3	0.993	0.993
Z	4	4
Mu (mm-1)	0.059	0.059
F000	2432.0	2432.0
F000’	2432.86	
h,k,lmax	17,32,23	17,32,23
Nref	13209	13200
Tmin,Tmax	0.981,0.992	0.874,0.992
Tmin’	0.960	

Correction method= MULTI-SCAN

Data completeness= 0.999 **Theta(max)= 25.030**

R(reflections)= 0.0654(7858) **wR2(reflections)= 0.1786(13200)**

S = 0.985 **Npar= 785**

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

PLAT412_ALERT_2_B Short Intra XH3 .. XHn H1C .. H4A .. 1.75 Ang.
PLAT412_ALERT_2_B Short Intra XH3 .. XHn H19B .. H22A .. 1.74 Ang.
PLAT412_ALERT_2_B Short Intra XH3 .. XHn H37C .. H40C .. 1.76 Ang.
PLAT412_ALERT_2_B Short Intra XH3 .. XHn H55B .. H58A .. 1.75 Ang.
PLAT049_ALERT_1_B Calculated Density less than 1.0 gcm-3 ..... 0.99

Alert level C

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.97 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.02 Ratio
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C13
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C16

Alert level G

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.69 mm
PLAT128_ALERT_4_G Non-standard setting of Space-group P21/c P21/n
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure !

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0 **ALERT level A** = In general: serious problem
5 **ALERT level B** = Potentially serious problem

4 **ALERT level C** = Check and explain
3 **ALERT level G** = General alerts; check

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: Complex_4d

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: **a=13.0543(11) b=26.647(2) c=16.4965(14)**
alpha=90 beta=91.218(1) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	5737.1(8)	5737.1(8)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	-P2yn
Moiety formula	C60 H80 Li4 N4 O4	C60 H80 Li4 N4 O4
Sum formula	C60 H80 Li4 N4 O4	C60 H80 Li4 N4 O4
Mr	949.04	949.04
Dx,g cm-3	1.099	1.099
Z	4	4
Mu (mm-1)	0.067	0.067
F000	2048.0	2048.0
F000’	2048.74	
h,k,lmax	16,34,21	16,34,21
Nref	13161	13161
Tmin,Tmax	0.982,0.985	0.902,0.984
Tmin’	0.974	

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 27.480

R(reflections)= 0.0532(8453) wR2(reflections)= 0.1478(13161)

S = 1.011 Npar= 673

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
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.40 mm

```
PLAT128_ALERT_4_G Non-standard setting of Space-group P21/c   ....      P21/n
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety        C59
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   0 ALERT level A = In general: serious problem
   0 ALERT level B = Potentially serious problem
   0 ALERT level C = Check and explain
   3 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Publication of your CIF in IUCr journals

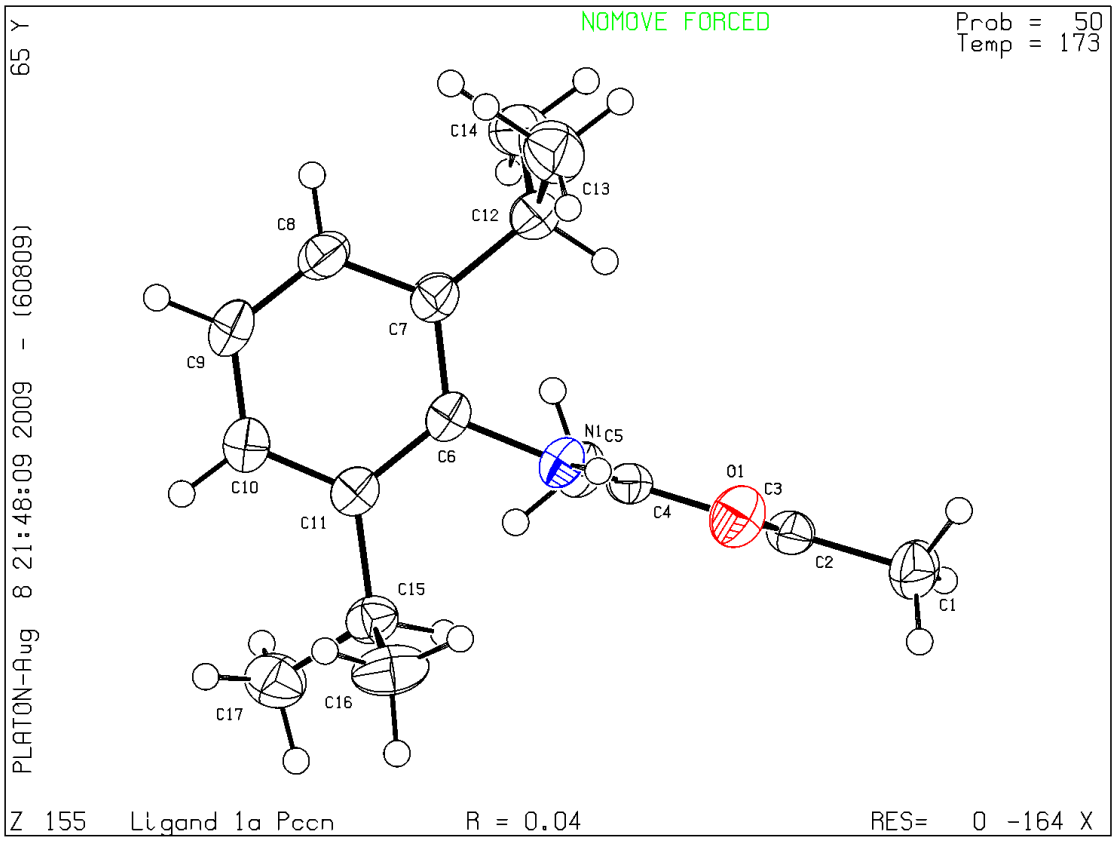
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

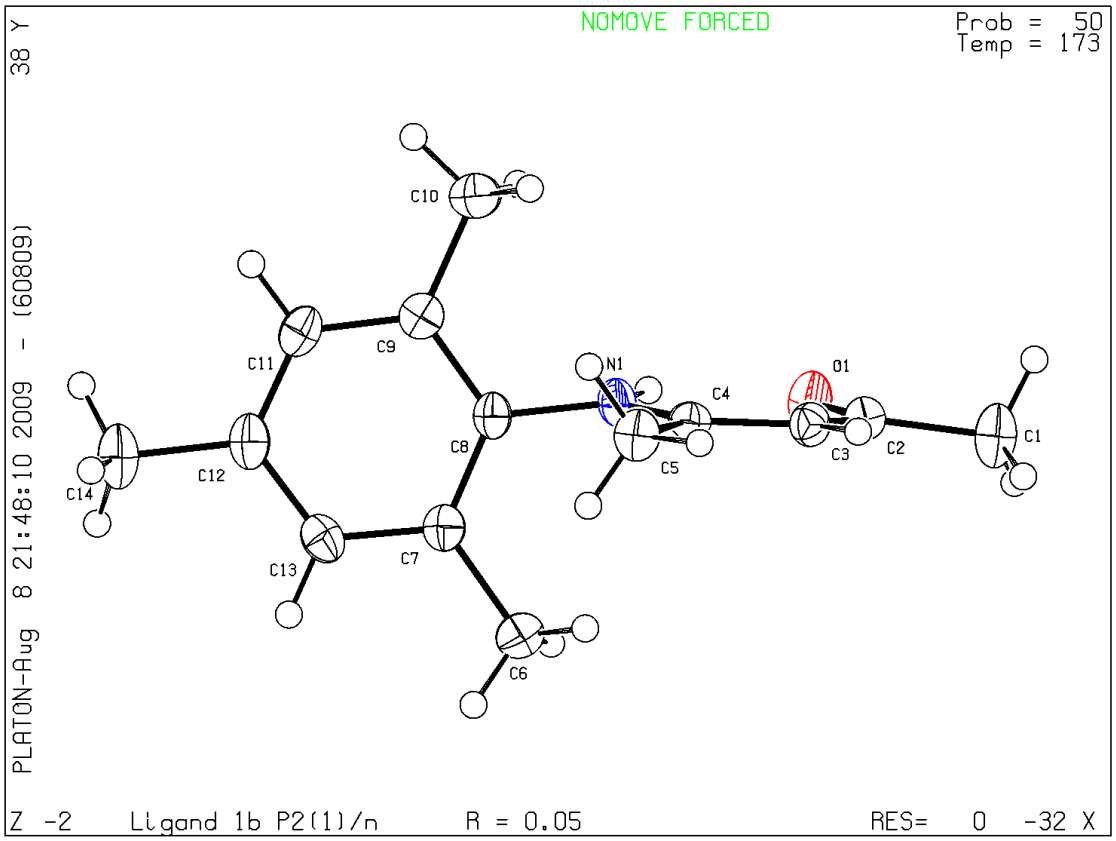
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/08/2009; check.def file version of 04/08/2009

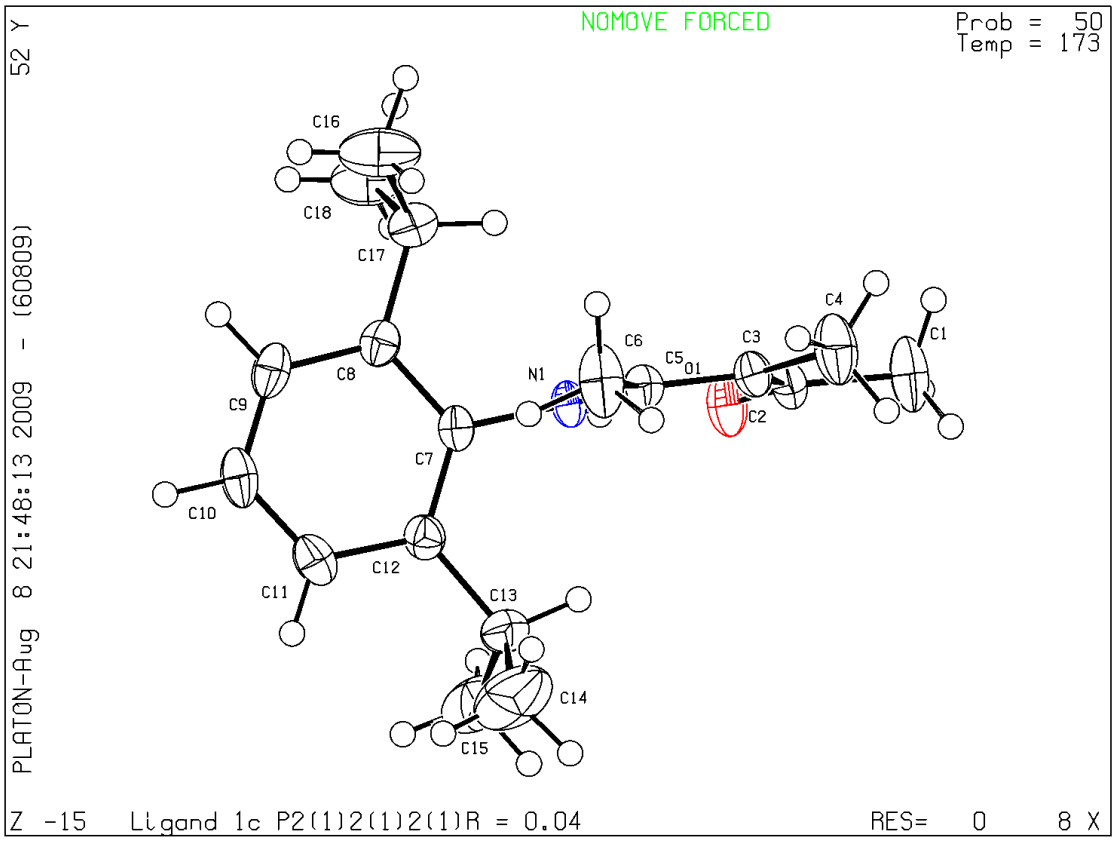
Datablock Ligand_1a - ellipsoid plot



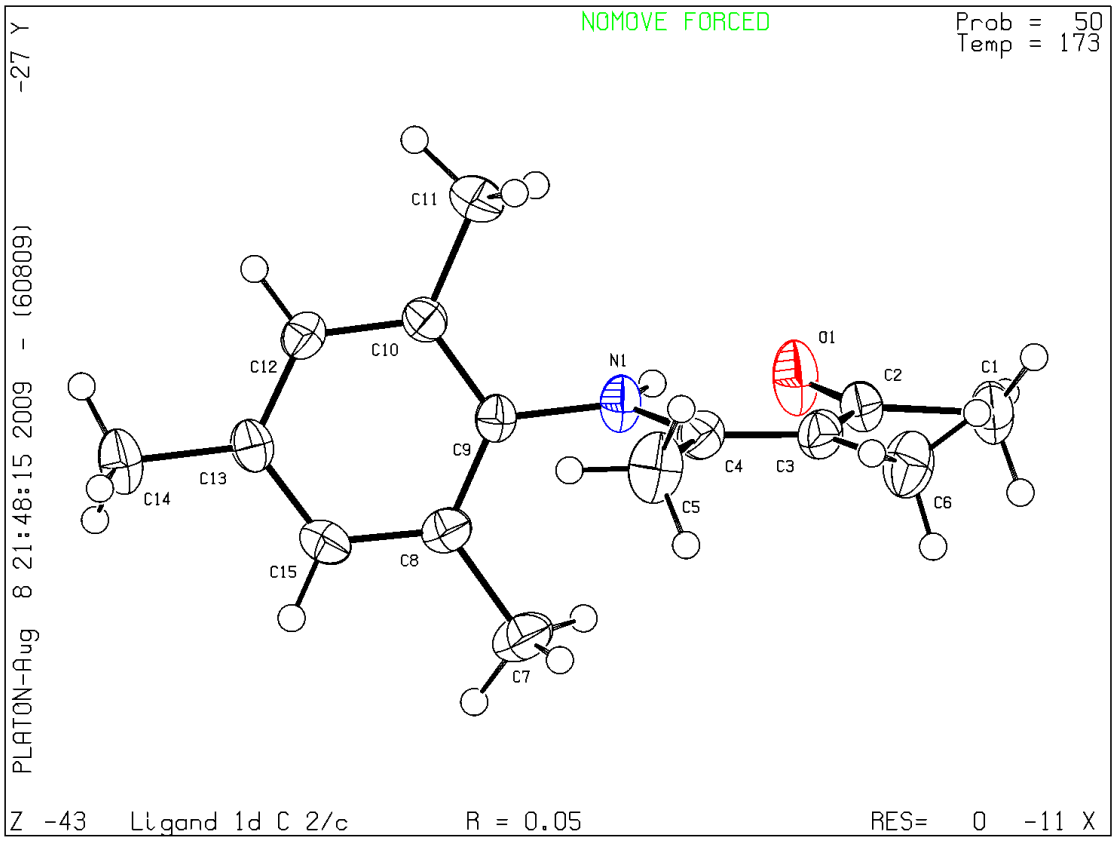
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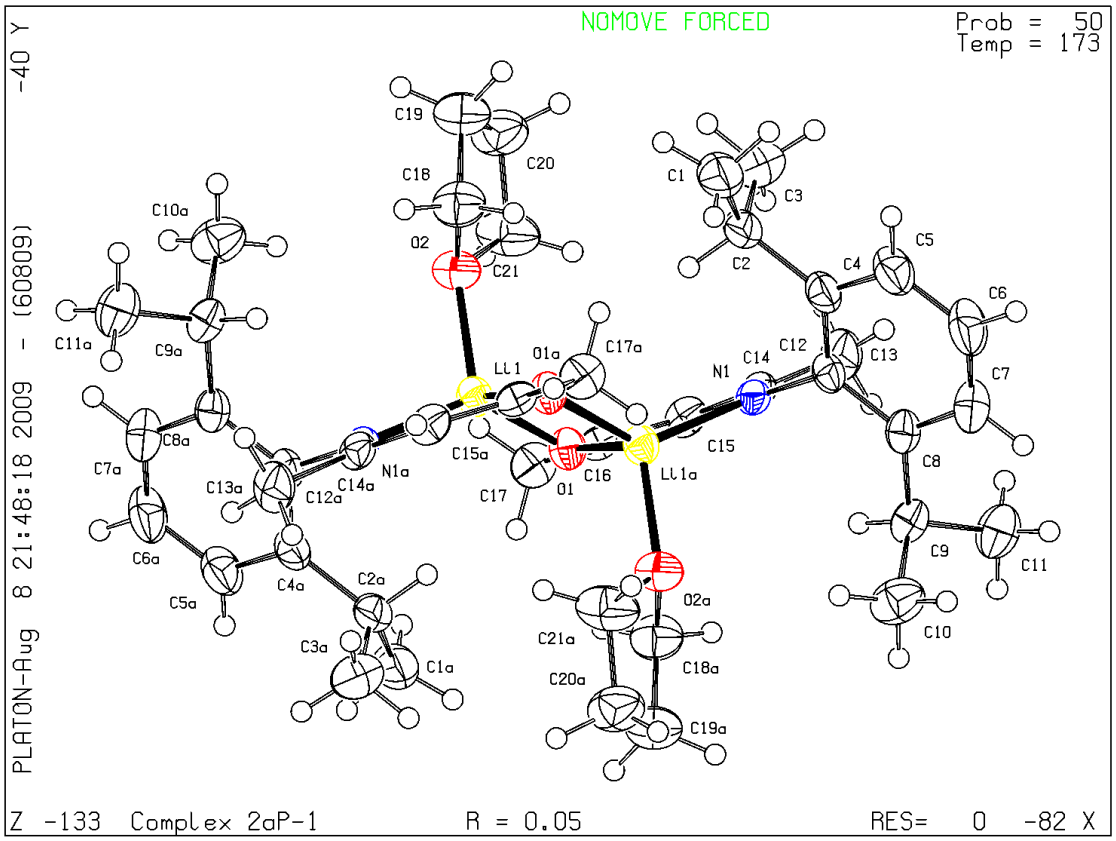
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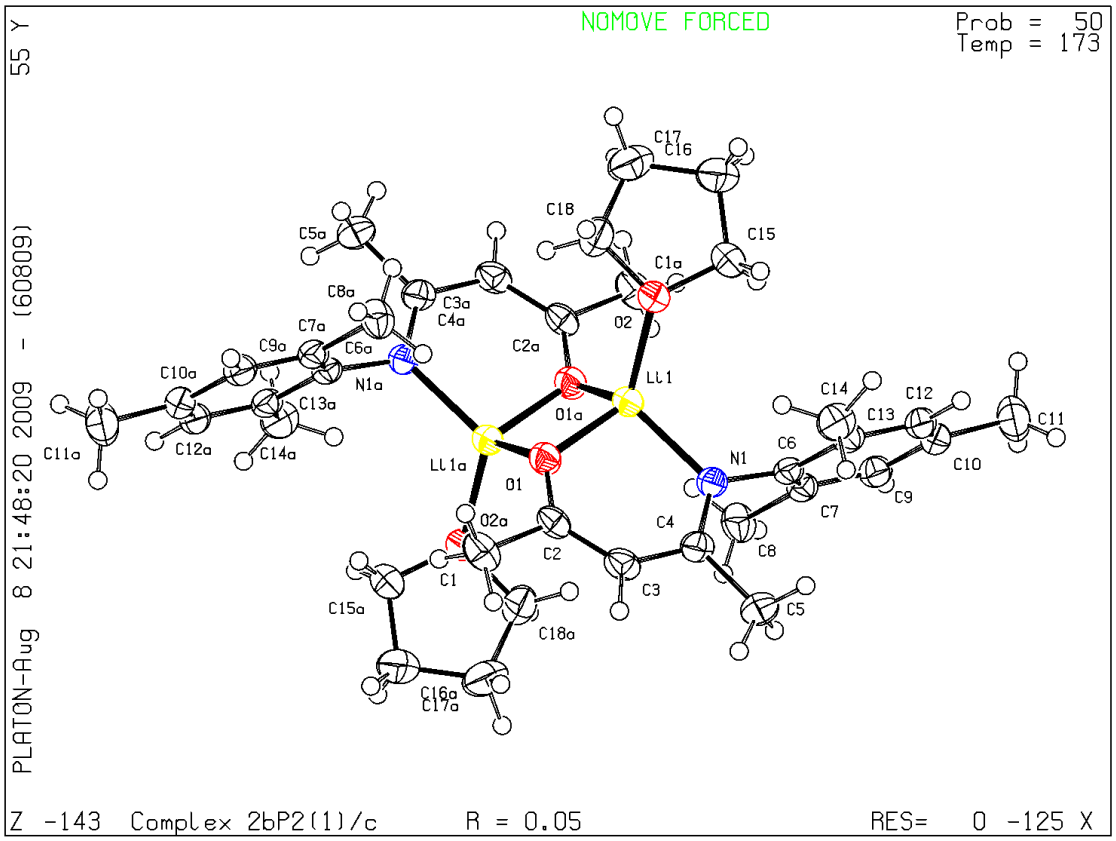
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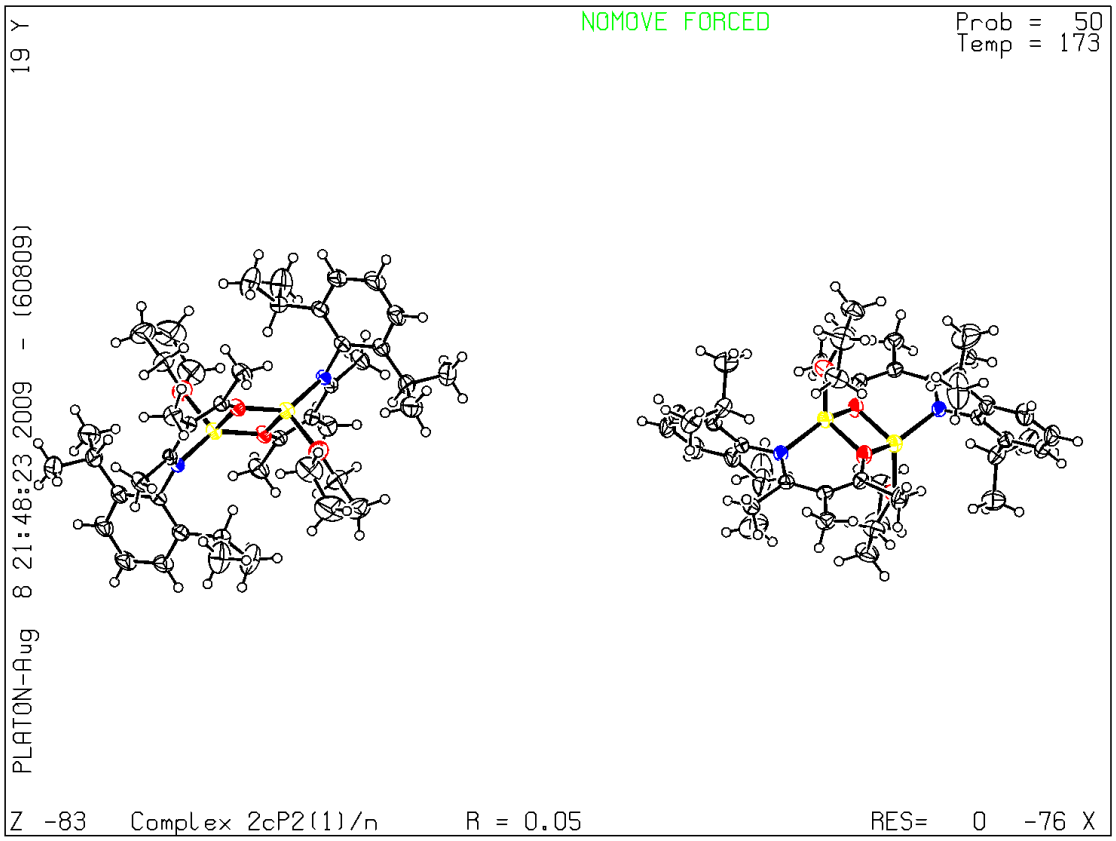
Datablock Complex_2a - ellipsoid plot



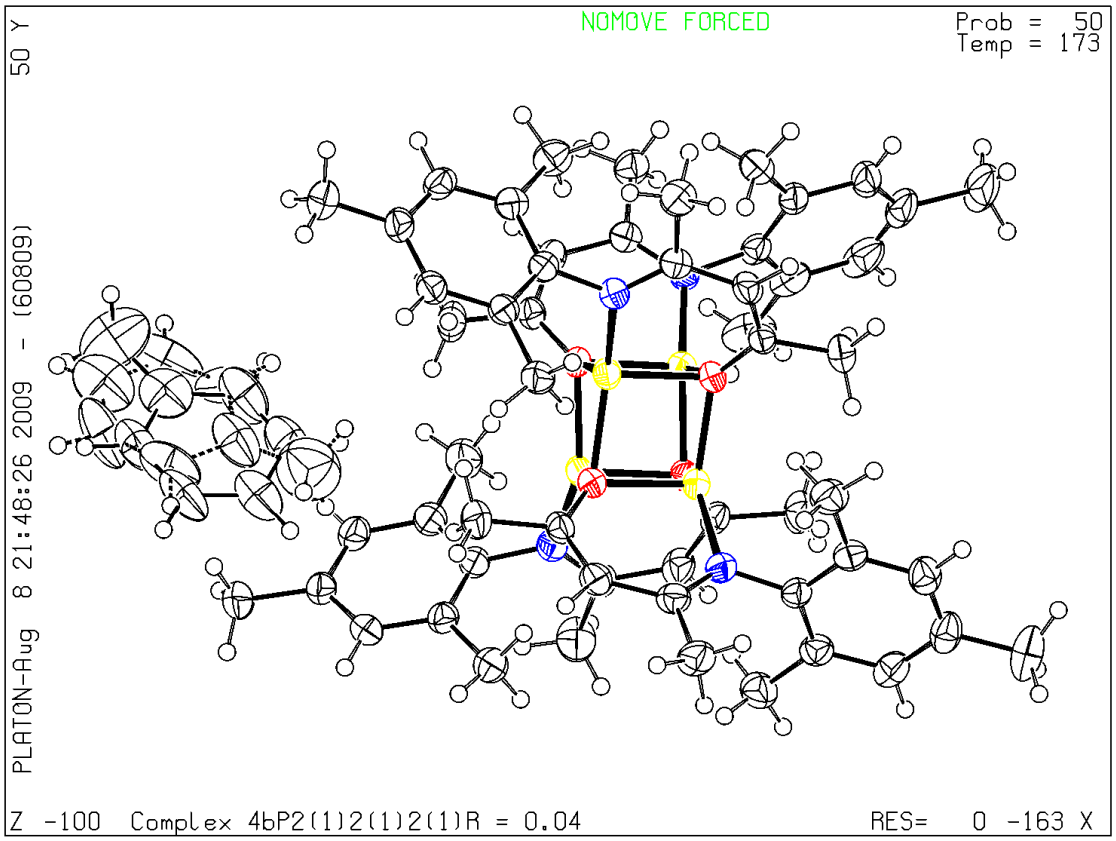
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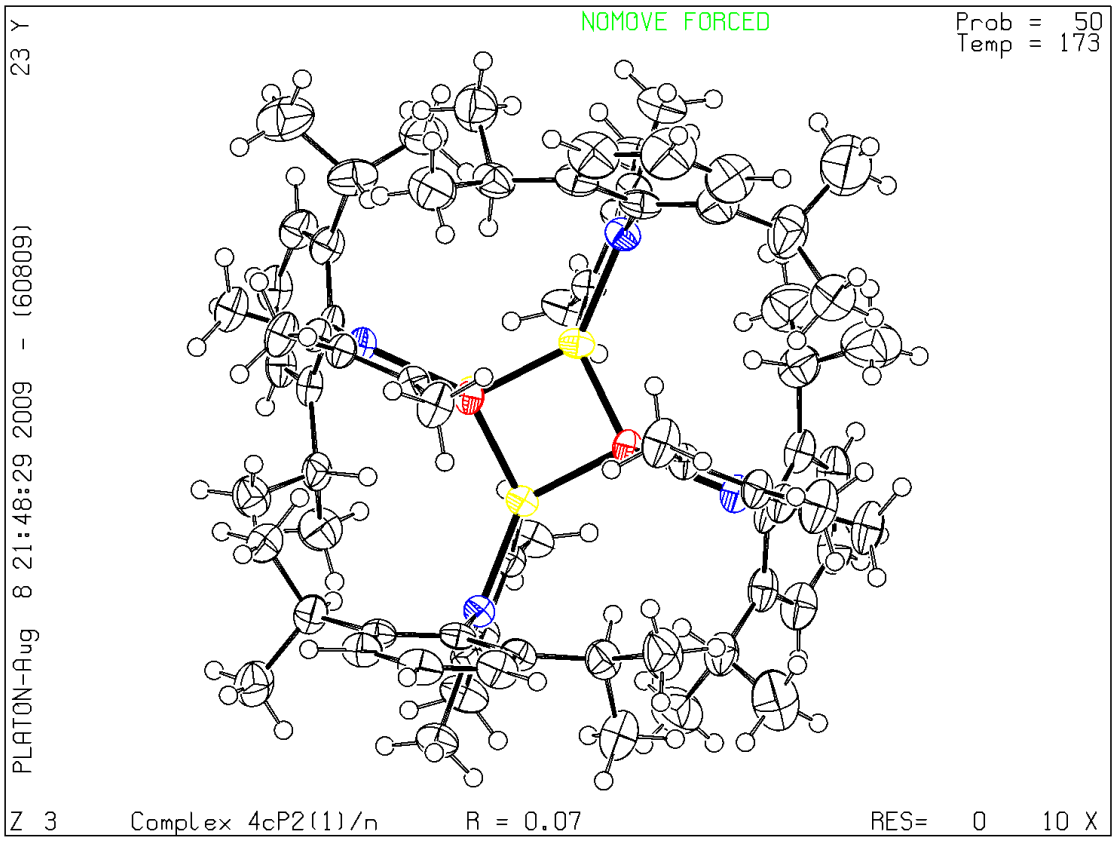
Datablock Complex_2c - ellipsoid plot



Datablock Complex_4b - ellipsoid plot



Datablock Complex_4c - ellipsoid plot



Datablock Complex_4d - ellipsoid plot

