checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2, 3, 3-decomposition, 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: 2

Bond precision: C-C = 0.0186 A Wavelength=0.71073

Cell: a=23.176(12) b=12.210(5) c=28.154(12)
alpha=90 beta=98.17(4) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	7886(6)	7886(6)
Space group	I 2/a	I 2/a
Hall group	-I 2ya	-I 2ya
Moiety formula	C36 H40 Bi Cl3 N2 [+ solvent]	C36 H40 Bi Cl3 N2
Sum formula	C36 H40 Bi Cl3 N2 [+ solvent]	C36 H40 Bi Cl3 N2
Mr	816.03	816.05
Dx,g cm-3	1.375	1.375
Z	8	8
Mu (mm-1)	4.698	4.698
F000	3232.0	3232.0
F000'	3204.23	
h,k,lmax	27,14,33	27,14,33
Nref	7222	7180
Tmin,Tmax	0.337,0.472	0.347,0.745
Tmin'	0.235	

Correction method= # Reported T Limits: Tmin=0.347 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 25.347

R(reflections)= 0.0788(4937) wR2(reflections)= 0.1991(7180)

S = 1.019 Npar= 379

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

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.265

Author Response: The investigated single crystal was of low quality and showed a poor diffracting power. Several experiments were performed on different batches, with the one of the highest quality being reported herein.

PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 ..... 0.265 Report

Author Response: The investigated single crystal was of low quality and showed a poor diffracting power. Several experiments were performed on different batches, with the one of the highest quality being reported herein.

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 12 Note
1 1 0, 2 0 0, -2 1 1, 0 1 1, 2 1 1, -2 0 2,
-1 1 2, 0 0 2, 1 1 2, 2 0 2, 0 1 3, 0 0 4,

Author Response: The crystal presents a large unit-cell causing reflections effected by the beamstop.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.89Ang From Bi1 2.60 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C4 --C5 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13 --C18 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22 --C24 . 0.20 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Bi1 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 C31 Check

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C34 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01861 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      6.355 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.243 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         30 Report
               26  0  0,  -6  0  2,  -2  4  2,  -2  0  4,  -2  2  4,  -2  1  5,
               -2  0  6, -10  0  8,  -2  0 10,  -8  0 12,  -6  0 12,  12  0 12,
               24  0 12,  -4  0 14,  10  4 14,  -6  4 16,   5  3 16, -14  5 17,
               -6  4 18, -16  0 20,  -6  2 20,  -2  0 20,  -1  1 20, -14  0 22,
              -10  0 22, -12  1 23, -14  0 24, -15  2 25, -14  1 25, -12  0 28,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.87Ang From Bi1             2.22 eA-3
```

Author Response: This residual density due to the presence of the Bi heavy atom.

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.98Ang From Bi1             1.69 eA-3
```

Author Response: This residual density due to the presence of the Bi heavy atom.

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.37Ang From Bi1            -1.70 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.42Ang From Bi1            -1.68 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15      .       -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H22      .       -0.72 eA-3
```

Alert level G

```
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)         293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)         293 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         176 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Bi1       (III)     .        2.95 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed           ! 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           8 Note
               1  1  0,   0  1  1,  -2  4  2,   2  1  1,   0  1  3,  -2  1  5,
               2  0  2,  -2  2  4,
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......      Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........        1.83 Note
             Predicted wR2: Based on SigI**2 10.89 or SHELX Weight 20.16
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.           0 Info
```

```
   2 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  19 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

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

Datablock: 3

Bond precision: C-C = 0.0325 A Wavelength=0.71073

Cell: a=10.539(5) b=11.459(5) c=12.812(6)
alpha=95.385(19) beta=113.799(16) gamma=98.125(18)
Temperature: 293 K

	Calculated	Reported
Volume	1381.9(11)	1382.0(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C60 H56 Bi2 Cl6 N4	C60 H56 Bi2 Cl6 N4
Sum formula	C60 H56 Bi2 Cl6 N4	C60 H56 Bi2 Cl6 N4
Mr	1463.75	1463.74
Dx,g cm-3	1.759	1.759
Z	1	1
Mu (mm-1)	6.692	6.691
F000	712.0	712.0
F000'	705.07	
h,k,lmax	12,14,15	12,14,15
Nref	5409	5348
Tmin,Tmax	0.286,0.343	0.400,0.745
Tmin'	0.241	

Correction method= # Reported T Limits: Tmin=0.400 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 25.970

R(reflections)= 0.1083(3654) wR2(reflections)= 0.2913(5348)

S = 1.065 Npar= 325

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.03Ang From Bi1 9.46 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.94Ang From Bi1 8.01 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Bi1 3.69 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.208

Author Response: The investigated single crystal was of low quality and showed a poor diffracting power. Several experiments were performed on different batches, with the one of the highest quality being reported herein.

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.208 Report

Author Response: The investigated single crystal was of low quality and showed a poor diffracting power. Several experiments were performed on different batches, with the one of the highest quality being reported herein.

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 9.82 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0325 Ang.

Author Response: The low bond precision on C-C bonds is due to weak and relatively imprecise diffraction data from the crystalline samples and limitations of the structural model, resulting in poor data quality.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.15Ang From Cl1 3.06 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.45Ang From Bi1 2.96 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.89Ang From Bi1   -3.40 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.82Ang From Bi1   -3.12 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.85Ang From Bi1   -3.01 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 1.51Ang From Bi1   -2.59 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT082_ALERT_2_C High R1 Value ....   0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ....   0.29 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.97 Report
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4   Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   5.514 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.01Ang From Cl1   2.42 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.62Ang From Cl1   2.35 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.48Ang From Bi1   2.33 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.87Ang From C7   2.16 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.37Ang From Cl2   2.06 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.54Ang From Cl1 1.88 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.86Ang From Cl2 1.83 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.84Ang From Bi1 -2.45 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.37Ang From Bi1 -2.20 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.83Ang From Bi1 -2.07 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.09Ang From Bi1 -1.80 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.43Ang From Bi1 -1.73 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.50Ang From Bi1 -1.69 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.78Ang From C27 -1.62 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.85Ang From Cl3 -1.59 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.49Ang From N2             -1.58 eA-3
```

Author Response: This residual density due to the presence of the Bi heavy atom.

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.51Ang From Bi1            -1.53 eA-3
```

Author Response: This residual density due to the presence of the Bi heavy atom.

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  2.31Ang From Cl3            -1.51 eA-3
```

Author Response: This residual density due to the presence of the Bi heavy atom.

```
PLAT977_ALERT_2_C Check Negative Difference Density on H26       .      -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H28       .      -0.53 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H29B      .      -0.79 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H29C      .      -0.44 eA-3
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      49.41 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C30      -H30B            1_555   1_555 ........     #   63 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Bi1       (III)     .       3.02 Info
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
               1  0  0,   0  1  0,  -1  0  1,   0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         56 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               0  1  0,
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       3.61 Note
             Predicted wR2: Based on SigI**2  8.06 or SHELX Weight 28.23
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

```
  3 ALERT level A = Most likely a serious problem - resolve or explain
 10 ALERT level B = A potentially serious problem, consider carefully
 28 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

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 38 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
  2 ALERT type 4 Improvement, methodology, query or suggestion
  3 ALERT type 5 Informative message, check
```

Datablock: 3-decomposition

Bond precision: C-C = 0.0180 A Wavelength=0.71073

Cell: a=16.076(5) b=7.1593(18) c=12.799(3)
alpha=90 beta=105.698(11) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1418.1(7)	1418.1(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	Bi2 Cl8, 2(C9 H14 N)	Bi2 Cl8, 2(C9 H14 N)
Sum formula	C18 H28 Bi2 Cl8 N2	C18 H28 Bi2 Cl8 N2
Mr	973.98	973.98
Dx,g cm-3	2.281	2.281
Z	2	2
Mu (mm-1)	13.157	13.157
F000	904.0	904.0
F000'	890.93	
h,k,lmax	20,9,16	20,9,16
Nref	3295	3244
Tmin,Tmax	0.027,0.072	0.110,0.178
Tmin'	0.014	

Correction method= # Reported T Limits: Tmin=0.110 Tmax=0.178
AbsCorr = MULTI-SCAN

Data completeness= 0.985 Theta(max)= 27.614

R(reflections)= 0.0581(2330) wR2(reflections)= 0.1462(3244)

S = 1.037 Npar= 136

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 1.29Ang From Bi1 3.56 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.82Ang From Bi1 3.52 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.76Ang From Bi1 -3.87 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_A Check Calcd Resid. Dens. 0.67Ang From Bi1 -3.71 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

Alert level B

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.83Ang From Bi1 3.24 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.28Ang From Bi1 3.05 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.85Ang From Bi1 2.79 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.43Ang From Bi1 2.77 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.43Ang From Bi1 2.67 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.85Ang From Bi1 2.59 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.93Ang From Bi1 2.56 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.91Ang From Bi1 2.51 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.76Ang From Bi1   -3.45 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.91Ang From Bi1   -3.34 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.83Ang From Bi1   -2.86 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
           Rint given   0.155
PLAT213_ALERT_2_C Atom C4   has ADP max/min Ratio .....   3.8 prolat
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.018 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   4.748 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.37Ang From Bi1   2.18 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.15Ang From Cl1   1.75 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.08Ang From Bi1   1.73 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.32Ang From Cl3   1.67 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.43Ang From Cl4   1.66 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.43Ang From Cl4   1.66 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.70Ang From Bi1   1.62 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.80Ang From Cl2   1.61 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.89Ang From Cl4   1.60 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.68Ang From N1   1.57 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.82Ang From Cl2   1.57 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.88Ang From Cl4   1.55 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.23Ang From Cl2   1.52 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.75Ang From Bi1   -2.49 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.41Ang From Bi1   -2.25 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.45Ang From Bi1   -2.10 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.62Ang From Cl2   -2.07 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.89Ang From Cl1   -1.88 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.70Ang From Bi1   -1.83 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.26Ang From Bi1   -1.81 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.23Ang From Cl4   -1.72 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 2.00Ang From Cl3   -1.66 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.30Ang From C6   -1.64 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.33Ang From Bi1   -1.56 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.65Ang From Bi1   -1.53 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.17Ang From Cl1   -1.51 eA-3

Author Response: This residual density due to the presence of the Bi heavy atom.

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.46Ang From Cl1           -1.51 eA-3
```

Author Response: This residual density due to the presence of the Bi heavy atom.

```
PLAT977_ALERT_2_C Check Negative Difference Density on H1B       .      -0.35 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H4        .      -0.49 eA-3
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
             H1A   H1B   H1C
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.155 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT480_ALERT_4_G Long H...A H-Bond Reported H9       ..CL4      .       2.94 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H9       ..CL4      .       2.94 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H9       ..CL4      .       2.94 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Bi1       (III)     .       3.19 Info
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).          2 Note
               1  0  0,   2  0  0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         49 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               2  0  0,
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       1.74 Note
             Predicted wR2: Based on SigI**2  8.41 or SHELX Weight 14.41
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
  11 ALERT level B = A potentially serious problem, consider carefully
  33 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  47 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
```

Datablock: 4

```
Bond precision:   C-C = 0.0113 A           Wavelength=0.71073

Cell:           a=11.9071(19)      b=12.515(2)       c=12.836(2)
                alpha=62.832(6)    beta=75.498(6)    gamma=89.515(7)
Temperature:    293 K
```

	Calculated	Reported
Volume	1635.0(5)	1635.0(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C60 H56 Bi2 Cl6 N4, 2(C H2 Cl2)	C60 H56 Bi2 Cl6 N4, 2(C H2 Cl2)
Sum formula	C62 H60 Bi2 Cl10 N4	C62 H60 Bi2 Cl10 N4
Mr	1633.60	1633.60
Dx,g cm-3	1.659	1.659
Z	1	1
Mu (mm-1)	5.823	5.823
F000	796.0	796.0
F000'	789.65	
h,k,lmax	16,17,17	16,16,17
Nref	8674	8389
Tmin,Tmax	0.340,0.497	0.479,0.746
Tmin'	0.168	

Correction method= # Reported T Limits: Tmin=0.479 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.967 Theta(max)= 28.968

R(reflections)= 0.0519(6134) wR2(reflections)= 0.1166(8389)

S = 1.101 Npar= 355

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

PLAT213_ALERT_2_C Atom C30 has ADP max/min Ratio ..... 3.5 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.1 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.1 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C26 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Bi1 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 C22 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C25 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C31 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl4 0.191 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C22 -C27 . 1.36 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01125 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C28 - C30 . 1.41 Ang.

```
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C1       - C11      .       1.53 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.676 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          5 Note
                  1  0  0,   0  1  0,   0  0  1,   1  0  1,   0  1  1,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         36 Report
                  2  0  0,  -3  1  0,  -2  1  0,   1  1  0,   0  2  0,   1  2  0,
                 -2  4  0,   2 -1  1,   3 -1  1,   4 -1  1,   5 -1  1,   2  0  1,
                  3  0  1,   2  1  1,  -1  2  1,  -1  4  1,  -2  0  2,   3  0  2,
                  4  0  2,   5  0  2,   0  1  2,   2  1  2,  -1  2  2,   0  4  2,
                 -1  5  2,   0  0  3,   5  0  3,  -2  1  3,   2  1  3,   3  1  3,
                  4  1  3,  -1  2  3,   0  5  3,  -1  1  4,   3  1  4,   4  1  4,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.81Ang From Bi1             1.93 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on       Bi1       1.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H31B      .      -0.42 eA-3
```

Alert level G

```
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Bi1      --Cl1      .        8.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Bi1      --Cl1_a    .       13.2 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Bi1       (III)     .       2.92 Info
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        238 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
                  0  4  2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         40 Note
                  1  0  0,   0  0  1,   0  1  1,   0  1  0,   4  0  2,   3  0  1,
                  3  1  4,   4  1  3,   2  0  1,  -2  1  0,   1  0  1,   3  0  2,
                 -1  4  1,   2  1  3,  -1  1  4,   3  1  3,   0  4  2,   2  0  0,
                 -3  1  0,   5  0  2,  -2  4  0,   4  1  4,   0  5  3,  -2  0  2,
                 -1  5  2,   2  1  1,   0  1  2,   4 -1  1,  -2  1  3,   1  1  0,
                  2 -1  1,   5  0  3,   2  1  2,  -1  2  3,   0  0  3,  -1  2  2,
                  0  2  0,   3 -1  1,   1  2  0,  -1  2  1,
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       2.78 Note
             Predicted wR2: Based on SigI**2  4.19 or SHELX Weight 10.82
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
   0 ALERT level B = A potentially serious problem, consider carefully
  23 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  22 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
   3 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

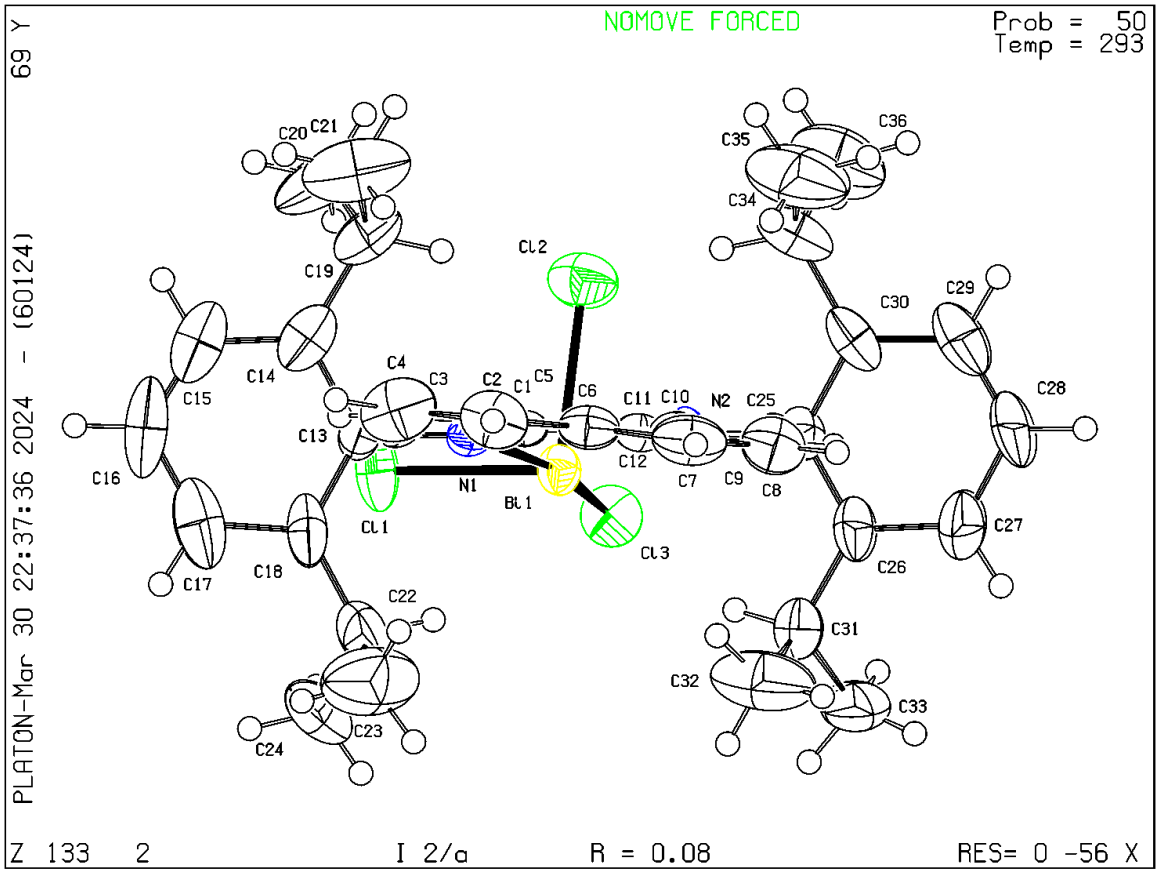
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

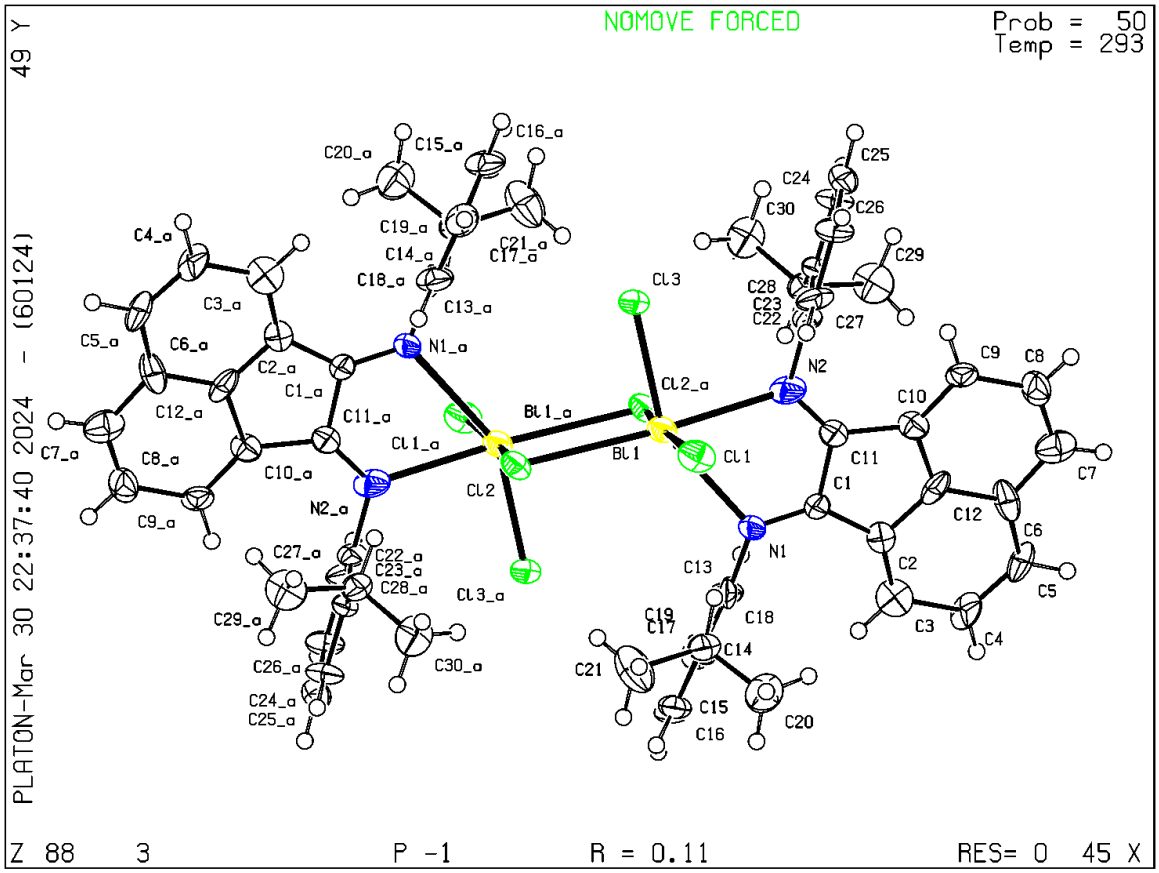
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/01/2024; check.def file version of 05/01/2024

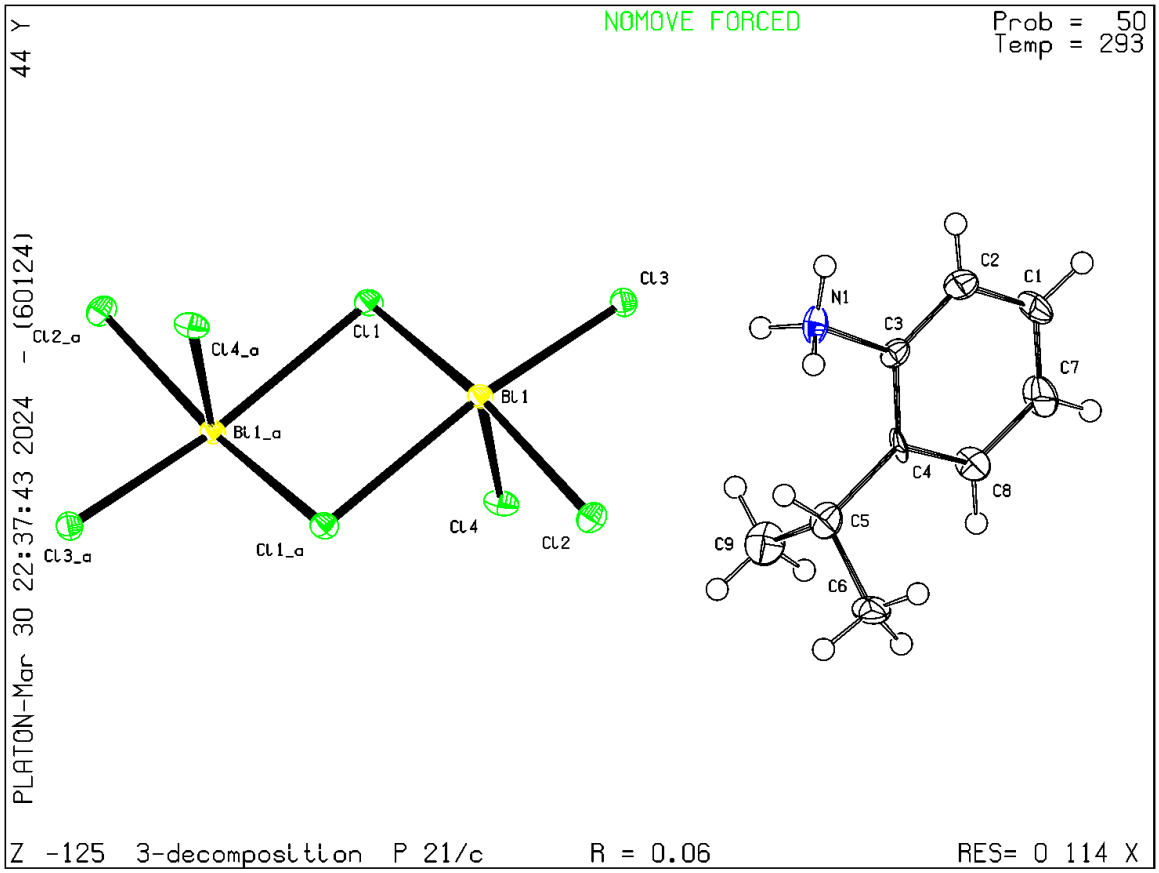
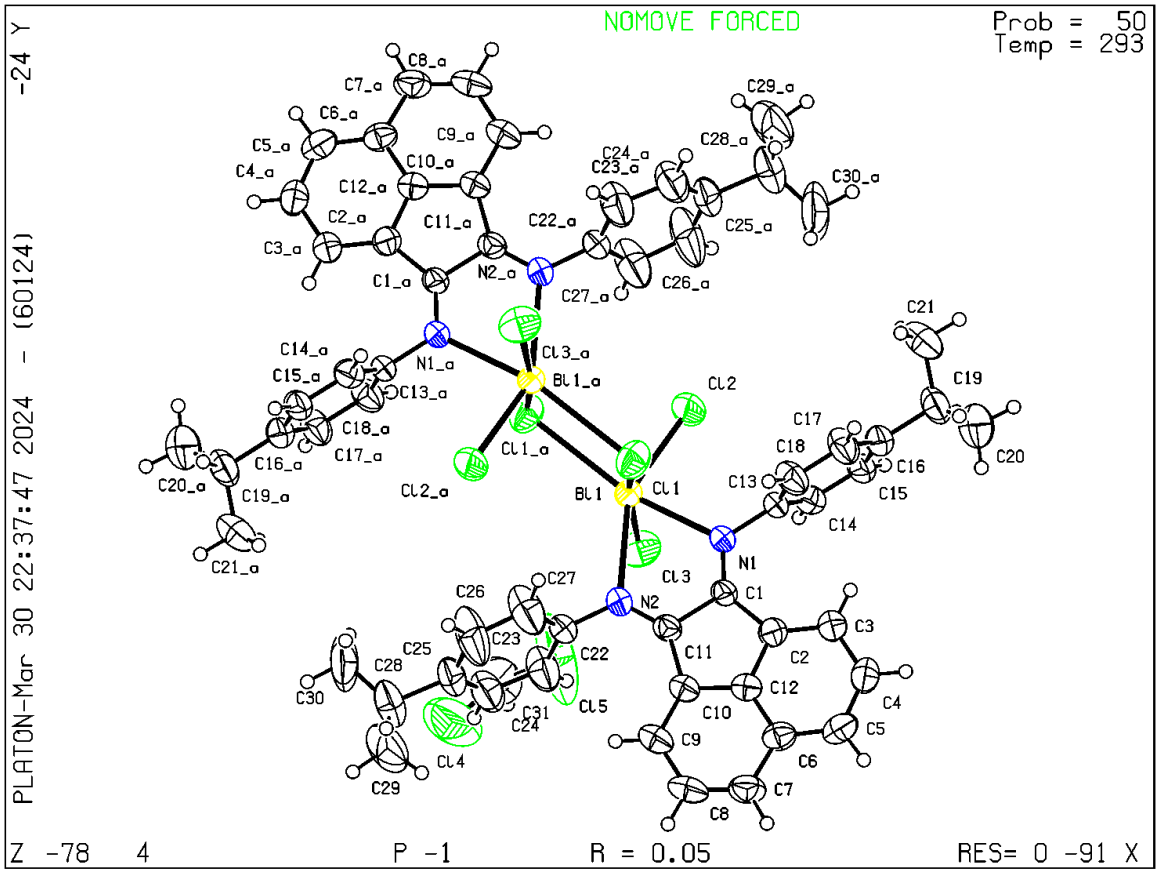
Datablock 2 - ellipsoid plot



Datablock 3 - ellipsoid plot



Datablock 3-decomposition - ellipsoid plot



Datablock 4 - ellipsoid plot