checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . . . . .
. . . . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) wa2586, wa2692, wa2904, wa2908, wa2933, wa2939, wa2985, wa2993, wa2996, wa3011, wa3013, wa3016

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
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: wa2996

```
Bond precision:        C-C = 0.0046 A                Wavelength=0.71073
Cell:        a=17.9787(6)      b=17.1205(8)      c=18.8527(7)
             alpha=90          beta=110.042(3)   gamma=90
Temperature: 173 K
                    Calculated                          Reported
Volume              5451.5(4)                           5451.5(4)
Space group         P 21/n                              P 21/n
Hall group          -P 2yn                              -P 2yn
Moiety formula      C50 H72 B2 Li N3 O2 [+ solvent]     C50 H72 B2 Li N3 O2
Sum formula         C50 H72 B2 Li N3 O2 [+ solvent]     C50 H72 B2 Li N3 O2
Mr                  775.67                              775.66
Dx,g cm-3           0.945                               0.945
Z                   4                                   4
Mu (mm-1)           0.056                               0.056
F000                1688.0                              1688.0
F000'               1688.57
h,k,lmax            21,20,23                            21,20,22
Nref                10380                               10225
Tmin,Tmax           0.984,0.987                         0.445,1.000
Tmin'               0.984
Correction method= # Reported T Limits: Tmin=0.445 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.985          Theta(max)= 25.710
R(reflections)= 0.0770( 6824)         wR2(reflections)= 0.2320( 10225)
S = 1.066               Npar= 555
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 21 Note

Alert level C

PLAT213_ALERT_2_C Atom C38' has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom C40' has ADP max/min Ratio ..... 3.5 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.7 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 9.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C37 --C38' . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C37 --C40 . 0.19 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C53 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N51 Check
And 4 other PLAT242 Alerts
More ...
PLAT245_ALERT_2_C U(iso) H1 Smaller than U(eq) B2 by 0.013 Ang**2
PLAT303_ALERT_2_C Full Occupancy Atom H1 with # Connections 2.00 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00459 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H13 ..H33 . 1.95 Ang.
x,y,z = 1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.527 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) . 1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 9 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 5% Note
PLAT395_ALERT_2_G Deviating X-O-Y Angle From 120 for O2 100.8 Degree
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H34 ..H40C . 1.89 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H36 ..H38D . 1.98 Ang.
x,y,z = 1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ..... ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 4 Check
O1 -C1 -LI1 1.555 1.555 1.555 35.45 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 18 Check
B1 -B2 -H1 1.555 1.555 1.555 30.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 28 Check
B2 -B1 -H1 1.555 1.555 1.555 32.10 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 72 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= 0.600 127 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 5 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
20 **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

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

Datablock: wa2985

```
Bond precision:        C-C = 0.0034 A                  Wavelength=0.71073
Cell:        a=15.5339(6)      b=20.0316(5)      c=18.0591(7)
             alpha=90          beta=108.566(3)   gamma=90
Temperature: 173 K
                     Calculated                          Reported
Volume               5327.0(3)                           5327.0(3)
Space group          P 21/c                              P 21/c
Hall group           -P 2ybc                             -P 2ybc
Moiety formula       C100 H144 B4 K2 N6 O4, 2(C4 H6 O)   C100 H144 B4 K2 N6 O4, 2(C4 H6 O)
Sum formula          C108 H156 B4 K2 N6 O6               C108 H156 B4 K2 N6 O6
Mr                   1755.83                             1755.82
Dx,g cm-3            1.095                               1.095
Z                    2                                   2
Mu (mm-1)            0.142                               0.142
F000                 1904.0                              1904.0
F000'                1905.45
h,k,lmax             18,24,22                            18,24,21
Nref                 10151                               9969
Tmin,Tmax            0.960,0.962                         0.482,1.000
Tmin'                0.960
Correction method= # Reported T Limits: Tmin=0.482 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.982          Theta(max)= 25.710
R(reflections)= 0.0600( 8336)         wR2(reflections)= 0.1686( 9969)
S = 1.060               Npar= 588
```

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

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 21 Note

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.40 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 5 Check
O61 C62' C63' C64 C65'
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 8.0 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N52 Check
And 3 other PLAT242 Alerts
More ...
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of O61 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C64 Check
PLAT303_ALERT_2_C Full Occupancy Atom H1 with # Connections 2.00 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.586 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 6 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.05A From O2 0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H62C -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H62A -0.33 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.04 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 5% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 60% Note
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H49A ..H62B . 2.02 Ang.
x,y,z = 1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H50C ..H62D . 1.84 Ang.
x,3/2-y,1/2+z = 2_565 Check
PLAT774_ALERT_1_G Check X-Y Bond in CIF: K1 --K1 .. 4.05 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 24 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 152 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 8 Info

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

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

Datablock: wa2692

Bond precision: C-C = 0.0062 A Wavelength=0.71073
Cell: a=11.4323(10) b=12.1113(13) c=22.6192(19)
alpha=85.878(8) beta=76.690(7) gamma=85.863(8)
Temperature: 173 K

	Calculated	Reported
Volume	3034.9(5)	3034.9(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C47 H63 B2 N2, C16 H32 Li O8	C47 H63 B2 N2, C16 H32 Li O8
Sum formula	C63 H95 B2 Li N2 O8	C63 H95 B2 Li N2 O8
Mr	1036.97	1036.96
Dx,g cm-3	1.135	1.135
Z	2	2
Mu (mm-1)	0.072	0.072
F000	1128.0	1128.0
F000'	1128.47	
h,k,lmax	13,14,27	13,14,27
Nref	11465	11346
Tmin,Tmax	0.990,0.991	0.577,1.000
Tmin'	0.986	

Correction method= # Reported T Limits: Tmin=0.577 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.990 Theta(max)= 25.635
R(reflections)= 0.1015(6372) wR2(reflections)= 0.1887(11346)
S = 1.211 Npar= 713

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

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 6.9 Ratio
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 24 Note

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.10 Report
PLAT213_ALERT_2_C Atom C20 has ADP max/min Ratio ..... 3.7 prolat
PLAT213_ALERT_2_C Atom C38 has ADP max/min Ratio ..... 3.1 prolat
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 8.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C17 --C18 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C27 --C29 . 0.17 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
And 3 other PLAT242 Alerts
More ...
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00624 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 33.848 Check
And 2 other PLAT906 Alerts
More ...
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 11 Report

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 6% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H24 ..H29A . 2.05 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H24 ..H29F . 2.14 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H26 ..H30B . 2.11 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H26 ..H30E . 2.14 Ang.
x,y,z = 1_555 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 36 Note
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 84 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.2 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
15 **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

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

Datablock: wa2904

```
Bond precision:        C-C = 0.0077 A                  Wavelength=0.71073
Cell:          a=12.2187(10)     b=16.2604(18)     c=16.2958(17)
               alpha=61.770(7)   beta=79.087(7)    gamma=82.091(8)
Temperature: 173 K
                      Calculated                          Reported
Volume                2796.7(5)                           2796.7(5)
Space group           P -1                                P -1
```

Hall group	-P 1	-P 1
Moiety formula	C55 H79 B2 N2 Na O2, 0.5(C6 H14)	C55 H79 B2 N2 Na O2, 0.5(C6 H14)
Sum formula	C58 H86 B2 N2 Na O2	C58 H86 B2 N2 Na O2
Mr	887.90	887.89
Dx,g cm-3	1.054	1.054
Z	2	2
Mu (mm-1)	0.068	0.068
F000	970.0	970.0
F000'	970.38	
h,k,lmax	14,19,19	14,19,19
Nref	9884	9836
Tmin,Tmax	0.989,0.994	0.670,1.000
Tmin'	0.986	

Correction method= # Reported T Limits: Tmin=0.670 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 25.027

R(reflections)= 0.0843(5056) wR2(reflections)= 0.1890(9836)

S = 1.005 Npar= 605

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

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 25 Note

---

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C17 --C19 . 0.16 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
And 2 other PLAT242 Alerts
More ...
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C72 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C71 0.181 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00772 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C71 - C72 . 1.39 Ang.
And 2 other PLAT360 Alerts
More ...
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 38.361 Check
And 2 other PLAT906 Alerts
More ...
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 23 Report

---

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 3% Note
PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C31 Check
PLAT344_ALERT_2_G Unusual sp3 Angle Range in Solvent/Ion for C72 Check
PLAT344_ALERT_2_G Unusual sp3 Angle Range in Solvent/Ion for C73 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.11 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 24 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully
16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: wa2933

```
Bond precision:        C-C = 0.0082 A                  Wavelength=0.71073
Cell:          a=35.9563(11)     b=15.1061(2)      c=23.4218(8)
               alpha=90          beta=121.286(2)   gamma=90
Temperature: 173 K
                      Calculated                          Reported
Volume                10871.9(6)                          10871.8(6)
Space group           C 2/c                               C 2/c
Hall group            -C 2yc                              -C 2yc
Moiety formula        C55 H79 B2 K N2 O2                  C55 H79 B2 K N2 O2
Sum formula           C55 H79 B2 K N2 O2                  C55 H79 B2 K N2 O2
Mr                    860.92                              860.92
Dx,g cm-3             1.052                               1.052
Z                     8                                   8
Mu (mm-1)             0.136                               0.136
F000                  3744.0                              3744.0
F000'                 3746.84
h,k,lmax              42,17,27                            42,17,27
Nref                  9603                                9582
Tmin,Tmax             0.933,0.957                         0.724,1.000
Tmin'                 0.933
Correction method= # Reported T Limits: Tmin=0.724 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.998           Theta(max)= 25.027
R(reflections)= 0.1090( 7689)         wR2(reflections)= 0.2877( 9582)
S = 1.102               Npar= 616
```

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

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 7.5 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for O61 --C62 . 10.7 s.u.
PLAT234_ALERT_4_B Large Hirshfeld Difference C64 --C65 . 0.27 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C63 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 21 Note

Alert level C

PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.29 Report
PLAT213_ALERT_2_C Atom C7 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C20 has ADP max/min Ratio ..... 3.1 prolat
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 7.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C17 --C18 . 5.3 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O51 --C52 . 0.17 Ang.

And 3 other PLAT234 Alerts
More ...
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O61 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5 Check
And 3 other PLAT242 Alerts
More ...
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00817 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C2 - C4 . 1.42 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C54 - C55 . 1.41 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 43 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 14.185 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.659 Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 5 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 10.09 Check

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 10 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 41.04 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C63 --C64 . 9.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C63 --C64' . 9.0 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 10% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H55A ..H65D . 2.05 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H46 ..H48B . 2.12 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 3 Note
PLAT722_ALERT_1_G Angle Calc 73.00, Rep 109.50 Dev... 36.50 Degree
C17 -C19 -H29C 1.555 1.555 1.555 # 171 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 60 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 61% Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
5 **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

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

Datablock: wa2939

Bond precision: C-C = 0.0070 A Wavelength=0.71073
Cell: a=35.3153(12) b=16.6312(6) c=23.2536(8)
alpha=90 beta=105.586(3) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	13155.5(8)	13155.5(8)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C55 H63 B2 N2, C12 H30 Li O6 [+ solvent]	C55 H63 B2 N2, C12 H30 Li O6
Sum formula	C67 H93 B2 Li N2 O6 [+ solvent]	C67 H93 B2 Li N2 O6
Mr	1050.99	1050.99

Dx,g cm-3	1.061	1.061
Z	8	8
Mu (mm-1)	0.066	0.066
F000	4560.0	4560.0
F000'	4561.79	
h,k,lmax	42,19,27	42,19,27
Nref	11970	11783
Tmin,Tmax	0.991,0.998	0.456,1.000
Tmin'	0.981	

Correction method= # Reported T Limits: Tmin=0.456 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.984 Theta(max)= 25.283

R(reflections)= 0.1143(7640) wR2(reflections)= 0.2192(11783)

S = 1.261 Npar= 761

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

PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C65 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C27 Check
And 4 other PLAT242 Alerts
More ...
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00704 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 17.891 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.347 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 131 Report

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Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 12 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 65.91 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 10% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H26 ..H30D . 2.10 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H34 ..H38D . 2.12 Ang.
x,y,z = 1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H44 ..H28D . 1.97 Ang.
1/2-x,3/2-y,1-z = 7_566 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 348 A**3
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 144 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 39% Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 50 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.6 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

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

Datablock: wa2993

```
Bond precision:        C-C = 0.0038 A                  Wavelength=0.71073
Cell:        a=18.5445(8)      b=16.8811(5)      c=19.3634(9)
             alpha=90          beta=118.010(3)   gamma=90
Temperature: 173 K
                     Calculated                          Reported
Volume               5351.7(4)                           5351.7(4)
Space group          P 21/c                              P 21/c
Hall group           -P 2ybc                             -P 2ybc
Moiety formula       C51 H77 B2 K N2 O2 Si2              C51 H77 B2 K N2 O2 Si2
Sum formula          C51 H77 B2 K N2 O2 Si2              C51 H77 B2 K N2 O2 Si2
Mr                   867.05                              867.04
Dx,g cm-3            1.076                               1.076
Z                    4                                   4
Mu (mm-1)            0.181                               0.181
F000                 1880.0                              1880.0
F000'                1882.01
h,k,lmax             22,20,23                            22,20,23
Nref                 10154                               10053
Tmin,Tmax            0.957,0.984                         0.442,1.000
Tmin'                0.957
Correction method= # Reported T Limits: Tmin=0.442 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.990          Theta(max)= 25.654
R(reflections)= 0.0600( 7764)         wR2(reflections)= 0.1355( 10053)
S = 1.091               Npar= 541
```

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

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 23 Note

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.2 Ratio
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 51 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 11.302 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.664 Check

Alert level G

PLAT722_ALERT_1_G Angle Calc 26.00, Rep 109.50 Dev... 83.50 Degree
C37 -C40 -H30C 1.555 1.555 1.555 # 250 Check
PLAT722_ALERT_1_G Angle Calc 67.00, Rep 109.50 Dev... 42.50 Degree
C47 -C50 -H40C 1.555 1.555 1.555 # 298 Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 77 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 7 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
5 **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

2 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
6 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: wa2908

```
Bond precision:        C-C = 0.0132 A                  Wavelength=0.71073
Cell:          a=9.6243(7)       b=14.9307(10)     c=20.6743(16)
               alpha=69.874(6)   beta=82.002(6)    gamma=73.617(6)
Temperature: 173 K
                      Calculated                          Reported
Volume                2673.3(4)                           2673.3(4)
Space group           P -1                                P -1
Hall group            -P 1                                -P 1
Moiety formula        C56 H80 B2 Li N O4                  C56 H80 B2 Li N O4
Sum formula           C56 H80 B2 Li N O4                  C56 H80 B2 Li N O4
Mr                    859.77                              859.77
Dx,g cm-3             1.068                               1.068
Z                     2                                   2
Mu (mm-1)             0.064                               0.064
F000                  936.0                               936.0
F000'                 936.35
h,k,lmax              11,18,25                            11,18,25
Nref                  10178                               10022
Tmin,Tmax             0.991,0.995                         0.469,1.000
Tmin'                 0.983
Correction method= # Reported T Limits: Tmin=0.469 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.985           Theta(max)= 25.691
R(reflections)= 0.1512( 5594)         wR2(reflections)= 0.4192( 10022)
S = 1.344               Npar= 625
```

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

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.42 Report
PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.29 eA-3
PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 7.7 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for O51 --C55 . 10.2 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C17 --C18 . 9.4 s.u.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C52 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01319 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C17 - C18 . 1.33 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 24 Note

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 ..... 0.15 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.50 Report
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 8.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C72 --C73 . 5.1 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C12 --C13 . 0.16 Ang.
And 10 other PLAT234 Alerts
More ...
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C54 Check
And 4 other PLAT241 Alerts
More ...
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O51 Check
And 4 other PLAT242 Alerts
More ...
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C63 - C64 . 1.43 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C73 - C74 . 1.43 Ang.
PLAT363_ALERT_2_C Long C(sp3)-C(sp2) Bond C15 - C17 . 1.70 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 40.760 Check
And 2 other PLAT906 Alerts
More ...
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 18 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 69 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.006 Degree
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 7 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C27 --C28' . 14.1 s.u.
And 4 other PLAT230 Alerts
More ...
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 8% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H63A ..H64B . 2.14 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H63B ..H64A . 2.14 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H24 ..H29F . 2.10 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H24 ..H30B . 1.90 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H26 ..H28C . 2.14 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H48C ..H28B . 2.12 Ang.
x,y,z = 1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H20A ..H53D . 1.46 Ang.
1+x,y,z = 1_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C20 ..C53' 2.99 Ang.
1+x,y,z = 1_655 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 21 Check
O1 -C1 -LI1 1.555 1.555 1.555 40.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 325 Check
O61 -C65 -LI1 1.555 1.555 1.555 40.40 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 484 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 124 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

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

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

Datablock: wa3013

Bond precision: C-C = 0.0093 A Wavelength=0.71073

Cell: a=13.0931(6) b=26.617(1) c=15.9341(8)
alpha=90 beta=103.292(4) gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	5404.3(4)	5404.3(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C53 H79 B2 N4 Na O	C53 H79 B2 N4 Na O
Sum formula	C53 H79 B2 N4 Na O	C53 H79 B2 N4 Na O
Mr	832.81	832.81
Dx,g cm-3	1.024	1.024
Z	4	4
Mu (mm-1)	0.067	0.067
F000	1816.0	1816.0
F000'	1816.68	
h,k,lmax	15,31,18	15,31,18
Nref	9549	9542
Tmin,Tmax	0.983,0.987	0.777,1.000
Tmin'	0.983	

Correction method= # Reported T Limits: Tmin=0.777 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.026

R(reflections)= 0.1348(6274) wR2(reflections)= 0.2857(9542)

S = 1.246 Npar= 582

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

PLAT082_ALERT_2_C High R1 Value ..... 0.13 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 .... 2.39 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.3 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C37 --C39 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C47 --C50 . 0.24 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
And 3 other PLAT242 Alerts
More ...
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00928 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 81 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 33.857 Check
And 2 other PLAT906 Alerts
More ...
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 2 Report

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 22.85 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 5% Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 23 Check
N1 -B2 -C1 1.555 1.555 1.555 39.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 25 Check
O1 -B2 -C1 1.555 1.555 1.555 41.20 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 48 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 40% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.5 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
18 **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

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

Datablock: wa3016

Bond precision: C-C = 0.0083 A Wavelength=0.71073
Cell: a=12.6458(5) b=18.8110(8) c=22.3127(9)
alpha=87.687(3) beta=82.704(3) gamma=77.661(3)
Temperature: 173 K

	Calculated	Reported
Volume	5142.7(4)	5142.7(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C88 H112 B4 K N2 O2, C12 H30 K O6 [+ solvent]	C100 H142 B4 K2 N2 O8
Sum formula	C100 H142 B4 K2 N2 O8 [+ solvent]	C100 H142 B4 K2 N2 O8
Mr	1621.60	1621.59
Dx,g cm-3	1.047	1.047
Z	2	2
Mu (mm-1)	0.143	0.143
F000	1756.0	1756.0
F000'	1757.45	
h,k,lmax	15,22,27	15,22,27
Nref	19644	19157
Tmin,Tmax	0.955,0.976	0.662,1.000
Tmin'	0.955	

Correction method= # Reported T Limits: Tmin=0.662 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.975 Theta(max)= 25.733
R(reflections)= 0.1158(12308) wR2(reflections)= 0.2736(19157)
S = 1.190 Npar= 1103

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

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 38 Note

Alert level C

PLAT082_ALERT_2_C High R1 Value ..... 0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.27 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.07 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.4 Ratio
PLAT221_ALERT_2_C Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 4.9 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.5 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range 5.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C83 --C84 . 6.9 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C27 --C29' . 0.24 Ang.
And 5 other PLAT234 Alerts
More ...
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of K1 Check
And 4 other PLAT241 Alerts
More ...
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
And 8 other PLAT242 Alerts
More ...
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00829 Ang.
PLAT359_ALERT_3_C Long (X,Y,Z)-B-H Distance B1A - H1A 1.23 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 15.115 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.862 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 94 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 3 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 13 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 17.42 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 3 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 6% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 11% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H24 ..H30A . 2.04 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H76B ..H74D . 2.14 Ang.
x,y,z = 1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ..... ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 7 Note
PLAT722_ALERT_1_G Angle Calc 88.00, Rep 109.50 Dev... 21.50 Degree
H28D -C28A -H28H 1.555 1.555 1.555 # 500 Check
PLAT722_ALERT_1_G Angle Calc 33.00, Rep 109.50 Dev... 76.50 Degree
C27A -C29A -H29D 1.555 1.555 1.555 # 504 Check
PLAT722_ALERT_1_G Angle Calc 83.00, Rep 109.50 Dev... 26.50 Degree
H29D -C29A -H29H 1.555 1.555 1.555 # 506 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.14 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C73' --C74' 1.88 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 73 Check
N1 -B2 -C1 1.555 1.555 1.555 40.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 74 Check
O1 -B2 -C1 1.555 1.555 1.555 41.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 395 Check
N1A -B2A -C1A 1.555 1.555 1.555 39.90 Deg.

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 396 Check
O1A -B2A -C1A 1.555 1.555 1.555 41.70 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 78 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= 0.600 356 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.3 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

---

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

Datablock: wa3011

Bond precision: C-C = 0.0048 A Wavelength=0.71073
Cell: a=12.0344(4) b=15.7136(5) c=27.0349(9)
alpha=86.859(3) beta=88.314(3) gamma=70.701(3)
Temperature: 173 K

	Calculated	Reported
Volume	4817.5(3)	4817.5(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C95 H127 B4 Li2 N3 O8 [+ solvent]	C95 H127 B4 Li2 N3 O8
Sum formula	C95 H127 B4 Li2 N3 O8 [+ solvent]	C95 H127 B4 Li2 N3 O8
Mr	1496.12	1496.11
Dx,g cm-3	1.031	1.031
Z	2	2
Mu (mm-1)	0.063	0.063
F000	1616.0	1616.0
F000'	1616.62	
h,k,lmax	14,19,33	14,19,33
Nref	18390	17955
Tmin,Tmax	0.978,0.983	0.613,1.000
Tmin'	0.973	

Correction method= # Reported T Limits: Tmin=0.613 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.976 Theta(max)= 25.732
R(reflections)= 0.0830(13344) wR2(reflections)= 0.1982(17955)
S = 1.198 Npar= 1029

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

Alert level B

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

Alert level C

PLAT213_ALERT_2_C Atom C19 has ADP max/min Ratio ..... 3.1 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.4 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N93 --C97' . 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C84 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C93 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N91 Check
And 5 other PLAT242 Alerts
More ...
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00482 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 9.480 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.118 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 58 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 5 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.79 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 4 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C83' --C84 . 7.0 s.u.
And 2 other PLAT230 Alerts
More ...
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 2% Note
PLAT397_ALERT_2_G Deviating B-O-B Angle From 120 for O4 131.0 Degree
PLAT410_ALERT_2_G Short Intra H...H Contact H94A ..H96B . 2.04 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H97A ..H99A . 1.86 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H98A ..H97D . 1.54 Ang.
x,y,z = 1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ..... ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 44 Check
O3 -B1 -LI2 1.555 1.555 1.555 44.70 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 48 Note
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 !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 361 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 5 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.6 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
21 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 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: wa2586

```
Bond precision:        C-C = 0.0037 A                  Wavelength=0.71073
Cell:        a=14.8315(7)      b=21.4829(7)      c=15.5290(7)
             alpha=90          beta=106.774(4)   gamma=90
Temperature: 173 K
                     Calculated                          Reported
Volume               4737.4(4)                           4737.4(4)
Space group          P 21/c                              P 21/c
Hall group           -P 2ybc                             -P 2ybc
Moiety formula       C52 H73 B2 Na O3                    C52 H73 B2 Na O3
Sum formula          C52 H73 B2 Na O3                    C52 H73 B2 Na O3
Mr                   790.71                              790.71
Dx,g cm-3            1.109                               1.109
Z                    4                                   4
Mu (mm-1)            0.073                               0.073
F000                 1720.0                              1720.0
F000'                1720.74
h,k,lmax             17,25,18                            17,25,18
Nref                 8376                                8363
Tmin,Tmax            0.982,0.987                         0.807,1.000
Tmin'                0.981
Correction method= # Reported T Limits: Tmin=0.807 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.998          Theta(max)= 25.026
R(reflections)= 0.0651( 6247)         wR2(reflections)= 0.1770( 8363)
S = 1.048               Npar= 631
```

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

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C74 Check
PLAT410_ALERT_2_B Short Intra H...H Contact H13 ..H43 . 1.89 Ang.
x,y,z = 1_555 Check

Alert level C

PLAT213_ALERT_2_C Atom C40 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C49' has ADP max/min Ratio ..... 3.1 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O71 --C75 . 0.18 Ang.
And 2 other PLAT234 Alerts
More ...
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C54 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Na1 Check
And 3 other PLAT242 Alerts
More ...
PLAT303_ALERT_2_C Full Occupancy Atom H1 with # Connections 2.00 Check
PLAT410_ALERT_2_C Short Intra H...H Contact H23 ..H33 . 1.95 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_C Short Intra H...H Contact H36 ..H46 . 1.99 Ang.
x,y,z = 1_555 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 15.058 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.681 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 8 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 5 Note
PLAT977_ALERT_2_C Check Negative Difference Density on H72B -0.35 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 25 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 23 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 6 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C17 --C18 . 5.3 s.u.
And 2 other PLAT230 Alerts
More ...
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 19% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H53A ..H54C . 2.14 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H53B ..H54D . 2.14 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H73A ..H74D . 2.13 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H73B ..H74C . 2.13 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H14 ..H19A . 2.12 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H16 ..H18A . 2.11 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H24 ..H29A . 2.05 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H26 ..H30D . 2.14 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H34 ..H48D . 1.85 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H36 ..H50D . 2.06 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 6 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C73 --C75 2.04 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 300 Check
C74 -C73 -C75 1.555 1.555 1.555 32.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . # 322 Check
C74 -C75 -C73 1.555 1.555 1.555 43.10 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 270 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 56% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

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9 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
0 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 worthwhi
In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structu

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 C checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts th are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspe 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

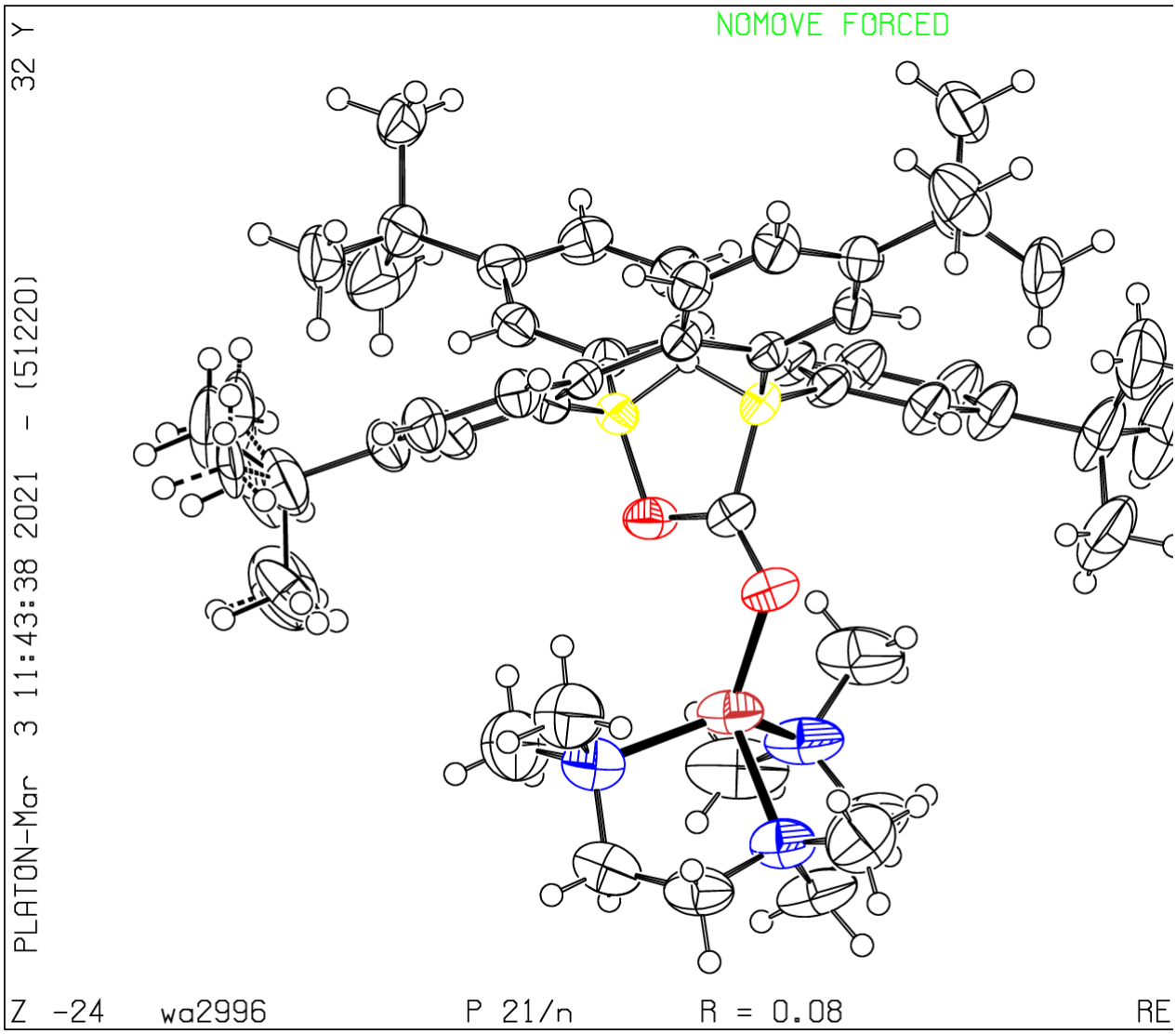
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if yo intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks ar run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

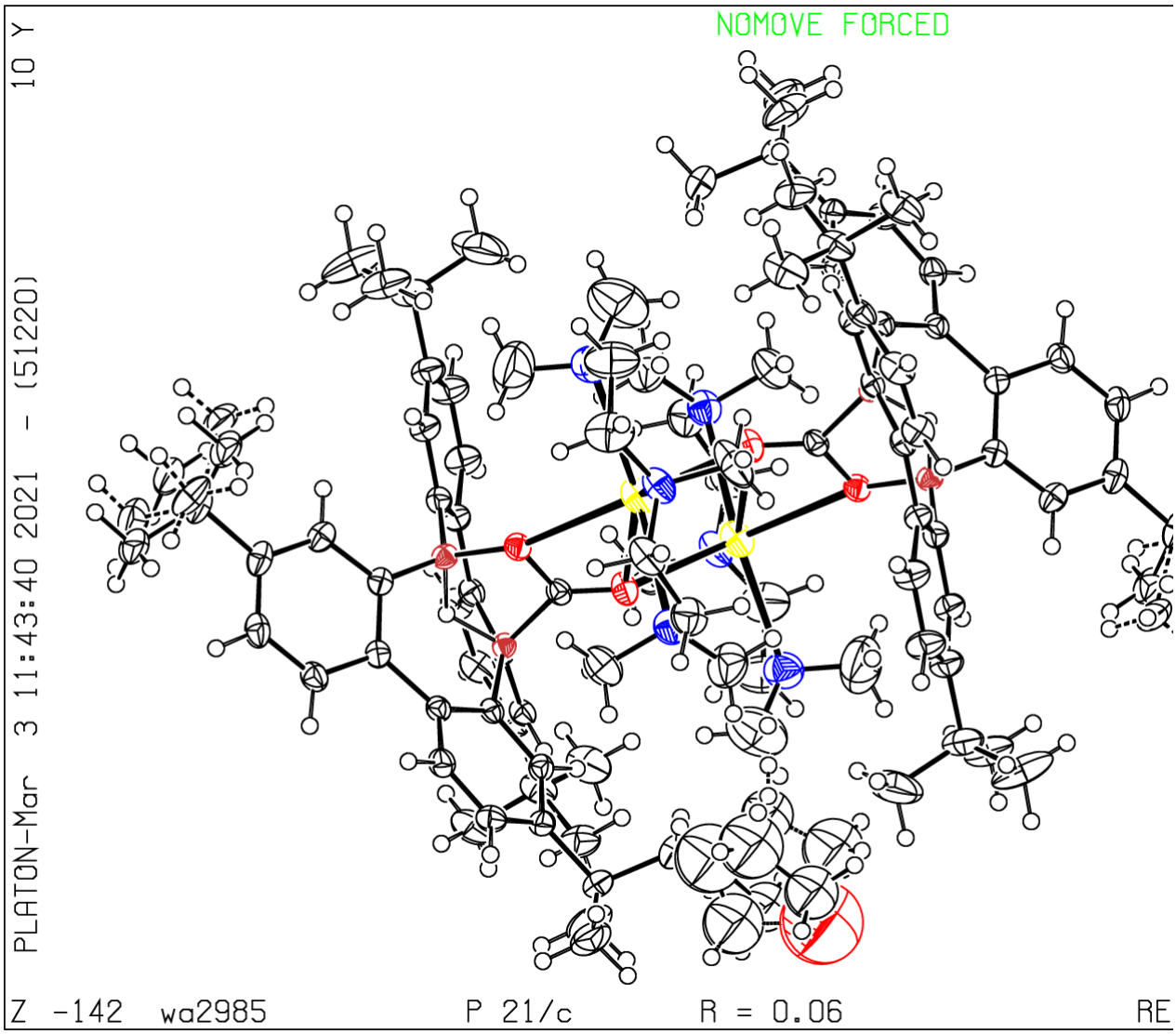
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 05/12/2020; check.def file version of 05/12/2020

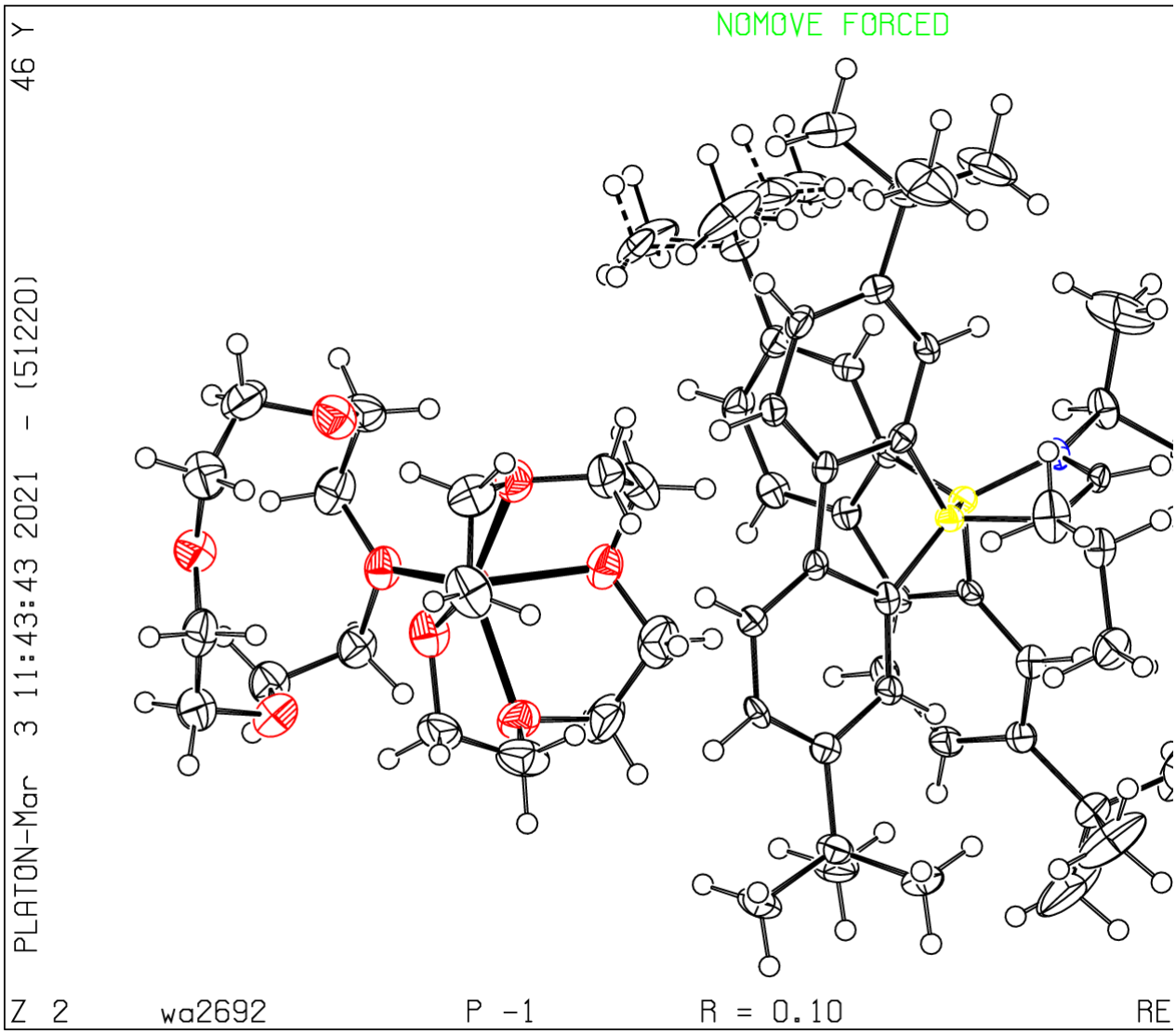
Datablock wa2996 - ellipsoid plot



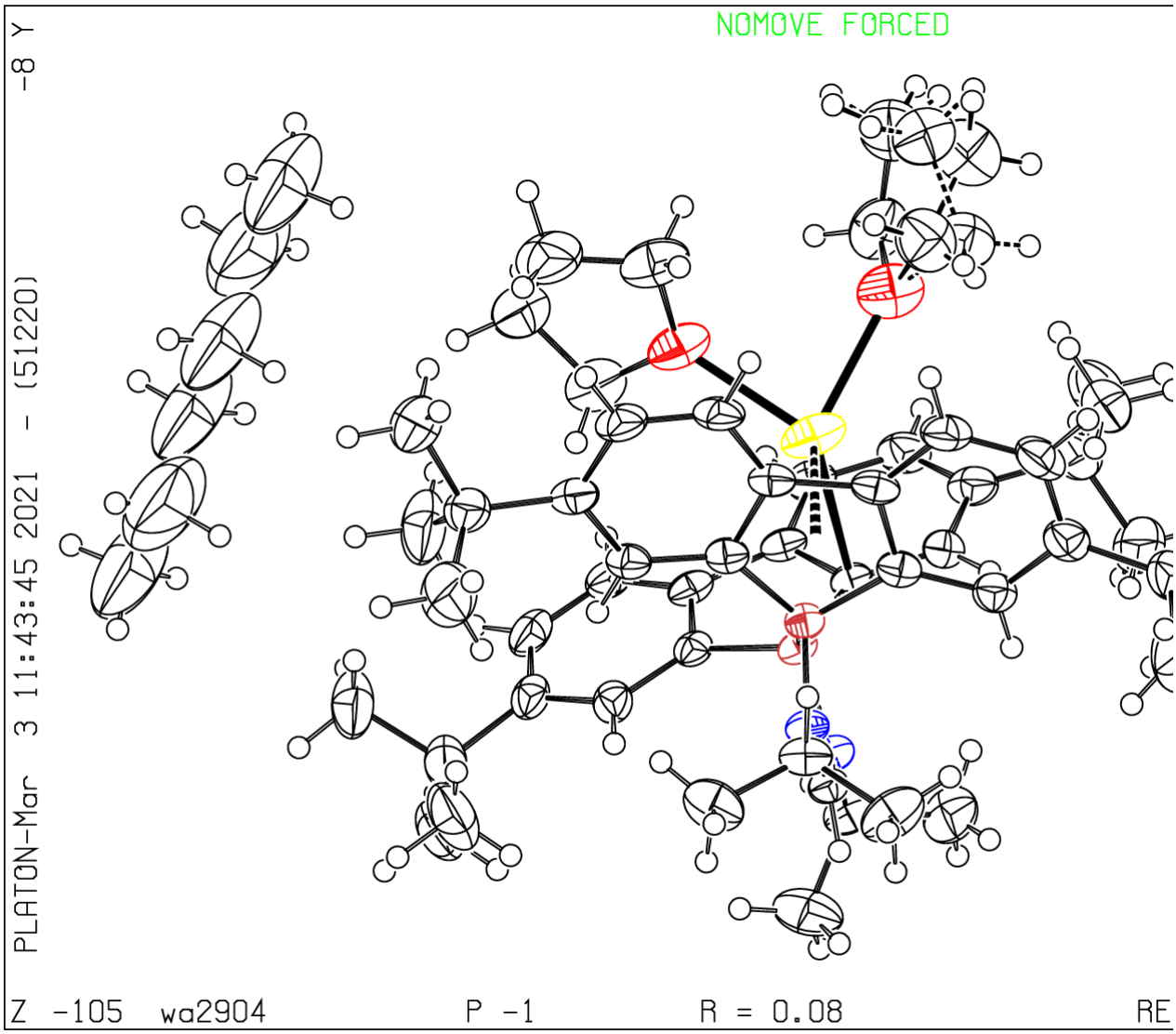
Datablock wa2985 - ellipsoid plot



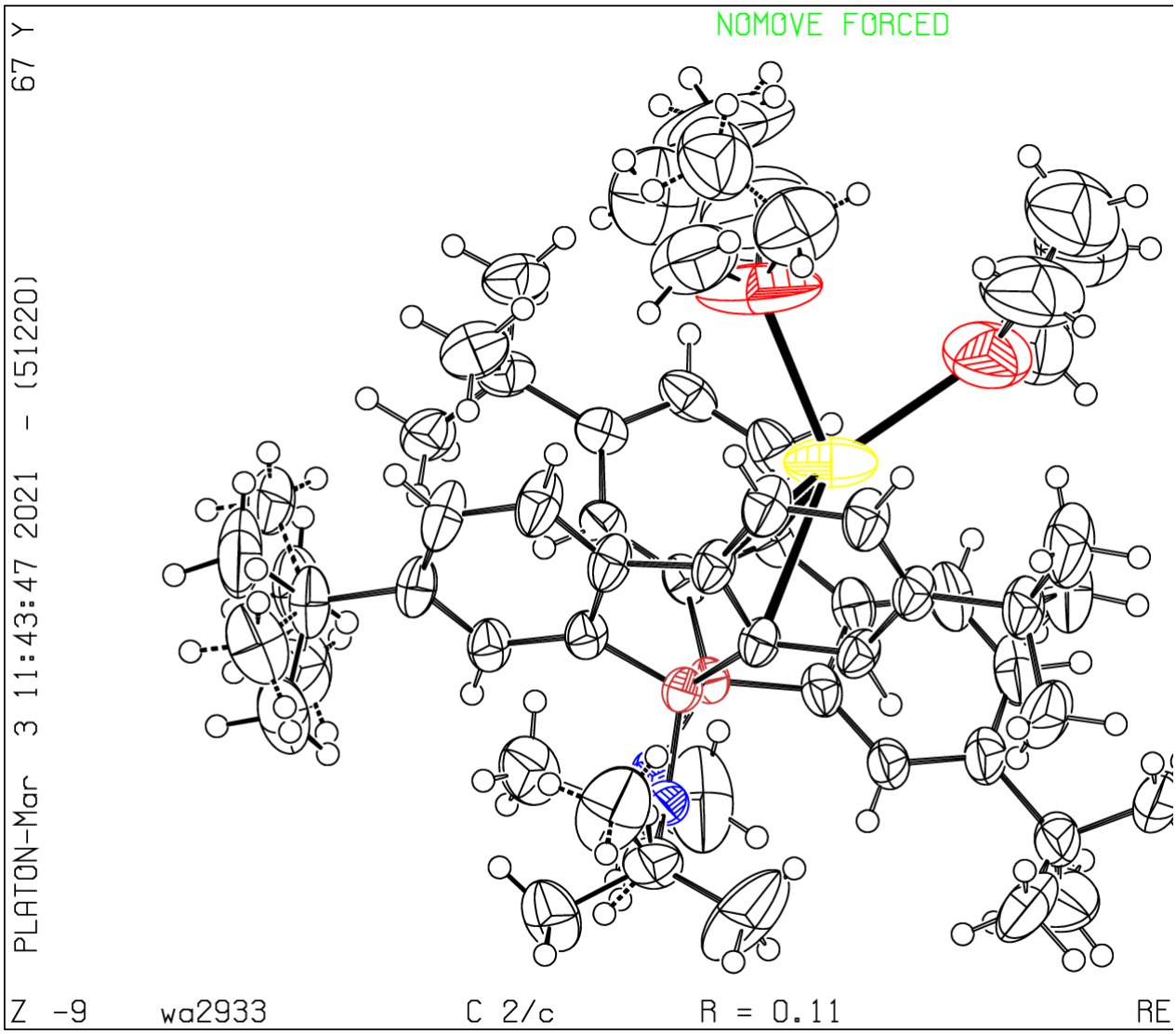
Datablock wa2692 - ellipsoid plot



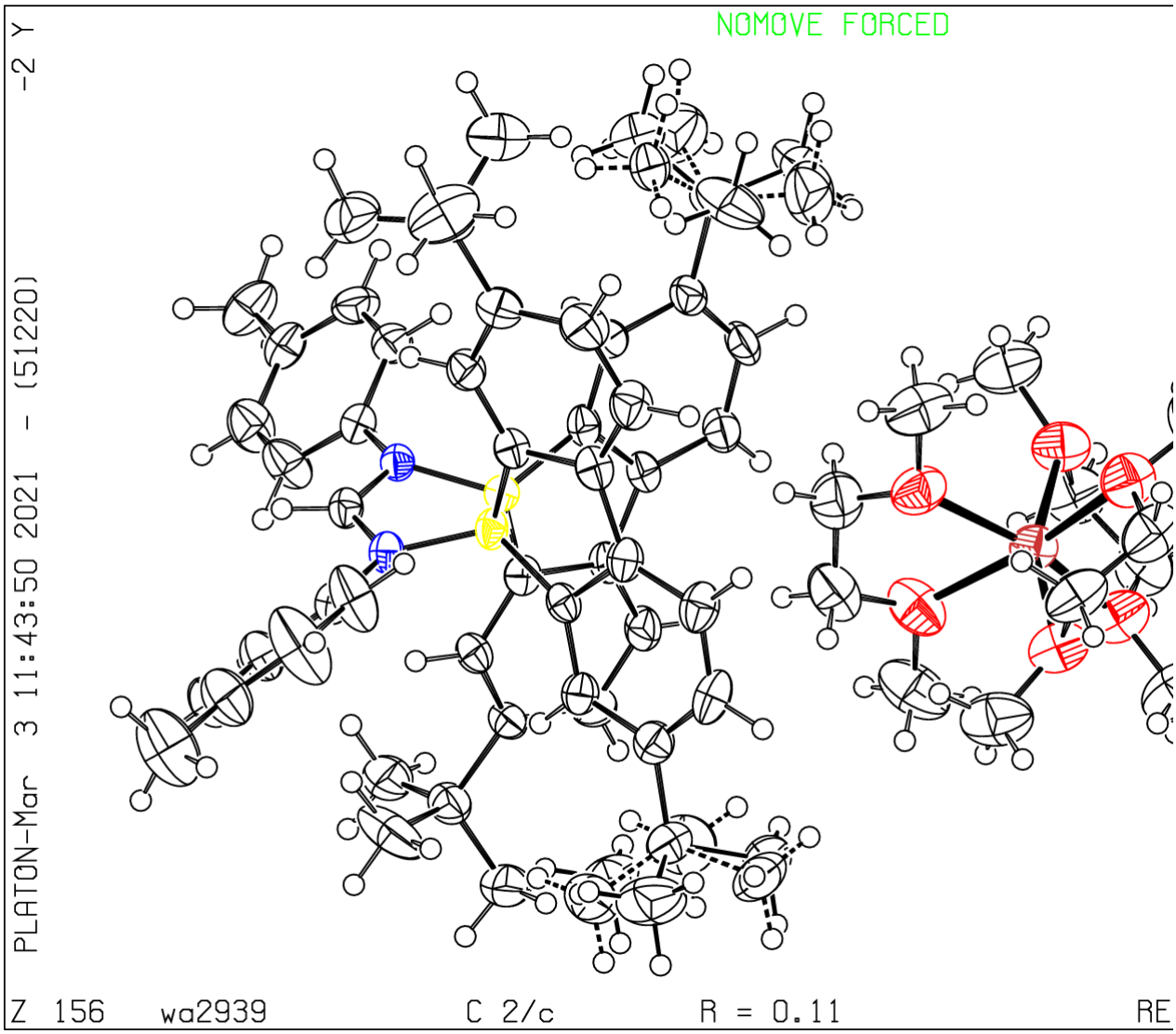
Datablock wa2904 - ellipsoid plot



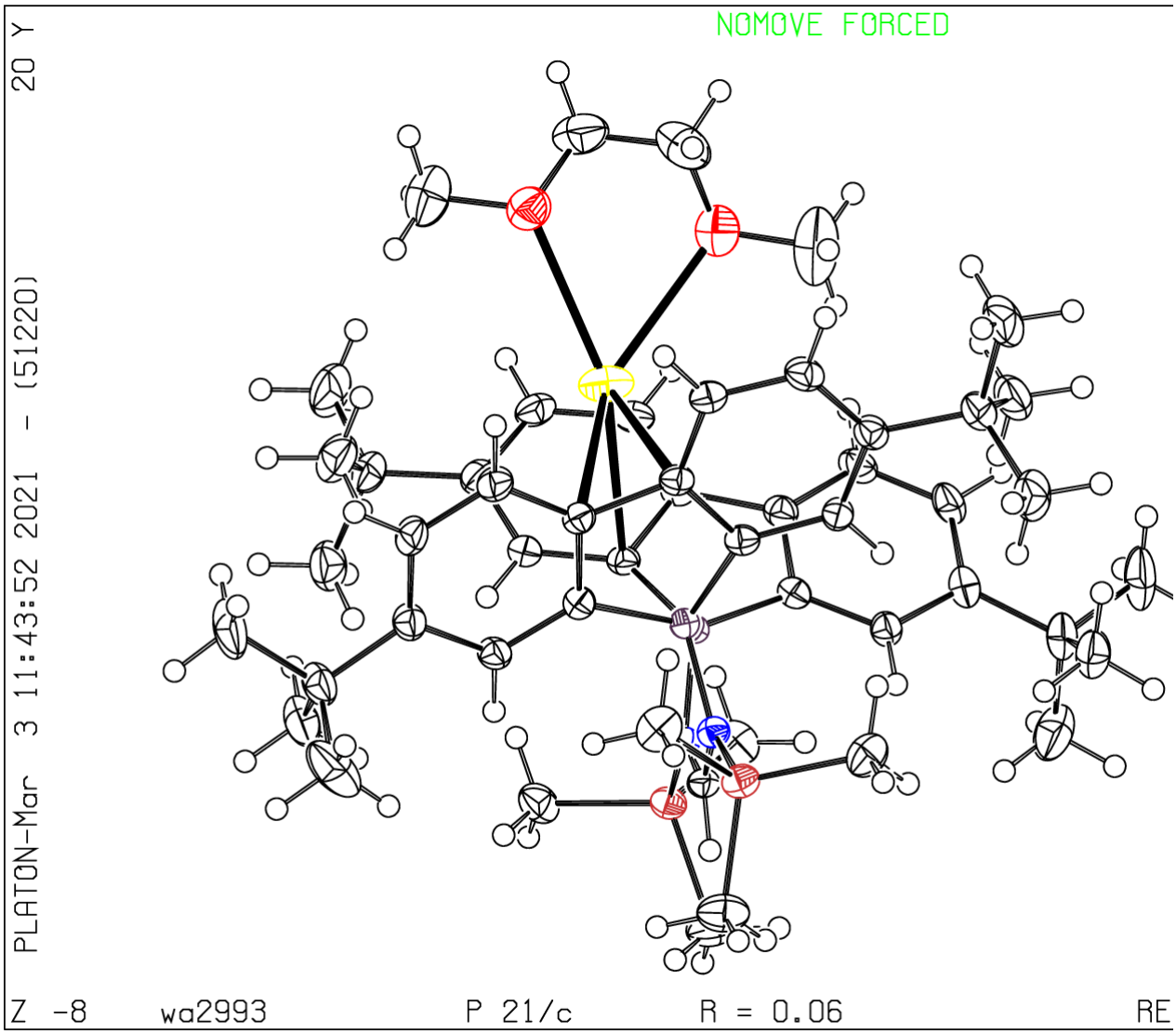
Datablock wa2933 - ellipsoid plot



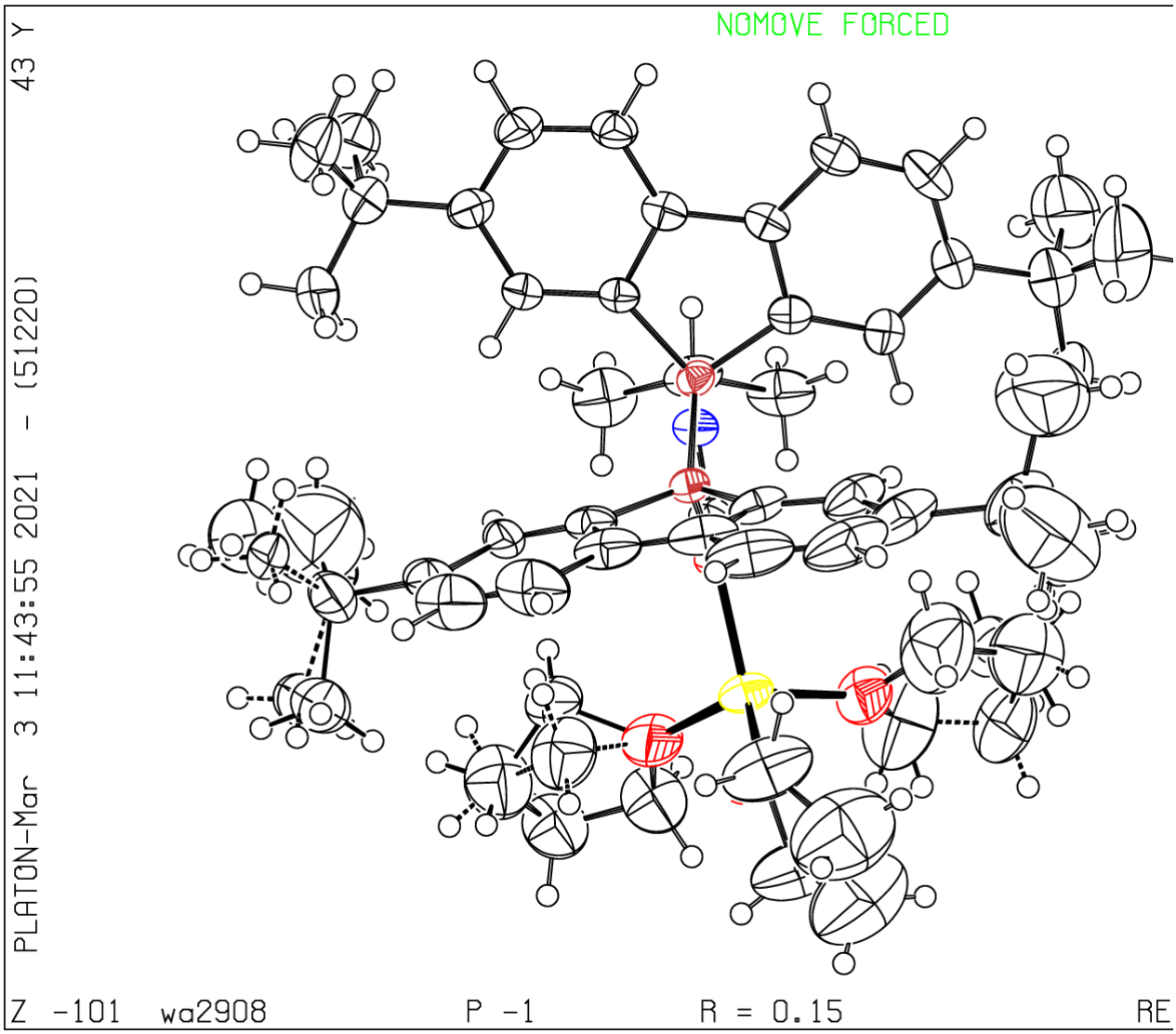
Datablock wa2939 - ellipsoid plot



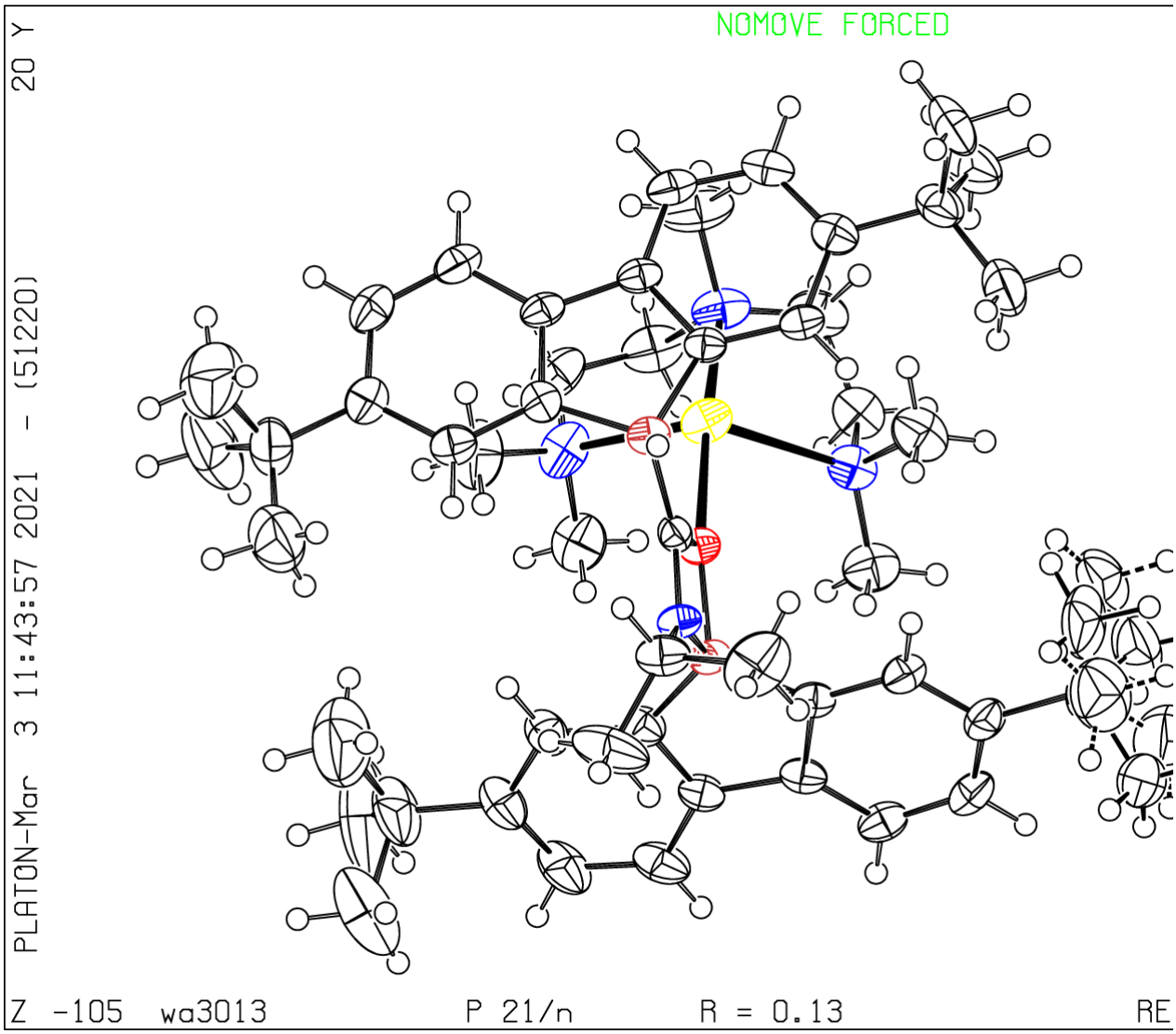
Datablock wa2993 - ellipsoid plot



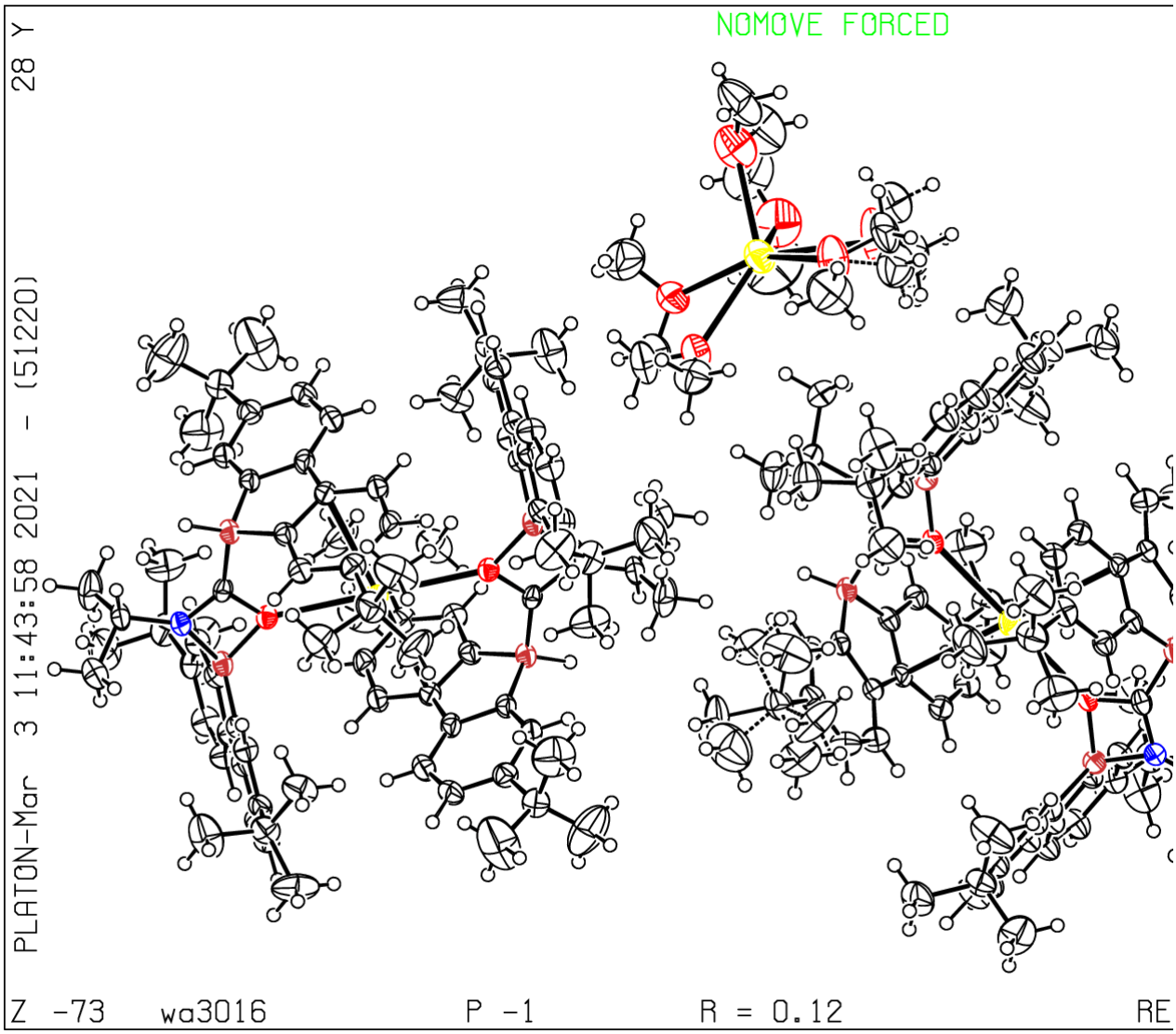
Datablock wa2908 - ellipsoid plot



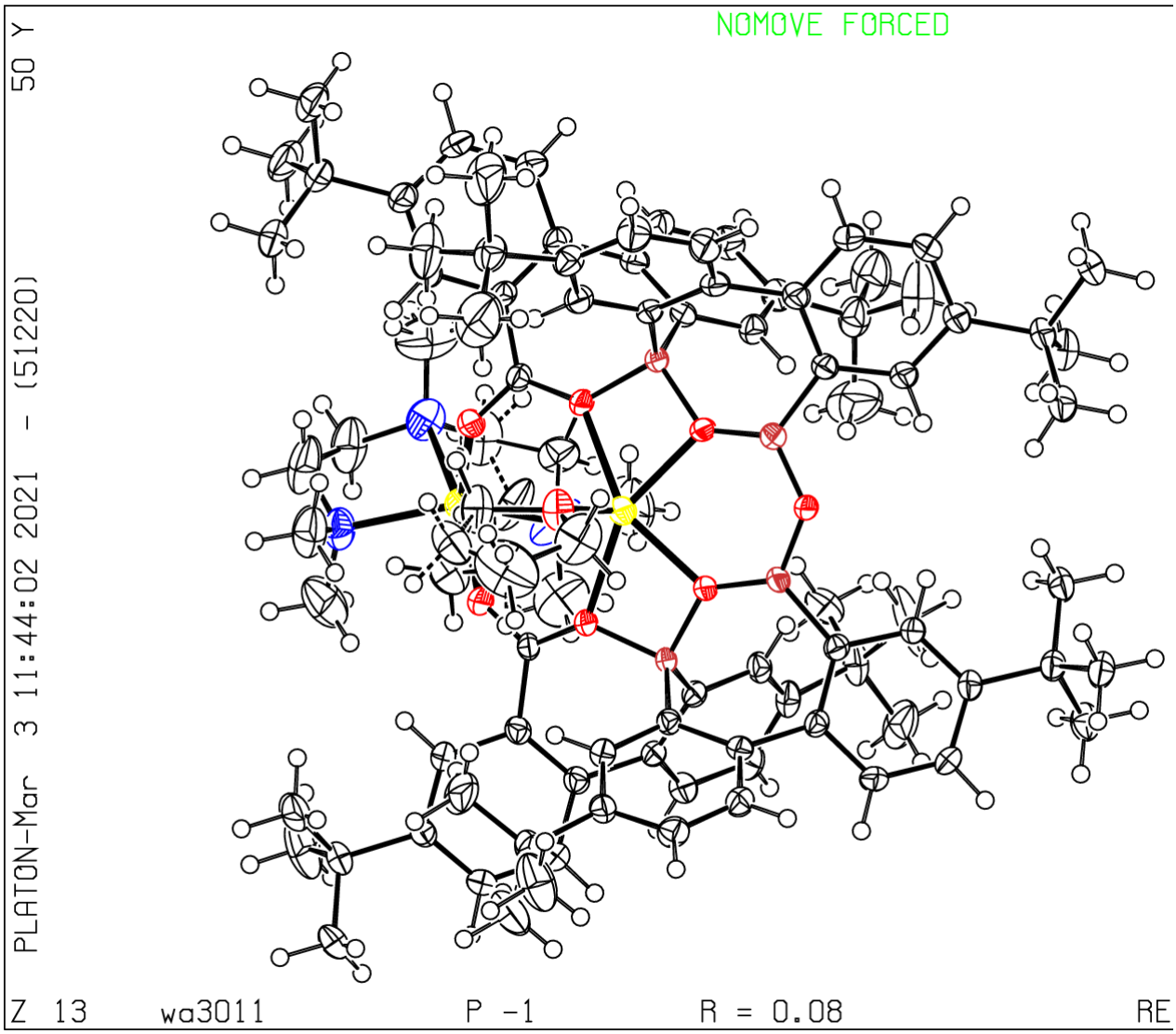
Datablock wa3013 - ellipsoid plot



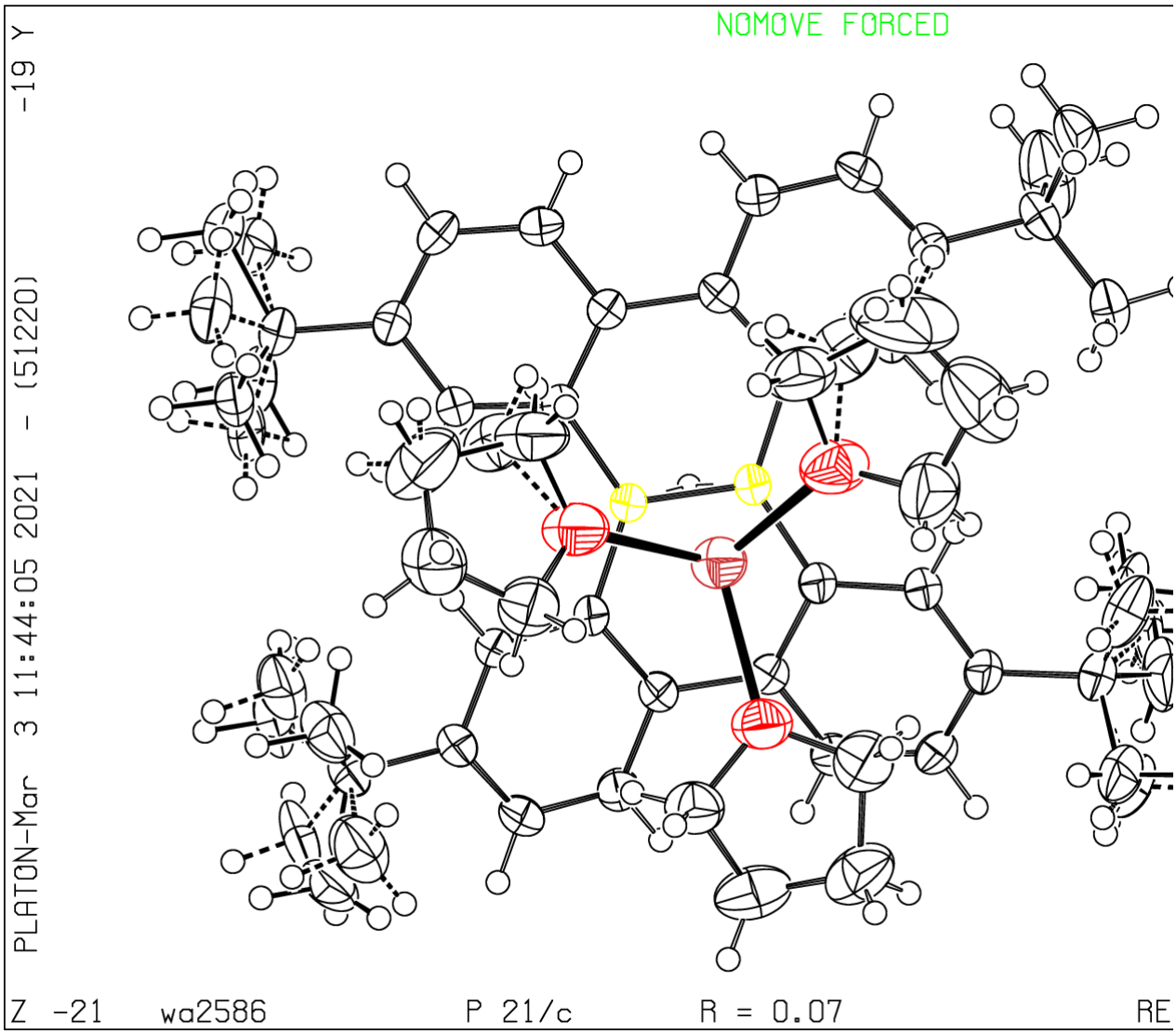
Datablock wa3016 - ellipsoid plot



Datablock wa3011 - ellipsoid plot



Datablock wa2586 - ellipsoid plot



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