checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2-Er, 2-Gd, 2-Ho, 2-Lu, 2-Tm, 2-Yb, 3, 4

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2-Gd

```
Bond precision:  = 0.0000 A              Wavelength=0.71073

Cell:            a=10.3257(4)    b=15.3846(6)       c=20.3749(8)
                 alpha=90        beta=99.152(3)     gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          3195.5(2)                 3195.5(2)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C34 H58 Cl Gd             C34 H58 Cl1 Gd1
Sum formula     C34 H58 Cl Gd             C34 H58 Cl Gd
Mr              659.50                    659.50
Dx,g cm-3       1.371                     1.371
Z               4                         4
Mu (mm-1)       2.179                     2.179
F000            1372.0                    1372.0
F000'           1372.23
h,k,lmax        12,18,24                  12,18,24
Nref            5854                      5819
Tmin,Tmax       0.685,0.836               0.763,1.000
Tmin'           0.672

Correction method= # Reported T Limits: Tmin=0.763 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.994          Theta(max)= 25.350

R(reflections)= 0.0479( 3809)     wR2(reflections)= 0.1215( 5819)

S = 0.964                 Npar= 639
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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

PLAT973_ALERT_2_B Check Calcd Positive Residual Density on Gd1A 1.53 eA-3

Author Response: The residual peak is placed in closed proximity of a strong absorber (Gd) and could not be modelled as any chemically sensible species.

Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.11 Note
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.235 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 33 Report
PLAT972_ALERT_2_C Check Calcd Residual Density 0.99A From Gd1A -1.61 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.04A From Gd1A -1.58 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 75 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 72 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1).. 100% Note
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 2).. 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (90.76) in Resd. # 1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (3.24) in Resd. # 2 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 18 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 94 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1070 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 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
5 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 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: 2-Ho

Bond precision: = 0.0000 A Wavelength=0.71073

Cell:	a=10.3275(3)	b=15.3654(5)	c=20.3014(5)
	alpha=90	beta=99.516(3)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	3177.22(16)	3177.22(16)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C0.43 H0.73 Cl0.01 Ho0.01, 0.988(C34 H58 Cl Ho)	C34 H58 Cl Ho
Sum formula	C34 H58 Cl Ho	C34 H58 Cl Ho
Mr	667.18	667.18
Dx,g cm-3	1.395	1.395
Z	4	4
Mu (mm-1)	2.594	2.594
F000	1384.0	1384.0
F000’	1384.05	
h,k,lmax	12,18,24	12,18,24
Nref	5828	5786
Tmin,Tmax	0.677,0.776	0.903,1.000
Tmin’	0.664	

Correction method= # Reported T Limits: Tmin=0.903 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.993 Theta(max)= 25.350

R(reflections)= 0.0258(4688) wR2(reflections)= 0.0587(5786)

S = 1.015 Npar= 638

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). 17 Note

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

Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.07 Note
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.248 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 20 Report

Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         72 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         72 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records          1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ho1A   --  Cl1A    ..        5.3 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..       100% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  2)..       100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         18 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         94 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1247 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          5 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.          9 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
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  17 ALERT level G = General information/check it is not something unexpected

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

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Bond precision:  C-C = 0.0046 A          Wavelength=1.54184

Cell:          a=10.40646(17)    b=15.8849(2)          c=19.9209(3)
               alpha=90          beta=103.3718(16)     gamma=90
Temperature:   100 K
```

	Calculated	Reported
Volume	3203.76(8)	3203.76(9)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C34 H58 Cl Er	C34 H58 Cl Er
Sum formula	C34 H58 Cl Er	C34 H58 Cl Er
Mr	669.51	669.51
Dx,g cm-3	1.388	1.388
Z	4	4
Mu (mm-1)	5.748	5.748
F000	1388.0	1388.0
F000’	1354.06	
h,k,lmax	12,19,23	12,19,23
Nref	2942	2940
Tmin,Tmax	0.431,0.795	0.837,0.945
Tmin’	0.238	

Correction method= # Reported T Limits: Tmin=0.837 Tmax=0.945
AbsCorr = ANALYTICAL

Data completeness= 0.999 Theta(max)= 68.239

R(reflections)= 0.0314(2768) wR2(reflections)= 0.0833(2940)

S = 1.094 Npar= 173

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
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3 Report

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Alert level G
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 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
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: 2-Tm

Bond precision: C-C = 0.0030 A Wavelength=1.54184

Cell: a=10.41842(7) b=15.91461(12) c=19.92036(15)
       alpha=90 beta=103.3115(8) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3214.16(4)	3214.16(4)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C34 H58 Cl Tm	C34 H58 Cl Tm
Sum formula	C34 H58 Cl Tm	C34 H58 Cl Tm
Mr	671.18	671.18
Dx,g cm-3	1.387	1.387
Z	4	4
Mu (mm-1)	6.053	6.053
F000	1392.0	1392.0
F000’	1363.66	
h,k,lmax	12,19,23	12,19,23
Nref	2952	2947
Tmin,Tmax	0.283,0.549	0.605,1.000
Tmin’	0.206	

Correction method= # Reported T Limits: Tmin=0.605 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.998 Theta(max)= 68.221

R(reflections)= 0.0182(2914) wR2(reflections)= 0.0439(2947)

S = 1.059 Npar= 173

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

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 5 Report

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Alert level G

PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..... 0.00012 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..... 0.00015 Ang.
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 11 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
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

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

Datablock: 2-Yb

Bond precision: C-C = 0.0053 A Wavelength=0.71073

Cell: a=10.4101(6) b=15.8845(7) c=19.9206(14)
alpha=90 beta=103.541(6) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3202.5(3)	3202.5(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C34 H58 Cl Yb	C34 H58 Cl Yb
Sum formula	C34 H58 Cl Yb	C34 H58 Cl Yb
Mr	675.29	675.29
Dx,g cm-3	1.401	1.401
Z	4	4
Mu (mm-1)	3.023	3.023
F000	1396.0	1396.0
F000’	1395.43	
h,k,lmax	12,19,23	12,19,23
Nref	2943	2933
Tmin,Tmax	0.485,0.685	0.640,1.000
Tmin’	0.457	

Correction method= # Reported T Limits: Tmin=0.640 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.997 Theta(max)= 25.349

R(reflections)= 0.0315(2806) wR2(reflections)= 0.0766(2933)

S = 1.080 Npar= 173

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
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.05 Report

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PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          9 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          2 Report
PLAT971_ALERT_2_C Check Calcd Residual Density  0.97A From     Yb1       2.16 eA-3
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Alert level G

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PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          5 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
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: 2-Lu

Bond precision: C-C = 0.0082 A Wavelength=0.71073

Cell: a=10.4265(4) b=15.9490(4) c=19.9604(8)
       alpha=90 beta=103.254(4) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	3230.9(2)	3230.84(19)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C34 H58 Cl Lu	C34 H58 Cl Lu
Sum formula	C34 H58 Cl Lu	C34 H58 Cl Lu
Mr	677.22	677.22
Dx,g cm-3	1.392	1.392
Z	4	4
Mu (mm-1)	3.158	3.158
F000	1400.0	1400.0
F000’	1399.09	
h,k,lmax	12,19,24	12,19,24
Nref	2969	2932
Tmin,Tmax	0.547,0.812	0.833,0.914
Tmin’	0.470	

Correction method= # Reported T Limits: Tmin=0.833 Tmax=0.914
AbsCorr = GAUSSIAN

Data completeness= 0.988 Theta(max)= 25.345

R(reflections)= 0.0408(2715) wR2(reflections)= 0.0954(2932)

S = 1.044 Npar= 173

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

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density	2.02	Report
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.00818	Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	8	Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600	29	Report
PLAT971_ALERT_2_C Check Calcd Residual Density 0.86A From Lu1	2.35	eA-3

Alert level G

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	1	Info

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

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

Datablock: 3

Bond precision: C-C = 0.0044 A Wavelength=0.71073

Cell:	a=19.4317(3)	b=18.0512(2)	c=19.4713(3)
	alpha=90	beta=109.572(2)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	6435.24(18)	6435.24(17)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C34 H58 Yb	C34 H58 Yb
Sum formula	C34 H58 Yb	C34 H58 Yb
Mr	639.84	639.84
Dx,g cm-3	1.321	1.321
Z	8	8
Mu (mm-1)	2.925	2.925
F000	2656.0	2656.0
F000'	2653.67	
h,k,lmax	23,21,23	23,21,23
Nref	11778	11694
Tmin,Tmax	0.433,0.580	0.357,1.000
Tmin'	0.168	

Correction method= # Reported T Limits: Tmin=0.357 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.993 Theta(max)= 25.350

R(reflections)= 0.0284(11107) wR2(reflections)= 0.0739(11694)

S = 1.072 Npar= 760

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). 31 Note

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

Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H67C .. H43E .. 2.01 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.240 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 51 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 4 Note
PLAT971_ALERT_2_C Check Calcd Residual Density 0.74A From Yb2 2.18 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.80A From Yb1 1.52 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.80A From Yb2 -1.58 eA-3

Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         57 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         79 Report
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....       0.61 mm
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      13.85 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..        17% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  2)..         9% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1855 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         2 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
   8 **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
  10 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
   0 ALERT type 5 Informative message, check

Datablock: 4

Bond precision: C-C = 0.0109 A Wavelength=0.71073

Cell:	a=13.9168(8)	b=8.9862(5)	c=18.5492(13)
	alpha=90	beta=99.580(6)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	2287.4(2)	2287.4(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C42 H74 I2 O2 Yb2	C42 H74 I2 O2 Yb2
Sum formula	C42 H74 I2 O2 Yb2	C42 H74 I2 O2 Yb2
Mr	1210.89	1210.89
Dx,g cm-3	1.758	1.758
Z	2	2
Mu (mm-1)	5.443	5.443
F000	1176.0	1176.0
F000’	1173.04	
h,k,lmax	16,10,22	16,10,22
Nref	4187	4152
Tmin,Tmax	0.755,0.863	0.825,1.000
Tmin’	0.337	

Correction method= # Reported T Limits: Tmin=0.825 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.992 Theta(max)= 25.347

R(reflections)= 0.0414(3105) wR2(reflections)= 0.0952(4152)

S = 1.029 Npar= 255

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

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

Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O1 -- C21B .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1 -- C21A .. 0.17 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01094 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.416 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 19 Report
PLAT977_ALERT_2_C Check the Negative Difference Density on H19C -0.39 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 7 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.06 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Yb1 -- I1B_a .. 15.9 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1).. 13% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 85 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 4 Note
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
1 **ALERT level B** = A potentially serious problem, consider carefully
9 **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

```
 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
  5 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 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

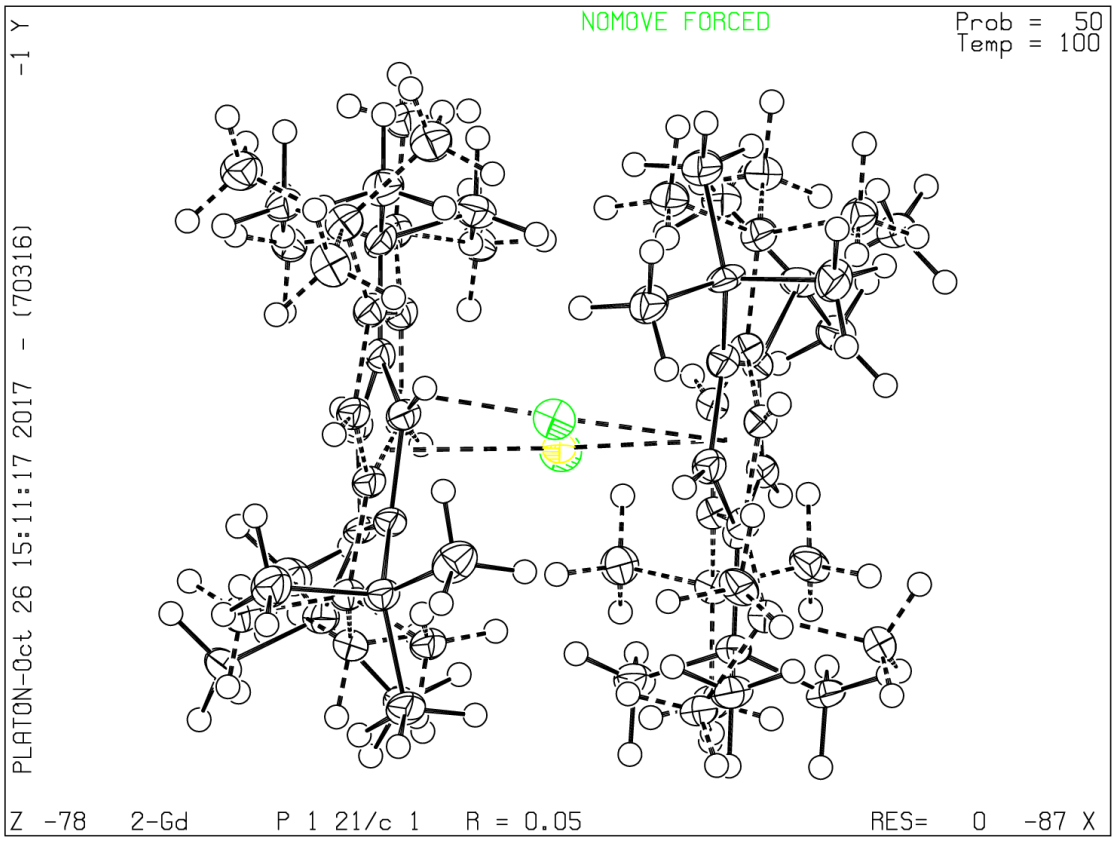
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

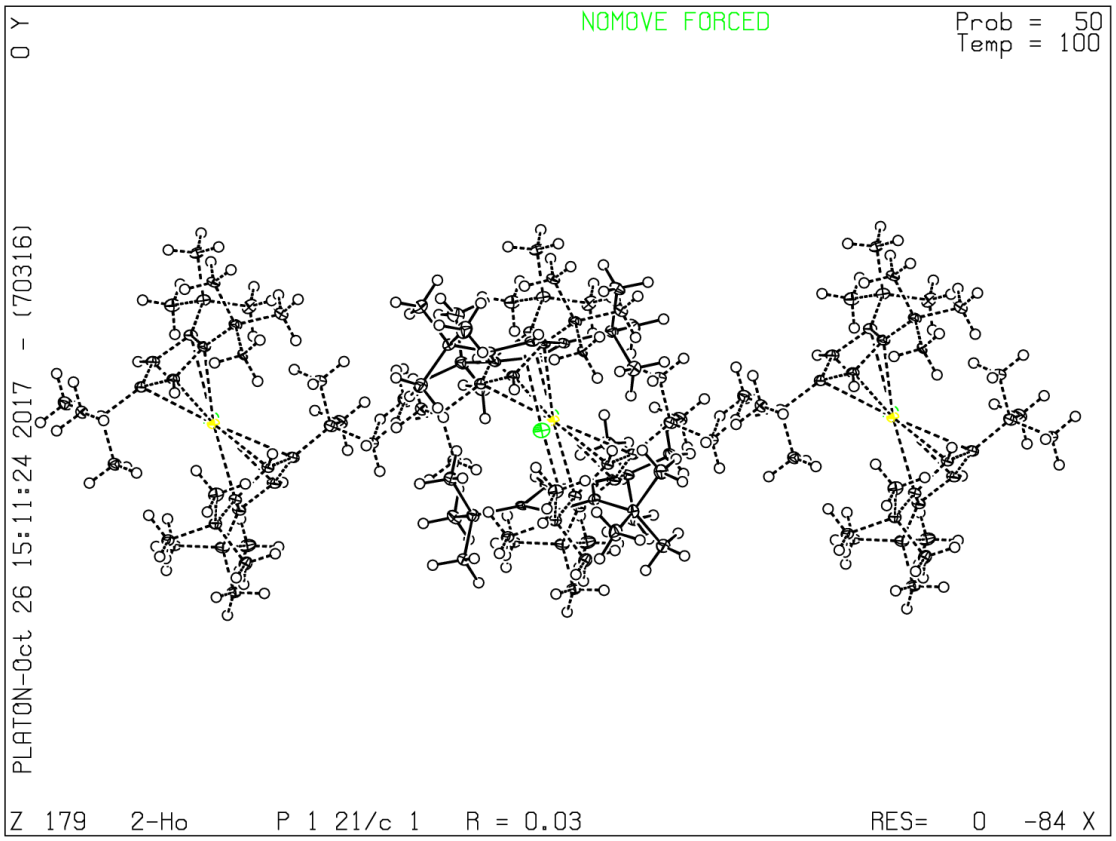
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

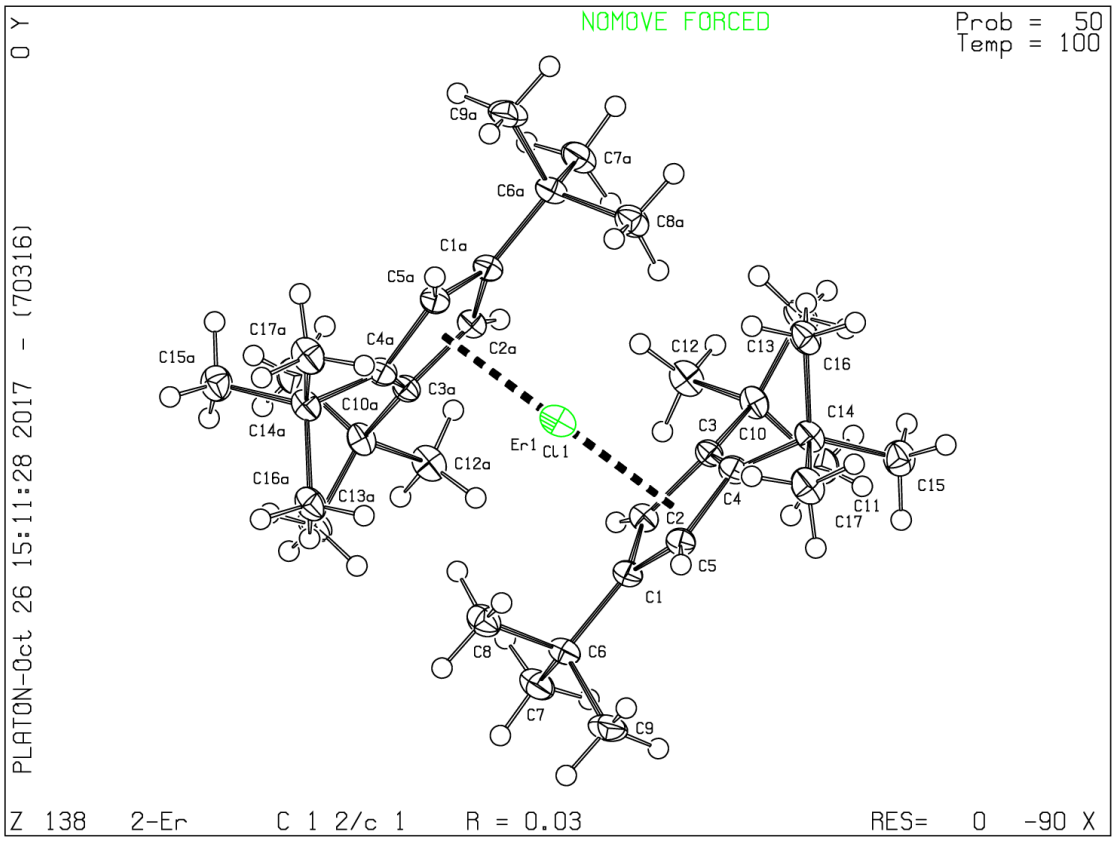
Datablock 2-Gd - ellipsoid plot



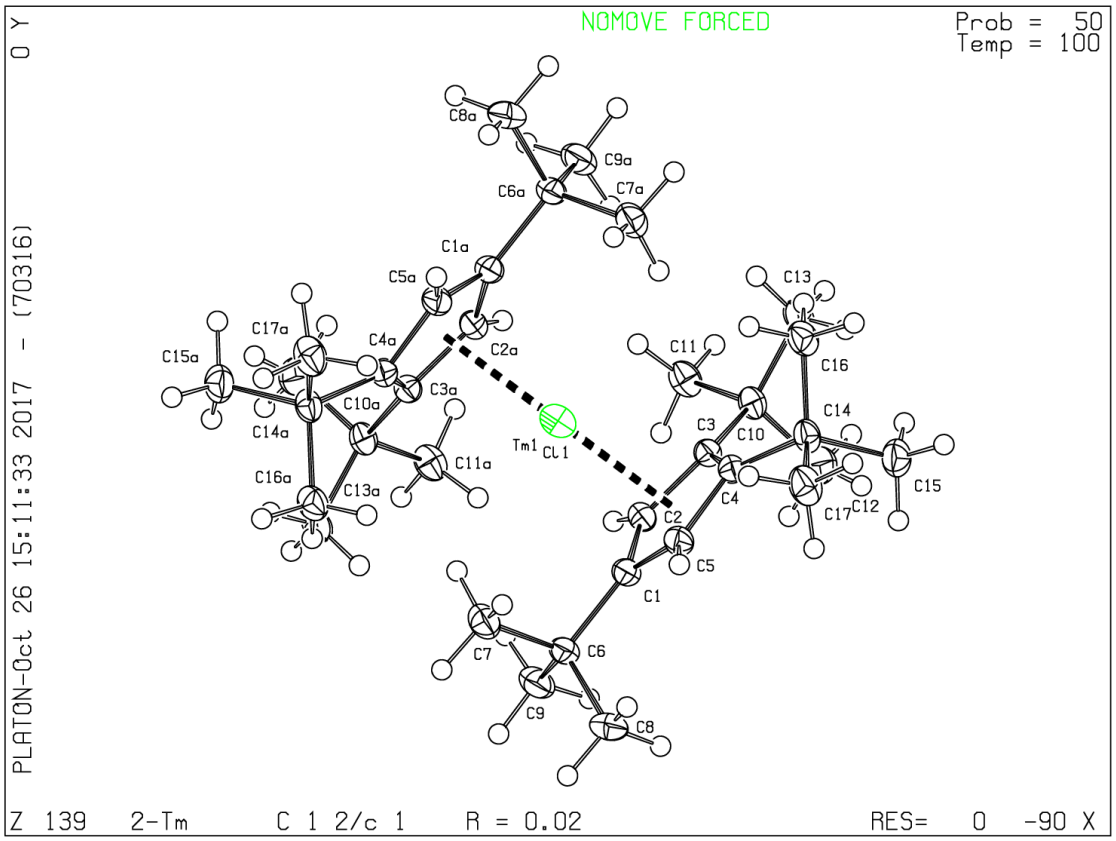
Datablock 2-Ho - ellipsoid plot



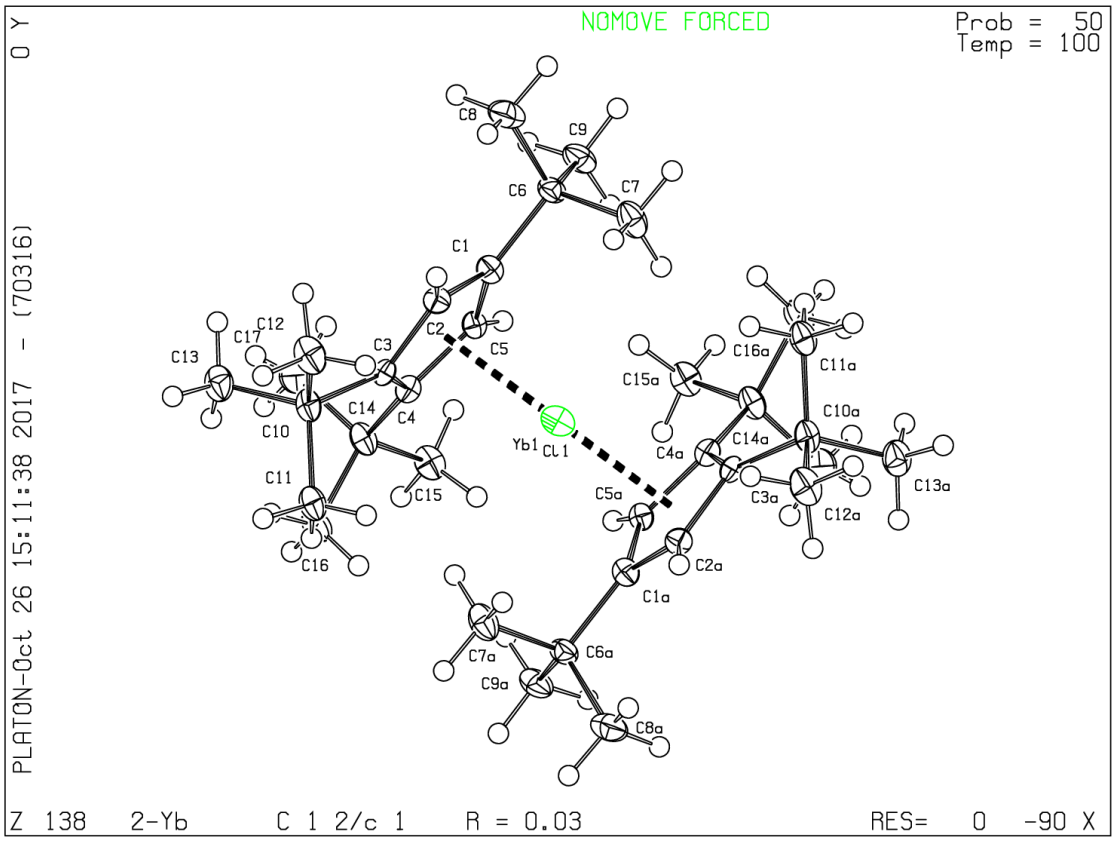
Datablock 2-Er - ellipsoid plot



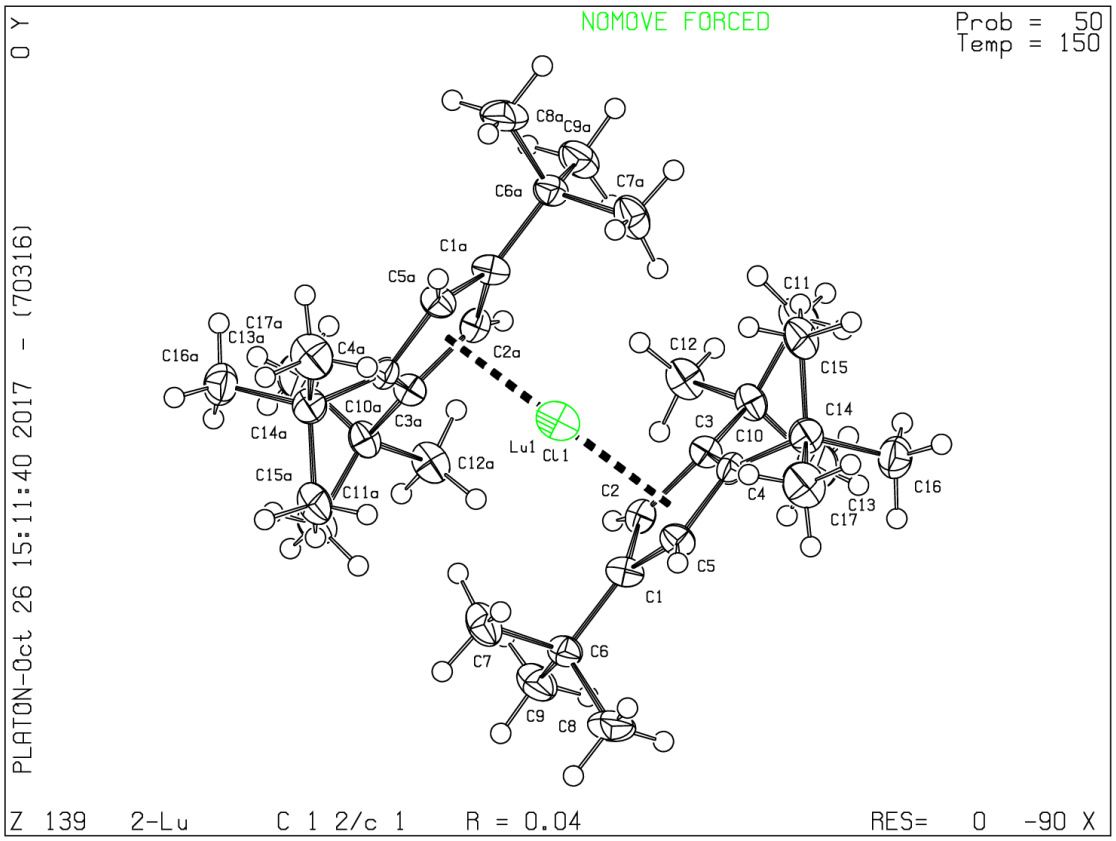
Datablock 2-Tm - ellipsoid plot



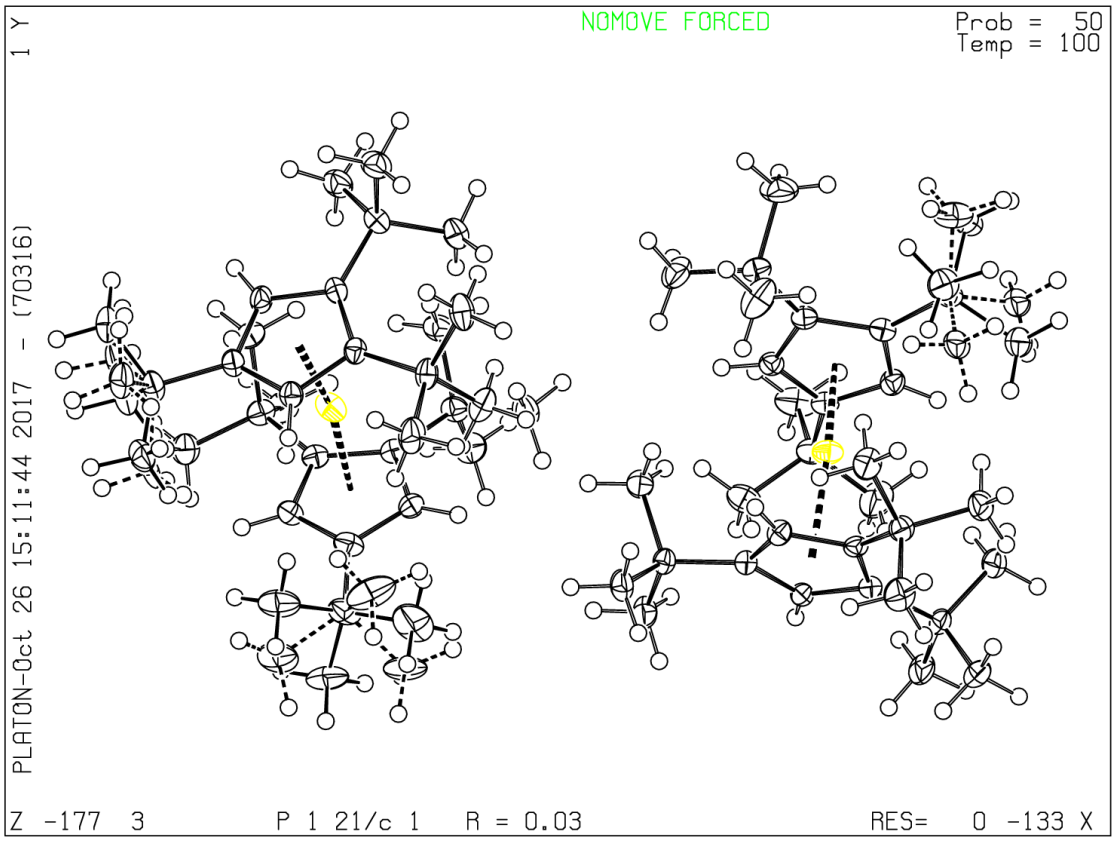
Datablock 2-Yb - ellipsoid plot



Datablock 2-Lu - ellipsoid plot



Datablock 3 - ellipsoid plot



Datablock 4 - ellipsoid plot

