checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1-Er-C6H6, 1-Er-CH2Cl2, 1-Gd-C6H6, 1-Gd-CH2Cl2, 1-Ho-CH2Cl2, 1-Lu-C6H14, 1-Tm-C6H14, 1-Yb-C6H14, 1-Yb-C6H6

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1-Gd-CH2Cl2

Bond precision: C-C = 0.0161 A Wavelength=0.71073

Cell: a=11.6943(4) b=12.4712(3) c=19.9988(9)
alpha=96.520(3) beta=90.614(3) gamma=100.760(3)
Temperature: 100 K

	Calculated	Reported
Volume	2845.33(18)	2845.33(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 B F20, C34 H58 Gd [+ solvent]	C34 H58 Gd, B C24 F20
Sum formula	C58 H58 B F20 Gd [+ solvent]	C58 H58 B F20 Gd
Mr	1303.10	1303.10
Dx,g cm-3	1.521	1.521
Z	2	2
Mu (mm-1)	1.268	1.268
F000	1310.0	1310.0
F000’	1310.57	
h,k,lmax	14,15,24	14,15,24
Nref	10406	10397
Tmin,Tmax	0.852,0.910	0.759,1.000
Tmin’	0.793	

Correction method= # Reported T Limits: Tmin=0.759 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.350

R(reflections)= 0.0966(9315) wR2(reflections)= 0.2242(10397)

S = 1.229 Npar= 740

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

PLAT930_ALERT_2_B Check Twin Law (0 0 1)[0 1 5] Estimated BASF 0.13

Author Response: A second component is indeed present and has been delt with. Please see refine_special_details section.

Alert level C

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.6	Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.8	Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.01614	Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance	7.938	Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance	2.341	Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	7	Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600	3	Report

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...	80	Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	69.87	Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree
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
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
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure	213	A**3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C34 H58 Gd	2	Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints	1260	Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed	!	Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..	!	Info
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 ...	2	Note

0	**ALERT level A** = Most likely a serious problem - resolve or explain
1	**ALERT level B** = A potentially serious problem, consider carefully
7	**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

2	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: 1-Gd-C6H6

Bond precision: C-C = 0.0068 A Wavelength=0.71073

Cell: a=11.8330(6) b=12.3634(5) c=21.0434(8)
alpha=79.470(3) beta=80.898(4) gamma=80.176(4)
Temperature: 100 K

	Calculated	Reported
Volume	2956.6(2)	2956.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 B F20, C34 H58 Gd, C6 H6	C34 H58 Gd, B C24 F20, C6 H6
Sum formula	C64 H64 B F20 Gd	C64 H64 B F20 Gd
Mr	1381.21	1381.21
Dx,g cm-3	1.551	1.551
Z	2	2
Mu (mm-1)	1.225	1.225
F000	1394.0	1394.0
F000’	1394.60	
h,k,lmax	14,14,25	14,14,25
Nref	10829	36057
Tmin,Tmax	0.898,0.972	0.898,1.000
Tmin’	0.871	

Correction method= # Reported T Limits: Tmin=0.898 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 3.330 Theta(max)= 25.350

R(reflections)= 0.0419(30485) wR2(reflections)= 0.1017(36057)

S = 0.977 Npar= 825

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

PLAT221_ALERT_2_C Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range 4.6 Ratio
PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of C14 Check
PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of C27 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 12 Report

---

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 16 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 20 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check

```
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 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    C14    --  C16B    ..        5.3 s.u.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..         9% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  F4     ..  C16A    ..       2.81 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F7     ..  C15B    ..       2.93 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       259 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
PLAT931_ALERT_5_G Found Twin Law ( 0 0  1)[       ] Estimated BASF      0.36 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         36 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   6 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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
   7 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: 1-Ho-CH2Cl2

Bond precision: C-C = 0.0071 A Wavelength=1.54184

Cell:	a=11.7004(4)	b=12.5068(4)	c=20.0756(6)
	alpha=82.939(2)	beta=89.866(3)	gamma=79.626(3)
Temperature:	150 K		

	Calculated	Reported
Volume	2867.23(16)	2867.23(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 B F20, C34 H58 Ho [+ solvent]	C34 H58 Ho, B C24 F20
Sum formula	C58 H58 B F20 Ho [+ solvent]	C58 H58 B F20 Ho
Mr	1310.78	1310.78
Dx,g cm-3	1.518	1.518
Z	2	2
Mu (mm-1)	3.484	3.484
F000	1316.0	1316.0
F000’	1290.92	
h,k,lmax	14,15,24	14,15,24
Nref	10486	10222
Tmin,Tmax	0.523,0.706	0.256,1.000
Tmin’	0.474	

Correction method= # Reported T Limits: Tmin=0.256 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.975 Theta(max)= 68.244

R(reflections)= 0.0639(8672) wR2(reflections)= 0.1777(10222)

S = 1.043 Npar= 749

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .	0.976	Note
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of	C14	Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance	2.590	Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600	251	Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.	0	Info

---

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	27	Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...	20	Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.10	Report
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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)..	9%	Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure	219	A**3
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters	1	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints	423	Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed	!	Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	13	Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	2	Note

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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
15 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: 1-Er-CH2Cl2

Bond precision: C-C = 0.0163 A Wavelength=0.71073

Cell:	a=10.9450(4)	b=11.4743(4)	c=12.7703(4)
	alpha=79.081(3)	beta=85.403(3)	gamma=72.146(3)
Temperature:	100 K		

	Calculated	Reported
Volume	1498.48(9)	1498.49(9)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C24 B F20, C34 H58 Er, 2(C H2 Cl2)	C34 H58 Er, 2(C H2 Cl2), B C24 F20
Sum formula	C60 H62 B Cl4 Er F20	C60 H62 B Cl4 Er F20
Mr	1482.97	1482.96
Dx,g cm-3	1.643	1.643
Z	1	1
Mu (mm-1)	1.680	1.680
F000	743.0	743.0
F000’	743.80	
h,k,lmax	13,13,15	13,13,15
Nref	10966[5483]	10880
Tmin,Tmax	0.821,0.932	0.723,1.000
Tmin’	0.753	

Correction method= # Reported T Limits: Tmin=0.723 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 1.98/0.99 Theta(max)= 25.348

R(reflections)= 0.0490(10757) wR2(reflections)= 0.1242(10880)

S = 1.023 Npar= 792

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

PLAT971_ALERT_2_B Check Calcd Residual Density 2.17A From C20 3.22 eA-3

Author Response: these electron density peak could not be modelled as any chemically sensible species. Their presence is likely due to the formation of ice during the collection and/or to imperfections in the absorption correction.

PLAT971_ALERT_2_B Check Calcd Residual Density 2.18A From C4 3.22 eA-3

Author Response: these electron density peak could not be modelled as any chemically sensible species. Their presence is likely due to the formation of ice during the collection and/or to imperfections in the absorption correction.

PLAT971_ALERT_2_B Check Calcd Residual Density 0.94A From Er1 2.85 eA-3

Author Response: these electron density peak could not be modelled as any chemically sensible species. Their presence is likely due to the formation of ice during the collection and/or to imperfections in the absorption correction.

PLAT971_ALERT_2_B Check Calcd Residual Density 0.93A From Er1 2.81 eA-3

Author Response: these electron density peak could not be modelled as any chemically sensible species. Their presence is likely due to the formation of ice during the collection and/or to imperfections in the absorption correction.

PLAT971_ALERT_2_B Check Calcd Residual Density 0.92A From Er1 2.53 eA-3

Author Response: these electron density peak could not be modelled as any chemically sensible species. Their presence is likely due to the formation of ice during the collection and/or to imperfections in the absorption correction.

Alert level C

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 6.92 Note
PLAT213_ALERT_2_C Atom F17 has ADP max/min Ratio ..... 3.6 oblate
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01626 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H25A .. H29C .. 1.87 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3 Report
PLAT971_ALERT_2_C Check Calcd Residual Density 0.82A From C18 2.00 eA-3

Author Response: these electron density peak could not be modelled as any chemically sensible species. Their presence is likely due to the formation of ice during the collection and/or to imperfections in the absorption correction.

PLAT971_ALERT_2_C Check Calcd Residual Density 0.76A From C1 1.87 eA-3

Author Response: these electron density peak could not be modelled as any chemically sensible species. Their presence is likely due to the formation of ice during the collection and/or to imperfections in the absorption correction.

```
PLAT972_ALERT_2_C Check Calcd Residual Density  0.95A From     Er1      -1.80 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.91A From     Er1      -1.77 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on     Er1       1.47 eA-3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        87 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.003 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3)..        33% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       901 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         3 Note
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
   5 ALERT level B = A potentially serious problem, consider carefully
  11 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: 1-Er-C6H6

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

Cell: a=11.8090(2) b=12.3393(2) c=21.0838(3)
       alpha=79.5390(14) beta=81.0030(14) gamma=80.4658(14)
Temperature: 100 K

	Calculated	Reported
Volume	2954.05(8)	2954.04(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 B F20, C34 H58 Er, C6 H6	C34 H58 Er, B C24 F20, C6 H6
Sum formula	C64 H64 B Er F20	C64 H64 B Er F20
Mr	1391.22	1391.22
Dx,g cm-3	1.564	1.564
Z	2	2
Mu (mm-1)	1.524	1.524
F000	1402.0	1402.0
F000’	1402.42	
h,k,lmax	14,14,25	14,14,25
Nref	10805	10795
Tmin,Tmax	0.812,0.878	0.679,1.000
Tmin’	0.710	

Correction method= # Reported T Limits: Tmin=0.679 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.999 Theta(max)= 25.350

R(reflections)= 0.0202(10168) wR2(reflections)= 0.0496(10795)

S = 1.050 Npar= 824

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
PLAT214_ALERT_2_C	Atom C34B (Anion/Solvent) ADP max/min Ratio	4.1 prolat
PLAT221_ALERT_2_C	Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range	4.6 Ratio
PLAT223_ALERT_4_C	Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range	5.0 Ratio
PLAT242_ALERT_2_C	Low ’MainMol’ Ueq as Compared to Neighbors of	C14 Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	7 Note
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	5 Report

---

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	27 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	89 Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT154_ALERT_1_G	The s.u.’s on the Cell Angles are Equal ..(Note)	0.0014 Degree
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1 Report
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3 Note
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1 Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C31 -- C34A ..	6.0 s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)..	9% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact F4 .. C33A ..	2.88 Ang.

```
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1050 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         13 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   7 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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
   6 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: 1-Tm-C6H14

Bond precision: C-C = 0.0049 A Wavelength=0.71073

Cell: a=11.5460(3) b=12.6736(3) c=21.1632(6)
alpha=82.831(2) beta=87.029(2) gamma=80.6448(19)
Temperature: 100 K

	Calculated	Reported
Volume	3030.15(14)	3030.14(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 B F20, C34 H58 Tm, C6 H14	C24 B F20, C34 H58 Tm, C6 H14
Sum formula	C64 H72 B F20 Tm	C64 H72 B F20 Tm
Mr	1400.96	1400.95
Dx,g cm-3	1.536	1.535
Z	2	2
Mu (mm-1)	1.565	1.565
F000	1420.0	1420.0
F000’	1420.31	
h,k,lmax	13,15,25	13,15,25
Nref	11098	11062
Tmin,Tmax	0.779,0.896	0.737,1.000
Tmin’	0.698	

Correction method= # Reported T Limits: Tmin=0.737 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.997 Theta(max)= 25.348

R(reflections)= 0.0337(9519) wR2(reflections)= 0.0700(11062)

S = 1.041 Npar= 795

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). 28 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
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 7 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

---

Alert level G
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
2 **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
2 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: 1-Yb-C6H14

Bond precision: C-C = 0.0153 A Wavelength=1.54184

Cell: a=11.6915(4) b=12.4956(4) c=20.0746(7)
alpha=96.913(3) beta=90.070(3) gamma=100.302(3)
Temperature: 150 K

	Calculated	Reported
Volume	2863.71(17)	2863.72(17)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 B F20, C34 H58 Yb [+ solvent]	C34 H58 Yb, B C24 F20
Sum formula	C58 H58 B F20 Yb [+ solvent]	C58 H58 B F20 Yb
Mr	1318.89	1318.89
Dx,g cm-3	1.530	1.530
Z	2	2
Mu (mm-1)	3.929	3.929
F000	1322.0	1322.0
F000’	1312.46	
h,k,lmax	13,14,23	13,14,23
Nref	10112	9717
Tmin,Tmax	0.655,0.675	0.496,1.000
Tmin’	0.434	

Correction method= # Reported T Limits: Tmin=0.496 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.961 Theta(max)= 66.601

R(reflections)= 0.0886(7977) wR2(reflections)= 0.2607(9717)

S = 1.120 Npar= 739

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full value Low .	0.961 Note
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.26 Report
PLAT242_ALERT_2_C	Low ’MainMol’ Ueq as Compared to Neighbors of	C14 Check
PLAT242_ALERT_2_C	Low ’MainMol’ Ueq as Compared to Neighbors of	C31 Check
PLAT334_ALERT_2_C	Small Average Benzene C-C Dist. C41 -C46	1.37 Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01528 Ang.
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn H25C .. H28C ..	1.87 Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	4.520 Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.595	395 Report
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0 Info

---

Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.15 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	19.70 Why ?
PLAT154_ALERT_1_G	The s.u.’s on the Cell Angles are Equal ..(Note)	0.003 Degree
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	217 A**3
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        69% 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 ...        11 Note
```

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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: 1-Yb-C6H6

Bond precision: C-C = 0.0122 A Wavelength=1.54184

Cell: a=11.8474(4) b=12.3523(5) c=21.1670(8)
       alpha=79.483(3) beta=80.994(3) gamma=80.564(3)
Temperature: 150 K

	Calculated	Reported
Volume	2978.7(2)	2978.67(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 B F20, C34 H58 Yb, C6 H6	C34 H58 Yb, B C24 F20, C6 H6
Sum formula	C64 H64 B F20 Yb	C64 H64 B F20 Yb
Mr	1397.00	1397.00
Dx,g cm-3	1.558	1.558
Z	2	2
Mu (mm-1)	3.814	3.814
F000	1406.0	1406.0
F000’	1396.66	
h,k,lmax	13,14,24	13,14,24
Nref	9810	9377
Tmin,Tmax	0.664,0.683	0.314,1.000
Tmin’	0.444	

Correction method= # Reported T Limits: Tmin=0.314 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.956 Theta(max)= 63.690

R(reflections)= 0.0676(6106) wR2(reflections)= 0.1489(9377)

S = 1.005 Npar= 803

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

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low . 0.956 Note

Author Response: Due to the very low diffracting power of the sample, the data was trimmed (SHEL) to 0.86, which impacted the completeness to a small degree. Multiple crystallisation solvents and ratios were tried from the small available range (DCM and benzene plus hexane, varying ratios), to give this sample as the largest single crystals we could synthesise.

Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5814
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01221 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.581 434 Report
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on Yb1 1.46 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H7B -0.31 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 22 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 89 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2).. 9% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact F12 .. C32A .. 2.82 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 209 Check
YB1 -C24 -H24A 1.555 1.555 1.555 44.00 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1102 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 48% 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
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
13 **ALERT level G** = General information/check it is not something unexpected

2 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
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

Datablock: 1-Lu-C6H14

Bond precision: C-C = 0.0111 A Wavelength=0.71073

Cell:	a=21.4141(4)	b=15.9006(2)	c=19.4449(3)
	alpha=90	beta=111.856(2)	gamma=90
Temperature:	150 K		

	Calculated	Reported
Volume	6145.04(19)	6145.04(19)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 B F20, C34 H58 Lu [+ solvent]	C34 H58 Lu, B C24 F20
Sum formula	C58 H58 B F20 Lu [+ solvent]	C58 H58 B F20 Lu
Mr	1320.82	1320.82
Dx,g cm-3	1.428	1.428
Z	4	4
Mu (mm-1)	1.702	1.702
F000	2648.0	2648.0
F000’	2647.95	
h,k,lmax	25,19,23	25,19,23
Nref	11250	20294
Tmin,Tmax	0.743,0.839	0.949,0.966
Tmin’	0.729	

Correction method= # Reported T Limits: Tmin=0.949 Tmax=0.966
AbsCorr = ANALYTICAL

Data completeness= 1.804 Theta(max)= 25.350

R(reflections)= 0.0665(15336) wR2(reflections)= 0.2139(20294)

S = 1.105 Npar= 740

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	2.11	Report
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0111	Ang.
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= 0.600	3	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	2	Check

---

Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.15	Report

```
PLAT434_ALERT_2_G Short Inter HL..HL Contact F5     ..  F18     ..       2.82 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          5 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
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
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   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
  10 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 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
```

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

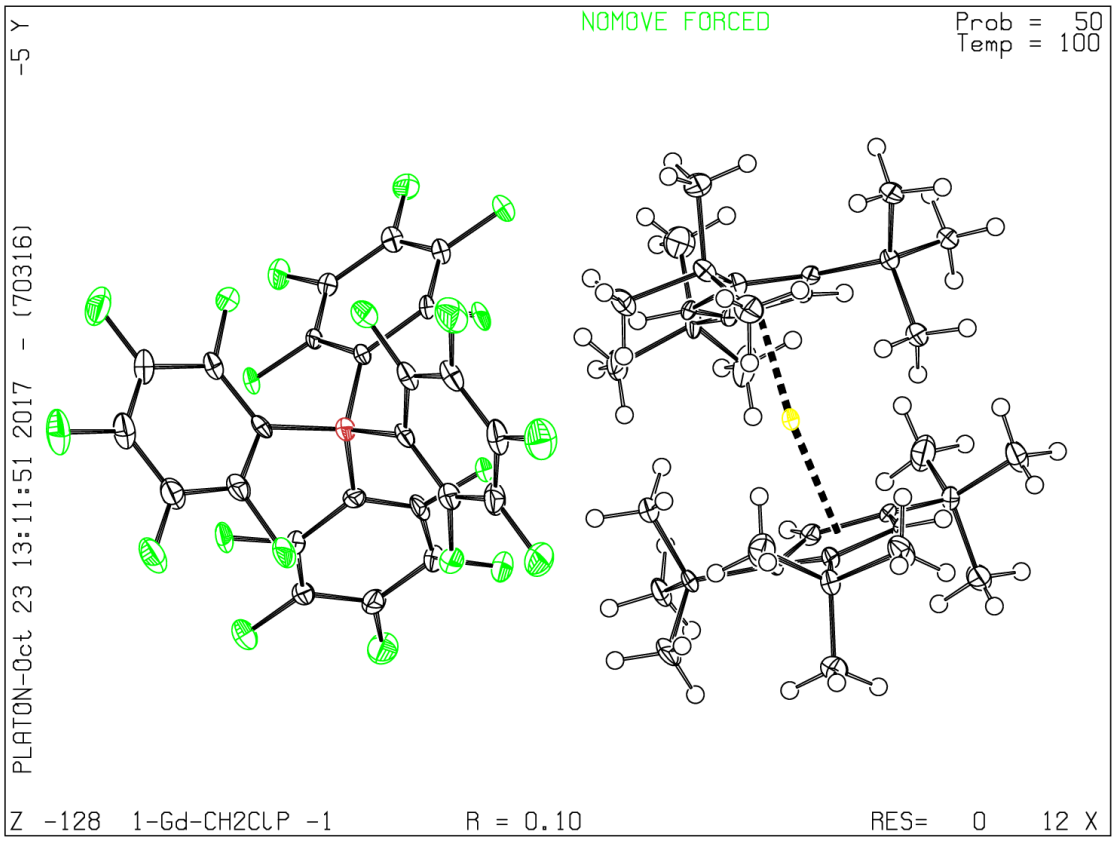
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

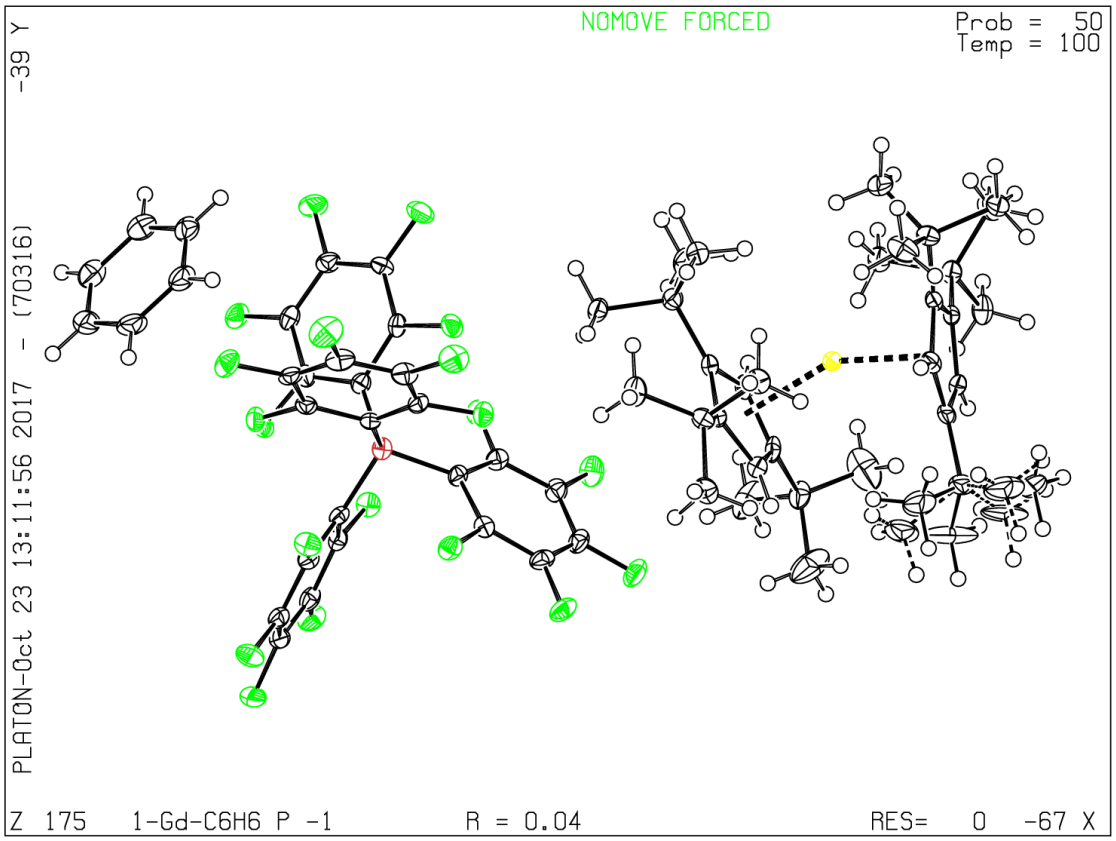
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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

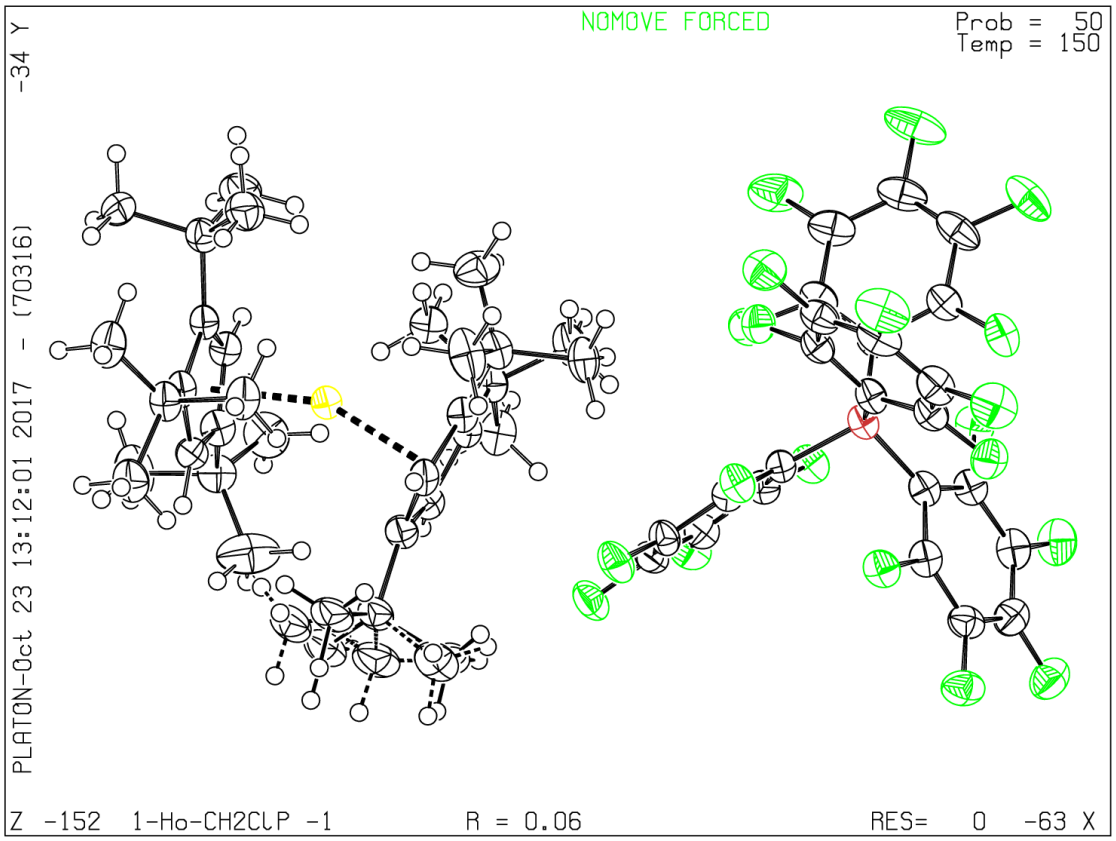
Datablock 1-Gd-CH2Cl2 - ellipsoid plot



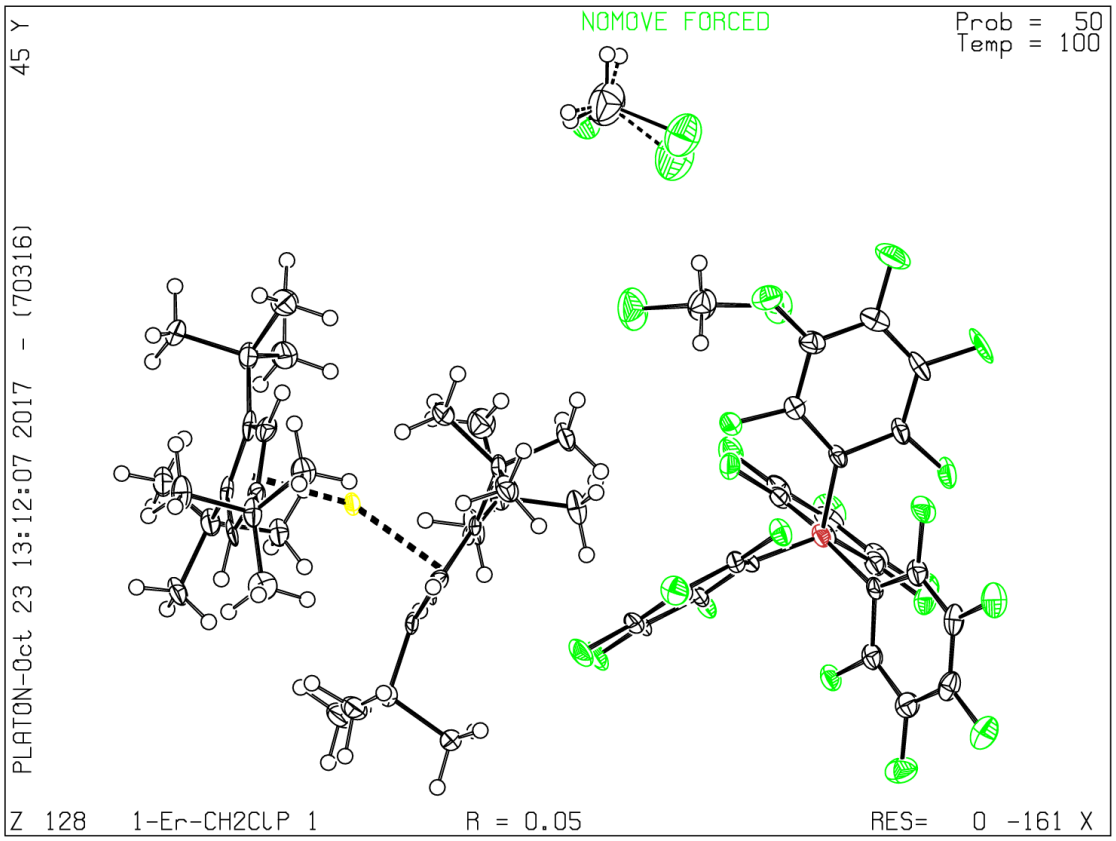
Datablock 1-Gd-C6H6 - ellipsoid plot



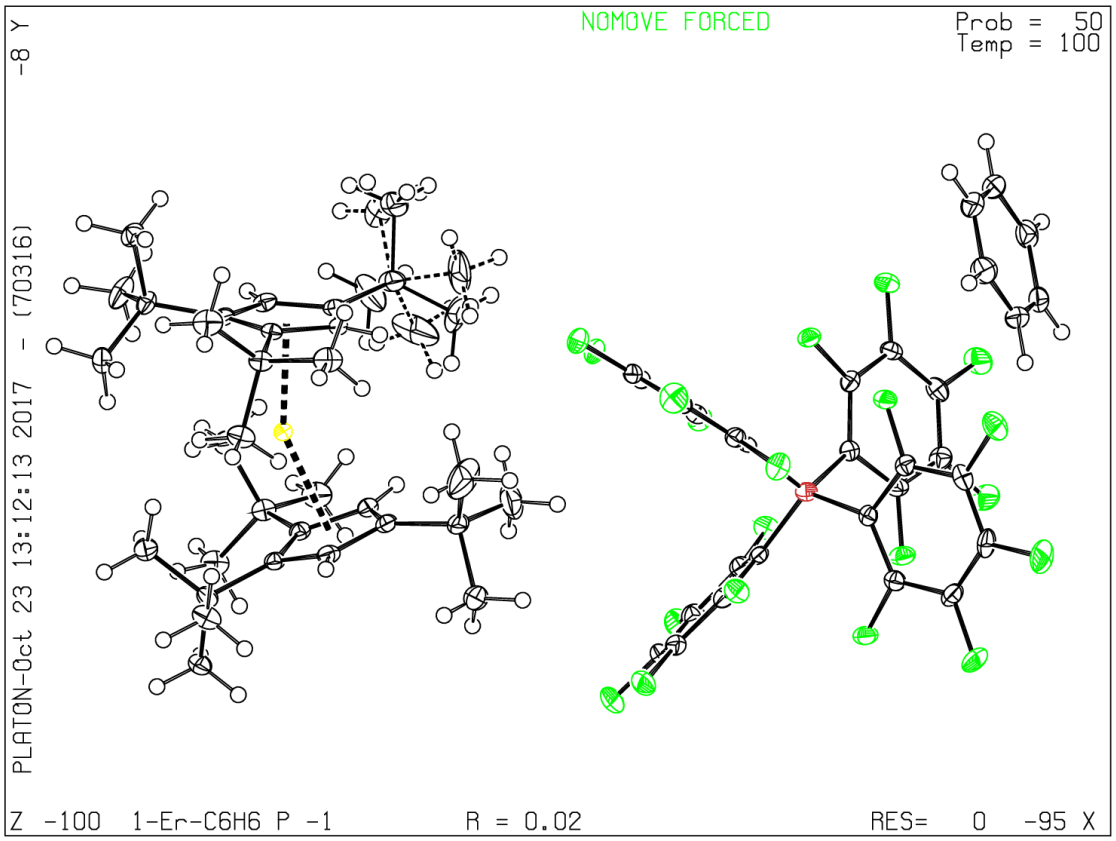
Datablock 1-Ho-CH2Cl2 - ellipsoid plot



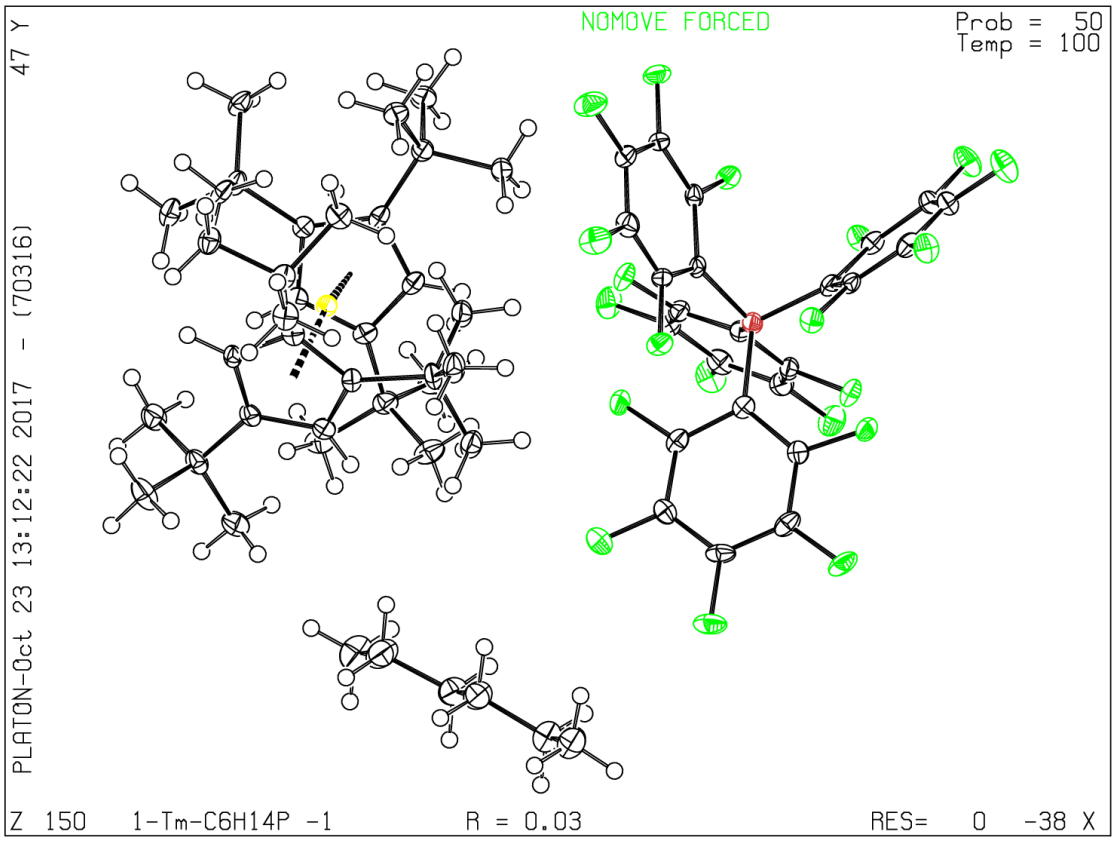
Datablock 1-Er-CH2Cl2 - ellipsoid plot



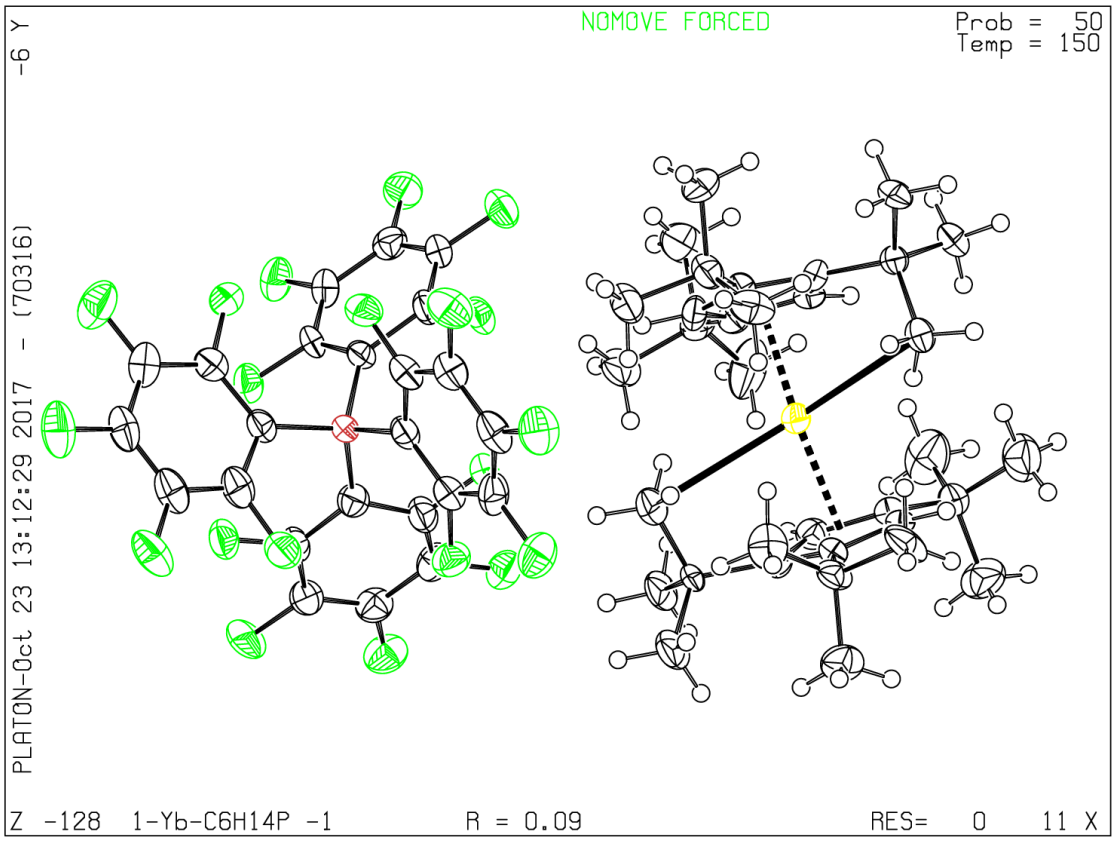
Datablock 1-Er-C6H6 - ellipsoid plot



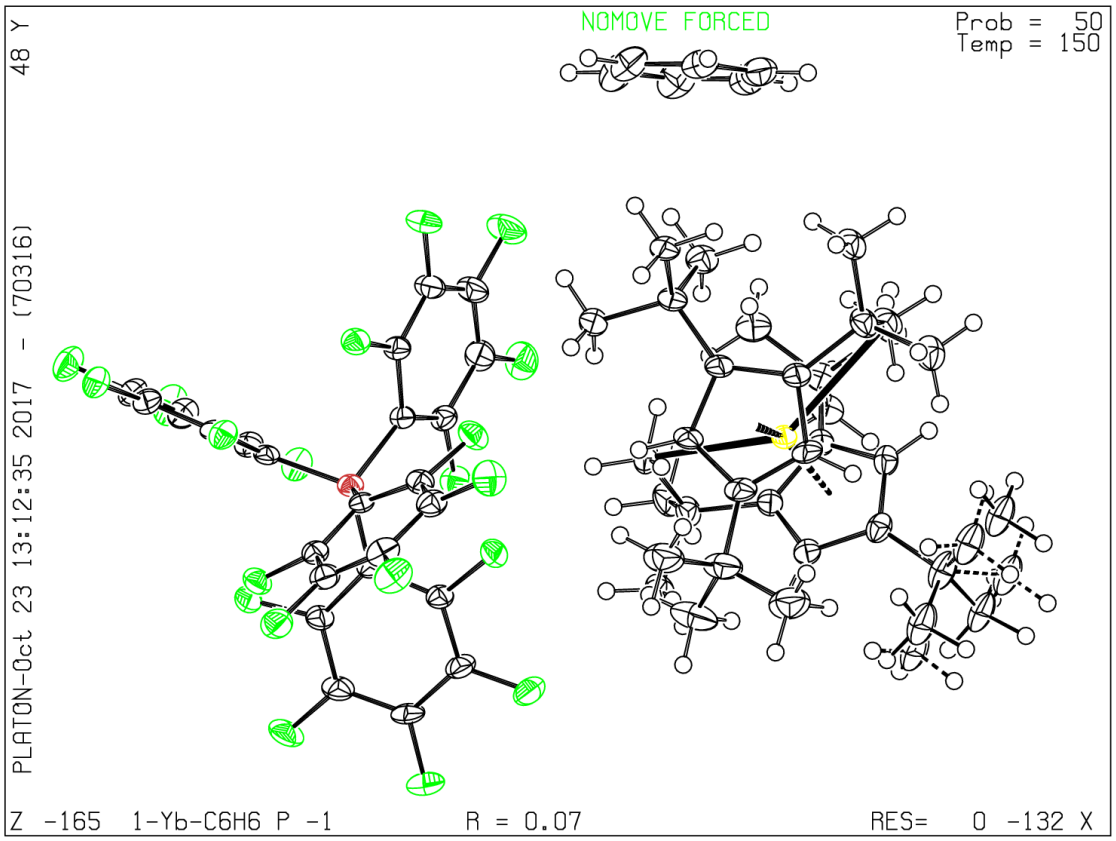
Datablock 1-Tm-C6H14 - ellipsoid plot



Datablock 1-Yb-C6H14 - ellipsoid plot



Datablock 1-Yb-C6H6 - ellipsoid plot



Datablock 1-Lu-C6H14 - ellipsoid plot

