# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

## Datablock: 01

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Bond precision: C-C = 0.0140 A Wavelength=0.71073

Cell: a=17.267(6) b=17.380(6) c=18.306(10)
alpha=102.659(5) beta=103.677(5) gamma=110.207(3)
Temperature: 223 K

| | Calculated | Reported |
|---|---|---|
| Volume | 4729(3) | 4729(3) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C42 H42 La2 N28 O26, 2(Cl4 Cu), 2(Cl) | C42 H66 La2 N28 O26, 2(Cu Cl4), 2Cl, 28(H2 O) |
| Sum formula | C42 H42 Cl10 Cu2 La2 N28 O26 | C42 H122 Cl10 Cu2 La2 N28 O54 |
| Mr | 2114.46 | 2643.08 |
| Dx,g cm-3 | 1.485 | 1.856 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.685 | 1.726 |
| F000 | 2080.0 | 2688.0 |
| F000’ | 2083.84 | |
| h,k,lmax | 20,20,21 | 20,20,21 |
| Nref | 16673 | 16672 |
| Tmin,Tmax | 0.634,0.696 | 0.653,0.713 |
| Tmin’ | 0.621 | |

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.000

R(reflections)= 0.0749( 9307) wR2(reflections)= 0.2528( 15597)

S = 1.004 Npar= 991

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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.

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**Alert level A**
CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as

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            calculated from the _atom_site* data lies outside
            the range 0.90 <> 1.10
           From the CIF: _cell_formula_units_Z                    2
           From the CIF: _chemical_formula_weight          2643.08
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01   42.00  504.46
           H         1.01   42.00   42.34
           N        14.01   28.00  392.20
           O        16.00   26.00  415.97
           Cl       35.45   10.00  354.53
           Cu       63.55    2.00  127.09
           La      138.91    2.00  277.81
           Calculated formula weight             2114.40
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low .......      0.936
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## Alert level C

```
RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.253
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.37 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT234_ALERT_4_C Large Hirshfeld Difference O4     --  C19     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O14    --  C40     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N22    --  C33     ..       0.18 Ang.
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        La1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        La2
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         Cu1
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         Cu2
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0140 Ang
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl4    ..  O8W     .       3.11 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl9    ..  O2W     .       3.09 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl9    ..  O4W     .       3.16 Ang.
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## Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C42 H122 Cl10 Cu2 La2 N28 O54
           Atom count from the _atom_site data:  C42 H42 Cl10 Cu2 La2 N28 O26
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C42 H122 Cl10 Cu2 La2 N28 O54
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         84.00     84.00    0.00
           H        244.00     84.00  160.00
           Cl        20.00     20.00    0.00
           Cu         4.00      4.00    0.00
           La         4.00      4.00    0.00
           N         56.00     56.00    0.00
           O        108.00     52.00   56.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ .............           ?
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PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.16
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....         ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....         ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....         ?
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       !
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          2
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C8      (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C9      (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C14     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C15     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C21     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C26     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C27     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C39     (Verify) ....         S
PLAT794_ALERT_5_G Note: Tentative Bond Valency for La1     (III)        3.21
PLAT794_ALERT_5_G Note: Tentative Bond Valency for La2     (III)        3.28
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed          !
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```
   2 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  16 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  30 ALERT level G = General information/check it is not something unexpected

  10 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
  22 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
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# Datablock: 02

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```
Bond precision:  C-C = 0.0087 A          Wavelength=0.71073

Cell:          a=17.2440(6)       b=17.3617(6)      c=18.1955(11)
               alpha=102.902(2)   beta=103.810(2)   gamma=110.459(1)
Temperature:   223 K
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| | Calculated | Reported |
|---|---|---|
| Volume | 4666.2(4) | 4666.2(4) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C42 H42 N28 Nd2 O26, 2(Cl4 Cu), 2(Cl) | C42 H66 Nd2 N28 O26, 2(Cu Cl4), 2Cl, 28(H2 O) |
| Sum formula | C42 H42 Cl10 Cu2 N28 Nd2 O26 | C42 H122 Cl10 Cu2 N28 Nd2 O54 |
| Mr | 2125.12 | 2653.74 |
| Dx,g cm-3 | 1.513 | 1.889 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.905 | 1.946 |
| F000 | 2092.0 | 2700.0 |
| F000’ | 2096.21 | |
| h,k,lmax | 20,20,21 | 20,20,21 |
| Nref | 16636 | 16427 |
| Tmin,Tmax | 0.552,0.591 | 0.584,0.622 |
| Tmin’ | 0.542 | |

Correction method= MULTI-SCAN

Data completeness= 0.987 Theta(max)= 25.100

R(reflections)= 0.0529( 13482) wR2(reflections)= 0.1756( 16427)

S = 1.110 Npar= 991

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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.

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**Alert level A**

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10

From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 2653.74
TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 42.00 | 504.46 |
| H | 1.01 | 42.00 | 42.34 |
| N | 14.01 | 28.00 | 392.20 |
| O | 16.00 | 26.00 | 415.97 |
| Cl | 35.45 | 10.00 | 354.53 |
| Nd | 144.24 | 2.00 | 288.48 |
| Cu | 63.55 | 2.00 | 127.09 |

Calculated formula weight 2125.07

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**Alert level C**

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.11 Perc.

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PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O4     --  C19     ..        5.2 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O12    --  C28     ..        5.7 su
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Nd1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Nd2
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         Cu1
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         Cu2
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0087 Ang
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl4    ..  O1W     .       3.13 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl9    ..  O8W     .       3.11 Ang.
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## Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C42 H122 Cl10 Cu2 N28 Nd2 O54
           Atom count from the _atom_site data:  C42 H42 Cl10 Cu2 N28 Nd2 O26
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C42 H122 Cl10 Cu2 N28 Nd2 O54
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         84.00     84.00    0.00
          H        244.00     84.00  160.00
          Cl        20.00     20.00    0.00
          Cu         4.00      4.00    0.00
          N         56.00     56.00    0.00
          Nd         4.00      4.00    0.00
          O        108.00     52.00   56.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ         ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ .............          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.11
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       5.45
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C8      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C9      (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C14     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C15     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C21     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C26     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C27     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C39     (Verify) ....          S
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

10 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
1 ALERT type 3 Indicator that the structure quality may be low
18 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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# Datablock: 03

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Bond precision: C-C = 0.0099 A Wavelength=0.71073

Cell: a=17.1376(9) b=17.4128(8) c=18.4104(9)
alpha=103.314(2) beta=103.349(2) gamma=110.196(2)
Temperature: 223 K

| | Calculated | Reported |
|---|---|---|
| Volume | 4718.9(4) | 4718.9(4) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C42 H42 La2 N28 O26, Cl4 Co, 4(Cl) | C42 H66 La2 N28 O26, Co Cl4, 4Cl, 31(H2 O) |
| Sum formula | C42 H42 Cl8 Co La2 N28 O26 | C42 H128 Cl8 Co La2 N28 O57 |
| Mr | 1975.39 | 2558.07 |
| Dx,g cm-3 | 1.390 | 1.800 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.362 | 1.407 |
| F000 | 1950.0 | 2618.0 |
| F000’ | 1952.67 | |
| h,k,lmax | 20,20,21 | 20,20,21 |
| Nref | 16812 | 16635 |
| Tmin,Tmax | 0.653,0.703 | 0.669,0.720 |
| Tmin’ | 0.640 | |

Correction method= MULTI-SCAN

Data completeness= 0.989 Theta(max)= 25.100

R(reflections)= 0.0567( 11474) wR2(reflections)= 0.1782( 16635)

S = 0.923 Npar= 964

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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.

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## Alert level A

```
CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
           calculated from the _atom_site* data lies outside
           the range 0.90 <> 1.10
          From the CIF: _cell_formula_units_Z                    2
          From the CIF: _chemical_formula_weight          2558.07
          TEST: Calculate formula weight from _atom_site_*
          atom     mass    num     sum
          C        12.01   42.00  504.46
          H         1.01   42.00   42.34
          N        14.01   28.00  392.20
          O        16.00   26.00  415.97
          Cl       35.45    8.00  283.62
          Co       58.93    1.00   58.93
          La      138.91    2.00  277.81
          Calculated formula weight             1975.34
```

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## Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       3.19 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N21    --  C31     ..        6.0 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N22    --  C35     ..        5.6 su
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        La1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        La2
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0099 Ang
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl2    ..  O1W     .       3.15 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl3    ..  O8W     .       3.14 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl5    ..  O8W     .       3.08 Ang.
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## Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C42 H128 Cl8 Co1 La2 N28 O57
           Atom count from the _atom_site data:  C42 H42 Cl8 Co1 La2 N28 O26
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C42 H128 Cl8 Co La2 N28 O57
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         84.00     84.00    0.00
          H        256.00     84.00  172.00
          Cl        16.00     16.00    0.00
          Co         2.00      2.00    0.00
          La         4.00      4.00    0.00
          N         56.00     56.00    0.00
          O        114.00     52.00   62.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.11
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........    0.00200 Deg.
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
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PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       !
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C8      (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C9      (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C14     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C15     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C21     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C26     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C27     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C39     (Verify) ....         S
PLAT794_ALERT_5_G Note: Tentative Bond Valency for La1     (III)        3.26
PLAT794_ALERT_5_G Note: Tentative Bond Valency for La2     (III)        3.29
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed          !
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```
   1 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  30 ALERT level G = General information/check it is not something unexpected

  11 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
   1 ALERT type 3 Indicator that the structure quality may be low
  16 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
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# Datablock: 04

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```
Bond precision:  C-C = 0.0086 A          Wavelength=0.71073

Cell:          a=17.0773(11)      b=17.3435(11)     c=18.243(2)
               alpha=103.410(3)   beta=103.249(3)   gamma=110.144(2)
Temperature:   223 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 4643.3(7) | 4643.2(7) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C42 H42 Ce2 N28 O26, Cl4 Co, 4(Cl) | C42 H66 Ce2 N28 O26, Co Cl4, 4Cl, 26(H2 O) |
| Sum formula | C42 H42 Ce2 Cl8 Co N28 O26 | C42 H118 Ce2 Cl8 Co N28 O52 |
| Mr | 1977.81 | 2470.41 |
| Dx,g cm-3 | 1.415 | 1.767 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.445 | 1.483 |
| F000 | 1954.0 | 2522.0 |
| F000’ | 1956.82 | |
| h,k,lmax | 20,20,21 | 20,20,21 |
| Nref | 16726 | 16543 |
| Tmin,Tmax | 0.610,0.650 | 0.632,0.673 |
| Tmin’ | 0.598 | |

Correction method= MULTI-SCAN

Data completeness= 0.989 Theta(max)= 25.200

R(reflections)= 0.0499( 12136) wR2(reflections)= 0.1568( 16543)

S = 1.027 Npar= 964

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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.

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**Alert level A**

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10

From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 2470.41
TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 42.00 | 504.46 |
| H | 1.01 | 42.00 | 42.34 |
| N | 14.01 | 28.00 | 392.20 |
| O | 16.00 | 26.00 | 415.97 |
| Cl | 35.45 | 8.00 | 283.62 |
| Ce | 140.12 | 2.00 | 280.24 |
| Co | 58.93 | 1.00 | 58.93 |

Calculated formula weight 1977.76

---

**Alert level C**

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.59 Perc.

```
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Ce1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Ce2
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0086 Ang
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl2    ..  O8W     .       3.13 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl3    ..  O1W     .       3.15 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl5    ..  O8W     .       3.12 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O6W     .       3.01 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O10W    .       3.04 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl8    ..  O1W     .       3.16 Ang.
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## Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C42 H118 Ce2 Cl8 Co1 N28 O52
           Atom count from the _atom_site data:  C42 H42 Ce2 Cl8 Co1 N28 O26
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C42 H118 Ce2 Cl8 Co N28 O52
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         84.00     84.00    0.00
          H        236.00     84.00  152.00
          Ce         4.00      4.00    0.00
          Cl        16.00     16.00    0.00
          Co         2.00      2.00    0.00
          N         56.00     56.00    0.00
          O        104.00     52.00   52.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ         ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ .............          ?
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....         ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....         ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....         ?
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3
            Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4
            Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6
            Cl
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C8      (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C9      (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C14     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C15     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C21     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C26     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C27     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C39     (Verify) ....         R
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

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

10 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
1 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

## Datablock: 05

Bond precision: C-C = 0.0129 A Wavelength=0.71073

Cell: a=17.0566(17) b=17.1421(17) c=20.041(3)
alpha=97.415(5) beta=112.647(5) gamma=111.089(4)
Temperature: 323 K

| | Calculated | Reported |
|---|---|---|
| Volume | 4795.8(10) | 4795.8(10) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C42 H42 Eu2 N28 O24, Cl4 Cu, 4(Cl0.50), 0.5(Cl) | C42 H62 Eu2 N28 O24, Cu Cl4, 4Cl, 39(H2 O) |
| Sum formula | C42 H42 Cl8 Cu Eu2 N28 O24 | C42 H140 Cl8 Cu Eu2 N28 O63 |
| Mr | 1974.13 | 2696.88 |
| Dx,g cm-3 | 1.367 | 1.868 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.803 | 1.859 |
| F000 | 1946.0 | 2766.0 |
| F000’ | 1949.09 | |
| h,k,lmax | 20,20,23 | 20,20,23 |
| Nref | 17091 | 16826 |
| Tmin,Tmax | 0.691,0.757 | 0.674,0.768 |
| Tmin’ | 0.646 | |

Correction method= MULTI-SCAN

Data completeness= 0.984 Theta(max)= 25.100

R(reflections)= 0.0822( 13121) wR2(reflections)= 0.2455( 16826)

S = 1.125 Npar= 932

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

---

## Alert level A

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 2696.88
TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 42.00 | 504.46 |
| H | 1.01 | 42.00 | 42.34 |
| N | 14.01 | 28.00 | 392.20 |
| O | 16.00 | 24.00 | 383.98 |
| Cl | 35.45 | 8.00 | 283.62 |
| Eu | 151.96 | 2.00 | 303.92 |
| Cu | 63.55 | 1.00 | 63.55 |

Calculated formula weight 1974.06

---

## Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.99 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.63
PLAT213_ALERT_2_C Atom C12 has ADP max/min Ratio ..... 3.3 oblat
PLAT230_ALERT_2_C Hirshfeld Test Diff for O1 -- C1 .. 5.3 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for N20 -- C30 .. 7.0 su
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Eu1
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Eu2
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Cu1
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0129 Ang
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl5 .. O1W . 3.11 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl6 .. O10W . 2.98 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl7 .. O5W . 3.11 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1
C42 H42 Eu2 N28 O24

---

## Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C42 H140 Cl8 Cu1 Eu2 N28 O63
Atom count from the _atom_site data: C42 H42 Cl8 Cu1 Eu2 N28 O24
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C42 H140 Cl8 Cu Eu2 N28 O63
TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|---|---|---|---|
| C | 84.00 | 84.00 | 0.00 |
| H | 280.00 | 84.00 | 196.00 |
| Cl | 16.00 | 16.00 | 0.00 |
| Cu | 2.00 | 2.00 | 0.00 |
| Eu | 4.00 | 4.00 | 0.00 |
| N | 56.00 | 56.00 | 0.00 |

```
          O        126.00     48.00   78.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         4
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....         2
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .         1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF         ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ         ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ .............          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.      0.16
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....         ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....         ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....         ?
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..................        11 Perc.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  Cl1    ..  Cl9     .      3.18 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  Cl3    ..  Cl9     .      3.33 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  Cl6    ..  Cl6     .      3.27 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2
             Cl4 Cu
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         3
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         4
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         5
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         6
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         7
             Cl0.50
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C15     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C39     (Verify) ....         S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        14
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed          !
```

---

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

10 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
2 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

---

# Datablock: 06

---

Bond precision:  C-C = 0.0167 A  Wavelength=0.71073

| | | | |
|---|---|---|---|
| Cell: | a=17.045(4) | b=17.080(4) | c=19.983(7) |
| | alpha=112.825(11) | beta=96.852(11) | gamma=111.574(8) |
| Temperature: | 223 K | | |

| | Calculated | Reported |
|---|---|---|
| Volume | 4748(2) | 4748(2) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C42 H42 Gd2 N28 O24, Cl4 Cu, 2.75(Cl0.50), 1.5(Cl) | C42 H62 Gd2 N28 O24, Cu Cl4, 4Cl, 43(H2 O) |
| Sum formula | C42 H42 Cl8 Cu Gd2 N28 O24 | C42 H148 Cl8 Cu Gd2 N28 O67 |
| Mr | 1984.69 | 2779.52 |
| Dx,g cm-3 | 1.388 | 1.944 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.897 | 1.959 |
| F000 | 1950.0 | 2850.0 |
| F000’ | 1953.05 | |
| h,k,lmax | 20,20,23 | 20,20,23 |
| Nref | 17105 | 16910 |
| Tmin,Tmax | 0.662,0.731 | 0.673,0.745 |
| Tmin’ | 0.643 | |

Correction method= MULTI-SCAN

Data completeness= 0.989 Theta(max)= 25.200

R(reflections)= 0.1009( 12439) wR2(reflections)= 0.3035( 16910)

S = 1.155 Npar= 911

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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 A**

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10

From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 2779.52
TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 42.00 | 504.46 |
| H | 1.01 | 42.00 | 42.34 |
| N | 14.01 | 28.00 | 392.20 |
| O | 16.00 | 24.00 | 383.98 |
| Cl | 35.45 | 8.00 | 283.62 |
| Gd | 157.25 | 2.00 | 314.50 |
| Cu | 63.55 | 1.00 | 63.55 |

Calculated formula weight 1984.64

## Alert level C

```
RFACG01_ALERT_3_C  The value of the R factor is > 0.10
           R factor given   0.101
RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.303
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       3.15 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT084_ALERT_2_C High wR2 Value ..............................        0.30
PLAT213_ALERT_2_C Atom O9             has ADP max/min Ratio .....        3.8 oblat
PLAT213_ALERT_2_C Atom O10W           has ADP max/min Ratio .....        3.1 prola
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O9     --  C1      ..        7.0 su
PLAT234_ALERT_4_C Large Hirshfeld Difference O11    --  C31     ..       0.16 Ang.
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Gd1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Gd2
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         Cu1
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0167 Ang
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl4    ..  O6W     .       3.16 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl5    ..  O6W     .       3.08 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O9W     .       3.06 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O9W     .       3.06 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1
             C42 H42 Gd2 N28 O24
```

## Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C42 H148 Cl8 Cu1 Gd2 N28 O67
           Atom count from the _atom_site data:  C42 H42 Cl8 Cu1 Gd2 N28 O24
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C42 H148 Cl8 Cu Gd2 N28 O67
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         84.00     84.00    0.00
          H        296.00     84.00  212.00
          Cl        16.00     16.00    0.00
          Cu         2.00      2.00    0.00
          Gd         4.00      4.00    0.00
          N         56.00     56.00    0.00
          O        134.00     48.00   86.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....          8
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.20
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................         22 Perc.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2
             Cl4 Cu
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7
```

```
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          9
             Cl
PLAT793_ALERT_4_G The Model has Chirality at C8      (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C9      (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C14     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C15     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C21     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....         R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        50
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed          !
```

---

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

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

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# Datablock: 07

---

Bond precision:  C-C = 0.0164 A  Wavelength=0.71073

| | | | |
|---|---|---|---|
| Cell: | a=16.979(3) | b=17.140(3) | c=20.168(3) |
| | alpha=97.223(7) | beta=113.441(6) | gamma=111.556(6) |
| Temperature: | 223 K | | |

| | Calculated | Reported |
|---|---|---|
| Volume | 4747.2(15) | 4747.3(14) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C42 H42 Dy2 N28 O24, Cl4 Co, 4.8(Cl0.20) | C42 H62 Dy2 N28 O24, Co Cl4, 4Cl, 39(H2 O) |
| Sum formula | C42 H42 Cl8 Co Dy2 N28 O24 | C42 H140 Cl8 Co Dy2 N28 O63 |
| Mr | 1990.57 | 2713.35 |
| Dx,g cm-3 | 1.393 | 1.898 |
| Z | 2 | 2 |
| Mu (mm-1) | 2.025 | 2.081 |
| F000 | 1954.0 | 2774.0 |
| F000’ | 1957.03 | |
| h,k,lmax | 20,20,24 | 20,20,24 |
| Nref | 16914 | 16666 |
| Tmin,Tmax | 0.694,0.747 | 0.669,0.759 |
| Tmin’ | 0.640 | |

Correction method= MULTI-SCAN

Data completeness= 0.985 Theta(max)= 25.100

R(reflections)= 0.0886( 12014) wR2(reflections)= 0.2524( 16666)

S = 1.022 Npar= 920

---

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

---

**Alert level A**

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10

From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 2713.35
TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 42.00 | 504.46 |
| H | 1.01 | 42.00 | 42.34 |
| N | 14.01 | 28.00 | 392.20 |
| O | 16.00 | 24.00 | 383.98 |
| Cl | 35.45 | 8.00 | 283.62 |
| Dy | 162.50 | 2.00 | 325.00 |
| Co | 58.93 | 1.00 | 58.93 |

Calculated formula weight 1990.53

PLAT434_ALERT_2_A Short Inter HL..HL Contact Cl8 .. Cl8 . 2.40 Ang.

---

**Alert level C**

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25

```
           Weighted R factor given   0.252
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.68 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT213_ALERT_2_C Atom O5              has ADP max/min Ratio .....        3.1 oblat
PLAT213_ALERT_2_C Atom O9              has ADP max/min Ratio .....        3.1 oblat
PLAT213_ALERT_2_C Atom C34             has ADP max/min Ratio .....        3.1 oblat
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Dy1    --  O2      ..        5.7 su
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Dy1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Dy2
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0164 Ang
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl5    ..  O7W     .       3.14 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O10W    .       3.04 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O10W    .       3.04 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl7    ..  O10W    .       3.16 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl8    ..  O5W     .       2.99 Ang.
```

---

## Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C42 H140 Cl8 Co1 Dy2 N28 O63
           Atom count from the _atom_site data:  C42 H42 Cl8 Co1 Dy2 N28 O24
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C42 H140 Cl8 Co Dy2 N28 O63
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         84.00     84.00    0.00
          H        280.00     84.00  196.00
          Cl        16.00     16.00    0.00
          Co         2.00      2.00    0.00
          Dy         4.00      4.00    0.00
          N         56.00     56.00    0.00
          O        126.00     48.00   78.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          5
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....          6
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.17
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................          5 Perc.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8
             Cl0.20
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....          R
```

```
PLAT793_ALERT_4_G The Model has Chirality at C15     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C39     (Verify) ....          S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         39
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

---

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

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 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
  15 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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# Datablock: 08

---

Bond precision:  C-C = 0.0257 A  Wavelength=0.71073

Cell:  a=17.085(4)  b=17.228(4)  c=20.219(6)
       alpha=97.325(10)  beta=113.561(7)  gamma=111.615(7)
Temperature:  223 K

| | Calculated | Reported |
|---|---|---|
| Volume | 4801(2) | 4801(2) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C42 H42 Er2 N28 O24, Cl4 Co, 2.5(Cl0.50), Cl0.50, Cl0.50, 1.5(C | C42 H62 Er2 N28 O24, Co Cl4, 4Cl, 47(H2 O) |
| Sum formula | C42 H42 Cl8 Co Er2 N28 O24 | C42 H156 Cl8 Co Er2 N28 O71 |
| Mr | 2000.09 | 2867.00 |
| Dx,g cm-3 | 1.384 | 1.983 |
| Z | 2 | 2 |
| Mu (mm-1) | 2.194 | 2.261 |
| F000 | 1962.0 | 2942.0 |
| F000’ | 1964.77 | |
| h,k,lmax | 20,20,24 | 20,20,24 |
| Nref | 16913 | 16592 |
| Tmin,Tmax | 0.672,0.745 | 0.673,0.758 |
| Tmin’ | 0.644 | |

Correction method= MULTI-SCAN

Data completeness= 0.981 Theta(max)= 25.000

R(reflections)= 0.1200( 10343) wR2(reflections)= 0.3393( 16592)

S = 1.114 Npar= 857

---

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

---

## Alert level A

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_weight 2867.00
TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 42.00 | 504.46 |
| H | 1.01 | 42.00 | 42.34 |
| N | 14.01 | 28.00 | 392.20 |
| O | 16.00 | 24.00 | 383.98 |
| Cl | 35.45 | 8.00 | 283.62 |
| Er | 167.26 | 2.00 | 334.52 |
| Co | 58.93 | 1.00 | 58.93 |

Calculated formula weight 2000.05

PLAT410_ALERT_2_A Short Intra H...H Contact H27 .. H30B .. 1.76 Ang.

---

## Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for N23 -- C30 .. 7.2 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for N25 -- C35 .. 7.4 su
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0257 Ang

---

## Alert level C

RFACG01_ALERT_3_C The value of the R factor is > 0.10
R factor given 0.120
RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.339
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.95 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT082_ALERT_2_C High R1 Value ..... 0.12
PLAT084_ALERT_2_C High wR2 Value ..... 0.34
PLAT213_ALERT_2_C Atom O9 has ADP max/min Ratio ..... 3.3 oblat
PLAT213_ALERT_2_C Atom O14 has ADP max/min Ratio ..... 3.1 prola
PLAT213_ALERT_2_C Atom C25 has ADP max/min Ratio ..... 3.2 prola
PLAT230_ALERT_2_C Hirshfeld Test Diff for N1 -- C1 .. 5.4 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for N1 -- C2 .. 6.6 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for N5 -- C5 .. 6.0 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for N5 -- C7 .. 7.0 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for N18 -- C27 .. 6.6 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for N20 -- C27 .. 6.7 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for N20 -- C28 .. 6.0 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for N20 -- C30 .. 5.1 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Er2 -- O6W .. 5.5 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Er2 -- O8W .. 9.0 su

```
PLAT234_ALERT_4_C Large Hirshfeld Difference N13    --  C20     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N14    --  C23     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N26    --  C37     ..       0.18 Ang.
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Er2
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C16
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C22
PLAT410_ALERT_2_C Short Intra H...H Contact  H29A   ..  H30B    ..       1.93 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl3    ..  O4W     .       3.16 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl5    ..  O4W     .       3.16 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O5W     .       3.05 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O5W     .       3.05 Ang.
```

---

## Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C42 H156 Cl8 Co1 Er2 N28 O71
           Atom count from the _atom_site data:  C42 H42 Cl8 Co1 Er2 N28 O24
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C42 H156 Cl8 Co Er2 N28 O71
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         84.00     84.00    0.00
           H        312.00     84.00  228.00
           Cl        16.00     16.00    0.00
           Co         2.00      2.00    0.00
           Er         4.00      4.00    0.00
           N         56.00     56.00    0.00
           O        142.00     48.00   94.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          8
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....         10
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.20
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................         26 Perc.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3
            Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8
            Cl
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C15     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C39     (Verify) ....          S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         65
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

---

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

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

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

---

# Datablock: 09

---

Bond precision: C-C = 0.0054 A Wavelength=0.71073

Cell: a=17.0739(11) b=27.7218(18) c=20.6280(14)
alpha=90 beta=97.558(2) gamma=90
Temperature: 223 K

| | Calculated | Reported |
|---|---|---|
| Volume | 9678.8(11) | 9678.8(11) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C42 H42 Eu2 N28 O24, Cl4 Co, 4(Cl0.50), 0.5(Cl) | C42 H62 Eu2 N28 O24, Co Cl4, 4Cl, 34(H2 O) |
| Sum formula | C42 H42 Cl8 Co Eu2 N28 O24 | C42 H130 Cl8 Co Eu2 N28 O58 |
| Mr | 1969.51 | 2602.19 |
| Dx,g cm-3 | 1.352 | 1.786 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.739 | 1.787 |
| F000 | 3884.0 | 5324.0 |
| F000’ | 3890.30 | |
| h,k,lmax | 20,33,24 | 20,33,24 |
| Nref | 17253 | 17146 |
| Tmin,Tmax | 0.580,0.617 | 0.607,0.644 |
| Tmin’ | 0.569 | |

Correction method= MULTI-SCAN

Data completeness= 0.994 Theta(max)= 25.100

R(reflections)= 0.0433( 12777) wR2(reflections)= 0.1243( 17146)

S = 1.016 Npar= 949

---

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

---

## Alert level A

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_weight 2602.19
TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 42.00 | 504.46 |
| H | 1.01 | 42.00 | 42.34 |
| N | 14.01 | 28.00 | 392.20 |
| O | 16.00 | 24.00 | 383.98 |
| Cl | 35.45 | 8.00 | 283.62 |
| Eu | 151.96 | 2.00 | 303.92 |
| Co | 58.93 | 1.00 | 58.93 |

Calculated formula weight 1969.45

---

## Alert level B

PLAT213_ALERT_2_B Atom C5 has ADP max/min Ratio ..... 4.2 prola
PLAT230_ALERT_2_B Hirshfeld Test Diff for N5 -- C7 .. 10.0 su

---

## Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.70 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.61
PLAT213_ALERT_2_C Atom N5 has ADP max/min Ratio ..... 3.6 prola
PLAT230_ALERT_2_C Hirshfeld Test Diff for N5 -- C5 .. 7.0 su
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Eu1
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Eu2
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.3
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl4 .. O6W . 3.16 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl5 .. O6W . 3.12 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl6 .. O9W . 3.03 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl6 .. O5W . 3.14 Ang.

---

## Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C42 H130 Cl8 Co1 Eu2 N28 O58
Atom count from the _atom_site data: C42 H42 Cl8 Co1 Eu2 N28 O24
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C42 H130 Cl8 Co Eu2 N28 O58
TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|---|---|---|---|
| C | 168.00 | 168.00 | 0.00 |
| H | 520.00 | 168.00 | 352.00 |
| Cl | 32.00 | 32.00 | 0.00 |
| Co | 4.00 | 4.00 | 0.00 |

```
           Eu         8.00      8.00    0.00
           N        112.00    112.00    0.00
           O        232.00     96.00  136.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ .............           ?
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..................          11 Perc.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  Cl6    ..  Cl8     .       2.89 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  Cl7    ..  Cl9     .       2.96 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2
           Cl4 Co
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5
           Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6
           Cl
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C39     (Verify) ....          S
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

---

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

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

---

# Datablock: 10

---

```
Bond precision:  C-C = 0.0050 A          Wavelength=0.71073

Cell:            a=17.0997(11)    b=27.7353(19)     c=20.6163(13)
                 alpha=90         beta=97.468(2)    gamma=90
Temperature:     223 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 9694.7(11) | 9694.7(11) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C42 H42 Gd2 N28 O24, Cl4 Co, 4(Cl0.50), 0.5(Cl) | C42 H62 Gd2 N28 O24, Co Cl4, 4Cl, 34(H2 O) |
| Sum formula | C42 H42 Cl8 Co Gd2 N28 O24 | C42 H130 Cl8 Co Gd2 N28 O58 |
| Mr | 1980.07 | 2612.77 |
| Dx,g cm-3 | 1.357 | 1.790 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.810 | 1.858 |
| F000 | 3892.0 | 5332.0 |
| F000’ | 3898.21 | |
| h,k,lmax | 20,33,24 | 20,33,24 |
| Nref | 17282 | 17169 |
| Tmin,Tmax | 0.589,0.640 | 0.615,0.664 |
| Tmin’ | 0.578 | |

Correction method= MULTI-SCAN

Data completeness= 0.993 Theta(max)= 25.100

R(reflections)= 0.0404( 12787) wR2(reflections)= 0.1217( 17169)

S = 0.951 Npar= 955

---

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

---

**Alert level A**

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10

From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_weight 2612.77
TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 42.00 | 504.46 |
| H | 1.01 | 42.00 | 42.34 |
| N | 14.01 | 28.00 | 392.20 |
| O | 16.00 | 24.00 | 383.98 |
| Cl | 35.45 | 8.00 | 283.62 |
| Gd | 157.25 | 2.00 | 314.50 |
| Co | 58.93 | 1.00 | 58.93 |

Calculated formula weight 1980.03

PLAT213_ALERT_2_A Atom N22 has ADP max/min Ratio ..... 5.3 prola

---

**Alert level B**

PLAT213_ALERT_2_B Atom C6 has ADP max/min Ratio ..... 4.4 prola

## Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.58 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.72
PLAT213_ALERT_2_C Atom C21             has ADP max/min Ratio .....        3.5 oblat
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N22    --  C22     ..        5.7 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N22    --  C41     ..        7.0 su
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Gd1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Gd2
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl4    ..  O6W     .       3.16 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl5    ..  O6W     .       3.14 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O10W    .       3.04 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O5W     .       3.14 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl7    ..  O5W     .       3.15 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1
             C42 H42 Gd2 N28 O24
```

## Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C42 H130 Cl8 Co1 Gd2 N28 O58
            Atom count from the _atom_site data:  C42 H42 Cl8 Co1 Gd2 N28 O24
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
             symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C42 H130 Cl8 Co Gd2 N28 O58
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        168.00    168.00    0.00
           H        520.00    168.00  352.00
           Cl        32.00     32.00    0.00
           Co         4.00      4.00    0.00
           Gd         8.00      8.00    0.00
           N        112.00    112.00    0.00
           O        232.00     96.00  136.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................         11 Perc.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  Cl2    ..  Cl9     .       3.31 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  Cl6    ..  Cl8     .       2.89 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7
             Cl0.50
PLAT793_ALERT_4_G The Model has Chirality at C23     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C24     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C25     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C26     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C27     (Verify) ....          R
```

PLAT793_ALERT_4_G The Model has Chirality at C28 (Verify) .... S
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed !

---

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

10 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
0 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

---

# Datablock: 11

---

Bond precision: C-C = 0.0140 A Wavelength=0.71073

Cell: a=17.084(2) b=27.493(4) c=20.428(3)
alpha=90 beta=99.261(4) gamma=90
Temperature: 223 K

| | Calculated | Reported |
|---|---|---|
| Volume | 9470(2) | 9470(2) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C42 H42 Dy2 N28 O24, Cl4 Cu, 4(Cl0.50), 0.5(Cl) | C42 H62 Dy2 N28 O24, Cu Cl4, 4Cl, 46(H2 O) |
| Sum formula | C42 H42 Cl8 Cu Dy2 N28 O24 | C42 H154 Cl8 Cu Dy2 N28 O70 |
| Mr | 1995.19 | 2844.07 |
| Dx,g cm-3 | 1.399 | 1.995 |
| Z | 4 | 4 |
| Mu (mm-1) | 2.080 | 2.146 |
| F000 | 3916.0 | 5836.0 |
| F000’ | 3921.95 | |
| h,k,lmax | 21,33,25 | 20,33,25 |
| Nref | 18611 | 18333 |
| Tmin,Tmax | 0.723,0.790 | 0.712,0.798 |
| Tmin’ | 0.687 | |

Correction method= MULTI-SCAN

Data completeness= 0.985 Theta(max)= 26.000

R(reflections)= 0.1016( 10670) wR2(reflections)= 0.2797( 18333)

S = 1.023 Npar= 955

---

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

---

## Alert level A

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_weight 2844.07
TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|---|---|---|---|
| C | 12.01 | 42.00 | 504.46 |
| H | 1.01 | 42.00 | 42.34 |
| N | 14.01 | 28.00 | 392.20 |
| O | 16.00 | 24.00 | 383.98 |
| Cl | 35.45 | 8.00 | 283.62 |
| Dy | 162.50 | 2.00 | 325.00 |
| Cu | 63.55 | 1.00 | 63.55 |

Calculated formula weight 1995.14

PLAT213_ALERT_2_A Atom Dy1 has ADP max/min Ratio ..... 7.7 oblat
PLAT213_ALERT_2_A Atom Dy2 has ADP max/min Ratio ..... 8.0 oblat

---

## Alert level B

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Dy1 -- O1 .. 12.1 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Dy1 -- O4W .. 11.0 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Dy2 -- O11 .. 14.5 su

---

## Alert level C

RFACG01_ALERT_3_C The value of the R factor is > 0.10
R factor given 0.102
RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.280
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.125
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 ..... 0.125
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 3.08 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT084_ALERT_2_C High wR2 Value ..... 0.28
PLAT213_ALERT_2_C Atom O2W has ADP max/min Ratio ..... 3.2 oblat
PLAT234_ALERT_4_C Large Hirshfeld Difference O9 -- C10 .. 0.16 Ang.
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Dy1
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Dy2
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Cu1
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0140 Ang
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl4 .. O8W . 3.15 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl5 .. O8W . 3.09 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl6 .. O4W . 3.01 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl6 .. O3W . 3.16 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl7 .. O4W . 3.06 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1
C42 H42 Dy2 N28 O24

---

## Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C42 H154 Cl8 Cu1 Dy2 N28 O70
           Atom count from the _atom_site data:  C42 H42 Cl8 Cu1 Dy2 N28 O24
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C42 H154 Cl8 Cu Dy2 N28 O70
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        168.00    168.00    0.00
           H        616.00    168.00  448.00
           Cl        32.00     32.00    0.00
           Cu         4.00      4.00    0.00
           Dy         8.00      8.00    0.00
           N        112.00    112.00    0.00
           O        280.00     96.00  184.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....         64
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT044_ALERT_1_G Calculated and Reported Dx Differ .............           ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.17
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1    --  O8_b    ..        6.2 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1    --  O14_b   ..        6.1 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy2    --  O6W     ..        5.5 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy2    --  O5_a    ..        7.5 su
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..................         11 Perc.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  Cl6    ..  Cl8     .       3.18 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2
           Cl4 Cu
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3
           Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5
           Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7
           Cl0.50
PLAT793_ALERT_4_G The Model has Chirality at C9      (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C14     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C26     (Verify) ....         S
PLAT793_ALERT_4_G The Model has Chirality at C27     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C33     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C38     (Verify) ....         R
PLAT793_ALERT_4_G The Model has Chirality at C39     (Verify) ....         S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        384
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

---

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

```
 10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 23 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
 18 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

---

## Datablock: 12

---

Bond precision: C-C = 0.0286 A Wavelength=0.71073

Cell: a=17.1162(13) b=27.675(2) c=20.4248(16)
alpha=90 beta=97.399(2) gamma=90
Temperature: 223 K

| | Calculated | Reported |
|---|---|---|
| Volume | 9594.5(13) | 9594.4(13) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C42 H42 Ho2 N28 O24, Cl4 Co, 3(Cl0.50), Cl0.50, 1.5(Cl0.50) | C42 H62 Ho2 N28 O24, Co Cl4, 4Cl, 55(H2 O) |
| Sum formula | C42 H42 Cl8 Co Ho2 N28 O24 | C42 H172 Cl8 Co Ho2 N28 O79 |
| Mr | 1995.43 | 3006.47 |
| Dx,g cm-3 | 1.381 | 2.081 |
| Z | 4 | 4 |
| Mu (mm-1) | 2.096 | 2.174 |
| F000 | 3916.0 | 6196.0 |
| F000’ | 3921.83 | |
| h,k,lmax | 21,34,25 | 21,33,25 |
| Nref | 18841 | 18676 |
| Tmin,Tmax | 0.648,0.722 | 0.658,0.736 |
| Tmin’ | 0.627 | |

Correction method= MULTI-SCAN

Data completeness= 0.991 Theta(max)= 26.000

R(reflections)= 0.0890( 10691) wR2(reflections)= 0.2583( 18676)

S = 1.030 Npar= 952

---

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

---

**Alert level A**

```
CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as
            calculated from the _atom_site* data lies outside
            the range 0.90 <> 1.10
           From the CIF: _cell_formula_units_Z                    4
           From the CIF: _chemical_formula_weight          3006.47
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01   42.00  504.46
           H         1.01   42.00   42.34
           N        14.01   28.00  392.20
           O        16.00   24.00  383.98
           Cl       35.45    8.00  283.62
           Ho      164.93    2.00  329.86
           Co       58.93    1.00   58.93
           Calculated formula weight             1995.39
```

---

## Alert level B

```
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ..............     0.0286 Ang
```

---

## Alert level C

```
RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
            Weighted R factor given   0.258
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       3.59 Perc.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT084_ALERT_2_C High wR2 Value ..............................       0.26
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.19
PLAT234_ALERT_4_C Large Hirshfeld Difference N16    --  C18     ..       0.17 Ang.
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Ho1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Ho2
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl6    ..  O7W     .       3.12 Ang.
PLAT431_ALERT_2_C Short Inter HL..A  Contact  Cl7    ..  O10W    .       2.99 Ang.
```

---

## Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C42 H172 Cl8 Co1 Ho2 N28 O79
            Atom count from the _atom_site data:  C42 H42 Cl8 Co1 Ho2 N28 O24
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C42 H172 Cl8 Co Ho2 N28 O79
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         168.00    168.00    0.00
           H         688.00    168.00  520.00
           Cl         32.00     32.00    0.00
           Co          4.00      4.00    0.00
           Ho          8.00      8.00    0.00
           N         112.00    112.00    0.00
           O         316.00     96.00  220.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....          6
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
```

```
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.15
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....          ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................         22 Perc.
PLAT434_ALERT_2_G Short Inter HL..HL Contact  Cl7    ..  Cl9     .       2.67 Ang.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4
             Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6
             Cl0.50
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7
             Cl
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C4      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C9      (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C10     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C22     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C28     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C40     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C44     (Verify) ....          R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         40
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

---

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

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  12 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
  15 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

---

# checkCIF publication errors

---

### Alert level A

```
PUBL004_ALERT_1_A  The contact author’s name and address are missing,
            _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
            _publ_contact_author_phone are all missing.
            At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. ’Acta Crystallographica Section C’
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

---

### Alert level G

```
PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
            missing. This is required for a full paper submission (but is
            optional for an electronic paper).
```

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

---

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   2 ALERT level G = General alerts. Data that may be required is missing
```

---

**Publication of your CIF**

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
```

;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_CHEMW03_01
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT029_01
;
PROBLEM: _diffrn_measured_fraction_theta_full Low .......      0.936
RESPONSE: ...
;
_vrf_CHEMW03_02
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_CHEMW03_03
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_CHEMW03_04
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_CHEMW03_05
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_CHEMW03_06
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_CHEMW03_07
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT434_07
;
PROBLEM: Short Inter HL..HL Contact  Cl8    ..  Cl8     .       2.40 Ang.
RESPONSE: ...
;
_vrf_CHEMW03_08
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT410_08

```
;
PROBLEM: Short Intra H...H Contact  H27    ..  H30B    ..       1.76 Ang.
RESPONSE: ...
;
_vrf_CHEMW03_09
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_CHEMW03_10
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT213_10
;
PROBLEM: Atom N22             has ADP max/min Ratio .....        5.3 prola
RESPONSE: ...
;
_vrf_CHEMW03_11
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT213_11
;
PROBLEM: Atom Dy1             has ADP max/min Ratio .....        7.7 oblat
RESPONSE: ...
;
_vrf_CHEMW03_12
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
# end Validation Reply Form
```

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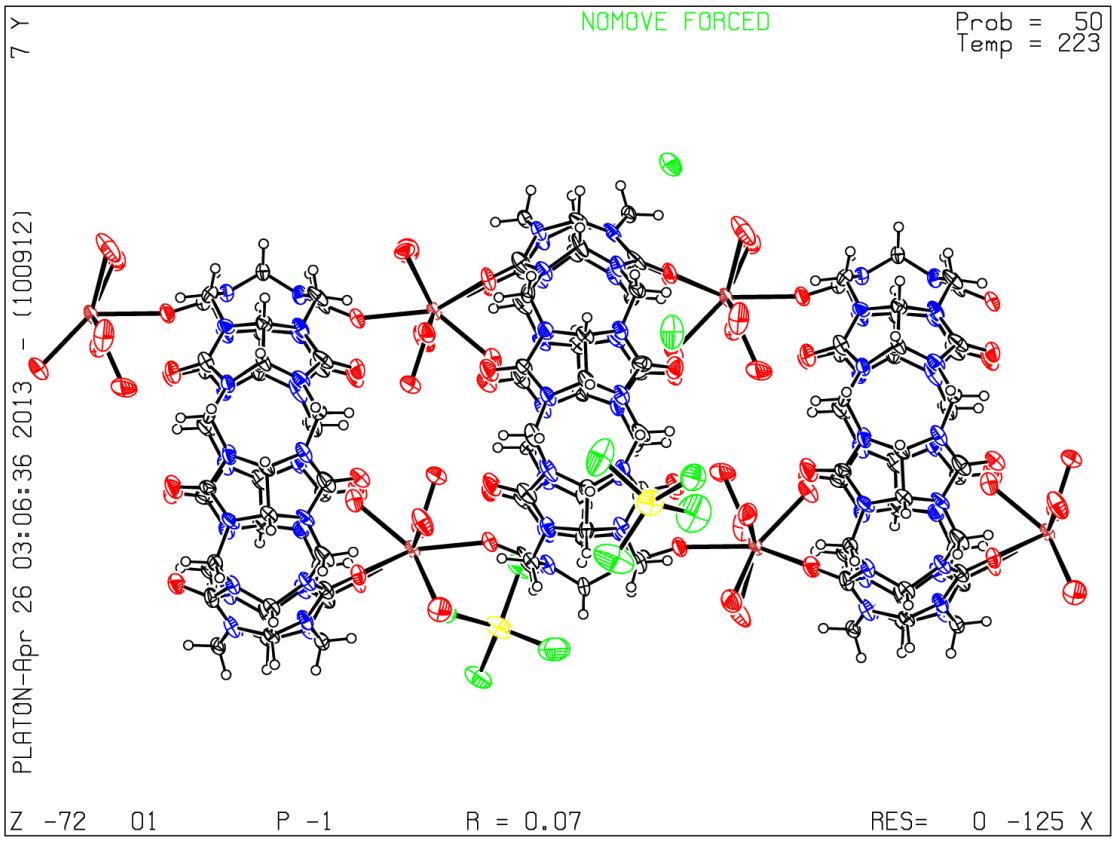
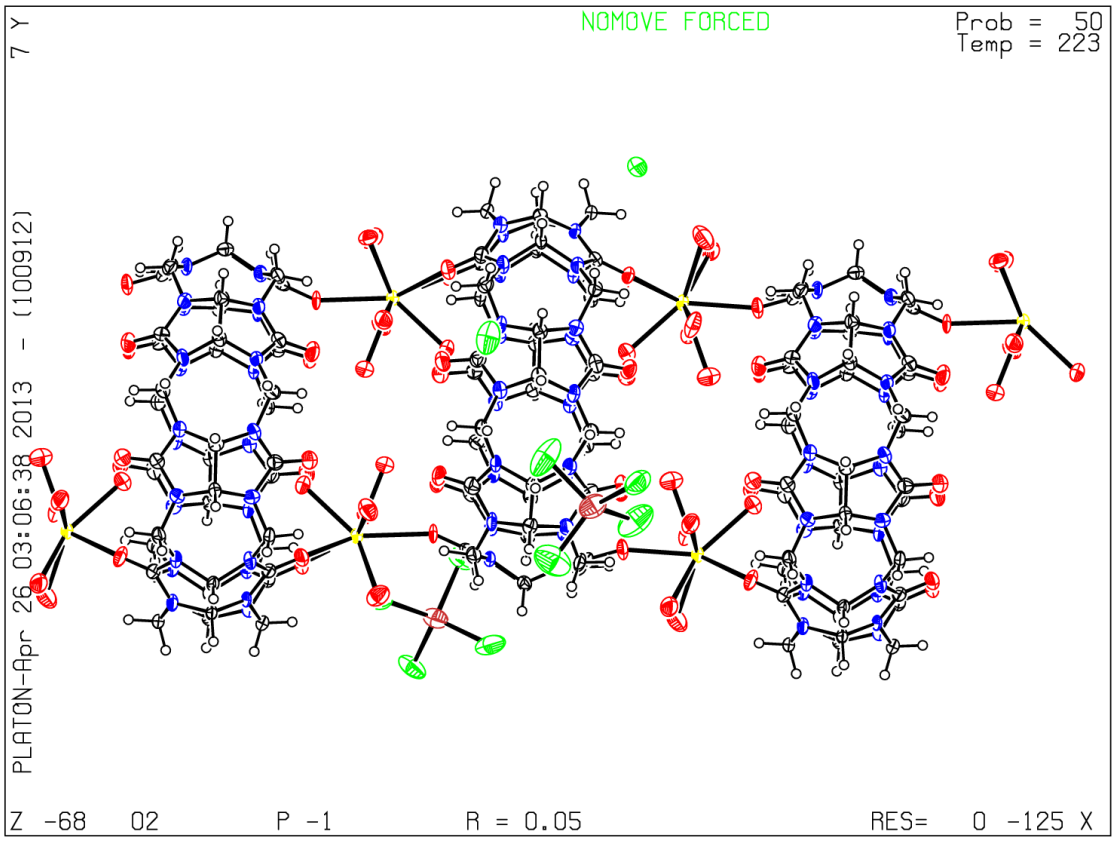
**PLATON version of 05/11/2012; check.def file version of 05/11/2012**

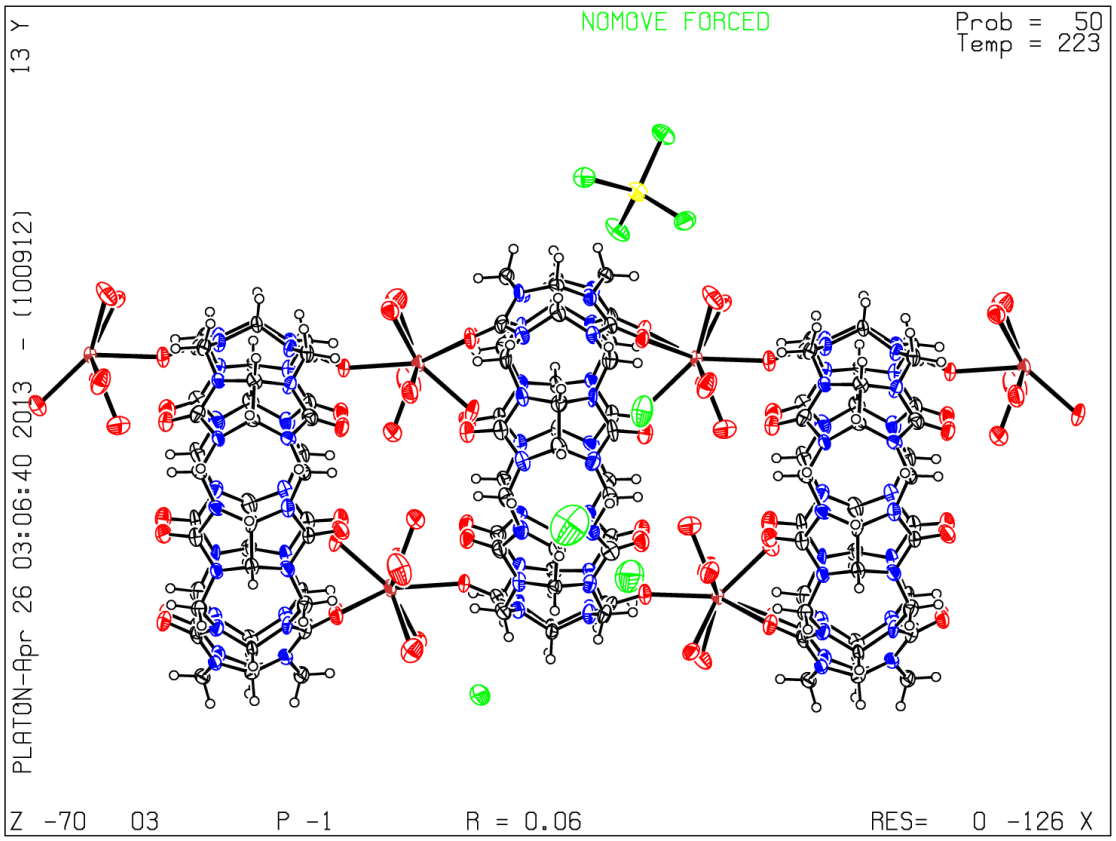
**Datablock 01** - ellipsoid plot



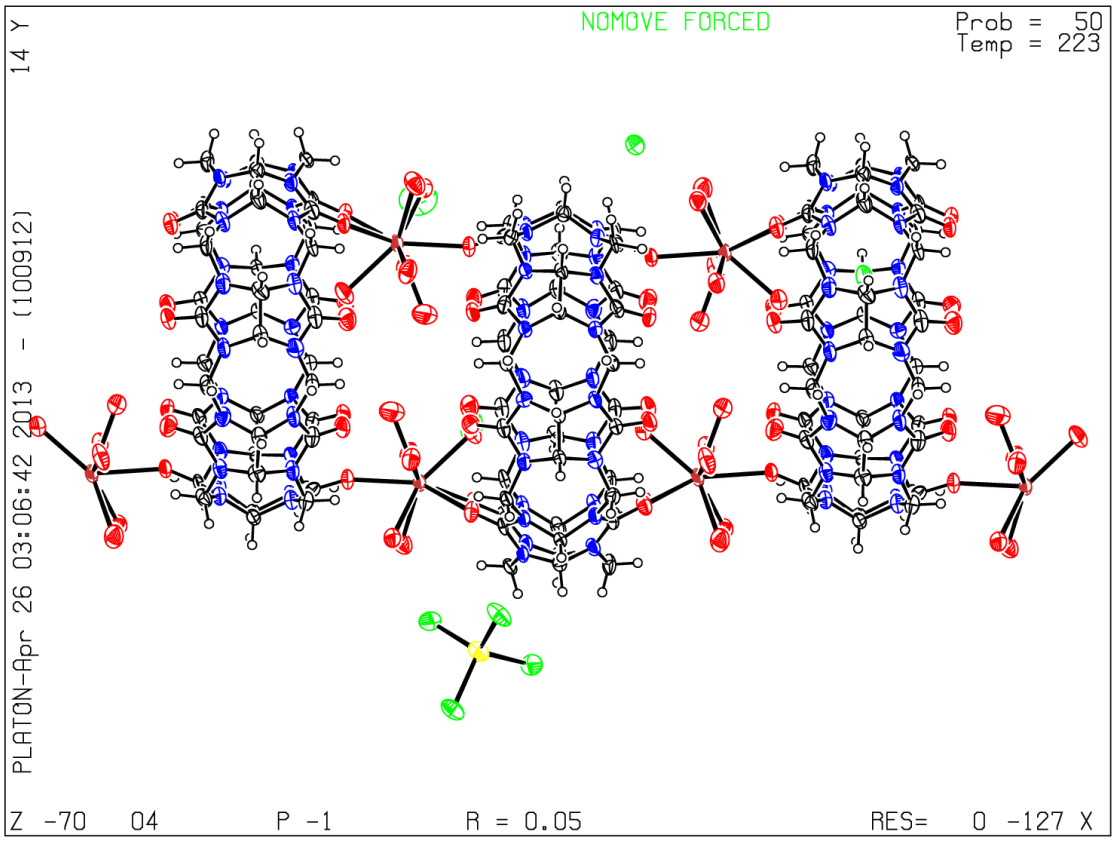
**Datablock 02** - ellipsoid plot



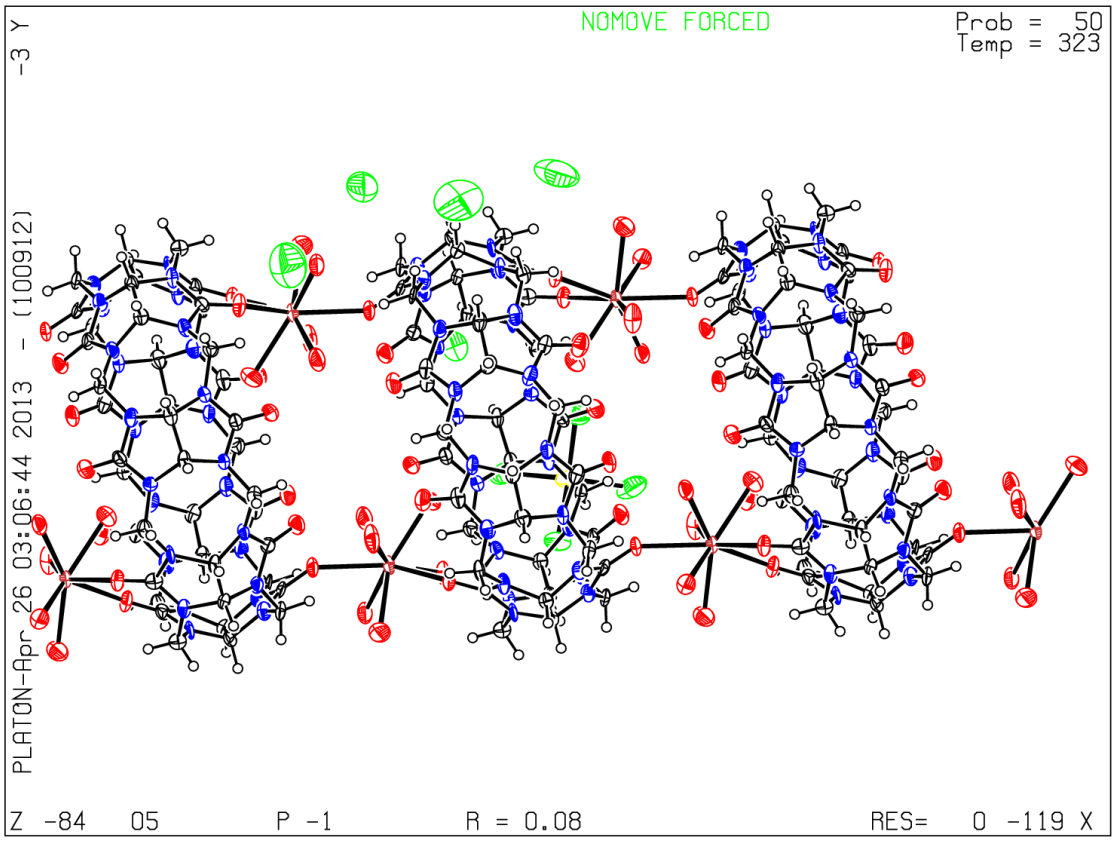
**Datablock 03** - ellipsoid plot



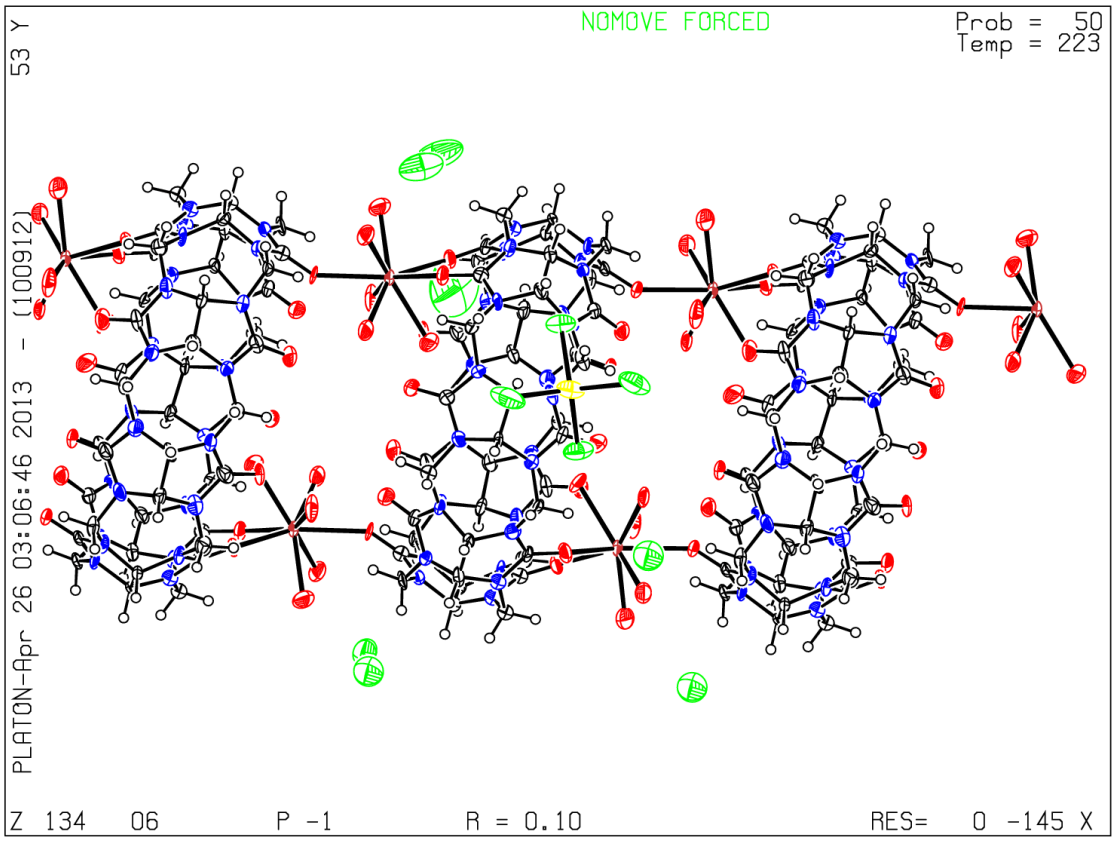
**Datablock 04** - ellipsoid plot



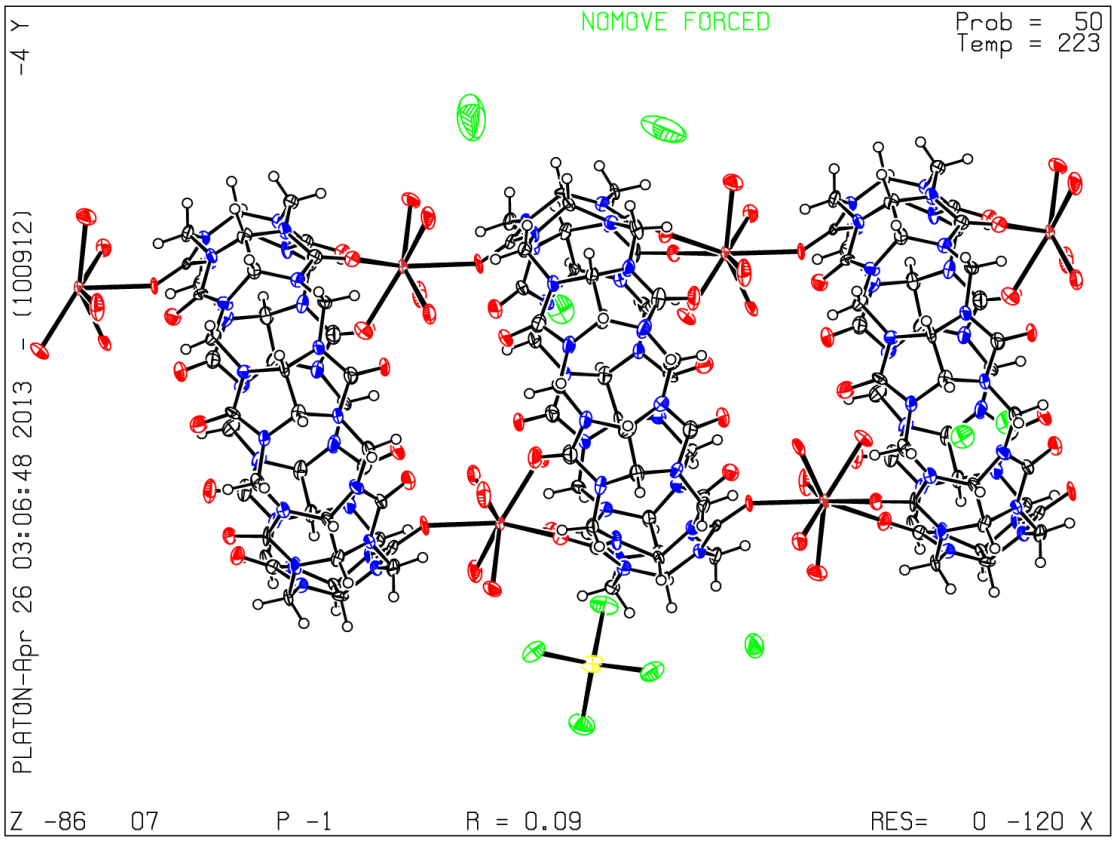
**Datablock 05** - ellipsoid plot



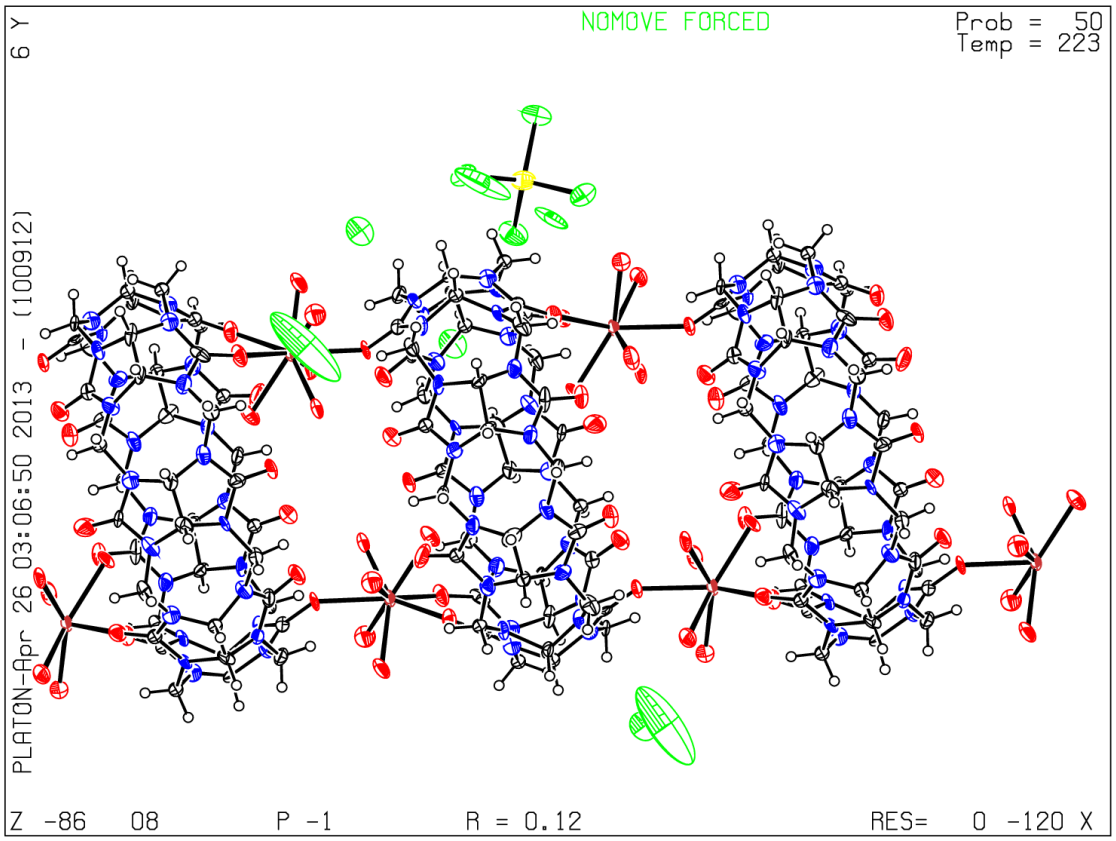
**Datablock 06** - ellipsoid plot



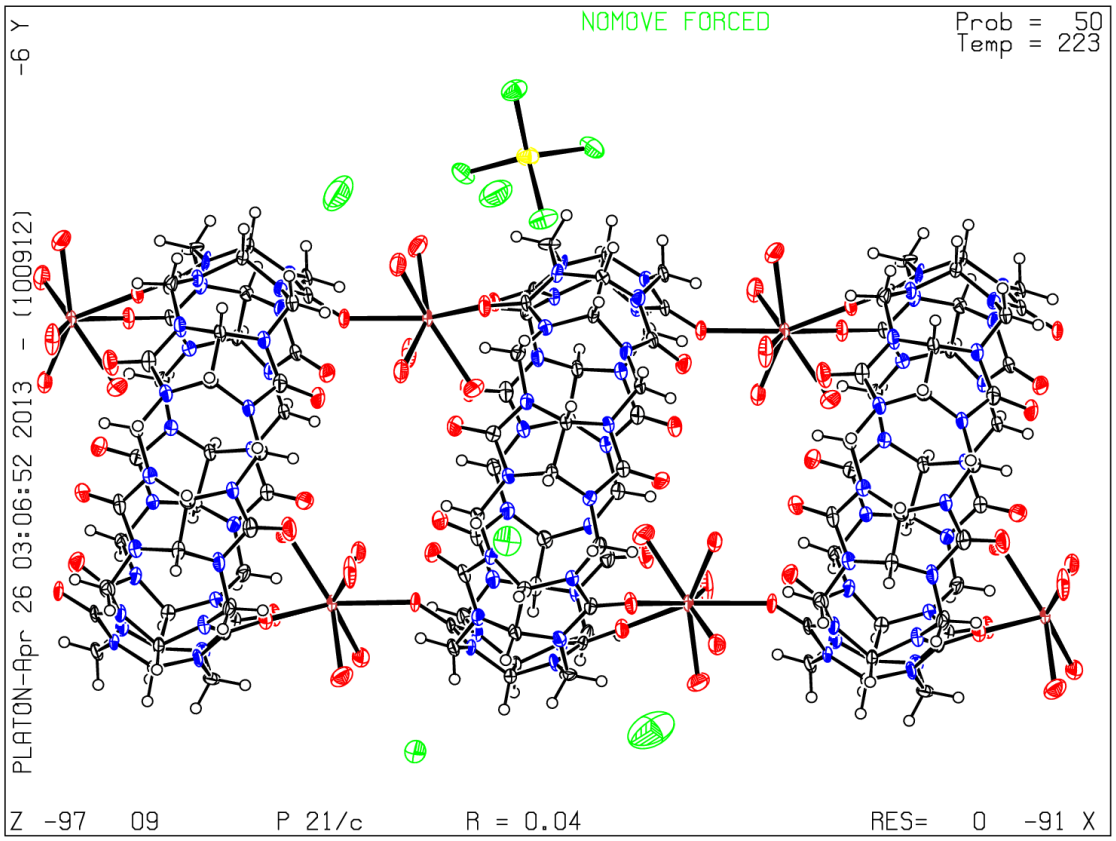
**Datablock 07** - ellipsoid plot



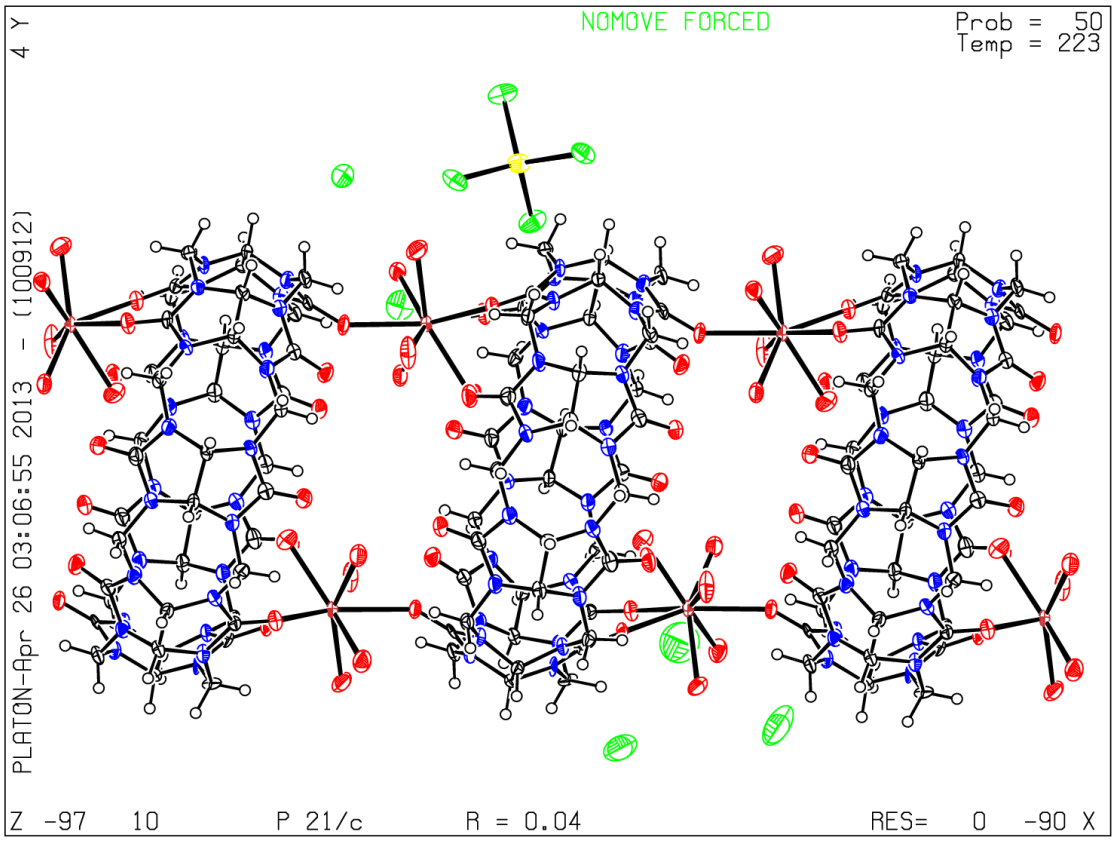
**Datablock 08** - ellipsoid plot



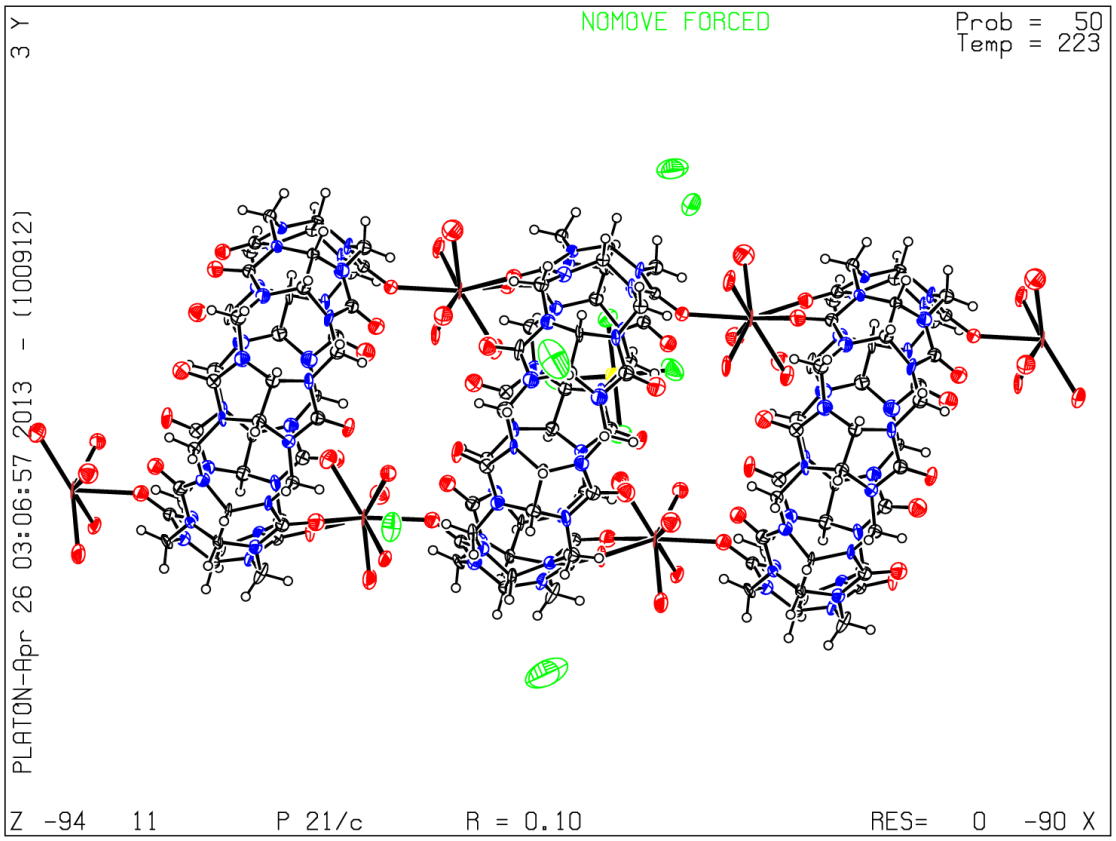
**Datablock 09** - ellipsoid plot



**Datablock 10** - ellipsoid plot



**Datablock 11** - ellipsoid plot



**Datablock 12** - ellipsoid plot