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: 1

```
Bond precision:  C-C = 0.0145 A          Wavelength=0.71073

Cell:          a=13.4863(18)      b=15.176(2)      c=20.111(3)
               alpha=84.901(10)   beta=76.434(9)   gamma=64.154(9)
Temperature:   273 K
```

	Calculated	Reported
Volume	3600.6(9)	3600.8(9)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C15 H27 Cu6 Gd2 N6 O32	?
Sum formula	C15 H27 Cu6 Gd2 N6 O32	C15 H72 Cl6 Cu6 Gd2 N6 O66
Mr	1499.23	2301.23
Dx,g cm-3	1.383	2.122
Z	2	2
Mu (mm-1)	3.612	3.901
F000	1434.0	2272.0
F000’	1437.94	
h,k,lmax	16,18,23	16,18,23
Nref	12656	12220
Tmin,Tmax	0.576,0.732	0.520,1.000
Tmin’	0.552	

```
Correction method= MULTI SCAN

Data completeness= 0.966          Theta(max)= 25.000

R(reflections)= 0.0558( 8137)     wR2(reflections)= 0.1468( 12220)

S = 0.976                 Npar= 546
```

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          2301.23
TEST: Calculate formula weight from _atom_site_*
atom     mass    num     sum
C        12.01   15.00  180.16
H         1.01   27.00   27.22
N        14.01    6.00   84.04
O        16.00   32.00  511.97
Cl       35.45    0.00    0.00
Cu       63.55    6.00  381.28
Gd      157.25    2.00  314.50
Calculated formula weight             1499.17
```

Alert level B

```
PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       7.41 %
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......          1
PLAT220_ALERT_2_B Large Non-Solvent    O     Ueq(max)/Ueq(min) ...        5.5 Ratio
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        O33
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        C11
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for        Gd1
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi scan
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.966
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT048_ALERT_1_C MoietyFormula Not Given ........................          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....          ?
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O16    --  C14     ..        5.3 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C5     --  C6      ..        5.1 su
PLAT234_ALERT_4_C Large Hirshfeld Difference Gd1    --  O31     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O9     --  C10     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O11    --  C12     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5     --  C9      ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N6     --  C11     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11    --  C12     ..       0.19 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O32
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O34
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C3
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C5
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C7
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0145 Ang
PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H1A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H1B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N4     -   H4A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N5     -   H5A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N5     -   H5B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6B    ...          ?
```

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:C15 H72 Cl6 Cu6 Gd2 N6 O66
           Atom count from the _atom_site data:  C15 H27 Cu6 Gd2 N6 O32
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  C15 H72 Cl6 Cu6 Gd2 N6 O66
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         30.00     30.00    0.00
           H        144.00     54.00   90.00
           Cl        12.00      0.00   12.00
           Cu        12.00     12.00    0.00
           Gd         4.00      4.00    0.00
           N         12.00     12.00    0.00
           O        132.00     64.00   68.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          5
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT007_ALERT_5_G Note: Number of Unrefined Donor-H Atoms ........         12
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        273 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        273 K
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT804_ALERT_5_G ARU-Pack Problem in PLATON Analysis ............          1 Times
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         18
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

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

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  25 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
   9 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
```

Datablock: 2

Bond precision: C-C = 0.0112 A Wavelength=0.71073

Cell: a=13.4763(8) b=15.1853(10) c=20.1435(13)
       alpha=84.725(4) beta=76.500(4) gamma=64.039(4)
Temperature: 293 K

	Calculated	Reported
Volume	3603.6(4)	3603.6(4)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C15 H27 Cu6 N6 O31.80 Tb2, O0.20	?
Sum formula	C15 H27 Cu6 N6 O32 Tb2	C15 H82 Cl6 Cu6 N6 O71 Tb2
Mr	1502.59	2394.65
Dx,g cm-3	1.385	2.207
Z	2	2
Mu (mm-1)	3.731	4.029
F000	1438.0	2376.0
F000'	1441.94	
h,k,lmax	16,18,23	16,18,23
Nref	12666	12392
Tmin,Tmax	0.552,0.754	0.520,1.000
Tmin'	0.541	

Correction method= MULTI SCAN

Data completeness= 0.978 Theta(max)= 25.000

R(reflections)= 0.0413(9063) wR2(reflections)= 0.1063(12392)

S = 0.918 Npar= 559

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 2394.65
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	15.00	180.16
H	1.01	27.00	27.22
N	14.01	6.00	84.04
O	16.00	32.00	511.97
Cl	35.45	0.00	0.00
Cu	63.55	6.00	381.28
Tb	158.93	2.00	317.85

Calculated formula weight 1502.52

PLAT414_ALERT_2_A Short Intra D-H..H-X H9BB .. H5A .. 1.71 Ang.

Alert level B

PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 7.39 %
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 1

```
PLAT220_ALERT_2_B Large Non-Solvent    O     Ueq(max)/Ueq(min) ...        4.4 Ratio
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        O26
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for         C5
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi scan
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.978
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ         ?
PLAT048_ALERT_1_C MoietyFormula Not Given ........................         ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...         ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....         ?
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O3     --  C4      ..        5.5 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O7     --  C8      ..        5.5 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu3    --  O26     ..        7.2 su
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O24
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C1
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C3
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C7
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Tb2
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C6
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.0112 Ang
PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H1A    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2A    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2B    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3C    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3D    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N4     -   H4A    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N4     -   H4B    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N5     -   H5B    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6A    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6B    ...         ?
```

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:C15 H82 Cl6 Cu6 N6 O71 Tb2
           Atom count from the _atom_site data:  C15 H27 Cu6 N6 O32 Tb2
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  C15 H82 Cl6 Cu6 N6 O71 Tb2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         30.00     30.00    0.00
          H        164.00     54.00  110.00
          Cl        12.00      0.00   12.00
          Cu        12.00     12.00    0.00
          N         12.00     12.00    0.00
          O        142.00     64.00   78.00
          Tb         4.00      4.00    0.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT007_ALERT_5_G Note: Number of Unrefined Donor-H Atoms ........         12
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............         ?
```

```
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .........    0.00400 Deg.
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................          3 %
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................        100 %
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O25'
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          4
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        248
             C9B  -N5   -C9A     1.555   1.555   1.555            26.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        317
             C9A  -C10  -C9B     1.555   1.555   1.555            25.70 Deg.
PLAT804_ALERT_5_G ARU-Pack Problem in PLATON Analysis ............          1 Times
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

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

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

Datablock: 3

Bond precision: C-C = 0.0083 A Wavelength=0.71073

Cell: a=13.4553(5) b=15.1834(5) c=20.1340(7)
       alpha=84.834(2) beta=76.451(2) gamma=64.080(2)
Temperature: 293 K

	Calculated	Reported
Volume	3596.2(2)	3596.2(2)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C15 H27 Cu6 Dy2 N6 O32	?
Sum formula	C15 H27 Cu6 Dy2 N6 O32	C15 H82 Cl6 Cu6 Dy2 N6 O71
Mr	1509.73	2401.81
Dx,g cm-3	1.394	2.218
Z	2	2
Mu (mm-1)	3.850	4.149
F000	1442.0	2380.0
F000'	1445.89	
h,k,lmax	15,18,23	15,18,23
Nref	12639	12586
Tmin,Tmax	0.584,0.718	0.548,1.000
Tmin'	0.510	

Correction method= MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.000

R(reflections)= 0.0355(10375) wR2(reflections)= 0.0966(12586)

S = 1.041 Npar= 550

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 2401.81

TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	15.00	180.16
H	1.01	27.00	27.22
N	14.01	6.00	84.04
O	16.00	32.00	511.97
Cl	35.45	0.00	0.00
Cu	63.55	6.00	381.28
Dy	162.50	2.00	325.00

Calculated formula weight 1509.67

Alert level B

PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 7.21 %
PLAT220_ALERT_2_B Large Non-Solvent O Ueq(max)/Ueq(min) ... 4.8 Ratio
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O25
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O26

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.
Absorption correction given as multi-scan

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT048_ALERT_1_C MoietyFormula Not Given ..... ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... ?
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu1 -- O24 .. 6.3 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu2 -- O25 .. 9.7 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu3 -- O4 .. 5.5 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu3 -- O26 .. 8.3 su
PLAT234_ALERT_4_C Large Hirshfeld Difference C5 -- C6 .. 0.16 Ang.
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O24
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C1
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C5
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C11
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Dy2
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0083 Ang

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PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H1A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N4     -   H4A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N4     -   H4B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N5     -   H5A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N5     -   H5B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6B    ...          ?
```

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:C15 H82 Cl6 Cu6 Dy2 N6 O71
           Atom count from the _atom_site data:  C15 H27 Cu6 Dy2 N6 O32
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  C15 H82 Cl6 Cu6 Dy2 N6 O71
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         30.00     30.00    0.00
           H        164.00     54.00  110.00
           Cl        12.00      0.00   12.00
           Cu        12.00     12.00    0.00
           Dy         4.00      4.00    0.00
           N         12.00     12.00    0.00
           O        142.00     64.00   78.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          9
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT007_ALERT_5_G Note: Number of Unrefined Donor-H Atoms ........         12
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........    0.00200 Deg.
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         36
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           !
```

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

  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  25 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Datablock: 4

Bond precision: C-C = 0.0195 A Wavelength=0.71073

Cell: a=38.074(10) b=38.074(10) c=24.316(13)
alpha=90 beta=90 gamma=120
Temperature: 293 K

	Calculated	Reported
Volume	30527(26)	30526(20)
Space group	R -3	R-3
Hall group	-R 3	?
Moiety formula	C15 H27 Cu6 Gd2 N6 O33	?
Sum formula	C15 H27 Cu6 Gd2 N6 O33	C15 H84 Cl6 Cu6 Gd2 N6 O72
Mr	1515.23	2409.32
Dx,g cm-3	1.484	2.359
Z	18	18
Mu (mm-1)	3.836	4.153
F000	13050.0	21528.0
F000’	13085.63	
h,k,lmax	45,45,28	45,45,28
Nref	11960	11945
Tmin,Tmax	0.742,0.847	0.515,1.000
Tmin’	0.559	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.000

R(reflections)= 0.0593(5712) wR2(reflections)= 0.1482(11945)

S = 0.984 Npar= 559

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 18
From the CIF: _chemical_formula_weight 2409.32
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	15.00	180.16
H	1.01	27.00	27.22
N	14.01	6.00	84.04
O	16.00	33.00	527.97
Cl	35.45	0.00	0.00
Cu	63.55	6.00	381.28
Gd	157.25	2.00	314.50

Calculated formula weight 1515.17

```
PLAT241_ALERT_2_A Check High      Ueq as Compared to Neighbors for        O23
```

Alert level B

```
PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       7.63 %
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        O22
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        O24
```

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.166
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....         48 %
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ         ?
PLAT048_ALERT_1_C MoietyFormula Not Given ........................         ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...         ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....         ?
PLAT220_ALERT_2_C Large Non-Solvent    O     Ueq(max)/Ueq(min) ...        3.4 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O1     --  C2      ..        6.4 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O2     --  C2      ..        6.5 su
PLAT234_ALERT_4_C Large Hirshfeld Difference Gd1    --  O32     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu2    --  O23     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O4     --  C4      ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O10    --  C10     ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O15    --  C14     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O17    --  C15     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1     --  C1      ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2     --  C3      ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5     --  C9      ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5     --  C6      ..       0.17 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         N6
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C1
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C3
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C5
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C7
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C9
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C13
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        Cu2
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0195 Ang
PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H1D    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2A    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2B    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3D    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N4     -   H4A    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N5     -   H5C    ...         ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6A    ...         ?
```

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:C15 H84 Cl6 Cu6 Gd2 N6 O72
           Atom count from the _atom_site data:  C15 H27 Cu6 Gd2 N6 O33
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   18
           From the CIF: _chemical_formula_sum  C15 H84 Cl6 Cu6 Gd2 N6 O72
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        270.00    270.00    0.00
           H       1512.00    486.00 1026.00
           Cl       108.00      0.00  108.00
           Cu       108.00    108.00    0.00
           Gd        36.00     36.00    0.00
           N        108.00    108.00    0.00
           O       1296.00    594.00  702.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         3
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        15
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .         3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF         ?
PLAT007_ALERT_5_G Note: Number of Unrefined Donor-H Atoms ........        12
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............         ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         6 Units
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature       293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature       293 K
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .     13324 A**3
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        48
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
   3 **ALERT level B** = A potentially serious problem, consider carefully
  37 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  15 **ALERT level G** = General information/check it is not something unexpected

  11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  26 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
  13 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check

Datablock: 5

Bond precision: C-C = 0.0142 A Wavelength=0.71073

Cell: a=38.002(5) b=38.002(5) c=24.348(6)
       alpha=90 beta=90 gamma=120
Temperature: 293 K

	Calculated	Reported
Volume	30451(13)	30452(10)
Space group	R -3	R-3
Hall group	-R 3	?
Moiety formula	C15 H27 Cu6 N6 O33 Tb2	?
Sum formula	C15 H27 Cu6 N6 O33 Tb2	C15 H80 Cl6 Cu6 N6 O70 Tb2
Mr	1518.59	2376.63
Dx,g cm-3	1.491	2.333
Z	18	18
Mu (mm-1)	3.976	4.289
F000	13086.0	21204.0
F000'	13121.64	
h,k,lmax	45,45,28	45,45,28
Nref	11920	11919
Tmin,Tmax	0.742,0.861	0.435,1.000
Tmin'	0.520	

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 24.990

R(reflections)= 0.0468(7348) wR2(reflections)= 0.1131(11919)

S = 0.975 Npar= 559

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 18

From the CIF: _chemical_formula_weight 2376.63

TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	15.00	180.16
H	1.01	27.00	27.22
N	14.01	6.00	84.04
O	16.00	33.00	527.97
Cl	35.45	0.00	0.00
Cu	63.55	6.00	381.28
Tb	158.93	2.00	317.85

Calculated formula weight 1518.52

PLAT241_ALERT_2_A Check High Ueq as Compared to Neighbors for O17

Alert level B

PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 7.30 %

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O16

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for C1

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ?
PLAT048_ALERT_1_C MoietyFormula Not Given .......................          ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....          ?
PLAT220_ALERT_2_C Large Non-Solvent    O     Ueq(max)/Ueq(min) ...        3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O5     --  C6      ..        5.2 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O6     --  C6      ..        5.7 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N3     --  C5      ..        6.9 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu2    --  O17     ..        8.3 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu4    --  O16     ..        6.0 su
PLAT234_ALERT_4_C Large Hirshfeld Difference O1     --  C2      ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O3     --  C4      ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O22    --  C13     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O25    --  C14     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C3     --  C4      ..       0.18 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O18
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C5
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C7
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C9
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C11
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Tb2
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Cu2
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0142 Ang
PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H1C    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3C    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N4     -   H4B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N5     -   H5D    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6B    ...          ?
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1
             C15 H27 Cu6 N6 O33 Tb2
```

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:C15 H80 Cl6 Cu6 N6 O70 Tb2
           Atom count from the _atom_site data:  C15 H27 Cu6 N6 O33 Tb2
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   18
          From the CIF: _chemical_formula_sum  C15 H80 Cl6 Cu6 N6 O70 Tb2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        270.00    270.00    0.00
          H       1440.00    486.00  954.00
          Cl       108.00      0.00  108.00
          Cu       108.00    108.00    0.00
          N        108.00    108.00    0.00
          O       1260.00    594.00  666.00
          Tb        36.00     36.00    0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          9
```

```
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT007_ALERT_5_G Note: Number of Unrefined Donor-H Atoms ........         12
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          3 Units
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .      13237 A**3
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         54
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
3 **ALERT level B** = A potentially serious problem, consider carefully
33 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
27 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
9 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Datablock: 6

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

Cell: a=20.9830(5) b=21.9555(5) c=25.6798(5)
alpha=75.639(1) beta=74.559(1) gamma=72.725(1)
Temperature: 296 K

	Calculated	Reported
Volume	10704.0(4)	10704.0(4)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C44 H76 Cu24 Gd6 N12 O94	?
Sum formula	C44 H76 Cu24 Gd6 N12 O94	C44 H280 Cl10 Cu24 Gd6 N12 O198
Mr	4745.84	6969.76
Dx,g cm-3	1.472	2.162
Z	2	2
Mu (mm-1)	4.222	4.414
F000	4512.0	6924.0
F000’	4527.74	
h,k,lmax	24,26,30	24,26,30
Nref	37682	37592
Tmin,Tmax	0.521,0.802	0.200,1.000
Tmin’	0.511	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.000

R(reflections)= 0.0470(23980) wR2(reflections)= 0.1222(37592)

S = 0.923 Npar= 1616

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 6969.76
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	44.00	528.48
H	1.01	76.00	76.61
N	14.01	12.00	168.08
O	16.00	94.00	1503.91
Cu	63.55	24.00	1525.10
Gd	157.25	6.00	943.50
Cl	35.45	0.00	0.00

Calculated formula weight 4745.69

PLAT241_ALERT_2_A Check High Ueq as Compared to Neighbors for O3D

Alert level B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) 2
PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 10.0 Ratio
PLAT220_ALERT_2_B Large Non-Solvent O Ueq(max)/Ueq(min) ... 5.7 Ratio
PLAT222_ALERT_3_B Large Non-Solvent H Uiso(max)/Uiso(min) .. 9.2 Ratio
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O1D
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O5D
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O31
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C8
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C32
PLAT412_ALERT_2_B Short Intra XH3 .. XHn H14A .. H15B .. 1.74 Ang.
PLAT414_ALERT_2_B Short Intra D-H..H-X H2B .. H5C .. 1.84 Ang.
PLAT414_ALERT_2_B Short Intra D-H..H-X H3A .. H8C .. 1.81 Ang.
PLAT414_ALERT_2_B Short Intra D-H..H-X H5A .. H14A .. 1.80 Ang.
PLAT414_ALERT_2_B Short Intra D-H..H-X H6A .. H17A .. 1.89 Ang.
PLAT414_ALERT_2_B Short Intra D-H..H-X H7A .. H20A .. 1.84 Ang.
PLAT414_ALERT_2_B Short Intra D-H..H-X H11B .. H32A .. 1.85 Ang.
PLAT414_ALERT_2_B Short Intra D-H..H-X H12B .. H35A .. 1.84 Ang.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
SHFSU01_ALERT_2_C The absolute value of parameter shift to su ratio > 0.05
Absolute value of the parameter shift to su ratio given 0.058
Additional refinement cycles may be required.
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?

```
PLAT048_ALERT_1_C MoietyFormula Not Given ........................          ?
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       4.35 %
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT080_ALERT_2_C Maximum Shift/Error ............................       0.06
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given .....          ?
PLAT213_ALERT_2_C Atom C9              has ADP max/min Ratio .....        3.6 prola
PLAT213_ALERT_2_C Atom C21             has ADP max/min Ratio .....        3.4 prola
PLAT213_ALERT_2_C Atom C23             has ADP max/min Ratio .....        3.4 prola
PLAT213_ALERT_2_C Atom C33             has ADP max/min Ratio .....        3.6 prola
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu20   --  O5D     ..        5.4 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cu22   --  O16W    ..        7.2 su
PLAT234_ALERT_4_C Large Hirshfeld Difference Cu8    --  O15W    ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O35    --  C42     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5     --  C6      ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C20    --  C21     ..       0.18 Ang.
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O2D
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O4D
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O6D
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         N6
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C5
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Cu8
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       Cu20
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       Cu22
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         N2
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        N12
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C4
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C7
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C11
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C13
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C17
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C19
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C22
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C25
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C26
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C28
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C34
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C40
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.0163 Ang
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C2     -   C3     ...       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C8     -   C9     ...       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C11    -   C12    ...       1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C17    -   C18    ...       1.38 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C20    -   C21    ...       1.37 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C23    -   C24    ...       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C35    -   C36    ...       1.38 Ang.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C14    -   C15    ...       1.38 Ang.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond  C32    -   C33    ...       1.38 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H5C    ..  H6E     ..       1.81 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H8C    ..  H9D     ..       1.89 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H20A   ..  H21B    ..       1.81 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H23A   ..  H24C    ..       1.86 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H35A   ..  H36C    ..       1.86 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H1B    ..  H2C     ..       1.92 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H4B    ..  H11C    ..       1.93 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H8B    ..  H23A    ..       1.90 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H9B    ..  H26A    ..       1.97 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H1A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N1     -   H1B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N2     -   H2B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N3     -   H3B    ...          ?
```

```
PLAT420_ALERT_2_C D-H Without Acceptor       N4     -   H4B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N5     -   H5A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N6     -   H6B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N7     -   H7A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N7     -   H7B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N8     -   H8A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N8     -   H8B    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N9     -   H9A    ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N10    -   H10A   ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N10    -   H10B   ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N11    -   H11A   ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N11    -   H11B   ...          ?
PLAT420_ALERT_2_C D-H Without Acceptor       N12    -   H12B   ...          ?
```

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:C44 H280 Cl10 Cu24 Gd6 N12 O19
           Atom count from the _atom_site data:  C44 H76 Cu24 Gd6 N12 O94
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  C44 H280 Cl10 Cu24 Gd6 N12 O198
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         88.00     88.00    0.00
           H        560.00    152.00  408.00
           Cl        20.00      0.00   20.00
           Cu        48.00     48.00    0.00
           Gd        12.00     12.00    0.00
           N         24.00     24.00    0.00
           O        396.00    188.00  208.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         22
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         36
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT007_ALERT_5_G Note: Number of Unrefined Donor-H Atoms ........         24
PLAT044_ALERT_1_G Calculated and Reported Dx Differ ..............          ?
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........    0.00100 Deg.
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................          1 %
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C5
PLAT343_ALERT_2_G Check         Angle Range in Main Residue for ..        C14
PLAT343_ALERT_2_G Check sp3     Angle Range in Main Residue for ..        C20
PLAT343_ALERT_2_G Check sp3     Angle Range in Main Residue for ..        C23
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C33
PLAT343_ALERT_2_G Check sp3     Angle Range in Main Residue for ..        C35
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        !
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.11 Ratio
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   GD1    --  CU4     ..       3.51 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   GD2    --  CU7     ..       3.52 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   GD3    --  CU12    ..       3.50 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   GD4    --  CU15    ..       3.50 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   GD5    --  CU24    ..       3.51 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   GD6    --  CU19    ..       3.52 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   CU7    --  GD2     ..       3.52 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   CU12   --  GD3     ..       3.50 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   CU16   --  GD5     ..       3.52 Ang.
```

```
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   CU24   --  GD5     ..       3.51 Ang.
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C8      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C11     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C17     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C23     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C26     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C32     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C35     (Verify) ....          R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        114
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
17 **ALERT level B** = A potentially serious problem, consider carefully
79 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
40 **ALERT level G** = General information/check it is not something unexpected

19 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
95 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
17 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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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.
```

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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

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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.

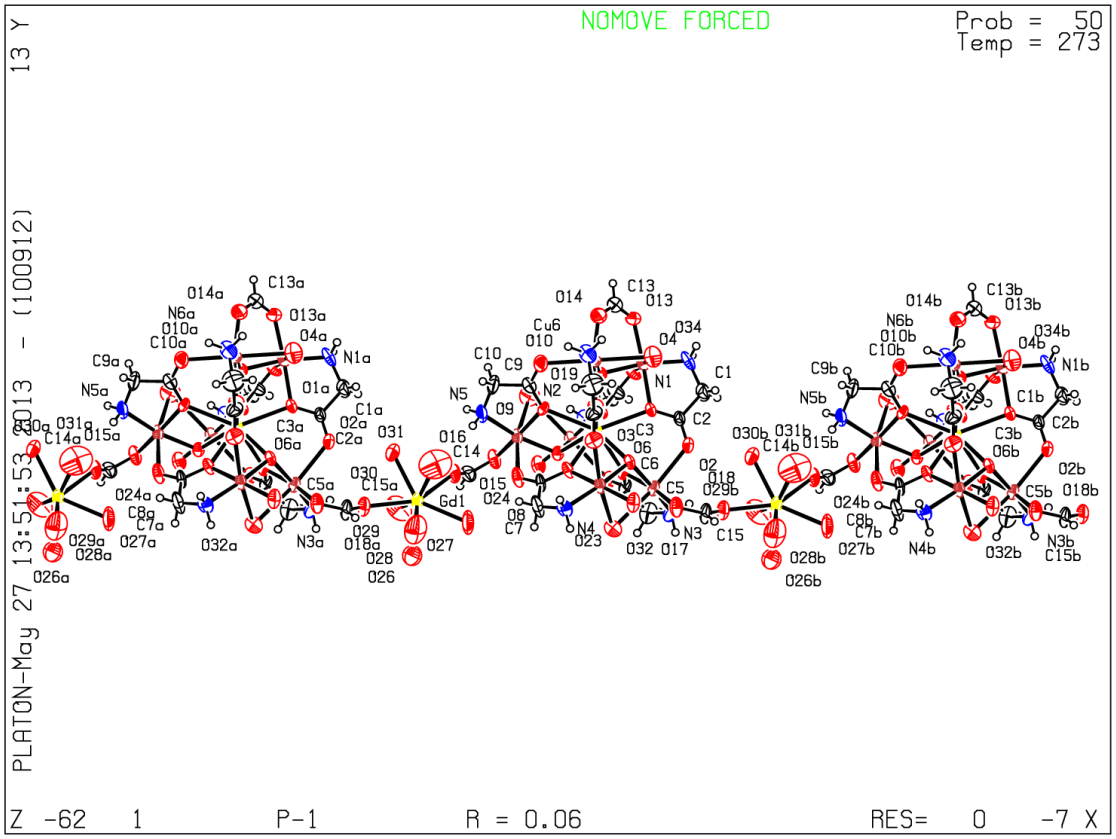
If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# 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.
```

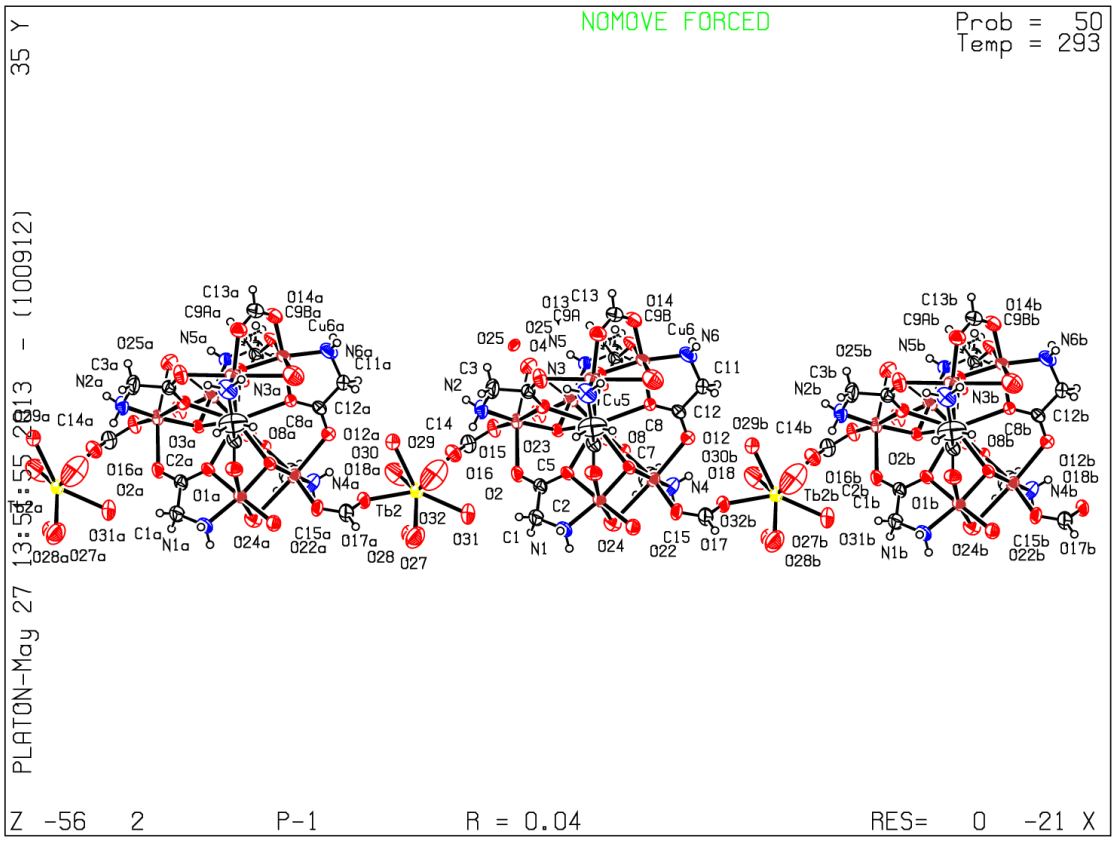
```
RESPONSE: ...
;
_vrf_CHEMW03_1
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_CHEMW03_2
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT414_2
;
PROBLEM: Short Intra D-H..H-X       H9BB   ..  H5A     ..       1.71 Ang.
RESPONSE: ...
;
_vrf_CHEMW03_3
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_CHEMW03_4
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT241_4
;
PROBLEM: Check High      Ueq as Compared to Neighbors for        O23
RESPONSE: ...
;
_vrf_CHEMW03_5
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT241_5
;
PROBLEM: Check High      Ueq as Compared to Neighbors for        O17
RESPONSE: ...
;
_vrf_CHEMW03_6
;
PROBLEM: ALERT: The ratio of given/expected molecular weight as
RESPONSE: ...
;
_vrf_PLAT241_6
;
PROBLEM: Check High      Ueq as Compared to Neighbors for        O3D
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 24/04/2013; check.def file version of 23/04/2013

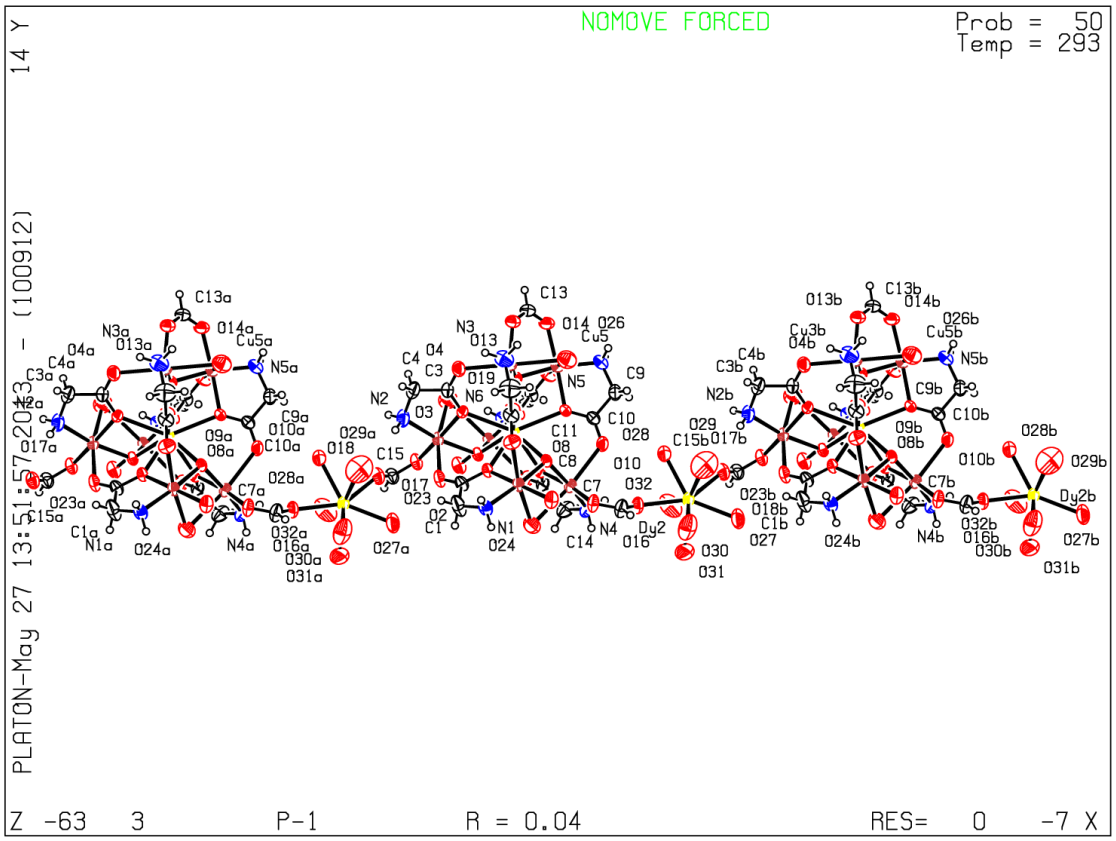
Datablock 1 - ellipsoid plot



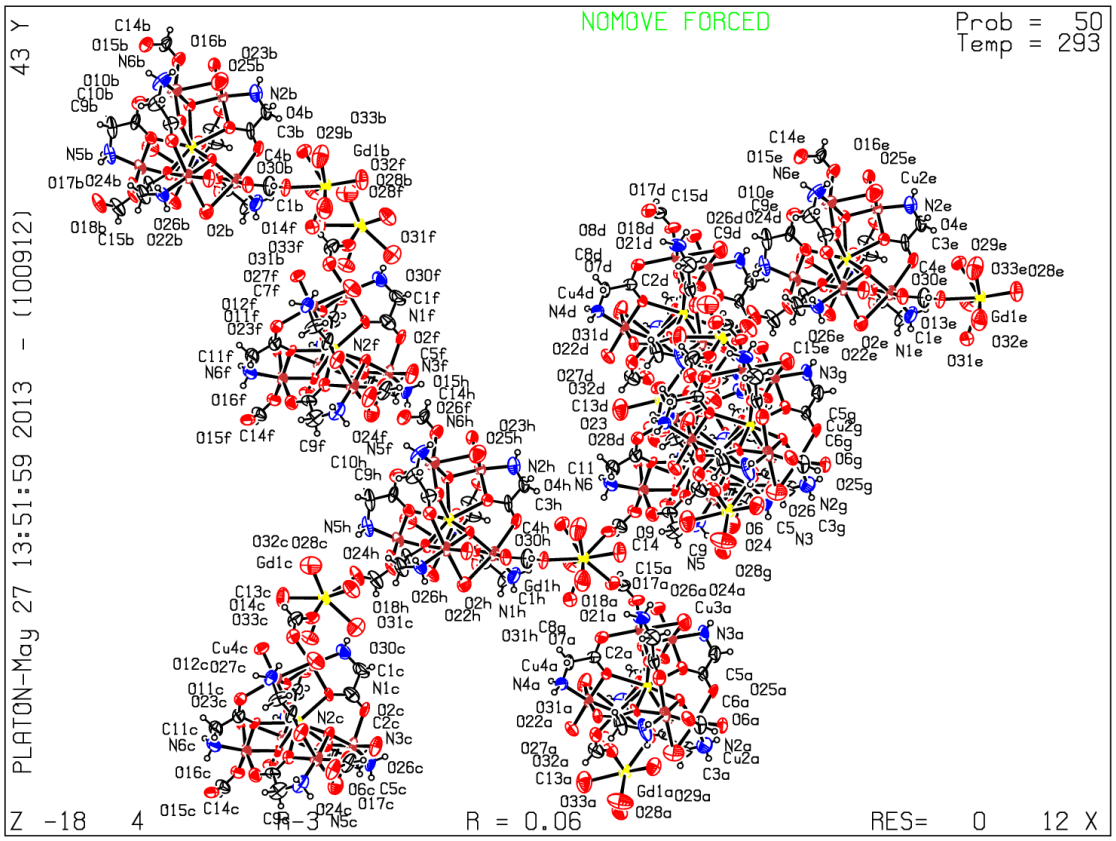
Datablock 2 - ellipsoid plot



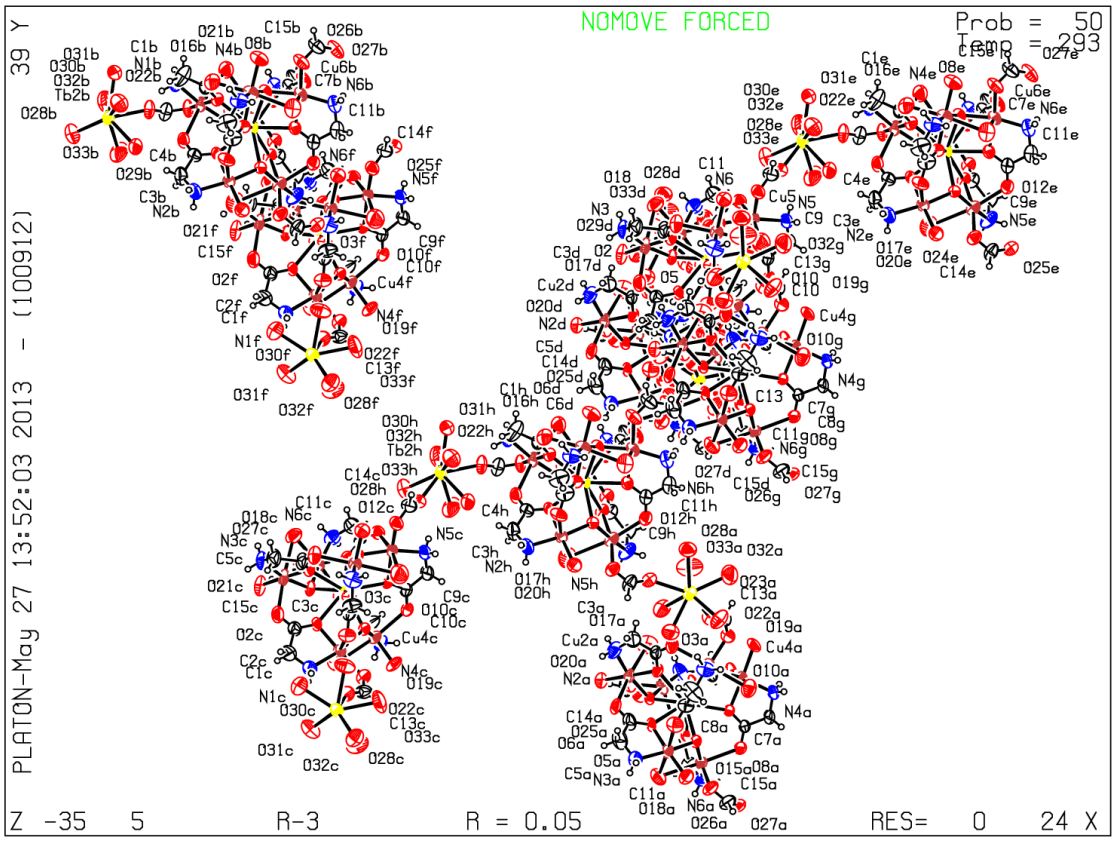
Datablock 3 - ellipsoid plot



Datablock 4 - ellipsoid plot



Datablock 5 - ellipsoid plot



Datablock 6 - ellipsoid plot