checkCIF/PLATON report

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

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

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: gd7_auto

```
Bond precision:    C-C = 0.0239 A          Wavelength=1.54184

Cell:              a=26.4695(2)     b=57.9994(6)       c=52.5818(6)
                   alpha=90         beta=98.283(1)     gamma=90
Temperature:       100 K

                 Calculated                        Reported
Volume           79882.3(14)                       79882.3(14)
Space group      P 21/n                            P 1 21/n 1
Hall group       -P 2yn                            -P 2yn
                 C206 H213 Gd7 N26 O36,            (C206 H214 Gd7 N26 O36),
Moiety formula   2(C206 H210 Gd7 N26 O36) [+ [NO3], 10[CH3OH],
                 solvent]                          10[CH3CN], 2[H2O]
                 C618 H633 Gd21 N78 O108 [+
Sum formula                                        C236 H288 Gd7 N37 O51
                 solvent]
Mr               14183.14                          5559.77
Dx,g cm-3        1.179                             1.387
Z                4                                 12
Mu (mm-1)        11.553                            11.692
F000             28380.0                           33828.0
F000'            27726.16
h,k,lmax         31,68,61                          31,67,61
Nref             137081                            133115
Tmin,Tmax        0.183,0.311                       0.699,1.000
Tmin'            0.064

Correction method= # Reported T Limits: Tmin=0.699 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.971             Theta(max)= 65.349
```

```
R(reflections)= 0.1210( 86336)                                wR2(reflections)=
                                                              0.3341(133115)
S = 1.073                     Npar= 7410
```

```
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

```
PLAT241_ALERT_2_A High   'MainMol' Ueq as Compared to Neighbors of        N36 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

Alert level B

```
PLAT220_ALERT_2_B NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        6.6 Ratio
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, leading to the Ueq(max)/Ueq(min) Range.

```
PLAT220_ALERT_2_B NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range       10.0 Ratio
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, leading to the Ueq(max)/Ueq(min) Range.

```
PLAT220_ALERT_2_B NonSolvent   Resd 2  N   Ueq(max)/Ueq(min) Range        7.9 Ratio
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, leading to the Ueq(max)/Ueq(min) Range.

```
PLAT220_ALERT_2_B NonSolvent   Resd 3  C   Ueq(max)/Ueq(min) Range        7.6 Ratio
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, leading to the Ueq(max)/Ueq(min) Range.

```
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         N5 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of       C194 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of       C270 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of       C507 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of       C540 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C240 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C267 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C268 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ...............    0.02395 Ang.
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, resulting in Low Bond Precision.

Alert level C

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
```

```
            Calculated sin(theta_max)/wavelength =    0.5895
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.971 Why?
PLAT082_ALERT_2_C High R1 Value ..................................       0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.33 Report
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Gd1        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Gd2        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for Gd3        .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O5         .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N11        .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C144       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C143       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C110       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C126       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C172       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C153       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C40        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C186       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C97        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C86        .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C94        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C45        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N17        .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C31        .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O37        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O46        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O45        .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C338       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C329       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C284       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O54        .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C246       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C272       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C292       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C404       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C405       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C230       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C278       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C350       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C215       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C369       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C205       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C216       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C411       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C391       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C358       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N47        .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C302       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C250       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C364       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C587       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C467       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O97        .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C576       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C604       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C554       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C458       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C613       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C532       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C503       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C535       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C549       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C521       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C577       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C543       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C498       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C441       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C476       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N60        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N72        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N76        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N59        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N75        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N53        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O88        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N71        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O102       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N63        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C586       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C593       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N67        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N58        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C527       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C454       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C428       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C421       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N68        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C494       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O90        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C436       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C422       .          6 Check
```

```
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C462       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N57        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N54        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C427       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C430       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C463       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C429       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O99        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N73        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C555       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C484       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C511       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C616       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C499       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C448       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C539       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C569       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N61        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C557       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N70        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C522       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C582       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C504       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C531       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C612       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C537       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C506       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C572       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C551       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C570       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C530       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C523       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C606       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N69        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C546       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C474       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C580       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C473       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C517       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C545       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C575       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C538       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C578       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C550       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C449       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C497       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C505       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C614       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C556       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C514       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C571       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C475       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C573       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C507       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C442       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C548       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C540       .          6 Check
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PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C581       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C481       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C547       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C574       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C482       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C607       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O105       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C276       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N31        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C161       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C240       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C30        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C29        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C242       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C95        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C267       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N143       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C268       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C508       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C168       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C408       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C96        .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C169       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C195       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C235       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C162       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C204       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C700       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C702       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C701       .          6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for C269       .          6 Check
PLAT220_ALERT_2_C NonSolvent   Resd 1  N   Ueq(max)/Ueq(min) Range        3.8 Ratio
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, leading to the Ueq(max)/Ueq(min) Range.

```
PLAT220_ALERT_2_C NonSolvent   Resd 2  C   Ueq(max)/Ueq(min) Range        5.8 Ratio
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, leading to the Ueq(max)/Ueq(min) Range.

```
PLAT220_ALERT_2_C NonSolvent   Resd 2  O   Ueq(max)/Ueq(min) Range        5.4 Ratio
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, leading to the Ueq(max)/Ueq(min) Range.

```
PLAT220_ALERT_2_C NonSolvent   Resd 3  N   Ueq(max)/Ueq(min) Range        3.7 Ratio
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, leading to the Ueq(max)/Ueq(min) Range.

```
PLAT220_ALERT_2_C NonSolvent   Resd 3  O   Ueq(max)/Ueq(min) Range        3.4 Ratio
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good, leading to the Ueq(max)/Ueq(min) Range.

```
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        8.4 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2  H   Uiso(max)/Uiso(min) Range        6.7 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 3  H   Uiso(max)/Uiso(min) Range        7.7 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O30 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        N13 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        N21 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        N22 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C12 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C21 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C31 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C33 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C35 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C40 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C62 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C166 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O57 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C218 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C232 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C234 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   ’MainMol’ Ueq as Compared to Neighbors of       C239 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   ’MainMol’ Ueq as Compared to Neighbors of       C241 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   ’MainMol’ Ueq as Compared to Neighbors of       C251 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   ’MainMol’ Ueq as Compared to Neighbors of       C259 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   ’MainMol’ Ueq as Compared to Neighbors of       C265 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   ’MainMol’ Ueq as Compared to Neighbors of       C273 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   ’MainMol’ Ueq as Compared to Neighbors of       C275 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   ’MainMol’ Ueq as Compared to Neighbors of       C317 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C382 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C407 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O105 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C489 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C523 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C578 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         O8 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N9 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N18 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        N25 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        C28 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        C29 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        C34 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        C38 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        C95 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C125 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C128 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C137 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C161 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C168 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C201 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        O60 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        N31 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       N143 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C231 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C247 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C301 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C403 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        N65 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of        N70 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C516 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

```
PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C580 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

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PLAT242_ALERT_2_C Low    ’MainMol’ Ueq as Compared to Neighbors of       C606 Check
```

Author Response: The single crystal X-ray diffraction data of the complex is not very good. The atom assignment is correct.

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PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C24      -C32      .       1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C90      -C98      .       1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C230     -C238     .       1.35 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C239     -C247     .       1.35 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C29      - C30      .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C162     - C194     .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C201     - C202     .       1.35 Ang.
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PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C275     - C276     .       1.39 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C700     - C701     .       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C474     - C475     .       1.36 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C507     - C508     .       1.41 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C36      - C37      .       1.67 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C95      - C96      .       1.66 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C18      - C19      .       1.39 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C23      - C24      .       1.40 Ang.
PLAT368_ALERT_2_C Short  C(sp2)-C(sp2) Bond  C232     - C234     .       1.23 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C24      - C32      .       1.53 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H18A     ..H183     .       1.96 Ang.
                                                      x,y,z  =     1_555 Check
PLAT410_ALERT_2_C Short Intra H...H Contact  H57D     ..H575     .       1.96 Ang.
                                                      x,y,z  =     1_555 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H43B     ..H70D     .       2.07 Ang.
                                                1-x,1-y,1-z  =     3_666 Check
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H43B     ..H70I     .       2.03 Ang.
                                                1-x,1-y,1-z  =     3_666 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H5E      ..H27C     .       1.98 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H9       ..H60A     .       1.91 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H10B     ..H14      .       1.93 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H13A     ..H93A     .       1.96 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H15A     ..H22      .       1.92 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H27D     ..H35      .       1.93 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H29C     ..H40A     .       1.90 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H33A     ..H43D     .       1.92 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H36H     ..H48I     .       1.93 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H37D     ..H47      .       1.94 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H39D     ..H51I     .       1.91 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H41V     ..H52A     .       1.97 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H43A     ..H57      .       1.93 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H45A     ..H58D     .       1.93 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H47A     ..H62      .       1.91 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H48A     ..H61      .       1.95 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H50A     ..H65      .       1.96 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H51D     ..H66      .       1.95 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H53A     ..H70      .       1.95 Ang.
                                                      x,y,z  =     1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X       H55A     ..H69      .       1.96 Ang.
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                                                      x,y,z  =      1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X      H58A     ..H74      .       1.94 Ang.
                                                      x,y,z  =      1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X      H60D     ..H77A     .       1.95 Ang.
                                                      x,y,z  =      1_555 Check
PLAT414_ALERT_2_C Short Intra D-H..H-X      H61C     ..H78A     .       1.94 Ang.
                                                      x,y,z  =      1_555 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N5       --H5D      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N5       --H5E      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N6       --H6D      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N6       --H6E      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N9       --H9       .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N10      --H10      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N13      --H13A     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N14      --H14      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N143     --H14A     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N17      --H17      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N18      --H18      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N21      --H21A     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N25      --H25      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N26      --H26      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N31      --H31D     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N35      --H35      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N36      --H36      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N39      --H39      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N40      --H40A     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N43      --H43D     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N44      --H44K     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N47      --H47      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N48      --H48I     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N51      --H51I     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N52      --H52A     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N57      --H57      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N58      --H58D     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N61      --H61      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N62      --H62      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N65      --H65      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N66      --H66      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N69      --H69      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N70      --H70      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N73      --H73A     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N74      --H74      .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N77      --H77A     .     Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N78      --H78A     .     Please Check
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C236 H288 Gd7 N37 O51
            Atom count from _chemical_formula_moiety:C206 H214 Gd7 N26 O36
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:C236 H288 Gd7 N37 O51
            Atom count from the _atom_site data:  C206 H211 Gd7 N26 O36
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
```

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CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z   12
           From the CIF: _chemical_formula_sum  C236 H288 Gd7 N37 O51
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C       2832.00   2472.00  360.00
           H       3456.00   2532.00  924.00
           Gd        84.00     84.00    0.00
           N        444.00    312.00  132.00
           O        612.00    432.00  180.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         87 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          1 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         38 Report
              H5D   H5E   H6D   H6E   H9    H10   H13A  H14   H17   H18   H21A
              H22   H25   H26   H14A  H31D  H35   H36   H39   H40A  H43D  H44K
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
              Calc: C206 H211 Gd7 N26 O36
              Rep.: C236 H288 Gd7 N37 O51
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: C206 H213 Gd7 N26 O36, 2(C206 H210 Gd7 N26 O36)
              Rep.: (C206 H214 Gd7 N26 O36),
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.333 Check
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       1.18 %
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    1077.95 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         40 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C24      -C32            0.27 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C33      -C41            0.22 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C230     -C238           0.28 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C263     -C271           0.19 Ang.
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for       C268 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for       C700 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C60 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C93 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C105 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C126 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C138 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C159 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C171 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C192 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C233 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C266 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C278 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C299 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C332 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C365 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C377 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C398 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C410 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C439 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C451 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C472 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C484 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C505 Check
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PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C517 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C538 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C550 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C583 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C604 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C616 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT608_ALERT_4_G ADDSYM Test Skipped (Too Time-consuming) .......          ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Gd1       (III)     .       3.59 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Gd8       (III)     .       3.56 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Gd15      (III)     .       3.59 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............          66 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........         2.3 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
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  1 ALERT level A = Most likely a serious problem - resolve or explain
 13 ALERT level B = A potentially serious problem, consider carefully
975 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 60 ALERT level G = General information/check it is not something unexpected

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

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

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

Publication of your CIF in other journals

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

PLATON version of 13/12/2023; check.def file version of 13/12/2023

Datablock gd7_auto - ellipsoid plot