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: gd_auto

```
Bond precision:    C-C = 0.0265 A              Wavelength=1.54184

Cell:              a=27.7525(9)        b=27.7525(9)        c=24.9438(7)
                   alpha=90            beta=90             gamma=90
Temperature:       173 K

                   Calculated                  Reported
Volume             19211.8(14)                 19211.7(13)
Space group        P 4/n                       P 4/n
Hall group         -P 4a                       -P 4a
                   C264 H272 Gd14 N48 O91,     C264 H272 Gd14 N48 O91,
Moiety formula     8(C2 H3 N), 9(O) [+         8(C2 H3 N), 9(H2 O),
                   solvent]                    1.5[CH3CN], 2[CH3
                   C280 H296 Gd14 N56 O100 [+
Sum formula        solvent]                    C285 H330.5 Gd14 N57.5 O104
Mr                 8247.25                     8427.05
Dx,g cm-3          1.426                       1.457
Z                  2                           2
Mu (mm-1)          15.984                      16.005
F000               8128.0                      8342.0
F000'              7909.51
h,k,lmax           34,34,31                    31,33,30
Nref               19516                       19020
Tmin,Tmax          0.107,0.091                 0.376,1.000
Tmin'              0.021

Correction method= # Reported T Limits: Tmin=0.376 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.975           Theta(max)= 73.942
```

R(reflections)= 0.0900(9251)   wR2(reflections)= 0.3012(19020)

S = 0.981   Npar= 1042

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

🟠 **Alert level B**
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ....   1 Report
            C70

> **Author Response: The Ueq value of C70 is too large, and isotropic refinement was carried out.**

PLAT220_ALERT_2_B NonSolvent   Resd 1 C   Ueq(max)/Ueq(min) Range   9.1 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.**

PLAT242_ALERT_2_B Low   'MainMol' Ueq as Compared to Neighbors of   C32 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   C63 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 ....   0.02653 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**
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..   49% Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ....   0.30 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.02 Report
PLAT213_ALERT_2_C Atom C1   has ADP max/min Ratio .....   3.1 oblate
PLAT213_ALERT_2_C Atom C4   has ADP max/min Ratio .....   3.5 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1 O   Ueq(max)/Ueq(min) Range   4.9 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.

```
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        10.0 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O8 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O10 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O11 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C12 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C45 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Gd1 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       Gd5 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        N7 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        C6 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       C25 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       C30 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       C54 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       C65 Check
```

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

```
PLAT244_ALERT_4_C Low     'Solvent' Ueq as Compared to Neighbors of        C64 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       N13      0.166 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       N14      0.173 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O1W      0.120 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O2W      0.150 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O3W      0.187 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O5W      0.223 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O4W      0.140 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C9        -C14       .     1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C49       -C54       .     1.37 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond C65       - C66       .     1.40 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond C25       - C29       .     1.41 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond C46       - C47       .     1.35 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N3        --H3       .     Please Check
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⬤ **Alert level G**

```
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:   C285 H330.5 Gd14 N57.5 O104
           Atom count from _chemical_formula_moiety:C283 H318.5 Gd14 N57.5 O100
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:C285 H330.5 Gd14 N57.5 O104
           Atom count from the _atom_site data:  C280 H296 Gd14 N56 O100
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  C285 H330.5 Gd14 N57.5 O104
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        570.00    560.00   10.00
           H        661.00    592.00   69.00
           Gd        28.00     28.00    0.00
           N        115.00    112.00    3.00
           O        208.00    200.00    8.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        9 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       11 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       10 Report
            H1    H3    H4    H4A   H7    H8    H21   H22   H23   H25
PLAT041_ALERT_1_G Calc. and Reported SumFormula   Strings  Differ    Please Check
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                  Calc: C280 H296 Gd14 N56 O100
                  Rep.: C285 H330.5 Gd14 N57.5 O104
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
                  Calc: C264 H272 Gd14 N48 O91, 8(C2 H3 N), 9(O)
                  Rep.: C264 H272 Gd14 N48 O91, 8(C2 H3 N), 9(H2 O),
                     1.5[CH3CN], 2[CH3OH], 2[H2O]
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       7 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records       1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records       5 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H1         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1W        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2W        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3W        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O5W        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4W        Constrained at     0.25 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)     100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    5)     100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    6)     100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    7)     100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    8)     100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    4)     0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    5)     0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    6)     0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    7)     0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    8)     0.25 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    O1W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    O2W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    O3W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    O5W Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....    O4W Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H1       ..H2     .     2.14 Ang.
                                             x,y,z  =     1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H4A      ..H35    .     2.13 Ang.
                                             x,y,z  =     1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O12      ..C69    .     2.97 Ang.
                                             x,y,z  =     1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........      ! Info
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      2 Note
           C2 H3 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      6 Note
           O
PLAT794_ALERT_5_G Tentative Bond Valency for Gd2       (III)    .     2.96 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Gd3       (III)    .     3.31 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Gd4       (III)    .     2.76 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     78 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 ...........    2.1 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      3 Units
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   0 ALERT level A = Most likely a serious problem – resolve or explain
   5 ALERT level B = A potentially serious problem, consider carefully
  39 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  49 ALERT level G = General information/check it is not something unexpected
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  6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 50 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
 26 ALERT type 4 Improvement, methodology, query or suggestion
  5 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