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: 170624g

Bond precision: C-C = 0.0165 A Wavelength=0.71073

Cell: a=14.2222(13) b=33.248(3) c=19.3213(17)
alpha=90 beta=105.913(3) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	8786.2(14)	8786.0(13)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	?
Moiety formula	2(C76 H56 Fe4 Gd N8 O20), 7(C5 H5 N), 2(C5 H6 N)	?
Sum formula	C197 H159 Fe8 Gd2 N25 O40	C98.50 H79.50 Fe4 Gd N12.50 O20
Mr	4277.80	2138.90
Dx,g cm-3	1.617	1.617
Z	2	4
Mu (mm-1)	1.472	1.472
F000	4344.0	4344.0
F000’	4350.51	
h,k,lmax	16,39,22	16,39,22
Nref	15496	15469
Tmin,Tmax	0.649,0.745	0.542,0.695
Tmin’	0.496	

Correction method= # Reported T Limits: Tmin=0.542 Tmax=0.695
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.020

R(reflections)= 0.0681(10476) wR2(reflections)= 0.1514(15469)

S = 1.082 Npar= 1225

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

Alert level C

```
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        4.0 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   N7       --C71       .        6.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference N8       --C76             0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N13      --C97             0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N13      --C99             0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C97      --C98             0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C98      --C99             0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C70 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C75 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C97 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C99 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C94 Check
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C90 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C93 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C95 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.6 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist C37      -C42           1.36 Ang.
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist C44      -C49           1.37 Ang.
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist C51      -C56           1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C1       -C6            1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C15      -C20           1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01649 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H26      ..H53             2.14 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H92      ..H97             2.12 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H96      ..H99             2.02 Ang.
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         35 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        137 Report
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      72.00 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of N13        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C98        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H98        Constrained at        0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        27% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  N12      ..C99             2.54 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  N12      ..C97             2.66 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C92      ..C97             3.13 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C96      ..C99             3.07 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
            C5 H5 N
PLAT794_ALERT_5_G Tentative Bond Valency for Gd1       (III)     .       3.69 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (III)     .       3.26 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (III)     .       3.29 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe3       (III)     .       3.27 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe4       (III)     .       3.24 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       4177 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2018 Note
```

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

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 21 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
 17 ALERT type 4 Improvement, methodology, query or suggestion
  7 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 23/04/2018; check.def file version of 23/04/2018

Datablock 170624g - ellipsoid plot