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: mo_d8v3223_0m

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Bond precision:   C-C = 0.0124 A            Wavelength=0.71073

Cell:          a=12.2312(9)      b=16.0108(12)      c=20.7089(16)
               alpha=90          beta=90            gamma=90
Temperature:   122 K

               Calculated              Reported
Volume         4055.5(5)               4055.5(5)
Space group    P 21 21 21              P 21 21 21
Hall group     P 2ac 2ab               P 2ac 2ab
Moiety formula C30 H24 F18 Fe Gd O12   C30 H24 F18 Fe Gd O12
Sum formula    C30 H24 F18 Fe Gd O12   C30 H24 F18 Fe Gd O12
Mr             1131.59                 1131.59
Dx,g cm-3      1.853                   1.853
Z              4                       4
Mu (mm-1)      2.117                   2.117
F000           2208.0                  2208.0
F000'          2210.60
h,k,lmax       14,19,24                14,19,24
Nref           7153[ 3996]             7119
Tmin,Tmax      0.834,0.890             0.576,0.745
Tmin'          0.834

Correction method= # Reported T Limits: Tmin=0.576 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.78/1.00      Theta(max)= 25.025

R(reflections)= 0.0344( 6777)     wR2(reflections)= 0.0838( 7119)

S = 1.254                  Npar= 579
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The following ALERTS were generated. Each ALERT has the format
　　　　test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full          ! Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       6.90 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.13 Report
PLAT213_ALERT_2_C Atom F13          has ADP max/min Ratio .....         3.2 prolat
PLAT213_ALERT_2_C Atom F16          has ADP max/min Ratio .....         3.4 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1  F   Ueq(max)/Ueq(min) Range     3.8 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference F19      --C6AA           0.18 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.01237 Ang.
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       2 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......  Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large   14.19 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records       2 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of    C3AA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of    C6AA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of    C0BA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of     C12 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of     C14 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of     C15 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )      5% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      31 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Gd1       (III)    .    3.42 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2       (III)    .    3.11 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      12 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...       5 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

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