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_d8v3317_0m

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Bond precision:   C-C = 0.0116 A            Wavelength=0.71073

Cell:             a=12.386(2)      b=15.853(2)       c=20.547(2)
                  alpha=90         beta=90           gamma=90
Temperature:      122 K

                  Calculated                 Reported
Volume            4034.5(9)                  4034.5(9)
Space group       P 21 21 21                 P 21 21 21
Hall group        P 2ac 2ab                  P 2ac 2ab
Moiety formula    C30 H24 F18 Ga Gd O12      C30 H24 F16.5 Ga Gd O12,
                                             1.5(F)
Sum formula       C30 H24 F18 Ga Gd O12      C30 H24 F18 Ga Gd O12
Mr                1145.46                    1145.46
Dx,g cm-3         1.886                      1.886
Z                 4                          4
Mu (mm-1)         2.437                      2.437
F000              2228.0                     2228.0
F000'             2230.11
h,k,lmax          16,20,27                   16,20,27
Nref              9738[ 5384]                9691
Tmin,Tmax         0.726,0.789                0.516,0.746
Tmin'             0.628

Correction method= # Reported T Limits: Tmin=0.516 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.80/1.00      Theta(max)= 27.981

R(reflections)= 0.0376( 8857)     wR2(reflections)= 0.0967( 9691)

S = 1.042                   Npar= 675
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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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PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       7.98 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.24 Report
PLAT215_ALERT_3_C Disordered F3#      has ADP max/min Ratio .....        4.0 Note
PLAT215_ALERT_3_C Disordered F4#      has ADP max/min Ratio .....        3.5 Note
PLAT215_ALERT_3_C Disordered F8#      has ADP max/min Ratio .....        3.2 Note
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range       4.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference F10      --C7BA             0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F6AA     --C5BA             0.20 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      F6AA Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01158 Ang.
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⬤ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      31 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       8 Report
PLAT012_ALERT_1_G No      _shelx_res_checksum Found in CIF ......  Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large   12.76 Why ?
PLAT153_ALERT_1_G The s.u.'s on the Cell Axes   are Equal ..(Note)   0.002 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records       4 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C5 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    C5AA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of    C7AA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of    C1BA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of     C14 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3        Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3AA      Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4AA      Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9        Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10       Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C0BA      Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9AA      Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4BA      Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17       Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6        Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8        Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11       Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9BA      Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5BA      Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6BA      Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8BA      Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C0CA      Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7BA      Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9AA      Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4BA      Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17       Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6        Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8        Constrained at      0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9BA      Constrained at      0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )      19% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  F1       ..C0AA          2.96 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      49 Note
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PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.23 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C17      --C8BA           1.98 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C3AA     --C6             1.91 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        97 Check
           C8BA -O0AA -C9      1.555   1.555   1.555        40.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        99 Check
           C3AA -O1AA -C6BA    1.555   1.555   1.555        43.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       114 Check
           C9   -C17  -C8BA    1.555   1.555   1.555        22.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       133 Check
           C6BA -C3AA -C6      1.555   1.555   1.555        43.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       159 Check
           C9   -C14  -C8BA    1.555   1.555   1.555        32.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       184 Check
           C6BA -C7AA -C3AA    1.555   1.555   1.555        34.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       207 Check
           C0BA -C1BA -C11     1.555   1.555   1.555        38.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       245 Check
           C7AA -C6BA -F5AA    1.555   1.555   1.555        42.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       250 Check
           C6BA -C6   -C3AA    1.555   1.555   1.555        27.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       257 Check
           C9   -C8BA -C17     1.555   1.555   1.555        37.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       263 Check
           C14  -C8BA -F11     1.555   1.555   1.555        42.80 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group #        36 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Ga2       (III)    .      3.31 Info
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and s.u.      0.02 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        75 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         1 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
 10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 61 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 16 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
 44 ALERT type 4 Improvement, methodology, query or suggestion
  1 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