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_d8v3299_0m

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Bond precision:   C-C = 0.0101 A              Wavelength=0.71073

Cell:              a=12.495(4)      b=15.905(5)       c=20.533(6)
                   alpha=90         beta=90           gamma=90
Temperature:       122 K

                   Calculated                 Reported
Volume             4081(2)                    4081(2)
Space group        P 21 21 21                 P 21 21 21
Hall group         P 2ac 2ab                  P 2ac 2ab
Moiety formula     C30 H24 F18 Ga O12 Pr      C30 H24 F18 Ga O12 Pr
Sum formula        C30 H24 F18 Ga O12 Pr      C30 H24 F18 Ga O12 Pr
Mr                 1129.12                    1129.12
Dx,g cm-3          1.838                      1.838
Z                  4                          4
Mu (mm-1)          1.978                      1.978
F000               2208.0                     2208.0
F000'              2209.92
h,k,lmax           17,22,29                   17,22,29
Nref               12568[ 6897]               12538
Tmin,Tmax          0.566,0.597                0.629,0.746
Tmin'              0.555

Correction method= # Reported T Limits: Tmin=0.629 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.82/1.00       Theta(max)= 30.619

R(reflections)= 0.0431( 11438)     wR2(reflections)= 0.1074( 12538)

S = 1.060                  Npar= 715
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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 B

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PLAT220_ALERT_2_B Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range       8.3 Ratio
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Alert level C

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PLAT213_ALERT_2_C Atom F18            has ADP max/min Ratio .....      3.1 prolat
PLAT213_ALERT_2_C Atom C8AA           has ADP max/min Ratio .....      3.2 prolat
PLAT213_ALERT_2_C Atom C7             has ADP max/min Ratio .....      3.2 prolat
PLAT215_ALERT_3_C Disordered F9       has ADP max/min Ratio .....      3.2 Note
PLAT220_ALERT_2_C Non-Solvent  Resd 1  F   Ueq(max)/Ueq(min) Range      3.9 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1   H   Uiso(max)/Uiso(min) Range     5.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference F4AA    --C7             0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O10     --C6BA           0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O12     --C2             0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C7      --C9AA           0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C9      --C7AA           0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     O19 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.01008 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #       1 Note
                  C30 H24 F18 Ga O12 Pr
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      24 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       3 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   13.17 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records       3 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for   O9      --C2BA     .      7.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   O9      --C9BA     .      5.4 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   F6AA    --C9       .      5.7 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C1AA    --C6AA     .      5.4 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C5      --C8AA     .      9.9 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of    C1AA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C3 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of    C8AA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C7 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9AA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8AA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7AA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F16       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5        Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6AA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7AA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1BA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9AA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C0BA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2BA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3BA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15       Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5BA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4BA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6BA      Constrained at     0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7BA      Constrained at     0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C8BA        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9BA        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C0CA        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H0BA        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3BA        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5BA        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4BA        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H15         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8BA        Constrained at       0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         29% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  F0AA      ..C11            2.97 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F6        ..C3BA           2.93 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F6        ..F9AA           2.71 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       47 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.26 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C5       --C4BA          2.00 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C15      --C4            2.03 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C2BA     --C0CA          1.74 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       77 Check
          C4   -O5   -C6AA    1.555   1.555   1.555          44.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      104 Check
          C14  -F4   -C0CA    1.555   1.555   1.555          18.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      105 Check
          F7AA -F4   -C14     1.555   1.555   1.555          42.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      140 Check
          F16  -C14  -F8AA    1.555   1.555   1.555          22.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      153 Check
          C0CA -C14  -F16     1.555   1.555   1.555           9.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      158 Check
          C0CA -C14  -F8AA    1.555   1.555   1.555          28.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      160 Check
          F7AA -C14  -F4      1.555   1.555   1.555          30.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      173 Check
          C0CA -F16  -C14     1.555   1.555   1.555           7.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      186 Check
          C6AA -C1AA -C4      1.555   1.555   1.555          34.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      196 Check
          C2   -C5   -C4BA    1.555   1.555   1.555          40.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      200 Check
          C14  -F9   -C0CA    1.555   1.555   1.555          21.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      201 Check
          C14  -F9   -F7AA    1.555   1.555   1.555          38.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      215 Check
          C2   -C8AA -C5      1.555   1.555   1.555          36.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      216 Check
          C6AA -C15  -C4      1.555   1.555   1.555          24.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      250 Check
          C9AA -C7   -C7BA    1.555   1.555   1.555          41.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      272 Check
          C14  -C2BA -C0CA    1.555   1.555   1.555          19.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      278 Check
          C3   -F10  -C6BA    1.555   1.555   1.555          42.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      298 Check
          C6AA -C4   -C15     1.555   1.555   1.555          37.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      304 Check
          C2   -C4BA -C5      1.555   1.555   1.555          27.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      308 Check
          C3   -C6BA -F10     1.555   1.555   1.555          44.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      334 Check
          C0CA -C9BA -C14     1.555   1.555   1.555          20.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      335 Check
          C0CA -C9BA -F16     1.555   1.555   1.555          28.90 Deg.
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PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       341 Check
          C0CA -F9AA -C14      1.555   1.555   1.555           24.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       342 Check
          C0CA -F9AA -F16      1.555   1.555   1.555           26.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       343 Check
          F16  -F8AA -C14      1.555   1.555   1.555           40.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       344 Check
          F16  -F8AA -C0CA     1.555   1.555   1.555           29.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       345 Check
          C0CA -F8AA -C14      1.555   1.555   1.555           11.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       354 Check
          C14  -C0CA -F7AA     1.555   1.555   1.555           37.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       360 Check
          F16  -C0CA -F8AA     1.555   1.555   1.555           31.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       377 Check
          F7AA -C0CA -F4       1.555   1.555   1.555           23.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       386 Check
          C14  -F7AA -C0CA     1.555   1.555   1.555           23.20 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        16 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Ga2        (III)    .       3.32 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        42 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         3 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  92 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  25 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
  74 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