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_d8v3322_0m

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Bond precision:   C-C = 0.0163 A            Wavelength=0.71073

Cell:           a=12.5084(11)     b=15.8220(13)      c=20.5746(18)
                alpha=90          beta=90            gamma=90
Temperature:    122 K

                Calculated                  Reported
Volume          4071.9(6)                   4071.9(6)
Space group     P 21 21 21                  P 21 21 21
Hall group      P 2ac 2ab                   P 2ac 2ab
                                            C30 H24 Cr F16.5 Gd O12,
Moiety formula  C30 H24 Cr F18 Gd O12       1.5(F)
Sum formula     C30 H24 Cr F18 Gd O12       C30 H24 Cr F18 Gd O12
Mr              1127.74                     1127.74
Dx,g cm-3       1.840                       1.840
Z               4                           4
Mu (mm-1)       2.019                       2.019
F000            2200.0                      2200.0
F000'           2202.51
h,k,lmax        15,19,25                    15,19,25
Nref            7787[ 4337]                 7736
Tmin,Tmax       0.704,0.820                 0.619,0.745
Tmin'           0.690

Correction method= # Reported T Limits: Tmin=0.619 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.78/0.99      Theta(max)= 25.735

R(reflections)= 0.0476( 7430)      wR2(reflections)= 0.1159( 7736)

S = 1.057                  Npar= 674
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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
PLAT234_ALERT_4_B Large Hirshfeld Difference F7A   --C0BA   0.28 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference O18   --C9BA   0.27 Ang.

🟡 Alert level C
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ....   6.43 Note
PLAT213_ALERT_2_C Atom F2AA   has ADP max/min Ratio .....   3.3 prolat
PLAT215_ALERT_3_C Disordered F7   has ADP max/min Ratio .....   3.7 Note
PLAT220_ALERT_2_C Non-Solvent Resd 1 C   Ueq(max)/Ueq(min) Range   4.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   F5AA   --C3AA   .   5.9 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F4   --C11   0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F4AA   --C0BA   0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F9   --C10   0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F20   --C11   0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O18   --C1BA   0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O19   --C6BA   0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C5AA   --C8   0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C11   --C1BA   0.23 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O0AA Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.01633 Ang.

⚪ Alert level G
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 ...   11 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   30.02 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   5 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   C6 Check
PLAT242_ALERT_2_G Low   'MainMol' Ueq as Compared to Neighbors of   C8 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   C10 Check
PLAT242_ALERT_2_G Low   'MainMol' Ueq as Compared to Neighbors of   C11 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4AA   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4AB   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7A   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8A   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 C4AA   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5AA   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9   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 C8AA   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 C2BA   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 C4BA   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7BA   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 C8BA   Constrained at   0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of C3BA        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20         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 C9BA        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1CA        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4AA        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8AA        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 H7BA        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H0CA        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20         Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        19% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....    C7AA Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      48 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .    1.20 Ratio
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C4AA     --C5BA         1.99 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C5AA     --C7BA         1.95 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      90 Check
          C5BA -O2  -C5     1.555   1.555   1.555            41.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #      95 Check
          C5AA -O4  -C8BA   1.555   1.555   1.555            43.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     126 Check
          C5   -C6  -C5BA   1.555   1.555   1.555            33.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     154 Check
          C5   -C4AA-C5BA   1.555   1.555   1.555            23.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     166 Check
          C8BA -C8  -C5AA   1.555   1.555   1.555            33.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     176 Check
          C2BA -C10 -C1CA   1.555   1.555   1.555            41.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     186 Check
          C8BA -C5AA-C7BA   1.555   1.555   1.555            41.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     233 Check
          C8BA -C7BA-C5AA   1.555   1.555   1.555            26.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     253 Check
          C5   -C5BA-C4AA   1.555   1.555   1.555            37.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #     261 Check
          C11  -C9BA-F3AA   1.555   1.555   1.555            41.90 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #      38 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cr2      (III)    .    3.22 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      90 Note
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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   2 **ALERT level B** = A potentially serious problem, consider carefully
  15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  62 **ALERT level G** = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 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
  56 ALERT type 4 Improvement, methodology, query or suggestion
   1 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