checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Cu-Gd-valen-dca

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: Cu-Gd-valen-dca

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Bond precision:   C-C = 0.0151 A          Wavelength=0.71073

Cell:             a=8.8191(7)     b=16.5598(14)       c=20.0787(18)
                  alpha=90        beta=91.748(2)      gamma=90
Temperature:      298 K

                 Calculated                  Reported
Volume           2931.0(4)                   2931.0(4)
Space group      P 21/n                      P 21/n
Hall group       -P 2yn                      -P 2yn
Moiety formula   C22 H28 Cl Cu Gd N6 O10     C22 H28 Cl Cu Gd N6 O10
Sum formula      C22 H28 Cl Cu Gd N6 O10     C22 H28 Cl Cu Gd N6 O10
Mr               792.75                      792.74
Dx,g cm-3        1.796                       1.797
Z                4                           4
Mu (mm-1)        3.121                       3.121
F000             1568.0                      1568.0
F000'            1569.81
h,k,lmax         10,19,23                    10,19,23
Nref             5174                        5137
Tmin,Tmax        0.255,0.305                 0.255,0.305
Tmin'            0.236

Correction method= # Reported T Limits: Tmin=0.255 Tmax=0.305
AbsCorr = MULTI-SCAN

Data completeness= 0.993           Theta(max)= 25.010

R(reflections)= 0.0822( 2559)                wR2(reflections)=
                                             0.2086( 5137)
S = 0.788                  Npar= 346
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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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PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on       Gd1       1.83 eA-3
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Author Response: Gd1 is a heavy atom and this alert is often found for molecules of this type.

Alert level C

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GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      0.788
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.176
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full          ! Check
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........      0.176 Report
PLAT213_ALERT_2_C Atom O7              has ADP max/min Ratio .....        3.1 oblate
PLAT234_ALERT_4_C Large Hirshfeld Difference O4       --C18      .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O6       --N3       .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C10      --C11      .       0.20 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         N5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C19 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C20 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01507 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.122 Report
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595        33 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.12Ang From Gd1            2.05 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.05Ang From Gd1            2.04 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.05Ang From Gd1            1.89 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.94Ang From O1       .      0.75 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H18C       .     -0.35 eA-3
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         1 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         4 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    150.00 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)       .      2.35 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         6 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        15 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       2.7 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged    Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..      50.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
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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
 20 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 13 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
  8 ALERT type 3 Indicator that the structure quality may be low
  4 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 28/11/2022; check.def file version of 28/11/2022

Datablock Cu-Gd-valen-dca - ellipsoid plot