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: w276

```
Bond precision:  C-C = 0.0126 A          Wavelength=0.71073

Cell:           a=12.4772(9)    b=9.7307(7)       c=21.9059(17)
                alpha=90        beta=93.201(2)    gamma=90
Temperature:    273 K

                Calculated                Reported
Volume          2655.5(3)                 2655.5(3)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C20 H21 Cu Dy N5 O15      C20 H21 Cu Dy N5 O15
Sum formula     C20 H21 Cu Dy N5 O15      C20 H22 Cu Dy N5 O15
Mr              797.47                    798.46
Dx,g cm-3       1.995                     1.997
Z               4                         4
Mu (mm-1)       3.677                     3.677
F000            1564.0                    1568.0
F000'           1565.32
h,k,lmax        16,12,28                  16,12,28
Nref            5936                      5889
Tmin,Tmax       0.569,0.667
Tmin'           0.511

Correction method= Not given

Data completeness= 0.992          Theta(max)= 27.222

R(reflections)= 0.0520( 5262)     wR2(reflections)= 0.1342( 5889)

S = 1.178                 Npar= 386
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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

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       0.99 Check
PLAT057_ALERT_3_C Correction for Absorption Required   RT(exp) ...       1.17 Do !
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O11 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N4 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for ..........         C8 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01259 Ang.
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Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C20 H22 Cu1 Dy1 N5 O15
           Atom count from _chemical_formula_moiety:C20 H21 Cu1 Dy1 N5 O15
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C20 H22 Cu1 Dy1 N5 O15
           Atom count from the _atom_site data:  C20 H21 Cu1 Dy1 N5 O15
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C20 H22 Cu Dy N5 O15
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         80.00     80.00    0.00
           H         88.00     84.00    4.00
           Cu         4.00      4.00    0.00
           Dy         4.00      4.00    0.00
           N         20.00     20.00    0.00
           O         60.00     60.00    0.00
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      39.81 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        273 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C8 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C7       - C8       .       1.56 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Dy1       (III)     .       2.94 Info
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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
  10 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   1 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 03/05/2019; check.def file version of 29/04/2019

Datablock w276 - ellipsoid plot