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: CoDy

Bond precision: C-C = 0.0057 A Wavelength=0.71073

Cell: a=11.3913(4) b=13.3809(5) c=15.4188(5)
alpha=103.070(3) beta=98.378(3) gamma=109.653(3)
Temperature: 104 K

	Calculated	Reported
Volume	2092.04(14)	2092.04(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C50 H92 Co2 Dy2 O22, 2(C6 H16 N), C2 N2	C50 H92 Co2 Dy2 O22, 2(C6 H16 N), C2 N2
Sum formula	C64 H124 Co2 Dy2 N4 O22	C64 H124 Co2 Dy2 N4 O22
Mr	1744.53	1744.52
Dx,g cm-3	1.385	1.385
Z	1	1
Mu (mm-1)	2.219	2.219
F000	898.0	898.0
F000’	898.68	
h,k,lmax	14,16,19	14,16,19
Nref	8565	8551
Tmin,Tmax	0.766,0.837	0.627,1.000
Tmin’	0.642	

Correction method= # Reported T Limits: Tmin=0.627 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.371

R(reflections)= 0.0315(7833) wR2(reflections)= 0.0752(8551)

S = 1.071 Npar= 478

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

```
PLAT213_ALERT_2_C Atom C3              has ADP max/min Ratio .....        3.6 prolat
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range       4.9 Ratio
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        O3 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C2 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       C11 Check
PLAT354_ALERT_3_C Short   O-H (X0.82,N0.98A) O1OH   -   H1OH   ...      0.62 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .        52 Ang3
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         2 Report
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........   0.00300 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1    --  O10_a   ..       6.0 su
PLAT300_ALERT_4_G Atom Site Occupancy of >C17    is Constrained at     0.564 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C18    is Constrained at     0.564 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C19    is Constrained at     0.564 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C17B   is Constrained at     0.436 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C18B   is Constrained at     0.436 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C19B   is Constrained at     0.436 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C17_a  is Constrained at     0.564 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C18_a  is Constrained at     0.564 Check
PLAT300_ALERT_4_G Atom Site Occupancy of >C19_a  is Constrained at     0.564 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C17B_a is Constrained at     0.436 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C18B_a is Constrained at     0.436 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <C19B_a is Constrained at     0.436 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =           8 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         2 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.16 Ratio
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2 Note
              C6 H16 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         3 Note
              C2 N2
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  20 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
  16 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*, 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 29/01/2015; check.def file version of 29/01/2015

Datablock CoDy - ellipsoid plot