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: shelx_Sam_AH179

```
Bond precision:  C-C = 0.0073 A          Wavelength=0.71073

Cell:            a=13.6849(3)     b=22.8267(6)       c=17.7221(4)
                 alpha=90         beta=98.349(2)     gamma=90
Temperature:     120 K
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	Calculated	Reported
Volume	5477.4(2)	5477.4(2)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C19.50 H21 Cl1.50 Dy N4.50 O9), 2(O2)	?
Sum formula	C39 H42 Cl3 Dy2 N9 O22	C39 H42 Cl3 Dy2 N9 O22
Mr	1420.17	1420.16
Dx,g cm-3	1.722	1.722
Z	4	4
Mu (mm-1)	2.936	2.936
F000	2792.0	2792.0
F000’	2793.56	
h,k,lmax	16,27,21	16,27,21
Nref	4849	4835
Tmin,Tmax	0.736,0.863	0.855,1.000
Tmin’	0.676	

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Correction method= # Reported T Limits: Tmin=0.855 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 25.035

R(reflections)= 0.0376( 4155)     wR2(reflections)= 0.0988( 4835)

S = 1.041                  Npar= 352
```

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 A

```
PLAT413_ALERT_2_A Short Inter XH3 .. XHn     H23C     ..H23C            1.69 Ang.
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Author Response: This alert is due to a disordered methyl group of DMF solvent molecule. Short contacts are then to be expected.

Alert level B

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O1W      ..N211            2.82 Ang.
```

Author Response: H-atoms from O1W crystallisation water molecule are missing. Thus, hydrogen bonds occur between the involved O-atoms referred to in the Alert.

Alert level C

```
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        4.8 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        4.1 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C12      - C13      .       1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C22      - C23      .       1.53 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H12C     ..H12C            2.00 Ang.
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Author Response: This alert is due to a disordered methyl group of DMF solvent molecule. Short contacts are then to be expected.

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PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         40 Ang**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 ...          3 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      47.22 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          4 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for   Cl1      --C1        .        8.3 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   Cl11     --C11       .        7.7 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   Cl21     --C21       .        6.3 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C1       --C100      .        8.3 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C11      --C111      .        7.7 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   C21      --C211      .        6.3 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl11       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl21       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N100       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N111       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N211       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C100       Constrained at        0.5 Check
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PLAT300_ALERT_4_G Atom Site Occupancy of C111       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C211       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        10% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C1       -C3_a            1.45 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist. C21      -C23_d           1.44 Ang.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C2D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C3D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C12D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C13D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C22D Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C23D Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          6 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         18 Note
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  32 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  19 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 30/01/2018; check.def file version of 30/01/2018

Datablock shelx_Sam_AH179 - ellipsoid plot