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: yp-cody

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Bond precision:   C-C = 0.0109 A           Wavelength=0.71073

Cell:             a=18.8802(6)     b=18.8802(6)     c=35.8782(15)
                  alpha=90         beta=90          gamma=120
Temperature:      180 K
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	Calculated	Reported
Volume	11075.8(8)	11075.8(8)
Space group	P -3 c 1	P -3 c 1
Hall group	-P 3 2"c	-P 3 2"c
Moiety formula	C78 H94 Co3 Dy3 N6 O25, 9(C2 H3 N), C2 N, 2(Cl)	C78 H94 Co3 Dy3 N6 O25, 2(Cl), 10(C2 H3 N)
Sum formula	C98 H121 Cl2 Co3 Dy3 N16 O25	C98 H124 Cl2 Co3 Dy3 N16 O25
Mr	2658.29	2661.31
Dx,g cm-3	1.594	1.596
Z	4	4
Mu (mm-1)	2.561	2.561
F000	5336.0	5348.0
F000'	5341.01	
h,k,lmax	23,23,43	23,23,43
Nref	7019	7016
Tmin,Tmax	0.530,0.631	0.506,0.581
Tmin'	0.471	

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Correction method= # Reported T Limits: Tmin=0.506 Tmax=0.581
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 25.674
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R(reflections)= 0.0367(4049)

wR2(reflections)= 0.0797(7016)

S = 0.825 Npar= 459

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
Calc: C98 H121 Cl2 Co3 Dy3 N16 O25
Rep.: C98 H124 Cl2 Co3 Dy3 N16 O25

Author Response: The methyl H-atoms on some of the lattice MeCN could not be modelled, but are included in the sum formula in the cif

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C78 H94 Co3 Dy3 N6 O25, 9(C2 H3 N), C2 N, 2(Cl
)
Rep.: C78 H94 Co3 Dy3 N6 O25, 2(Cl), 10(C2 H3 N)

Author Response: The methyl H-atoms on some of the lattice MeCN could not be modelled, but are included in the sum formula in the cif

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.02 Check

Author Response: The methyl H-atoms on some of the lattice MeCN could not be modelled, but are included in the sum formula in the cif

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check

Author Response: The methyl H-atoms on some of the lattice MeCN could not be modelled, but are included in the sum formula in the cif

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C31 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C33 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N31 0.147 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N32 0.121 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01092 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS <= 36 Ang**3

Alert level G

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:C98 H124 Cl2 Co3 Dy3 N16 O25
Atom count from the _atom_site data: C98.00480 H121 Cl2.004900 Co3 Dy

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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  C98 H124 Cl2 Co3 Dy3 N16 O25
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        392.00    392.00    0.00
           H        496.00    484.00   12.00
           Cl         8.00      8.00    0.00
           Co        12.00     12.00    0.00
           Dy        12.00     12.00    0.00
           N         64.00     64.00    0.00
           O        100.00    100.00   -0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         16 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0200 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
              N33A    C35A    C36A    H36A    H36B    H36C    N33B    C35B
              C36B    H36D    H36E    H36F
PLAT300_ALERT_4_G Atom Site Occupancy of N41        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C41        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C42        Constrained at     0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2        Constrained at     0.3333 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    4)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    5)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    6)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    8)        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    7)        0.33 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd    8)        0.33 Check
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing).         C42 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H14      ..H36B     .        2.10 Ang.
                                               y,1-x+y,1-z  =      8_566 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn     H18A     ..H36F     .        1.92 Ang.
                                               y,1-x+y,1-z  =      8_566 Check
PLAT480_ALERT_4_G Long H...A H-Bond Reported H34A     ..N32      .        2.65 Ang.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #           3 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Dy1       (III)     .        2.96 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (III)     .        3.27 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers          1 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         16 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
              -1  2  0,   0  1  0,
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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
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
29 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 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
18 ALERT type 4 Improvement, methodology, query or suggestion
2 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 19/12/2024; check.def file version of 19/12/2024

Datablock yp-cody - ellipsoid plot