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: ps75

Bond precision: C-C = 0.0116 A Wavelength=1.54180

Cell: a=16.231(3) b=9.431(3) c=24.107(3)
alpha=90 beta=108.22(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	3505.2(15)	3505.2(14)
Space group	P 2/c	P 2/c
Hall group	-P 2yc	?
Moiety formula	C42 H18 Ca3 Dy2 N6 O36, 10(O0.50)	?
Sum formula	C42 H18 Ca3 Dy2 N6 O45	C21 H32 Ca1.50 Dy N3 O23
Mr	1771.86	917.12
Dx,g cm-3	1.679	1.738
Z	2	4
Mu (mm-1)	14.139	14.158
F000	1728.0	1836.0
F000’	1697.74	
h,k,lmax	18,10,27	18,10,27
Nref	5725	5642
Tmin,Tmax	0.117,0.120	0.080,0.131
Tmin’	0.005	

Correction method= REFDELF

Data completeness= 0.986 Theta(max)= 63.450

R(reflections)= 0.0620(3767) wR2(reflections)= 0.1888(5642)

S = 1.006 Npar= 445

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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PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O7W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O8W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O9W
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......       O10W
PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of .        158 Ang3
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Alert level C

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CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
            calculated from the _atom_site* data lies outside
            the range 0.99 <> 1.01
           From the CIF: _cell_formula_units_Z                    4
           From the CIF: _chemical_formula_weight           917.12
           TEST: Calculate formula weight from _atom_site_*
           atom     mass    num     sum
           C        12.01   21.00  252.23
           H         1.01    9.00    9.07
           N        14.01    3.00   42.02
           O        16.00   22.50  359.98
           Dy      162.50    1.00  162.50
           Ca       40.08    1.50   60.12
           Calculated formula weight              885.92
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
            Calculated sin(theta_max)/wavelength =    0.5802
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ          ? Check
PLAT043_ALERT_1_C Check Reported Molecular Weight .............     917.12
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ? Check
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O10
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         C4
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Ca1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        Ca2
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds .............     0.0116 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C8     -   C9     ...       1.54 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C13    -   C14    ...       1.53 Ang.
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Alert level G

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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:C21 H32 Ca1.5 Dy1 N3 O23
            Atom count from the _atom_site data:  C21 H9 Ca1.5 Dy1 N3 O22.5
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C21 H32 Ca1.50 Dy N3 O23
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         84.00     84.00    0.00
           H        128.00     36.00   92.00
           Ca         6.00      6.00    0.00
           Dy         4.00      4.00    0.00
           N         12.00     12.00    0.00
           O         92.00     90.00    2.00
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .          3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ? Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by .............       0.50 Ratio
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.13
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed
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PLAT153_ALERT_1_G The su’s on the Cell Axes   are Equal .........    0.00300 Ang.
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature       293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature       293 K
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................        11 %
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H’s ?) .....       O11W
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        17
            O4  -CA2 -O4  -C7    146.00 59.00   3.666   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        61
            O12 -CA3 -O12 -C21     5.00  0.00   3.566   1.555   1.555   1.555
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         2
              O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #         3
              O
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   5 ALERT level B = A potentially serious problem, consider carefully
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  17 ALERT level G = General information/check it is not something unexpected

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   2 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*, 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 01/06/2013; check.def file version of 24/05/2013

Datablock ps75 - ellipsoid plot