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: 1

Bond precision: Dy- O = 0.0001 A Wavelength=1.15450

Cell: a=5.30945(10) b=5.30945(10) c=5.30945(10)
alpha=90 beta=90 gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	149.675(8)	149.674(8)
Space group	F -4 3 m	F -4 3 m
Hall group	F -4 2 3	F -4 2 3
Moiety formula	Dy2 O2, 2(H)	?
Sum formula	Dy2 H2 O2	H O Dy
Mr	359.02	179.51
Dx,g cm-3	7.966	7.966
Z	2	4
Mu (mm-1)	0.000	0.000
F000	75.9	0.0
F000’	299.87	
h,k,lmax	9,9,9	
Nref	62[37]	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.00/0.00 Theta(max)=

R(reflections)= wR2(reflections)=

S = Npar=

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

PLAT305_ALERT_2_A Isolated Hydrogen Atom (Outside Bond Range ??) H2 Check

Ionic hydride, therefore isolated hydride ion

Alert level B

PLAT111_ALERT_2_B ADDSYM Detects New (Pseudo) Centre of Symmetry . 100 %Fit
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem 41 100 %Fit
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem 41 100 %Fit
PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem 43 100 %Fit
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Fd-3m Check

We checked, but Fd-3m is not possible because Z=4 in the current model cannot be realized in Fd-3m (smallest multiplicity is 8) and there are no hints for loss of translational symmetry.

Alert level C

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

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Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT778_ALERT_2_G Check O..H..X Bond in CIF: H2 --O3 2.65 Ang.
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PLAT778_ALERT_2_G Check O..H..X Bond in CIF: O3 --H2 2.65 Ang.

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

3 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
0 ALERT type 3 Indicator that the structure quality may be low
0 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 16/05/2021; check.def file version of 13/05/2021

Datablock 1 - ellipsoid plot