

## 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: I

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Bond precision:	= 0.0000 A	Wavelength=0.71359	
Cell:	a=7.0187 (14) alpha=90	b=7.0187 (14) beta=90	c=6.2385 (11) gamma=90
Temperature:	379 K		
	Calculated	Reported	
Volume	307.32 (13)	307.32 (10)	
Space group	I 41/a m d:	I 41/a m d	
Hall group	I 4bw 2bw -	-I 4bd;-2	
Moiety formula	As3.34 Dy0.29 Er0.15 Gd0.16 Ho0.14 Lu0.06 O16 P0.66 Y3 ? Yb0.10		
Sum formula	As3.34 Dy0.29 Er0.15 Gd0.16 O4 As0.82 P0.17 Y0.76 Ho0.14 Lu0.06 O16 P0.66 Y3 Gd0.04 Er0.04 Ho0.03 Dy0.07 Yb0.10	Yb0.04 Lu0.02	
Mr	943.43	238.00	
Dx, g cm-3	5.098	5.144	
Z	1	4	
Mu (mm-1)	28.944	30.698	
F000	426.1	426.0	
F000'	418.25		
h, k, lmax	9, 9, 8	9, 9, 8	
Nref	122	123	
Tmin, Tmax			
Tmin'			
Correction method=	Not given		
Data completeness=	1.008	Theta (max)= 29.290	

R(reflections)= 0.0932( 94)

wR2(reflections)=

wR= 0.1198( 123)

S = 7.870

Npar= 11

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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.

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### Alert level A

EXPT005\_ALERT\_1\_A \_exptl\_crystal\_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR\_01

GOODF01\_ALERT\_2\_A The least squares goodness of fit parameter lies outside the range 0.40 <> 6.00

Goodness of fit given = 7.870

PLAT183\_ALERT\_1\_A Missing \_cell\_measurement\_reflns\_used Value .... Please Do !

PLAT184\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_min Value ..... Please Do !

PLAT185\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_max Value ..... Please Do !

PLAT699\_ALERT\_1\_A Missing \_exptl\_crystal\_description Value ..... Please Do !

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### Alert level B

RINTA01\_ALERT\_3\_B The value of Rint is greater than 0.18

Rint given 0.194

PLAT020\_ALERT\_3\_B The Value of Rint is Greater Than 0.12 ..... 0.194 Report

PLAT051\_ALERT\_1\_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 5.72 %

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### Alert level C

ABSMU01\_ALERT\_1\_C The ratio of given/expected absorption coefficient lies outside the range 0.99 <> 1.01

Calculated value of mu = 29.381

Value of mu given = 30.698

RADNW01\_ALERT\_1\_C The radiation wavelength lies outside the expected range for the supplied radiation type. Expected range 0.71065-0.71075

Wavelength given = 0.71359

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check

Calc: As0.83 Dy0.07 Er0.04 Gd0.04 Ho0.03 Lu0.02 O4 P0.17 Y0.75 Yb0

Rep.: O4 As0.82 P0.17 Y0.76 Gd0.04 Er0.04 Ho0.03 Dy0

.07 Yb0.04 Lu0.02

PLAT043\_ALERT\_1\_C Calculated and Reported Mol. Weight Differ by .. 8.57 Check

PLAT052\_ALERT\_1\_C Info on Absorption Correction Method Not Given Please Do !

PLAT053\_ALERT\_1\_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054\_ALERT\_1\_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055\_ALERT\_1\_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077\_ALERT\_4\_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 2.27 Report

PLAT127\_ALERT\_1\_C Implicit Hall Symbol Inconsistent with Explicit -I 4bd;-2 Check

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### 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: As0.82 Dy.07 Er.04 Gd.04 Ho.03 L  
 Atom count from the \_atom\_site data: As0.8349 Dy.0735 Er.0379 Gd.0393  
 CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
 CELLZ01\_ALERT\_1\_G ALERT: check formula stoichiometry or atom site occupancies.  
 From the CIF: \_cell\_formula\_units\_Z 4  
 From the CIF: \_chemical\_formula\_sum O4 As0.82 P0.17 Y0.76 Gd0.04 Er0.0  
 TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
O	16.00	16.00	0.00
As	3.28	3.34	-0.06
P	0.68	0.66	0.02
Y	3.04	3.01	0.03
Gd	0.16	0.16	0.00
Er	0.16	0.15	0.01
Ho	0.12	0.14	-0.02
Dy	0.28	0.29	-0.01
Yb	0.16	0.10	0.06
Lu	0.08	0.06	0.02

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF	Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...	0.250 Check
PLAT120_ALERT_1_G Reported I41/amd Inconsistent with Explicit	I41/amd Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...	3 Units
PLAT300_ALERT_4_G Atom Site Occupancy of Lu Constrained at	0.0151 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Yb Constrained at	0.0261 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Er Constrained at	0.0379 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ho Constrained at	0.0348 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Dy Constrained at	0.0735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Gd Constrained at	0.0393 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Y Constrained at	0.7517 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As Constrained at	0.8349 Check
PLAT300_ALERT_4_G Atom Site Occupancy of P Constrained at	0.1651 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1)	79% Note
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....	! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0 Sig(I)
PLAT982_ALERT_1_G The As-f' = 0.0511 Deviates from IT-value =	0.0499 Check
PLAT982_ALERT_1_G The Dy-f' = -0.1320 Deviates from IT-value =	-0.1892 Check
PLAT982_ALERT_1_G The Er-f' = -0.2056 Deviates from IT-value =	-0.2586 Check
PLAT982_ALERT_1_G The Gd-f' = -0.0996 Deviates from IT-value =	-0.1653 Check
PLAT982_ALERT_1_G The Ho-f' = -0.1634 Deviates from IT-value =	-0.2175 Check
PLAT982_ALERT_1_G The Lu-f' = -0.4188 Deviates from IT-value =	-0.4720 Check
PLAT982_ALERT_1_G The P-f' = 0.1048 Deviates from IT-value =	0.1023 Check
PLAT982_ALERT_1_G The Y-f' = -2.9793 Deviates from IT-value =	-2.7962 Check
PLAT982_ALERT_1_G The Yb-f' = -0.3326 Deviates from IT-value =	-0.3850 Check
PLAT983_ALERT_1_G The As-f'' = 2.0283 Deviates from IT-Value =	2.0058 Check
PLAT983_ALERT_1_G The Dy-f'' = 4.4885 Deviates from IT-Value =	4.4098 Check
PLAT983_ALERT_1_G The Er-f'' = 5.0438 Deviates from IT-Value =	4.9576 Check
PLAT983_ALERT_1_G The Gd-f'' = 3.9799 Deviates from IT-Value =	3.9035 Check
PLAT983_ALERT_1_G The Ho-f'' = 4.7604 Deviates from IT-Value =	4.6783 Check
PLAT983_ALERT_1_G The Lu-f'' = 5.9646 Deviates from IT-Value =	5.8584 Check
PLAT983_ALERT_1_G The P-f'' = 0.0969 Deviates from IT-Value =	0.0942 Check
PLAT983_ALERT_1_G The Y-f'' = 3.5765 Deviates from IT-Value =	3.5667 Check
PLAT983_ALERT_1_G The Yb-f'' = 5.6460 Deviates from IT-Value =	5.5486 Check

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

39 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 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  
10 ALERT type 4 Improvement, methodology, query or suggestion  
5 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.

Datablock 1 - ellipsoid plot

