

## 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=0.41066	
Cell:	a=7.0150(2)	b=7.0150(2)	c=6.2590(3)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	308.01(2)	308.007(19)	
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 <sup>-3</sup>	5.086	5.132	
Z	1	4	
Mu (mm <sup>-1</sup> )	6.695	6.875	
F000	426.1	426.0	
F000'	427.02		
h, k, lmax	11, 11, 10	3, 11, 10	
Nref	210	97	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.462      Theta(max)= 19.920

R(reflections)= 0.0325( 85)

wR2(reflections)=

wR= 0.0371( 97)

S = 2.120

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

PLAT027_ALERT_3_A _diffrn_reflths_theta_full value (too) Low .....	10.52 Degree
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .	0.740 Why?
PLAT183_ALERT_1_A Missing _cell_measurement_reflths_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 C

GOODF01\_ALERT\_2\_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00

Goodness of fit given = 2.120

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

PLAT051\_ALERT\_1\_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.62 %

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

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

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu

not performed for this radiation type.

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
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O	16.00	16.00	0.00
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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
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.41066	Ang.
PLAT120_ALERT_1_G	Reported I41/amd Inconsistent with Explicit	I41/amd	Check
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3	Note
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature ..... (K)	293	Check
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 !
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	8	Units
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0	Sig(I)
PLAT984_ALERT_1_G	The As-f' = 0.2878 Deviates from the B&C-Value	0.2864	Check
PLAT984_ALERT_1_G	The Dy-f' = -0.6999 Deviates from the B&C-Value	-0.6916	Check
PLAT984_ALERT_1_G	The Er-f' = -0.6332 Deviates from the B&C-Value	-0.6207	Check
PLAT984_ALERT_1_G	The Gd-f' = -0.7802 Deviates from the B&C-Value	-0.7780	Check
PLAT984_ALERT_1_G	The Ho-f' = -0.6648 Deviates from the B&C-Value	-0.6545	Check
PLAT984_ALERT_1_G	The Lu-f' = -0.5571 Deviates from the B&C-Value	-0.5418	Check
PLAT984_ALERT_1_G	The Y-f' = 0.2097 Deviates from the B&C-Value	0.2116	Check
PLAT984_ALERT_1_G	The Yb-f' = -0.5804 Deviates from the B&C-Value	-0.5650	Check
PLAT985_ALERT_1_G	The As-f" = 0.7669 Deviates from the B&C-Value	0.7641	Check
PLAT985_ALERT_1_G	The Dy-f" = 1.7292 Deviates from the B&C-Value	1.7162	Check
PLAT985_ALERT_1_G	The Er-f" = 1.9570 Deviates from the B&C-Value	1.9421	Check
PLAT985_ALERT_1_G	The Gd-f" = 1.5225 Deviates from the B&C-Value	1.5097	Check
PLAT985_ALERT_1_G	The Ho-f" = 1.8406 Deviates from the B&C-Value	1.8265	Check
PLAT985_ALERT_1_G	The Lu-f" = 2.3386 Deviates from the B&C-Value	2.3193	Check
PLAT985_ALERT_1_G	The Yb-f" = 2.2053 Deviates from the B&C-Value	2.1884	Check

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- 7 **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
  - 42 **ALERT level G** = General information/check it is not something unexpected

36 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

2 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  
12 ALERT type 4 Improvement, methodology, query or suggestion  
6 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.

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**PLATON version of 13/05/2024; check.def file version of 04/05/2024**

Datablock I - ellipsoid plot

