

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

Bond precision:	= 0.0000 A	Wavelength=0.71359	
Cell:	a=7.0220 (14)	b=7.0220 (14)	c=6.2433 (11)
	alpha=90	beta=90	gamma=90
Temperature:	523 K		
	Calculated	Reported	
Volume	307.85 (13)	307.85 (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	5.089	5.135	
Z	1	4	
Mu (mm ⁻¹)	28.894	30.646	
F000	426.1	426.0	
F000'	418.25		
h, k, lmax	9, 9, 8	9, 9, 8	
Nref	123	111	
Tmin, Tmax			
Tmin'			
Correction method=	Not given		
Data completeness=	0.902	Theta (max)=	29.280

R(reflections)= 0.0593(83)

wR2(reflections)=

wR= 0.0658(111)

S = 3.960

Npar= 11

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

EXPT005_ALERT_1_A _exptl_crystal_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR_01

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 !

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18

Rint given 0.192

PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 5.72 %

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 = 29.330

Value of mu given = 30.646

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies

outside the range 0.80 <> 2.00

Goodness of fit given = 3.960

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 2.04 Report

PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -I 4bd;-2 Check

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 !
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12	0.192	Report
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

5 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
41 **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

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

Datablock I - ellipsoid plot

