

## 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=0.41029	
Cell:	a=6.8043(2)	b=6.8043(2)	c=6.0161(1)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	278.536(17)	278.536(12)	
Space group	I 41/a m d:	I 41/a m d	
Hall group	I 4bw 2bw -	-I 4bd;-2	
	As0.42 Dy0.29 Er0.16 Gd0.19		
Moiety formula	Ho0.15 O16 P3.58 Y3.07	?	
	Yb0.14		
	As0.42 Dy0.29 Er0.16 Gd0.19	As0.11 Dy0.07 Er0.05 Gd0.05	
Sum formula	Ho0.15 O16 P3.58 Y3.07	Ho0.04 O4 P0.89 Y0.77	
	Yb0.14	Yb0.03	
Mr	824.33	207.70	
Dx, g cm <sup>-3</sup>	4.914	4.952	
Z	1	4	
Mu (mm <sup>-1</sup> )	5.653	5.781	
F000	377.4	377.0	
F000'	377.66		
h, k, lmax	11, 11, 10	5, 10, 10	
Nref	214	127	
Tmin, Tmax		0.637, 1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.637 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.593

Theta(max)= 20.710

R(reflections)= 0.0292( 122)

wR2(reflections)=

wR= 0.0346( 127)

S = 2.700

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

PLAT029\_ALERT\_3\_A \_diffrn\_measured\_fraction\_theta\_full value Low . 0.830 Why?

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 = 2.700

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

Calc: As0.11 Dy0.07 Er0.04 Gd0.05 Ho0.04 O4 P0.89 Y0.77 Yb0.03

Rep.: As0.11 Dy0.07 Er0.05 Gd0.05 Ho0.04 O4 P0.89 Y0

.77 Yb0.03

PLAT043\_ALERT\_1\_C Calculated and Reported Mol. Weight Differ by .. 6.47 Check

PLAT051\_ALERT\_1\_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 2.22 %

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

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 As0.11 Dy0.07 Er0.05 Gd0.05 Ho0.04

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
As	0.44	0.42	0.02
Dy	0.28	0.29	-0.01
Er	0.20	0.16	0.04
Gd	0.20	0.19	0.01
Ho	0.16	0.15	0.01
O	16.00	16.00	0.00
P	3.56	3.58	-0.02
Y	3.08	3.07	0.01
Yb	0.12	0.14	-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
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.41029	Ang.
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 ...	5	Units
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Yb	Constrained at	0.0343 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Er	Constrained at	0.0408 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ho	Constrained at	0.038 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Dy	Constrained at	0.0734 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Gd	Constrained at	0.0464 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Y	Constrained at	0.7671 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of As	Constrained at	0.106 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of P	Constrained at	0.894 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	80%	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	6	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' = 0.2876 Deviates from the B&C-Value	0.2862	Check
PLAT984_ALERT_1_G	The Dy-f' = -0.7013 Deviates from the B&C-Value	-0.6931	Check
PLAT984_ALERT_1_G	The Er-f' = -0.6345 Deviates from the B&C-Value	-0.6220	Check
PLAT984_ALERT_1_G	The Gd-f' = -0.7818 Deviates from the B&C-Value	-0.7795	Check
PLAT984_ALERT_1_G	The Ho-f' = -0.6662 Deviates from the B&C-Value	-0.6559	Check
PLAT984_ALERT_1_G	The Y-f' = 0.2101 Deviates from the B&C-Value	0.2121	Check
PLAT984_ALERT_1_G	The Yb-f' = -0.5816 Deviates from the B&C-Value	-0.5663	Check
PLAT985_ALERT_1_G	The As-f" = 0.7656 Deviates from the B&C-Value	0.7629	Check
PLAT985_ALERT_1_G	The Dy-f" = 1.7265 Deviates from the B&C-Value	1.7135	Check
PLAT985_ALERT_1_G	The Er-f" = 1.9539 Deviates from the B&C-Value	1.9391	Check
PLAT985_ALERT_1_G	The Gd-f" = 1.5201 Deviates from the B&C-Value	1.5073	Check
PLAT985_ALERT_1_G	The Ho-f" = 1.8377 Deviates from the B&C-Value	1.8236	Check
PLAT985_ALERT_1_G	The Yb-f" = 2.2018 Deviates from the B&C-Value	2.1850	Check

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

32 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 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  
10 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.

Datablock I - ellipsoid plot

