

## 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=6.219 (9)      b=6.4574 (12)      c=6.0699 (12)	alpha=90      beta=102.91 (6)      gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	237.6 (4)	237.6 (4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yabc
Moiety formula	As0.42 Dy0.29 Er0.16 Gd0.19 Ho0.15 O16 P3.58 Y3.07 Yb0.14	?
Sum formula	As0.42 Dy0.29 Er0.16 Gd0.19 Ho0.15 O16 P3.58 Y3.07 Yb0.14	As0.11 Dy0.07 Er0.05 Gd0.05 Ho0.04 O4 P0.89 Y0.77 Yb0.03
Mr	824.33	207.70
Dx, g cm <sup>-3</sup>	5.761	5.805
Z	1	4
Mu (mm <sup>-1</sup> )	6.627	6.777
F000	377.4	377.0
F000'	377.66	
h, k, lmax	10, 11, 10	4, 10, 10
Nref	1300	298
Tmin, Tmax		0.430, 1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.430 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.229

Theta (max)= 20.850

R(reflections)= 0.1146( 205)

wR2(reflections)=

wR= 0.1318( 298)

S = 3.170

Npar= 30

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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 _diffn_refl_theta_full value (too) Low .....	12.46 Degree
PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low .	0.390 Why?
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value .....	Please Do !

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### Alert level B

PLAT149_ALERT_3_B s.u. on the beta Angle is Too Large .....	0.06 Degree
P O1 O2 O3 O4	

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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 = 3.170

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
PLAT082_ALERT_2_C High R1 Value .....	0.11 Report
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit	-P 2yabc Check
PLAT148_ALERT_3_C s.u. on the a - Axis is (Too) Large ....	0.009 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	O3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)	2.8 Note

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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.
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)			33% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact As ..04 .			2.96 Ang.
	1/2-x,-1/2+y,3/2-z =			2_546 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact P ..04 .			2.96 Ang.
	1/2-x,-1/2+y,3/2-z =			2_546 Check
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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- 4 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
13 **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

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

6 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 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.

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

Datablock I - ellipsoid plot

