

## 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=6.343 (7)   | b=6.5530 (11)  | c=6.1430 (12) |
|                        | alpha=90  | beta=103.56 (5)  | gamma=90      |
| Temperature:           | 293 K   |  |               |
|                        | Calculated  | Reported   |               |
| Volume                 | 248.2 (3)   | 248.2 (3)  |               |
| 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<br>Ho0.15 O16 P3.58 Y3.07<br>Yb0.14 | ?  |               |
| Sum formula            | As0.42 Dy0.29 Er0.16 Gd0.19<br>Ho0.15 O16 P3.58 Y3.07<br>Yb0.14 | As0.11 Dy0.07 Er0.05 Gd0.05<br>Ho0.04 O4 P0.89 Y0.77<br>Yb0.03 |               |
| Mr                     | 824.33  | 207.70   |               |
| Dx, g cm <sup>-3</sup> | 5.515   | 5.556  |               |
| Z                      | 1   | 4  |               |
| Mu (mm <sup>-1</sup> ) | 6.344   | 6.487  |               |
| F000                   | 377.4   | 377.0  |               |
| F000'                  | 377.66  |  |               |
| h, k, lmax             | 10, 11, 10  | 5, 10, 10  |               |
| Nref                   | 1341  | 295  |               |
| Tmin, Tmax             |   | 0.353, 1.000   |               |
| Tmin'                  |   |  |               |

Correction method= # Reported T Limits: Tmin=0.353 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.220

Theta (max)= 20.760

R(reflections)= 0.1158( 213)

wR2(reflections)=

wR= 0.1326( 295)

S = 3.290

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 \_diffrn\_reflns\_theta\_full value (too) Low ..... 8.45 Degree

PLAT029\_ALERT\_3\_A \_diffrn\_measured\_fraction\_theta\_full value Low . 0.400 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 = 3.290

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 . 2.21 %

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 ..... 0.12 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 .... 0.007 Ang.

PLAT250\_ALERT\_2\_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 3.8 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                     | .                           | 3.08 Ang.     |
|                   |  | $1/2-x, -1/2+y, 3/2-z =$ |                             | 2_546 Check   |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact P                      | ..04                     | .                           | 3.08 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  |                          |                             | 5 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  
0 **ALERT level B** = A potentially serious problem, consider carefully  
12 **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  
5 ALERT type 2 Indicator that the structure model may be wrong or deficient  
4 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

