

## 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: p1**

Bond precision:	C-C = 0.0199 A	Wavelength=1.54184		
Cell:	a=21.3246 (2)	b=21.3246 (2)	c=21.3246 (2)	
	alpha=90	beta=90	gamma=90	
Temperature:	100 K			

	Calculated	Reported
Volume	9697.1(3)	9697.1(3)
Space group	P 21 3	P 21 3
Hall group	P 2ac 2ab 3	P 2ac 2ab 3
Moiety formula	C90 H75 Co3 Dy N6 O12	C90 H75 Co3 Dy1 N6 O12
Sum formula	C90 H75 Co3 Dy N6 O12	C90 H75 Co3 Dy N6 O12
Mr	1771.85	1771.85
Dx, g cm <sup>-3</sup>	1.214	1.214
Z	4	4
Mu (mm <sup>-1</sup> )	8.445	8.445
F000	3600.0	3600.0
F000'	3542.39	
h, k, lmax	26, 26, 26	26, 26, 26
Nref	6587[ 3565]	6587
Tmin, Tmax	0.417, 0.509	0.417, 0.509
Tmin'	0.316	

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Correction method= # Reported T Limits: Tmin=0.417 Tmax=0.509
AbsCorr = MULTI-SCAN
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Data completeness= 1.85/1.00      Theta (max)= 73.858

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R(reflections)= 0.0986( 4592)      wR2(reflections)=
S = 1.051                          0.2660( 5934)
Npar= 331
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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

PLAT602\_ALERT\_2\_A Solvent Accessible VOID(S) in Structure ..... ! Check

**Author Response: Highly disordered solvent. There is likely other components in the disorder that could not be modeled.**

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### Alert level C

CRYSC01\_ALERT\_1\_C The word below has not been recognised as a standard identifier.

crimson

CRYSC01\_ALERT\_1\_C No recognised colour has been given for crystal colour.

DIFMN02\_ALERT\_2\_C The minimum difference density is < -0.1\*ZMAX\*0.75

\_refine\_diff\_density\_min given = -6.077

Test value = -4.950

DIFMN03\_ALERT\_1\_C The minimum difference density is < -0.1\*ZMAX\*0.75

The relevant atom site should be identified.

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C90 H75 Co3 Dy N6 O12

Rep.: C90 H75 Co3 Dy1 N6 O12

PLAT084\_ALERT\_3\_C High wr2 Value (i.e. > 0.25) ..... 0.27 Report

PLAT098\_ALERT\_2\_C Large Reported Min. (Negative) Residual Density -6.08 eA-3

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.2 Ratio

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of Dy01 Check

PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.01993 Ang.

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### Alert level G

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 38 Report

PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check

PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.19 Report

PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 1 Report

PLAT177\_ALERT\_4\_G The CIF-Embedded .res File Contains DELU Records 2 Report

PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 6 Report

PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 2 Report

PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0200 Report

PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT192\_ALERT\_3\_G A Non-default DELU Restraint Value for SecondPar 0.0200 Report

PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Dy01 --O2 . 7.3 s.u.

PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Dy01 --O3 . 8.0 s.u.

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 1 Note  
Dy01

PLAT794\_ALERT\_5\_G Tentative Bond Valency for Dy01 (III) . 3.64 Info

PLAT794\_ALERT\_5\_G Tentative Bond Valency for Col (III) . 3.24 Info

PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 370 Note

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 15 Note

-1 1 5, 3 3 4, -3 3 4, 2 3 3, 0 0 6, 2 1 3,

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      0 0 14,   2 0 3,   0 1 1,  -4 5 6,   0 2 2,   0 0 4,
      1 1 5,  -2 1 3,   0 5 7,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....      3.8 Low

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 1 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
19 ALERT level G = General information/check it is not something unexpected

 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
 8 ALERT type 3 Indicator that the structure quality may be low
 5 ALERT type 4 Improvement, methodology, query or suggestion
 2 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.

