

## 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: p3

Bond precision:	C-C = 0.0191 Å	Wavelength=1.54184	
Cell:	a=21.217(2)	b=21.217(2)	c=21.217(2)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	9551(3)	9551(3)	
Space group	P 21 3	P 21 3	
Hall group	P 2ac 2ab 3	P 2ac 2ab 3	
Moiety formula	C90 H78 Co3 Dy N6 O12	C90 H78 Co3 Dy N6 O12	
Sum formula	C90 H78 Co3 Dy N6 O12	C90 H78 Co3 Dy N6 O12	
Mr	1774.88	1774.88	
Dx, g cm-3	1.234	1.234	
Z	4	4	
Mu (mm-1)	8.574	8.574	
F000	3612.0	3612.0	
F000'	3554.39		
h, k, lmax	26, 26, 26	26, 26, 26	
Nref	6487[ 3513]	6487	
Tmin, Tmax	0.411, 0.504	0.420, 0.511	
Tmin'	0.311		

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Correction method= # Reported T Limits: Tmin=0.420 Tmax=0.511
AbsCorr = MULTI-SCAN
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Data completeness= 1.85/1.00      Theta (max)= 73.928

R(reflections)= 0.0896( 4499)	wR2(reflections)= 0.2403( 5944)
S = 0.993	Npar= 337

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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.

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C27 --C28 . 0.16 Ang.

PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.01907 Ang.

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### Alert level G

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report

PLAT012\_ALERT\_1\_G N.O.K. \_shelx\_res\_checksum Found in CIF ..... Please Check

PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.18 Report

PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 2 Report

PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 3 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

PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Dyl --O2 . 7.0 s.u.

PLAT721\_ALERT\_1\_G Bond Calc 0.96000, Rep 0.97000 Dev... 0.01 Ang.

C30 -H30A 1\_555 1\_555 ..... # 36 Check

PLAT721\_ALERT\_1\_G Bond Calc 0.96000, Rep 0.97000 Dev... 0.01 Ang.

C30 -H30B 1\_555 1\_555 ..... # 37 Check

PLAT721\_ALERT\_1\_G Bond Calc 0.96000, Rep 0.97000 Dev... 0.01 Ang.

C15 -H15A 1\_555 1\_555 ..... # 68 Check

PLAT721\_ALERT\_1\_G Bond Calc 0.96000, Rep 0.97000 Dev... 0.01 Ang.

C15 -H15B 1\_555 1\_555 ..... # 69 Check

PLAT794\_ALERT\_5\_G Tentative Bond Valency for Dyl (III) . 3.40 Info

PLAT794\_ALERT\_5\_G Tentative Bond Valency for Col (III) . 3.39 Info

PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 48 Note

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 5 Note

-1 2 4, 0 2 2, 1 1 5, 1 0 7, 2 0 3,

PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 4.0 Low

PLAT982\_ALERT\_1\_G The Dy-f' = -8.8380 Deviates from IT-value = -9.8046 Check

PLAT983\_ALERT\_1\_G The Dy-f" = 11.9157 Deviates from IT-Value = 9.8477 Check

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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  
5 **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

9 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  
3 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.

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**PLATON version of 06/01/2024; check.def file version of 05/01/2024**

