

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) d772

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: d772

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Bond precision:	C-C = 0.0068 A	Wavelength=0.71070	
Cell:	a=12.6372(2)	b=13.68094(19)	c=26.7692(5)
	alpha=90	beta=103.494(2)	gamma=90
Temperature:	294 K		
	Calculated	Reported	
Volume	4500.33(13)	4500.33(14)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C39 H41 Ho N4 O17 Zn2, C H2 Cl2	C39 H41 Ho N4 O17 Zn2, C H2 Cl2	
Sum formula	C40 H43 Cl2 Ho N4 O17 Zn2	C40 H43 Cl2 Ho N4 O17 Zn2	
Mr	1218.40	1218.35	
Dx, g cm <sup>-3</sup>	1.798	1.798	
Z	4	4	
Mu (mm <sup>-1</sup> )	2.995	2.995	
F000	2432.0	2432.0	
F000'	2435.63		
h,k,lmax	15,16,33	15,16,33	
Nref	8837	8584	
Tmin,Tmax	0.365,0.395	0.846,1.000	
Tmin'	0.337		

Correction method= # Reported T Limits: Tmin=0.846 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.971      Theta(max)= 25.993

R(reflections)= 0.0337( 7124)      wR2(reflections)= 0.0814( 8584)

S = 1.040      Npar= 604

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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 C**

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	Low	.....	0.970	Note
PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min) Range	3.6	Ratio
PLAT242_ALERT_2_C	Low		Ueq as Compared to Neighbors for	.....	C37 Check
PLAT244_ALERT_4_C	Low		'Solvent' Ueq as Compared to Neighbors of		C40 Check
PLAT410_ALERT_2_C	Short Intra H...H Contact	H10	.. H13 ..	1.94	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H16	.. H21 ..	1.96	Ang.

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			4	Note
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details		in the CIF		Please Do !
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT		Unusually Large.	7.81	Why ?
PLAT333_ALERT_2_G	Check Large Av C6-Ring C-C Dist.	C11	-C20	1.42	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C24	.. C30 ..	3.17	Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		.....	3	Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 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  
1 ALERT type 4 Improvement, methodology, query or suggestion  
1 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*, 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 21/06/2015; check.def file version of 21/06/2015**

