

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) BM495-1\_a

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: BM495-1\_a

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Bond precision:	C-C = 0.0048 A	Wavelength=0.71073	
Cell:	a=50.9980(12)	b=10.2764(2)	c=15.3569(4)
	alpha=90	beta=90	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	8048.2(3)	8048.2(3)	
Space group	F d d 2	F d d 2	
Hall group	F 2 -2d	F 2 -2d	
Moiety formula	C28 H18 I10 N2 O4 Zn	?	
Sum formula	C28 H18 I10 N2 O4 Zn	C28 H18 I10 N2 O4 Zn	
Mr	1780.83	1780.81	
Dx, g cm <sup>-3</sup>	2.940	2.939	
Z	8	8	
Mu (mm <sup>-1</sup> )	8.316	8.316	
F000	6336.0	6336.0	
F000'	6303.11		
h, k, lmax	72, 14, 21	72, 14, 21	
Nref	6155[ 3184]	6155	
Tmin, Tmax	0.257, 0.401	0.642, 0.746	
Tmin'	0.234		

Correction method= # Reported T Limits: Tmin=0.642 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.93/1.00      Theta(max)= 30.538

R(reflections)= 0.0135( 6088)	wR2(reflections)=
S = 0.985	0.0364( 6155)
Npar= 204	

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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

ABSTY02\_ALERT\_1\_C An \_exptl\_absorpt\_correction\_type has been given without  
a literature citation. This should be contained in the  
\_exptl\_absorpt\_process\_details field.

Absorption correction given as multi-scan

PLAT369\_ALERT\_2\_C Long C(sp2)-C(sp2) Bond C1 - C2 . 1.53 Ang.

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### Alert level G

PLAT431\_ALERT\_2\_G Short Inter HL..A Contact I2 ..02 . 3.04 Ang.

3/4-x,-1/4+y,1/4+z = 16\_545 Check

PLAT431\_ALERT\_2\_G Short Inter HL..A Contact I4 ..02 . 3.32 Ang.

x,1/2+y,1/2+z = 5\_555 Check

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact I2 ..C2 . 3.43 Ang.

3/4-x,-1/4+y,1/4+z = 16\_545 Check

PLAT767\_ALERT\_4\_G INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

PLAT794\_ALERT\_5\_G Tentative Bond Valency for Zn1 (II) . 1.90 Info

PLAT850\_ALERT\_4\_G Check Flack Parameter Exact Value 0.00 with s.u. 0.01 Check

PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !

PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 1 Note

PLAT965\_ALERT\_2\_G The SHELXL WEIGHT Optimisation has not Converged Please Check

PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 5 Info

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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

2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

11 **ALERT level G** = General information/check it is not something unexpected

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

7 ALERT type 2 Indicator that the structure model may be wrong or deficient

1 ALERT type 3 Indicator that the structure quality may be low

2 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* 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.

