

# 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: 20171225lzw122\_0m\_a\_sq

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Bond precision:    C-C = 0.0105 A

Wavelength=0.71073

Cell:                a=13.4501(6)                b=18.6963(9)                c=19.6467(8)  
                      alpha=72.745(1)        beta=72.528(1)        gamma=88.801(2)  
Temperature:        296 K

	Calculated	Reported
Volume	4487.9(3)	4487.9(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H30 Br4 N4 O9 Zn2, C31 H30 Br4 N4 O8 Zn2 [+ solvent]	C32 H30 Br4 N4 O9 Zn2, C31 H30 Br4 N4 O8 Zn2
Sum formula	C63 H60 Br8 N8 O17 Zn4 [+ solvent]	C63 H60 Br8 N8 O17 Zn4
Mr	2101.95	2101.95
Dx,g cm-3	1.556	1.555
Z	2	2
Mu (mm-1)	4.675	4.675
F000	2060.0	2060.0
F000'	2058.70	
h,k,lmax	15,22,23	15,22,23
Nref	15809	15711
Tmin,Tmax	0.379,0.452	
Tmin'	0.344	

Correction method= Not given

Data completeness= 0.994

Theta(max)= 25.010

R(reflections)= 0.0523( 10738)

wR2(reflections)= 0.1557( 15711)

S = 1.049

Npar= 909

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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.



### Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT057_ALERT_3_C	Correction for Absorption Required	RT(exp) ...	1.19 Do !
PLAT221_ALERT_2_C	Solv./Anion Resd 2 C	Ueq(max)/Ueq(min) Range	5.7 Ratio
PLAT223_ALERT_4_C	Solv./Anion Resd 2 H	Ueq(max)/Ueq(min) Range	6.4 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O15 --C63	5.1 s.u.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	O15	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C36	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....		0.01046 Ang.
PLAT431_ALERT_2_C	Short Inter HL..A Contact	Br1 ..O13	3.25 Ang.



### Alert level G

PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O1	110.9 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O2	110.7 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O5	110.4 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O6	111.5 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O10	109.7 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O11	109.5 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O12	112.0 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y	Angle From 120 for O13	110.0 Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Br4 ..C44	3.32 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O1 ..C31	2.98 Ang.
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure		! Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		! Info
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		4 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
16 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  
3 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

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 30/01/2018; check.def file version of 30/01/2018**

