

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zncn2cy2bc

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: zncn2cy2bcat**

Bond precision:	C-C = 0.0112 A	Wavelength=1.54178	
Cell:	a=12.1946 (4)	b=18.2169 (6)	c=20.8605 (6)
	alpha=90	beta=90	gamma=90
Temperature:	298 K		

	Calculated	Reported
Volume	4634.1(3)	4634.1(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C48 H67 B N4 O2 Zn	C48 H67 B N4 O2 Zn
Sum formula	C48 H67 B N4 O2 Zn	C48 H67 B N4 O2 Zn
Mr	808.26	808.23
Dx, g cm <sup>-3</sup>	1.158	1.158
Z	4	4
Mu (mm <sup>-1</sup> )	1.035	1.035
F000	1736.0	1736.0
F000'	1733.89	
h, k, lmax	14, 21, 25	14, 21, 25
Nref	8497[ 4721]	7698
Tmin, Tmax	0.952, 0.980	0.655, 1.000
Tmin'	0.911	

Correction method= # Reported T Limits: Tmin=0.655 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.63/0.91      Theta (max)= 68.263

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R(reflections)= 0.0679( 6073)      wR2(reflections)=
S = 0.980                          0.1768( 7698)
Npar= 515
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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

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C6	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C11	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C31	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C34	Check
PLAT341_ALERT_3_C	Low	Bond Precision on C-C Bonds .....	0.0112	Ang.
PLAT601_ALERT_2_C		Unit Cell Contains Solvent Accessible VOIDS of .	47	Ang**3
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L= 0.600	19	Report
	12 12 0,	12 12 4, 6 18 5, 5 20 5, 11 13 6,	7 17 6,	
	6 19 6,	11 13 7, 9 16 7, 10 14 8, 9 15 9,	4 14 15,	
	7 14 15,	6 15 15, 9 7 18, 0 15 18, 1 15 18,	0 14 19,	
	1 14 19,			

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#### Alert level G

PLAT072_ALERT_2_G	SHELXL First	Parameter in WGHT Unusually Large	0.12	Report
PLAT395_ALERT_2_G	Deviating	X-O-Y Angle From 120 for O2 .	105.0	Degree
PLAT883_ALERT_1_G	No Info/Value for	_atom_sites_solution_primary .	Please	Do !
PLAT912_ALERT_4_G	Missing # of	FCF Reflections Above STh/L= 0.600	25	Note
PLAT941_ALERT_3_G	Average	HKL Measurement Multiplicity .....	3.8	Low
PLAT969_ALERT_5_G	The 'Henn et al.'	R-Factor-gap value .....	2.104	Note
		Predicted wR2: Based on SigI**2 8.40 or SHELX Weight 18.03		
PLAT978_ALERT_2_G	Number	C-C Bonds with Positive Residual Density.	0	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  
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected
- 1 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  
3 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* 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.

