

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: jwjw001

Bond precision: C-C = 0.0055 A Wavelength=0.71073

Cell: a=8.4825(13) b=20.092(3) c=13.5846(18)
 alpha=90 beta=93.405(9) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	2311.1(6)	2311.1(6)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C23 H17 Br N4 O4 Zn	C23 H17 Br N4 O4 Zn
Sum formula	C23 H17 Br N4 O4 Zn	C23 H17 Br N4 O4 Zn
Mr	558.70	558.69
Dx,g cm-3	1.606	1.606
Z	4	4
Mu (mm-1)	2.829	2.829
F000	1120.0	1120.0
F000'	1120.40	
h,k,lmax	11,26,17	10,26,17
Nref	5274	5240
Tmin,Tmax	0.558,0.601	0.588,0.630
Tmin'	0.547	

Correction method= # Reported T Limits: Tmin=0.588 Tmax=0.630
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 27.460

R(reflections)= 0.0411(3302) wR2(reflections)= 0.1134(5240)

S = 1.034 Npar= 366

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N2	--C10	.	7.0 s.u.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		O1 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C4 Check

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				2 Report
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF				Please Do !
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.				17 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II)				1.94 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				1 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL/				2018 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **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
4 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
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.

PLATON version of 16/05/2021; check.def file version of 13/05/2021

Datablock jwjw001 - ellipsoid plot

