

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zxk-20240425-drxl\_auto

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: zxk-20240425-drxl\_auto

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Bond precision: C-C = 0.0040 Å Wavelength=1.54184

Cell: a=7.3007(2) b=9.1847(2) c=21.3007(5)  
alpha=90 beta=89.975(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1428.31(6)	1428.31(6)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H13 Br O2	C18 H13 Br O2
Sum formula	C18 H13 Br O2	C18 H13 Br O2
Mr	341.18	341.19
Dx, g cm <sup>-3</sup>	1.587	1.587
Z	4	4
μ (mm <sup>-1</sup> )	3.930	3.930
F000	688.0	688.0
F000'	686.93	
h, k, lmax	9,11,26	9,11,26
Nref	2982	2898
Tmin, Tmax	0.431, 0.456	0.634, 1.000
Tmin'	0.326	

Correction method= # Reported T Limits: Tmin=0.634 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.972 Theta (max)= 75.560

R(reflections)= 0.0418( 2846) wR2 (reflections)=  
0.1052( 2898)  
S = 1.076 Npar= 190

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

PLAT157\_ALERT\_4\_C Non-standard Monoclinic Beta Angle less 90 Deg 89.97 Degree  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.191 Check

### • Alert level G

PLAT398\_ALERT\_2\_G Deviating C-O-C Angle From 120 for O1 . 109.8 Degree  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 83 Note  
 PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 1 Note  
 2 0 2,  
 PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 5.19 Note  
 Predicted wR2: Based on SigI\*\*2 2.03 or SHELX Weight 10.11  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 7 Info

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

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

5 **ALERT LEVEL 3** GENERAL INFORMATION: CHECK TO SEE IF SCREENING UNEXPECTED

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

2 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

2 ALERT type 4 Improvement, methodology, query or suggestion

1 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 06/01/2024; check.def file version of 05/01/2024**

Datablock zxk-20240425-drxl\_auto - ellipsoid plot

