checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zxk-20231019_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-20231019_auto

```
Bond precision:   C-C = 0.0067 A           Wavelength=1.54184

Cell:          a=9.9225(2)        b=11.6881(3)      c=15.1944(3)
               alpha=110.104(2)   beta=102.399(2)   gamma=100.788(2)
Temperature:   100 K
```

	Calculated	Reported
Volume	1549.40(7)	1549.39(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H15 Br O2	C20 H15 Br O2
Sum formula	C20 H15 Br O2	C20 H15 Br O2
Mr	367.22	367.23
Dx,g cm-3	1.574	1.574
Z	4	4
Mu (mm-1)	3.670	3.670
F000	744.0	744.0
F000'	743.06	
h,k,lmax	11,13,17	11,13,17
Nref	5283	5193
Tmin,Tmax	0.676,0.746	0.592,1.000
Tmin'	0.549	

```
Correction method= # Reported T Limits: Tmin=0.592 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.983           Theta(max)= 65.089

R(reflections)= 0.0541( 4479)                    wR2(reflections)=
                                                 0.1412( 5193)
S = 1.052                  Npar= 415
```

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

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5882
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00675 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C20 H15 Br O2
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.048 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         90 Report
              -11  1  0,  -7 12  0,  -2 12  0,   2-13  1,   3-13  1,   4-13  1,
               10 -9  1,  -9 -5  1,  11 -3  1,  11 -2  1,  10 -1  1, -11  0  1,
                5  6  1,   6  8  1,  -1 10  1,  -2 11  1,   1-13  2,   2-13  2,
                3-13  2,   9-10  2,  11 -5  2, -11 -1  2,  10  0  2,  -9 10  2,
               -3 12  2, -10 -4  3,  10 -1  3,  10  0  3,   8  3  3,   4  4  3,
                8  4  3,   0  6  3,  -3-12  4,  10 -2  4,  10 -1  4,   7  5  4,
               -2 -9  5,  -1 -9  5,  -2 -8  5,  10 -7  5,  10 -3  5, -11 -2  5,
              -11 -1  5, -11  6  5,  -4 11  5,  -3 11  5,   6  5  6,   3  8  6,
               -6-10  7,  -7 -9  7,   8  1  7,  -4 10  7,  -5-10  8,   9 -5  8,
              -11  3  8,   5  4  8,   2  7  8,   0  0  9,   7-10 10,   8 -6 10,
              -10 -4 10,   4  4 10,   3  5 10,   2-13 11, -10 -3 11,   7 -3 11,
              -10 -2 11,  -5  7 11, -10 -2 12, -10 -1 12,   5  0 12,  -6  6 12,
               -5  6 12,  -1-12 13,  -9 -4 13,  -9  1 13,  -6  5 13,  -5  5 13,
                4 -8 14,   5 -5 14,  -7  3 14,  -4  4 14,  -4 -9 15,  -7 -6 15,
                4 -6 15,   4 -5 15,   2 -3 16,  -6  0 16,  -5  1 16,   1 -5 17,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.90Ang From Br22            1.84 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3        .      -0.32 eA-3
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Alert level G

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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.97 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O9       .      109.2 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O32      .      109.6 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  Br22     ..C35      .       3.29 Ang.
                                                    x,y,z  =      1_555 Check
PLAT793_ALERT_4_G Model has Chirality at C6          (Centro SpGr)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C29         (Centro SpGr)          R Verify
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        76% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
              4  4  3,  10 -1  1,  10 -1  3,  10  0  2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.9 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.500 Note
           Predicted wR2: Based on SigI**2  5.65 or SHELX Weight 13.42
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 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
12 **ALERT level G** = General information/check it is not something unexpected

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

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  8 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
  3 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.

PLATON version of 22/08/2024; check.def file version of 21/08/2024

Datablock zxk-20231019_auto - ellipsoid plot