checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zxk-20240425-drxlys-3_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-drxlys-3_auto

```
Bond precision:   C-C = 0.0158 A           Wavelength=1.54184

Cell:           a=9.6930(4)        b=9.7666(3)       c=14.6505(4)
                alpha=87.001(2)    beta=86.137(3)    gamma=75.644(3)
Temperature:    100 K

                Calculated                 Reported
Volume          1339.66(8)                 1339.66(8)
Space group     P -1                       P -1
Hall group      -P 1                       -P 1
Moiety formula  C18 H11 Br O2              2(C18 H11 Br O2)
Sum formula     C18 H11 Br O2              C36 H22 Br2 O4
Mr              339.17                     678.35
Dx,g cm-3       1.682                      1.682
Z               4                          2
Mu (mm-1)       4.190                      4.190
F000            680.0                      680.0
F000'           678.93
h,k,lmax        11,11,17                   11,11,17
Nref            4754                       4732
Tmin,Tmax       0.288,0.433                0.676,1.000
Tmin'           0.185

Correction method= # Reported T Limits: Tmin=0.676 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.995           Theta(max)= 66.592

R(reflections)= 0.1056( 4084)                    wR2(reflections)=
                                                 0.2837( 4732)
S = 1.190                  Npar= 379
```

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 B

```
PLAT341_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.01585 Ang.
```

Author Response: This is likely related to the weak diffraction of the crystal.

Alert level C

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C18 H11 Br O2
             Rep.: 2(C18 H11 Br O2)
PLAT082_ALERT_2_C High R1 Value ..................................       0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.28 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     16.781 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.667 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         22 Report
                8 -4  1,   1  2  1,   4  3  2,   6 11  2,   1  0  3,   6 11  3,
                2  3  4,  -1 10  5,  -7  6  6,  -5  8  6,  -9  2  7,   5 10  8,
                4 -5  9,   8 -3  9,   3  8 11,  -5 -3 12,  -5 -4 13,  -5  2 13,
                7  2 13,   1  8 13,   7  3 14,  -3  2 16,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.00Ang From O42              2.32 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.12Ang From Br20             2.25 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.99Ang From Br41             2.08 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.07Ang From Br20             1.98 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From Br41             1.81 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.03Ang From Br20            -1.93 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.92Ang From O21     .        0.73 eA-3
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          42 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...           2 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       34.71 Why ?
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records           2 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par      0.0100 Report
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar      0.0200 Report
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O34      .       110.0 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  O13      ..C33      .        2.84 Ang.
                                                    x,y,z  =      1_555 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         354 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still          69% Note
PLAT930_ALERT_2_G FCF-based   Twin Law ( 1-1 0)         Est.d BASF        0.10 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 1-1 0)         Est.d BASF        0.10 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          7 Note
                1  0  3,   1  2  1,   2  3  4,   3  8 11,   3 11  7,   4  3  2,
                5 10  8,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........         4.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........        5.18 Note
             Predicted wR2: Based on SigI**2  5.47 or SHELX Weight 24.85
```

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

---

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
15 ALERT type 2 Indicator that the structure model may be wrong or deficient
10 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

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

Datablock zxk-20240425-drxlys-3_auto - ellipsoid plot