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: shelx

```
Bond precision:   C-C = 0.0142 A           Wavelength=0.71073

Cell:               a=14.282(2)      b=16.526(2)      c=17.662(2)
                    alpha=90         beta=90          gamma=90
Temperature:        296 K

                 Calculated                  Reported
Volume           4168.7(9)                   4168.9(10)
Space group      P b c a                     P b c a
Hall group       -P 2ac 2ab                  -P 2ac 2ab
Moiety formula   C12 H28 N, Br4 Fe           ?
Sum formula      C12 H28 Br4 Fe N            C12 H28 Br4 Fe N
Mr               561.80                      561.84
Dx,g cm-3        1.790                       1.790
Z                8                           8
Mu (mm-1)        8.380                       8.379
F000             2184.0                      2184.0
F000'            2179.11
h,k,lmax         17,20,21                    17,20,21
Nref             3958                        3935
Tmin,Tmax        0.310,0.285                 0.383,0.745
Tmin'            0.261

Correction method= # Reported T Limits: Tmin=0.383 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.994            Theta(max)= 25.668

R(reflections)= 0.0512( 1926)                    wR2(reflections)=
                                                 0.1633( 3935)
S = 1.002                  Npar= 170
```

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

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Fe Check

Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 49% Check
PLAT234_ALERT_4_C Large Hirshfeld Difference N --C10 . 0.17 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Br1 0.112 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01425 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C4 - C5 . 1.43 Ang.

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 16.89 Why ?
PLAT480_ALERT_4_G Long H...A H-Bond Reported H7A ..BR2 . 3.01 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H4B ..BR2 . 3.03 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H11A ..BR3 . 3.11 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Fe (II) . 3.00 Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 16 Note
1 0 2, 2 0 0, 0 0 2, 0 2 1, 1 1 1, 0 2 0,
1 1 2, 13 1 9, 3 6 15, 1 2 1, 4 0 0, 2 0 6,
2 1 1, 0 12 8, 0 2 15, 2 8 0,
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
4 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.

PLATON version of 04/06/2025; check.def file version of 30/05/2025

Datablock shelx - ellipsoid plot