

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: xulij_1023

Bond precision: C-C = 0.0108 Å Wavelength=1.54184

Cell: a=7.0790 (6) b=11.0184 (11) c=11.2355 (9)
 alpha=62.588 (9) beta=71.771 (8) gamma=75.318 (8)
Temperature: 294 K

| | Calculated | Reported |
|------------------------|------------------|------------------|
| Volume | 732.67 (13) | 732.67 (13) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C17 H13 Fe N3 O2 | C17 H13 Fe N3 O2 |
| Sum formula | C17 H13 Fe N3 O2 | C17 H13 Fe N3 O2 |
| Mr | 347.15 | 347.15 |
| Dx, g cm ⁻³ | 1.574 | 1.574 |
| Z | 2 | 2 |
| Mu (mm ⁻¹) | 8.370 | 8.370 |
| F000 | 356.0 | 356.0 |
| F000' | 354.72 | |
| h, k, lmax | 8, 13, 13 | 8, 13, 13 |
| Nref | 2774 | 2709 |
| Tmin, Tmax | 0.703, 0.846 | 0.625, 1.000 |
| Tmin' | 0.627 | |

Correction method= # Reported T Limits: Tmin=0.625 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.977 Theta(max)= 69.962

| | |
|--------------------------------|----------------------------------|
| R(reflections)= 0.0714 (2278) | wR2(reflections)= 0.2196 (2709) |
| S = 1.082 | Npar= 208 |

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

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree



Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.79 Report
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Fe1 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.01082 Ang.



Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (II) . 2.15 Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.7 Low

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

- 1 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
2 ALERT type 3 Indicator that the structure quality may be low
0 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.

