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: 01

```
Bond precision:   C-C = 0.0094 A          Wavelength=1.54178

Cell:             a=18.0793(11)      b=24.9505(17)      c=14.994(1)
                  alpha=90           beta=90            gamma=90
Temperature:      302 K

                 Calculated                Reported
Volume           6763.6(8)                 6763.6(8)
Space group      A b a 2                   A e a 2
Hall group       A 2 -2ac                  A 2 -2ac
Moiety formula   C84 H52 Fe2 N12 O         C84 H52 Fe2 N12 O
Sum formula      C84 H52 Fe2 N12 O         C84 H52 Fe2 N12 O
Mr               1357.08                   1357.07
Dx,g cm-3        1.333                     1.333
Z                4                         4
Mu (mm-1)        3.901                     3.901
F000             2800.0                    2800.0
F000'            2798.24
h,k,lmax         21,30,18                  21,30,18
Nref             6233[ 3250]               6105
Tmin,Tmax        0.585,0.602               0.643,0.753
Tmin'            0.530

Correction method= # Reported T Limits: Tmin=0.643 Tmax=0.753
AbsCorr = NONE

Data completeness= 1.88/0.98        Theta(max)= 68.573

R(reflections)= 0.0447( 4428)                    wR2(reflections)=
                                                 0.1141( 6105)
S = 0.983                  Npar= 447
```

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

```
PLAT987_ALERT_1_B The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
```

Alert level C

```
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       7.27 Note
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C23      --C24      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C29      --C30      .       0.20 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C23 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C27 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C30 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C38 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C27      --C32      .       1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00936 Ang.
```

Alert level G

```
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (III)     .       2.95 Info
```

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT987_01
;
PROBLEM: The Flack x is >> 0 -  Do a BASF/TWIN Refinement     Please Check
RESPONSE: ...
;
_vrf_PLAT090_01
;
PROBLEM: Poor Data / Parameter Ratio (Zmax > 18) ........       7.27 Note
RESPONSE: ...
;
```

```
_vrf_PLAT220_01
;
PROBLEM: NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
RESPONSE: ...
;
_vrf_PLAT234_01
;
PROBLEM: Large Hirshfeld Difference C23      --C24      .       0.16 Ang.
RESPONSE: ...
;
_vrf_PLAT241_01
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of        C23 Check
RESPONSE: ...
;
_vrf_PLAT242_01
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of        C21 Check
RESPONSE: ...
;
_vrf_PLAT331_01
;
PROBLEM: Small Aver Phenyl C-C Dist C27      --C32      .       1.37 Ang.
RESPONSE: ...
;
_vrf_PLAT341_01
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.00936 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

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 01 - ellipsoid plot