checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 0790_cg

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: 0790_cg

```
Bond precision:    C-C = 0.0020 A             Wavelength=0.71073

Cell:              a=18.0135(10)    b=15.4791(10)      c=17.8598(9)
                   alpha=90         beta=100.554(2)    gamma=90
Temperature:       150 K

                   Calculated                Reported
Volume             4895.7(5)                 4895.6(5)
Space group        P 21/c                    P 1 21/c 1
Hall group         -P 2ybc                   -P 2ybc
Moiety formula     C20 H41 Fe O P3           C20 H41 Fe O P3
Sum formula        C20 H41 Fe O P3           C20 H41 Fe O P3
Mr                 446.29                    446.29
Dx,g cm-3          1.211                     1.211
Z                  8                         8
Mu (mm-1)          0.818                     0.818
F000               1920.0                    1920.0
F000'              1925.62
h,k,lmax           24,20,24                  24,20,24
Nref               12762                     12593
Tmin,Tmax          0.899,0.958               0.899,0.994
Tmin'              0.778

Correction method= # Reported T Limits: Tmin=0.899 Tmax=0.994
AbsCorr = MULTI-SCAN

Data completeness= 0.987          Theta(max)= 28.791

R(reflections)= 0.0295( 10794)     wR2(reflections)= 0.0724( 12593)

S = 1.055                    Npar= 506
```

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

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PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          4 Report
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7 Note
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for      P6         --C40A    .      9.1 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for      P6         --C38B    .      9.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1         --O1      .      5.2 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       12% Note
PLAT793_ALERT_4_G Model has Chirality at C7          (Centro SPGR)         S Verify
PLAT793_ALERT_4_G Model has Chirality at C27         (Centro SPGR)         R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600         158 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          6 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          1 Check
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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
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   0 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
   4 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 07/08/2019; check.def file version of 30/07/2019

NOMOVE FORCED

Prob = 50
Temp = 150

-8 Y

PLATON-Oct 16 12:11:56 2019 - (70316)

Z 156   0790_cg   P 1 21/c 1   R = 0.03   RES=   0   -62 X