checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lcam16

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: lcam16

```
Bond precision:  C-C = 0.0271 A          Wavelength=1.54184

Cell:            a=6.8570(9)     b=25.484(3)          c=13.743(2)
                 alpha=90        beta=92.460(14)      gamma=90
Temperature:     100 K

                Calculated                 Reported
Volume          2399.3(5)                  2399.3(6)
Space group     P 21/c                     P 1 21/c 1
Hall group      -P 2ybc                    -P 2ybc
Moiety formula  C21 H9 Fe O6 [+ solvent]   C21 H9 Fe O6
Sum formula     C21 H9 Fe O6 [+ solvent]   C21 H9 Fe O6
Mr              413.13                     413.13
Dx,g cm-3       1.144                      1.144
Z               4                          4
Mu (mm-1)       5.288                      5.288
F000            836.0                      836.0
F000'           834.17
h,k,lmax        6,23,12                    6,23,12
Nref            1865                       1853
Tmin,Tmax       0.948,0.948                0.249,1.000
Tmin'           0.948

Correction method= # Reported T Limits: Tmin=0.249 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994          Theta(max)= 44.312

R(reflections)= 0.1525( 1022)     wR2(reflections)= 0.4306( 1853)

S = 1.426                  Npar= 197
```

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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.4531

Author Response: Crystals diffracted to 1.1 A of resolution, so the data had to be trimmed accordigly

---

Alert level B

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ..... 0.43 Report

Author Response: Due to the poor resolution of the data adquired, the model was based on ill shaped electrondensity map. As consequence the wR2 and R1 values are larger than normal values

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 8 Report
C2 C3 C4 C5 C6 C7 etc.

Author Response: In order to maximize the data/parameter ratio, the disordered atoms were refined isotrophically

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02706 Ang.

Author Response: It is caused by the low resolution data.

Alert level C

PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full ! Check
PLAT082_ALERT_2_C High R1 Value ..... 0.15 Report
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 9.41 Note
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C16 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C8 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
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C20 - C20_b . 1.53 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.604 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.453 13 Report
PLAT922_ALERT_1_C wR2 in the CIF and FCF Differ by ..... 0.0028 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H6 -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H16 -0.33 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

---

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 18 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 34 Report

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C23        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C24        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C25        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C26        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H23        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H24        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H25        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H26        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H27        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        21% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C14              2.98 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C2       ..C14              3.14 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C17              3.12 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C4       ..C18              3.20 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C5       ..C10              2.94 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C5       ..C9               3.14 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C7       ..C12              3.10 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C7       ..C13              3.12 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C8       ..C13              3.17 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C9       ..C13              3.17 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C18      ..C14              3.16 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C19      ..C24              3.17 Ang.
                                            -1+x,y,z  =      1_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C21      ..C25              3.16 Ang.
                                          2-x,1-y,1-z  =      3_766 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C23      ..C27              3.16 Ang.
                                          2-x,1-y,1-z  =      3_766 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (III)     .       3.58 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        289 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        30% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          4 Note
PLAT954_ALERT_1_G Reported (CIF) and Actual (FCF) Kmax Differ by .          1 Units
```

---

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

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

```
 29 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
 15 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

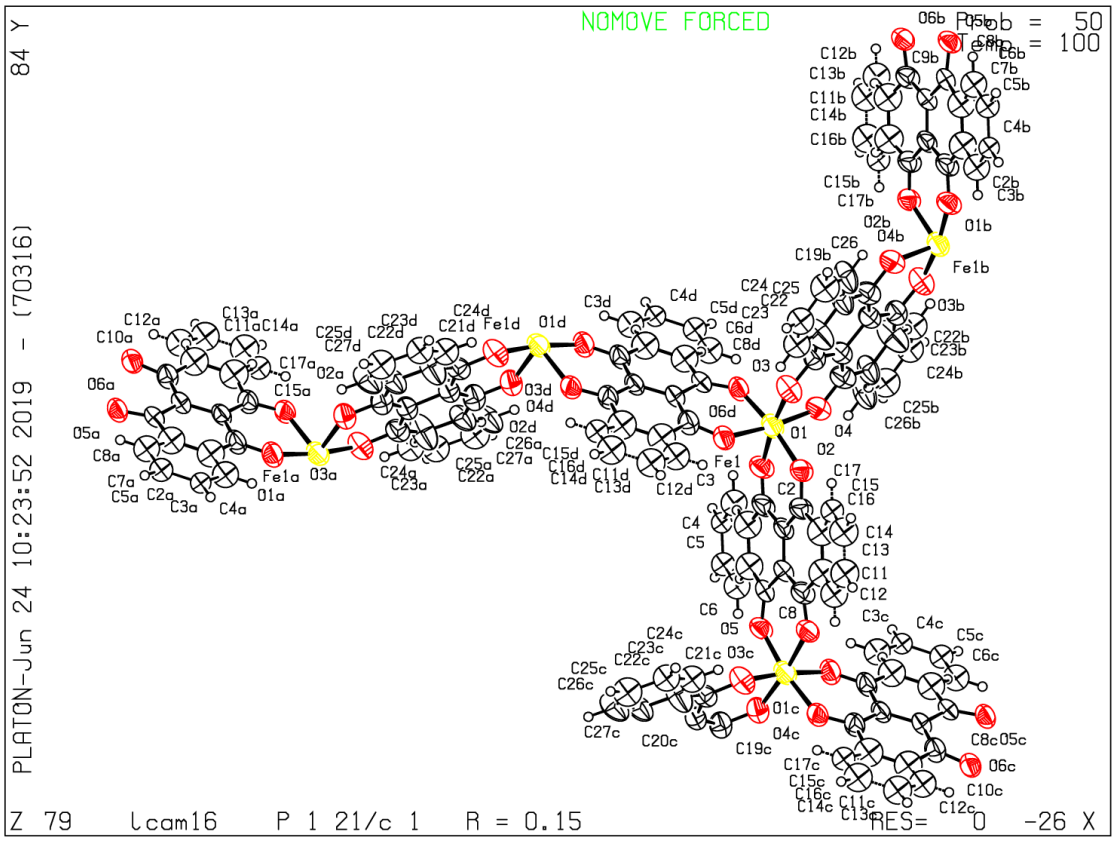
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 03/05/2019; check.def file version of 29/04/2019

Datablock lcam16 - ellipsoid plot