checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cb9block

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: cb9block

```
Bond precision:  C-C = 0.0057 A          Wavelength=0.77490

Cell:            a=8.7293(4)     b=8.7613(5)         c=38.725(2)
                 alpha=90        beta=91.950(3)      gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	2960.0(3)	2960.0(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C30 H22 Fe N6, 2(Cl O4), O	C30 H22 Fe N6, 2(Cl O4), H2 O
Sum formula	C30 H22 Cl2 Fe N6 O9	C30 H24 Cl2 Fe N6 O9
Mr	737.29	739.30
Dx,g cm-3	1.655	1.659
Z	4	4
Mu (mm-1)	0.954	0.898
F000	1504.0	1512.0
F000’	1507.64	
h,k,lmax	12,12,54	12,12,54
Nref	8677	8630
Tmin,Tmax	0.914,0.931	0.645,0.747
Tmin’	0.914	

```
Correction method= MULTI-SCAN

Data completeness= 0.995          Theta(max)= 33.072

R(reflections)= 0.0785( 7493)     wR2(reflections)= 0.1800( 8630)

S = 1.231                  Npar= 433
```

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

```
PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       6.21 %
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        O1W Check
```

Author Response: Hydrogens on the lattice oxygen O1W could not be found nor fixed. The presence of these hydrogens is clearly indicated by short contact of O1W with O2 and O3, corresponding to hydrogen bonds. However refinement of hydrogen atoms at the corresponding approximate coordinates with distance restraints did not converge and these hydrogens are thus omitted in the structural model, although taken into account in the formula.

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O1W    ..  O3      ..       2.69 Ang.
```

Author Response: Hydrogens on the lattice oxygen O1W could not be found nor fixed. The presence of these hydrogens is clearly indicated by short contact of O1W with O2 and O3, corresponding to hydrogen bonds. However refinement of hydrogen atoms at the corresponding approximate coordinates with distance restraints did not converge and these hydrogens are thus omitted in the structural model, although taken into account in the formula.

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O1W    ..  O2      ..       2.84 Ang.
```

Author Response: Hydrogens on the lattice oxygen O1W could not be found nor fixed. The presence of these hydrogens is clearly indicated by short contact of O1W with O2 and O3, corresponding to hydrogen bonds. However refinement of hydrogen atoms at the corresponding approximate coordinates with distance restraints did not converge and these hydrogens are thus omitted in the structural model, although taken into account in the formula.

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       2.01 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         Cl2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
```

Alert level G

```
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      19.22 Why ?
PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag Ka ..     0.7749 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1W    ..  C15     ..       2.92 Ang.
PLAT984_ALERT_1_G The Fe-f'=     0.358 Deviates from the B&C-Value      0.356 Check
```

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully

```
  5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  5 ALERT level G = General information/check it is not something unexpected

  6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  6 ALERT type 2 Indicator that the structure model may be wrong or deficient
  0 ALERT type 3 Indicator that the structure quality may be low
  2 ALERT type 4 Improvement, methodology, query or suggestion
  0 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*, 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 20/08/2014; check.def file version of 18/08/2014

Datablock cb9block - ellipsoid plot