

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:	C-C = 0.0055 A	Wavelength=0.71075
Cell:	a=16.9178(13)	b=13.6023(10)      c=12.8848(10)
	alpha=90	beta=108.530(3)      gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	2811.4(4)	2811.3(4)
Space group	P 2/c	P 2/c
Hall group	-P 2yc	-P 2yc
Moiety formula	F18 Fe4, 2.5(C4 H12 N2), C2 H6 N, 2(O)	?
Sum formula	C12 H36 F18 Fe4 N6 O2	C12 H40 F18 Fe4 N6 O2
Mr	861.87	865.90
Dx,g cm-3	2.036	2.046
Z	4	4
Mu (mm-1)	2.167	2.167
F000	1728.0	1744.0
F000'	1734.84	
h,k,lmax	20,16,15	20,16,15
Nref	4961	4952
Tmin,Tmax	0.746,0.823	0.737,1.000
Tmin'	0.731	

Correction method= # Reported T Limits: Tmin=0.737 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.998      Theta(max)= 25.000

R(reflections)= 0.0331( 3648)      wR2(reflections)= 0.0913( 4952)

S = 1.006      Npar= 399

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**test-name\_ALERT\_alert-type\_alert-level.**  
Click on the hyperlinks for more details of the test.

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	4.03	Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.6	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595	7 Report
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.85A	From O2S'	0.51 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.80A	From O2S'	0.40 eA-3

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FORMU001_ALERT_2_G There is a discrepancy between the atom counts in the
    _chemical_formula_sum and the formula from the _atom_site* data.
    Atom count from _chemical_formula_sum: C12 H40 F18 Fe4 N6 O2
    Atom count from the _atom_site data:  C12 H36 F18 Fe4 N6 O2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
    From the CIF: _cell_formula_units_Z      4
    From the CIF: _chemical_formula_sum  C12 H40 F18 Fe4 N6 O2
    TEST: Compare cell contents of formula and atom_site data

    atom      Z*formula    cif sites diff
    C          48.00        48.00      0.00
    H          160.00       144.00     16.00
    F           72.00        72.00      0.00
    Fe          16.00        16.00      0.00
    N           24.00        24.00      0.00
    O           8.00         8.00      0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....          12 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )      100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  9  )      100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      01S Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      02S Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      01S' Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      02S' Check
PLAT431_ALERT_2_G Short Inter HL..A Contact   F3      ..01S'      .      2.86 Ang.
                                x,y,1+z =      1_556 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact   F9      ..02S      .      2.85 Ang.
                                x,y,z  =      1_555 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact   F18     ..01S      .      2.42 Ang.
                                x,y,z  =      1_555 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact   F18     ..01S'      .      2.48 Ang.
                                x,y,z  =      1_555 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          2 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1      (III)      .      2.99 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2      (III)      .      3.04 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe3      (III)      .      3.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe4      (III)      .      3.02 Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still      61% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....          4.7 Low

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
14 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 ALERT type 3 Indicator that the structure quality may be low  
5 ALERT type 4 Improvement, methodology, query or suggestion  
6 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.

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