

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) al_bf5a

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: al_bf5a

Bond precision: C-C = 0.0030 Å Wavelength=0.71073

Cell: a=8.9379 (8) b=17.9291 (16) c=13.4514 (13)
 alpha=90 beta=91.562 (4) gamma=90

Temperature: 273 K

	Calculated	Reported
Volume	2154.8 (3)	2154.8 (3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C30 H34 Fe N18 O2, 2 (B F4), 4 (H2 O)	C30 H34 Fe N18 O2, 4 (H2 O), 2 (B F4)
Sum formula	C30 H42 B2 F8 Fe N18 O6	C30 H42 B2 F8 Fe N18 O6
Mr	980.29	980.28
Dx, g cm ⁻³	1.511	1.511
Z	2	2
Mu (mm ⁻¹)	0.449	0.449
F000	1008.0	1008.0
F000'	1009.23	
h, k, lmax	11, 23, 17	11, 23, 17
Nref	4955	4915
Tmin, Tmax	0.898, 0.914	
Tmin'	0.799	

Correction method= Not given

Data completeness= 0.992

Theta (max)= 27.524

R(reflections)= 0.0435 (4082)

wR2(reflections)=
0.1381 (4915)

S = 1.055

Npar= 341

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT234_ALERT_4_C	Large Hirshfeld Difference F3A --B1 .	0.17 Ang.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	B1 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including F1A	0.153 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O3	0.102 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	38 Report



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	13 Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	5 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	273 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	273 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	80% Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (II) .	2.02 Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.1 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

14 **ALERT level G** = General information/check it is not something unexpected

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

4 ALERT type 2 Indicator that the structure model may be wrong or deficient

3 ALERT type 3 Indicator that the structure quality may be low

7 ALERT type 4 Improvement, methodology, query or suggestion

3 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.

