

checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) km0803

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](#)
Please wait while processing [Interpreting this report](#)

Structure factor report

Datablock: km0803

Bond precision: C-C = 0.0040 Å Wavelength=0.71069
Cell: a=9.3120(2) b=18.7523(3) c=17.9380(4)
alpha=90 beta=99.974(1) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	3085.02(11)	3085.02(11)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H34 Fe2 N2 O6 P2	C28 H34 Fe2 N2 O6 P2
Sum formula	C28 H34 Fe2 N2 O6 P2	C28 H34 Fe2 N2 O6 P2
Mr	668.21	668.21
Dx, g cm-3	1.439	1.439
Z	4	4
Mu (mm-1)	1.086	1.086
F000	1384.0	1384.0
F000'	1388.05	
h,k,lmax	11,23,22	11,23,22
Nref	6314	6303
Tmin,Tmax	0.710,0.796	0.705,0.814
Tmin'	0.588	

Correction method= # Reported T Limits: Tmin=0.705 Tmax=0.814 AbsCorr = ANALYTICAL
Data completeness= 0.998 Theta(max)= 26.370
R(reflections)= 0.0381(4622) wR2(reflections)= 0.0912(6303)
S = 1.025 Npar= 375

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

[PLAT420_ALERT_2_C](#) D-H Bond Without Acceptor N1 --H1 . Please Check
[PLAT420_ALERT_2_C](#) D-H Bond Without Acceptor N2 --H2 . Please Check
[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 2.145 Check
[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 9 Report

Alert level G

[PLAT230_ALERT_2_G](#) Hirshfeld Test Diff for O5 --C5 . 5.5 s.u.
[PLAT232_ALERT_2_G](#) Hirshfeld Test Diff (M-X) Fe1 --C1 . 6.5 s.u.

And 5 other PLAT232 Alerts

[More ...](#)

[PLAT480_ALERT_4_G](#) Long H...A H-Bond Reported H2 ..O1 . 2.66 Ang.
[PLAT710_ALERT_4_G](#) Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 43 Do !
O1 -C1 -FE1 -C3 -117.00 14.00 1_555 1_555 1_555 1_555

And 29 other PLAT710 Alerts

[More ...](#)

[PLAT912_ALERT_4_G](#) Missing # of FCF Reflections Above STh/L= 0.600 2 Note
[PLAT913_ALERT_3_G](#) Missing # of Very Strong Reflections in FCF 2 Note

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 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
32 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

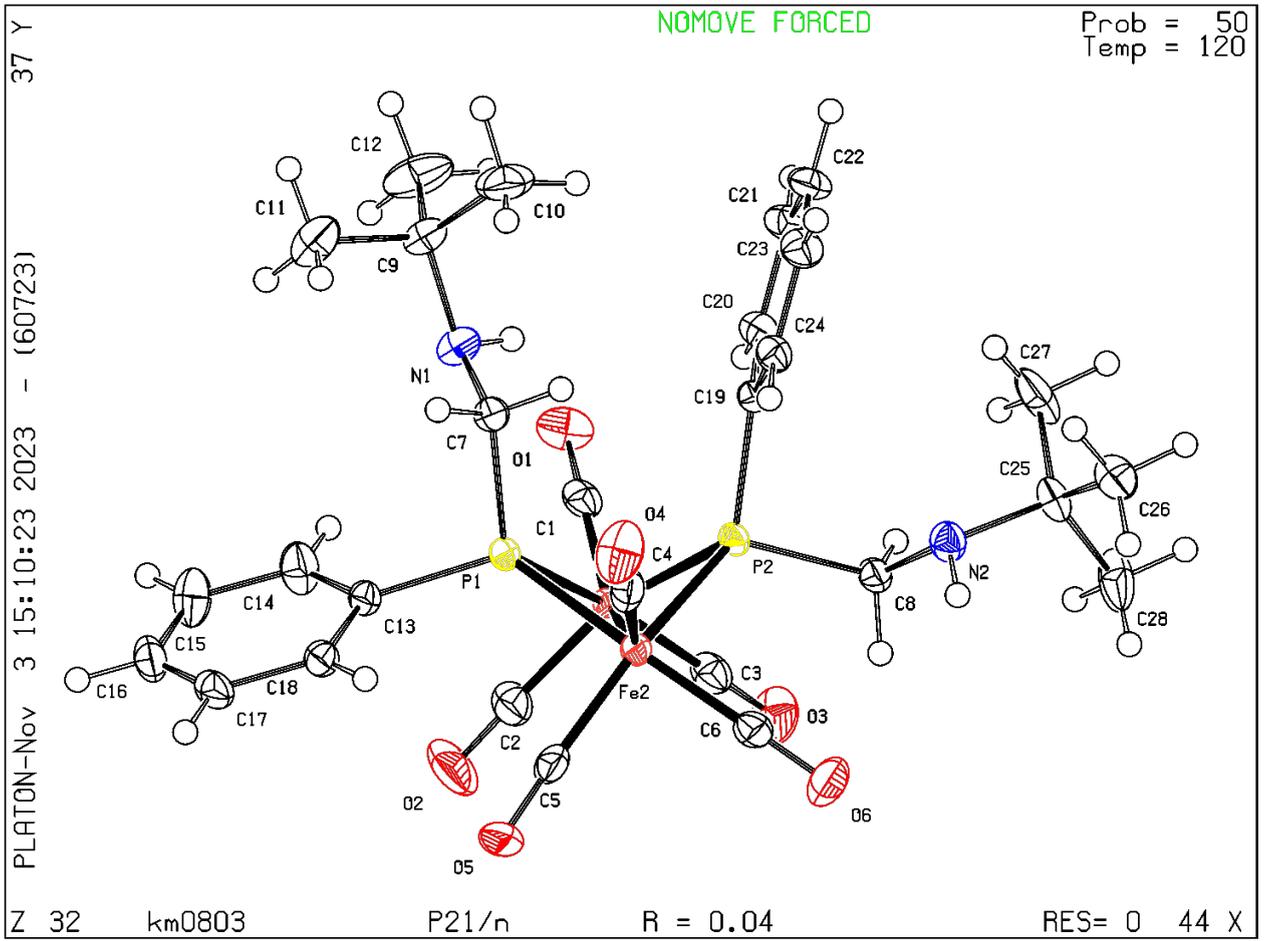
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* 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 06/07/2023; check.def file version of 30/06/2023

Datablock km0803 - ellipsoid plot



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