

checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) km1403

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: km1403

Bond precision:	C-C = 0.0039 Å	Wavelength=0.71073
Cell:	a=27.4929(5) b=13.2772(2) c=13.9398(2)	
	alpha=90 beta=90 gamma=90	
Temperature: 100 K		
	Calculated	Reported
Volume	5088.43(14)	5088.43(14)
Space group	P b c n	Pbcn
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C24 H23 Fe2 N O6 P2	C24 H23 Fe2 N O6 P2
Sum formula	C24 H23 Fe2 N O6 P2	C24 H23 Fe2 N O6 P2
Mr	595.07	595.07
Dx, g cm-3	1.554	1.554
Z	8	8
Mu (mm-1)	1.306	1.306
F000	2432.0	2432.0
F000'	2440.02	
h,k,lmax	32,15,16	32,15,16
Nref	4502	4265
Tmin,Tmax	0.631,0.694	0.502,0.698
Tmin'	0.502	
Correction method= # Reported T Limits: Tmin=0.502 Tmax=0.698 AbsCorr =		
MULTI-SCAN		
Data completeness= 0.947	Theta(max)= 25.020	
R(reflections)= 0.0356(3866)	wR2(reflections)= 0.0988(4265)	
S = 1.039	Npar= 319	

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

[PLAT029_ALERT_3_B_diffn_measured_fraction_theta_full](#) value Low . 0.947 Why?

Alert level C

[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.595 237 Report

[PLAT913_ALERT_3_C](#) Missing # of Very Strong Reflections in FCF 20 Note

Alert level G

[PLAT066_ALERT_1_G](#) Predicted and Reported Tmin&Tmax Range Identical ? Check

[PLAT083_ALERT_2_G](#) SHELXL Second Parameter in WGHT Unusually Large 5.32 Why ?

[PLAT230_ALERT_2_G](#) Hirshfeld Test Diff for O4 --C4 . 5.4 s.u.

[PLAT232_ALERT_2_G](#) Hirshfeld Test Diff (M-X) Fe1 --C1 . 8.1 s.u.

And 5 other PLAT232 Alerts

More ...

[PLAT909_ALERT_3_G](#) Percentage of I>2sig(I) Data at Theta(Max) Still 82% Note

[PLAT933_ALERT_2_G](#) Number of HKL-OMIT Records in Embedded .res File 1 Note

[PLAT941_ALERT_3_G](#) Average HKL Measurement Multiplicity 4.7 Low

[PLAT978_ALERT_2_G](#) Number C-C Bonds with Positive Residual Density. 6 Info

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 10 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
 - 0 ALERT type 4 Improvement, methodology, query or suggestion
 - 0 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

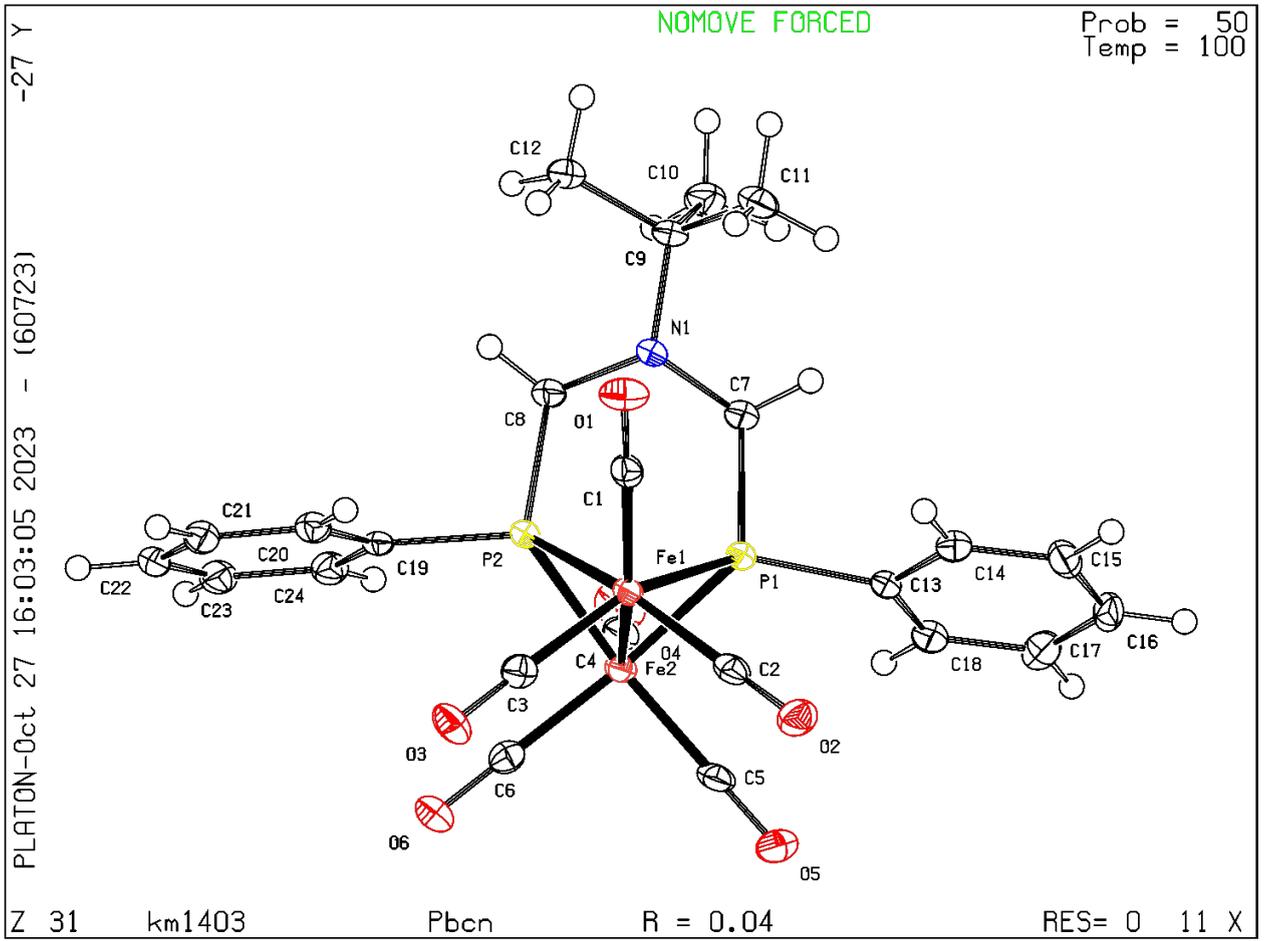
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock km1403 - ellipsoid plot



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