

checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. [CIF dictionary](#)

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

Structure factor report

Datablock: high

Bond precision:	C-C = 0.0030 Å	Wavelength=0.71073
Cell:	a=20.368(1) b=6.2757(4) c=29.5214(14)	
	alpha=90 beta=101.024(5) gamma=90	
Temperature: 100 K		
	Calculated	Reported
Volume	3703.9(4)	3703.9(4)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C22 H17 Fe N O4	C22 H17 Fe N O4
Sum formula	C22 H17 Fe N O4	C22 H17 Fe N O4
Mr	415.22	415.21
Dx, g cm ⁻³	1.489	1.489
Z	8	8
Mu (mm ⁻¹)	0.843	0.843
F000	1712.0	1712.0
F000'	1715.47	
h,k,lmax	24,7,35	24,7,35
Nref	3318	3303
Tmin,Tmax	0.809,0.874	0.775,0.899
Tmin'	0.720	
Correction method=	# Reported T Limits: Tmin=0.775 Tmax=0.899 AbsCorr =	
ANALYTICAL		
Data completeness=	0.995	Theta(max)= 25.121
R(reflections)=	0.0359(2867)	wR2(reflections)= 0.0905(3303)
S =	1.063	Npar= 257

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

[PLAT410_ALERT_2_C](#) Short Intra H...H Contact H15 ..H22 . 1.98 Ång.
x,y,z = 1_555 Check

● Alert level G

[PLAT005_ALERT_5_G](#) No Embedded Refinement Details Found in the CIF Please Do !

[PLAT230_ALERT_2_G](#) Hirshfeld Test Diff for O4 --C10 . 6.8 s.u.

[PLAT232_ALERT_2_G](#) Hirshfeld Test Diff (M-X) Fe1 --C8 . 7.8 s.u.

And 2 other PLAT232 Alerts

More ...

[PLAT793_ALERT_4_G](#) Model has Chirality at C6 (Centro SpGr) R Verify

[PLAT794_ALERT_5_G](#) Tentative Bond Valency for Fe1 (II) . 2.00 Info

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

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

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

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

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

5 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

1 ALERT type 4 Improvement, methodology, query or suggestion

2 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

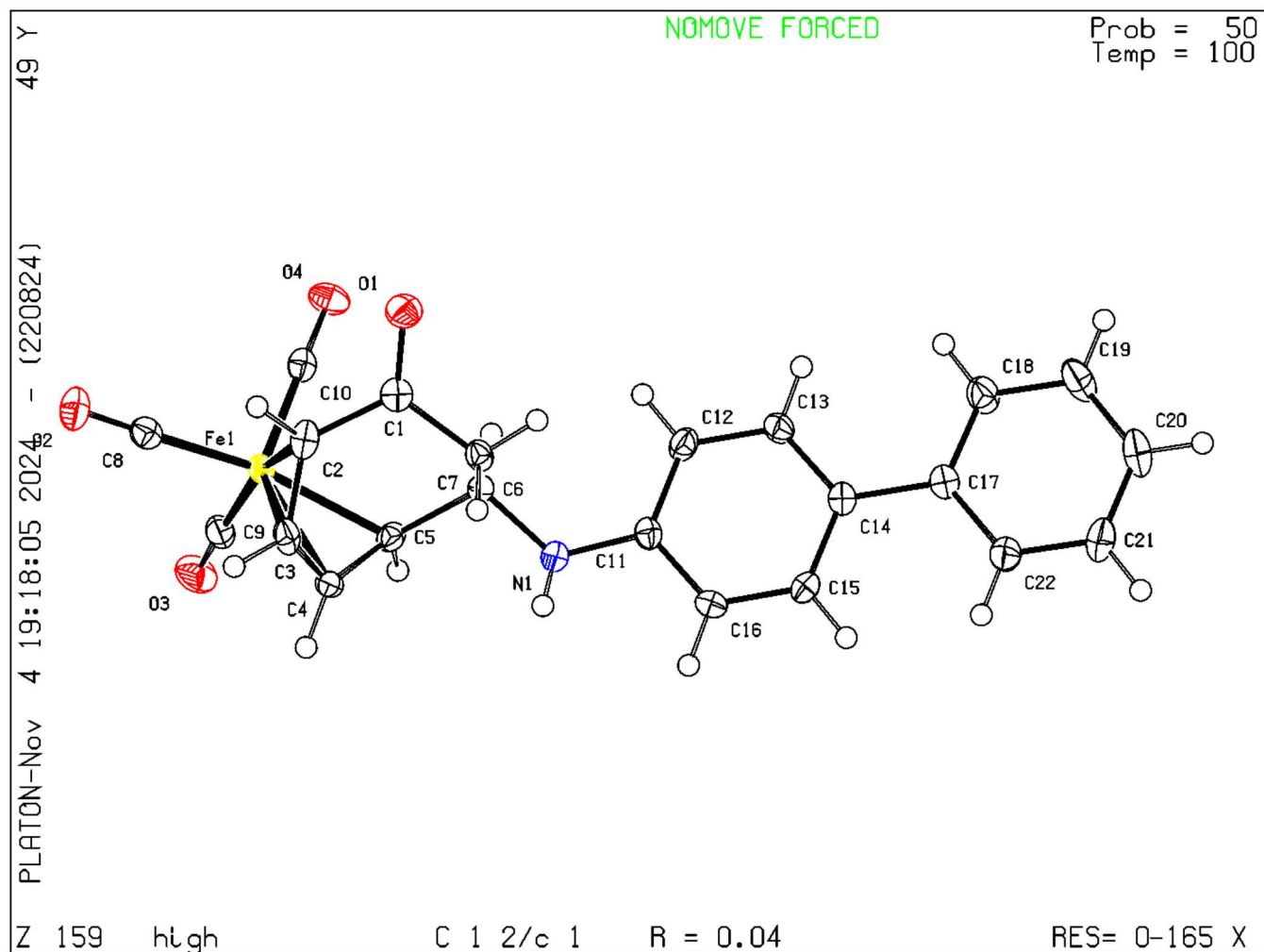
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 22/08/2024; check.def file version of 21/08/2024

Datablock high - ellipsoid plot



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