

# checkCIF (basic structural check) running

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## checkCIF/PLATON (basic structural check)

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

No syntax errors found.  
Please wait while processing ....

[CIF dictionary](#)  
[Interpreting this report](#)

[Structure factor report](#)

### Datablock: xcalibur

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Bond precision:	C-C = 0.0016 Å	Wavelength=0.71073
Cell:	a=9.7325 (4)    b=15.4375 (6)    c=11.7681 (4)	
	alpha=90    beta=100.832 (3)    gamma=90	
Temperature:	123 K	
Volume	Calculated 1736.60 (12)	Reported 1736.60 (12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H20 N2	C24 H20 N2
Sum formula	C24 H20 N2	C24 H20 N2
Mr	336.42	336.44
Dx, g cm <sup>-3</sup>	1.287	1.287
Z	4	4
Mu (mm <sup>-1</sup> )	0.075	0.075
F000	712.0	712.0
F000'	712.24	
h, k, lmax	14, 22, 16	13, 21, 16
Nref	5426	4481
Tmin, Tmax	0.949, 0.978	0.580, 0.978
Tmin'	0.949	
Correction method=	# Reported T Limits: Tmin=0.580 Tmax=0.978	

AbsCorr = MULTI-SCAN  
Data completeness= 0.826                      Theta(max)= 30.790  
R(reflections)= 0.0456( 3777)                      wR2(reflections)= 0.1300( 4481)  
S = 1.102                      Npar= 315

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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.

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#### ● Alert level A

[PLAT029\\_ALERT\\_3\\_A](#) \_diffn\_measured\_fraction\_theta\_full value Low .                      0.826 Why?

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#### ● Alert level G

[CHEMS02\\_ALERT\\_1\\_G](#) Please check that you have entered the correct  
\_publ\_requested\_category classification of your compound;  
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;  
FO or CO or EO for organic.  
From the CIF: \_publ\_requested\_category    CHOOSE FI FM FO CI CM CO or A  
From the CIF: \_chemical\_formula\_sum :C24 H20 N2  
[PLAT005\\_ALERT\\_5\\_G](#) No Embedded Refinement Details Found in the CIF                      Please Do !  
[PLAT063\\_ALERT\\_4\\_G](#) Crystal Size Possibly too Large for Beam Size ..                      0.70 mm  
[PLAT882\\_ALERT\\_1\\_G](#) No Datum for \_diffn\_reflns\_av\_unetI/netI .....                      Please Do !

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

2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
0 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
1 **ALERT type 3** Indicator that the structure quality may be low  
1 **ALERT type 4** Improvement, methodology, query or suggestion  
1 **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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**PLATON version of 18/09/2020; check.def file version of 20/08/2020**

**Datablock xcalibur - ellipsoid plot**

