

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) TT-CCH

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: TT-CCH

---

Bond precision:	C-C = 0.0019 A	Wavelength=1.54184
Cell:	a=13.35072 (15)	b=4.63511 (4)      c=16.41198 (19)
	alpha=90	beta=96.7803 (11)      gamma=90
Temperature:	296 K	
	Calculated	Reported
Volume	1008.504 (19)	1008.504 (19)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C11 H6 N6	C11 H6 N6
Sum formula	C11 H6 N6	C11 H6 N6
Mr	222.22	222.22
Dx, g cm <sup>-3</sup>	1.464	1.464
Z	4	4
Mu (mm <sup>-1</sup> )	0.805	0.805
F000	456.0	456.0
F000'	457.38	
h, k, lmax	17, 5, 20	17, 5, 20
Nref	2194	2177
Tmin, Tmax	0.849, 0.923	0.595, 1.000
Tmin'	0.773	

Correction method= # Reported T Limits: Tmin=0.595 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.992      Theta(max)= 80.142

R(reflections)= 0.0420 ( 2010)	wR2(reflections)= 0.1164 ( 2177)
S = 1.050	Npar= 154

---

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**

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.195 Check

---



#### **Alert level G**

PLAT142\_ALERT\_4\_G s.u. on b - Axis Small or Missing ..... 0.00004 Ang.  
PLAT371\_ALERT\_2\_G Long C(sp2)-C(sp1) Bond C2 - C10 . 1.41 Ang.  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact C11 ..C11 . 3.20 Ang.  
2-x,2-y,1-z = 3\_776 Check  
PLAT899\_ALERT\_4\_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note  
PLAT899\_ALERT\_4\_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 17 Note  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 4.25 Note  
Predicted wR2: Based on SigI\*\*2 2.74 or SHELX Weight 11.51  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info  
PLAT992\_ALERT\_5\_G Repd & Actual \_reflns\_number\_gt Values Differ by 2 Check

---

- 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  
9 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 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  
4 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 06/01/2024; check.def file version of 05/01/2024**

