

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

Bond precision:	C-C = 0.0043 Å	Wavelength=0.71073	
Cell:	a=11.132 (5)	b=12.623 (6)	c=14.347 (6)
	alpha=90	beta=110.582 (14)	gamma=90
Temperature:	300 K		

	Calculated	Reported
Volume	1887.4 (15)	1887.1 (15)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C25 H25 N	C25 H25 N
Sum formula	C25 H25 N	C25 H25 N
Mr	339.46	339.46
Dx, g cm <sup>-3</sup>	1.195	1.195
Z	4	4
Mu (mm <sup>-1</sup> )	0.068	0.068
F000	728.0	728.0
F000'	728.25	
h, k, lmax	13, 15, 17	13, 15, 17
Nref	3516	3502
Tmin, Tmax	0.984, 0.988	0.622, 0.746
Tmin'	0.984	

Correction method= # Reported T Limits: Tmin=0.622 Tmax=0.746  
AbsCorr = ?

Data completeness= 0.996                      Theta (max)= 25.500

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R(reflections)= 0.0610( 2089)      wR2(reflections)=
S = 1.032                        0.1896( 3502)
Npar= 235
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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 C

PLAT052\_ALERT\_1\_C Info on Absorption Correction Method Not Given Please Do !  
PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C13 --C18 . 7.0 s.u.  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0043 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.557 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 13 Report  
-5 4 1, -2 0 2, 2 4 2, -2 6 3, 1 6 4, -3 0 11,  
-2 0 12, -3 0 13, -2 0 14, -3 0 15, -1 0 15, -2 0 16,  
-2 1 16,

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### ● Alert level G

PLAT793\_ALERT\_4\_G Model has Chirality at C13 (Centro SpGr) S Verify  
PLAT793\_ALERT\_4\_G Model has Chirality at C17 (Centro SpGr) S Verify  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note  
-1 0 1,  
PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 1 Note  
-2 0 2,  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 5 Note  
-1 0 1, 2 4 2, -2 6 3, 1 6 4, -5 4 1,  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 4.9 Low  
PLAT967\_ALERT\_5\_G Note: Two-Theta Cutoff Value in Embedded .res .. 51.0 Degree  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 2.580 Note  
Predicted wR2: Based on SigI\*\*2 7.35 or SHELX Weight 18.37  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
5 **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

- 1 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  
6 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

