

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

## Datablock: 2c

Bond precision:	C-C = 0.0053 Å	Wavelength=0.71073
Cell:	a=5.1616(4)      b=6.6616(5)      c=19.2655(14)	
	alpha=90      beta=92.600(3)      gamma=90	
Temperature:	294 K	

  

	Calculated	Reported
Volume	661.75(9)	661.75(9)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C16 H18 N2 O	C16 H18 N2 O
Sum formula	C16 H18 N2 O	C16 H18 N2 O
Mr	254.32	254.32
Dx, g cm <sup>-3</sup>	1.276	1.276
Z	2	2
Mu (mm <sup>-1</sup> )	0.081	0.081
F000	272.0	272.0
F000'	272.10	
h, k, lmax	6, 8, 24	6, 8, 24
Nref	2737[ 1491]	2725
Tmin, Tmax	0.984, 0.992	0.910, 0.990
Tmin'	0.976	

Correction method= # Reported T Limits: Tmin=0.910  
Tmax=0.990 AbsCorr = MULTI-SCAN

Data completeness= 1.83/1.00      Theta(max)= 26.410

R(reflections)= 0.0524( 2250)      wR2(reflections)=  
0.1409( 2725)

S = 1.149      Npar= 176

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 A

[PLAT939 ALERT 3 A](#) Large Value of Not (SHELXL) Weight Optimized S . 1162.40 Check

### Alert level C

[STRVA01 ALERT 4 C](#) Flack test results are ambiguous.  
From the CIF: `_refine_ls_abs_structure_Flack` 0.400  
From the CIF: `_refine_ls_abs_structure_Flack_su` 0.900

[PLAT340 ALERT 3 C](#) Low Bond Precision on C-C Bonds ..... 0.00531 Ang.  
[PLAT906 ALERT 3 C](#) Large K Value in the Analysis of Variance ..... 2.090 Check  
[PLAT918 ALERT 3 C](#) Reflection(s) with I(obs) much Smaller I(calc) . 1 Check  
[PLAT934 ALERT 3 C](#) Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check  
[PLAT977 ALERT 2 C](#) Check Negative Difference Density on H10 -0.31 eA-3  
[PLAT977 ALERT 2 C](#) Check Negative Difference Density on H14A -0.33 eA-3

### Alert level G

[PLAT002 ALERT 2 G](#) Number of Distance or Angle Restraints on AtSite 2 Note  
[PLAT032 ALERT 4 G](#) Std. Uncertainty on Flack Parameter Value High . 0.900 Report  
[PLAT172 ALERT 4 G](#) The CIF-Embedded .res File Contains DFIX Records 1 Report  
[PLAT860 ALERT 3 G](#) Number of Least-Squares Restraints ..... 2 Note  
[PLAT910 ALERT 3 G](#) Missing # of FCF Reflection(s) Below Theta(Min). 2 Note  
[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density. 0 Info

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
7 ALERT type 3 Indicator that the structure quality may be low

3 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.

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PLATON version of 13/07/2021; check.def file version of 13/07/2021

## **Datablock 2c - ellipsoid plot**

