

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

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

## Datablock: TH07R2\_01\_a

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Bond precision: C-C = 0.0047 Å Wavelength=0.71073  
Cell: a=15.193(2) b=21.892(4) c=6.8654(13)  
alpha=90 beta=90 gamma=90  
Temperature: 153 K

	Calculated	Reported
Volume	2283.5(7)	2283.4(7)
Space group	I b a 2	I b a 2
Hall group	I 2 -2c	I 2 -2c
Moiety formula	C15 H14	C15 H14
Sum formula	C15 H14	C15 H14
Mr	194.26	194.26
Dx, g cm <sup>-3</sup>	1.130	1.130
Z	8	8
Mu (mm <sup>-1</sup> )	0.063	0.063
F000	832.0	832.0
F000'	832.29	
h,k,lmax	19,27,8	19,27,8
Nref	2378[ 1297]	2242
Tmin,Tmax	0.969,0.972	
Tmin'	0.969	

Correction method= Not given

Data completeness= 1.73/0.94 Theta(max)= 26.500

R(reflections)= 0.0495( 1871) wR2(reflections)=  
0.1462( 2242)

S = 1.188 Npar= 139

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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

[STRVA01 ALERT 4 C](#) Flack parameter is too small

From the CIF: `_refine_ls_abs_structure_Flack` -7.200

From the CIF: `_refine_ls_abs_structure_Flack_su` 1.000

[PLAT031 ALERT 4 C](#) Refined Extinction Parameter Within Range of ... 2.789 Sigma

[PLAT340 ALERT 3 C](#) Low Bond Precision on C-C Bonds ..... 0.00471 Ang.

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### ● Alert level G

[PLAT032 ALERT 4 G](#) Std. Uncertainty on Flack Parameter Value High . 1.000

Report

[PLAT883 ALERT 1 G](#) No Info/Value for `_atom_sites_solution_primary` . Please Do !

[PLAT899 ALERT 4 G](#) SHELXL2018 is Outdated and Succeeded by SHELXL 2019/3 Note

[PLAT910 ALERT 3 G](#) Missing # of FCF Reflection(s) Below Theta(Min). 3 Note

2 0 0, 1 1 0, 0 2 0,

[PLAT916 ALERT 2 G](#) Hooft y and Flack x Parameter Values Differ by . 7.10 Check

[PLAT967 ALERT 5 G](#) Note: Two-Theta Cutoff Value in Embedded .res .. 53.0

Degree

[PLAT969 ALERT 5 G](#) The 'Henn et al.' R-Factor-gap value ..... 6.171 Note

Predicted wR2: Based on SigI\*\*2 2.37 or SHELX Weight 12.31

[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

3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
8 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 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

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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 22/08/2024; check.def file version of 21/08/2024**

## **Datablock TH07R2\_01\_a - ellipsoid plot**

