

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

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

## Datablock: TH41\_02fin

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Bond precision:	C-C = 0.0043 Å	Wavelength=0.71073
Cell:	a=11.503(4)    b=14.280(4)    c=19.347(7)	
	alpha=108.93(2) beta=104.87(2) gamma=91.12(2)	
Temperature:	123 K	

  

	Calculated	Reported
Volume	2887.0(17)	2887.2(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C15 H14 O2), C7 H8	4(C15 H14, 2(C7 H8)
Sum formula	C37 H36 O4	C74 H72 O8
Mr	544.66	1089.31
Dx, g cm <sup>-3</sup>	1.253	1.253
Z	4	2
Mu (mm <sup>-1</sup> )	0.080	0.080
F000	1160.0	1160.0
F000'	1160.52	
h,k,lmax	14,18,24	14,18,24
Nref	12618	12395
Tmin,Tmax	0.989,0.995	
Tmin'	0.976	
Correction method=	Not given	
Data completeness=	0.982	Theta(max)= 27.000
R(reflections)=	0.0576( 6800)	wR2(reflections)= 0.1524( 12395)
S =	1.064	Npar= 773

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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.

### Alert level B

[PLAT910 ALERT 3 B](#) Missing # of FCF Reflection(s) Below Theta(Min) . 15 Note

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

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### Alert level C

[PLAT042 ALERT 1 C](#) Calc. and Reported MoietyFormula Strings Differ Please Check

Calc.: 2(C15 H14 O2), C7 H8  
Rep.: 4(C15 H14, 2(C7 H8)

[PLAT245 ALERT 2 C](#) U(iso) H1C Smaller than U(eq) O1C by 0.012  
Ang\*\*2

[PLAT340 ALERT 3 C](#) Low Bond Precision on C-C Bonds ..... 0.00434 Ang.

[PLAT414 ALERT 2 C](#) Short Intra D-H..H-X H2B ..H15D . 1.96 Ang.

x,y,z = 1\_555 Check

[PLAT414 ALERT 2 C](#) Short Intra D-H..H-X H2D ..H15G . 1.99 Ang.

x,y,z = 1\_555 Check

[PLAT906 ALERT 3 C](#) Large K Value in the Analysis of Variance ..... 2.931 Check

[PLAT911 ALERT 3 C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 172

Report

-2	2	0,	-2	4	0,	-2	5	0,	-3	6	0,	-2	6	0,	-4	7	0,
-3	7	0,	-2	7	0,	-4	8	0,	-3	8	0,	-2	8	0,	-4	9	0,
-3	9	0,	-3	10	0,	-2	10	0,	-3	11	0,	-2	11	0,	-3	12	0,
-2	13	0,	2	-8	1,	2	-7	1,	2	-6	1,	-2	-4	1,	-1	-4	1,
0	-4	1,	-3	-3	1,	-2	-3	1,	-1	-3	1,	0	-3	1,	-4	-2	1,

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-3 -2 1, -1 -2 1, -2 -1 1, -3 0 1, -4 1 1, 11 3 1,
-3 6 1, -4 7 1, -3 7 1, -5 8 1, -4 8 1, -3 8 1,
-5 9 1, -4 9 1, -3 9 1, -6 10 1, -5 10 1, -4 10 1,
-3 10 1, -4 11 1, -3 11 1, -5 12 1, -4 12 1, -3 12 1,
-3 13 1, -2 13 1, -3 14 1, -3 -6 2, -5 -4 2, -6 -3 2,
-5 -3 2, -4 -3 2, -6 -2 2, -5 -2 2, -4 -2 2, -3 -2 2,
-5 8 2, -4 8 2, -6 9 2, -5 9 2, -4 9 2, -6 10 2,
-5 10 2, -4 10 2, -3 10 2, -6 11 2, -5 11 2, -4 11 2,
-3 11 2, -5 12 2, -4 12 2, -3 12 2, -6 13 2, -4 13 2,
-3 13 2, -5 14 2, -3 14 2, -6 9 3, -5 9 3, -4 9 3,
-7 10 3, -6 10 3, -5 10 3, -4 10 3, -7 11 3, -6 11 3,

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## ●Alert level G

[FORMU01 ALERT 1 G](#) There is a discrepancy between the atom counts in the  
 \_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
 usually due to the moiety formula being in the wrong format.  
 Atom count from \_chemical\_formula\_sum: C74 H72 O8  
 Atom count from \_chemical\_formula\_moiety: C74 H72

[PLAT002 ALERT 2 G](#) Number of Distance or Angle Restraints on AtSite 16 Note  
[PLAT045 ALERT 1 G](#) Calculated and Reported Z Differ by a Factor ... 2 Check  
[PLAT154 ALERT 1 G](#) The s.u.'s on the Cell Angles are Equal ..(Note) 0.02  
 Degree

[PLAT172 ALERT 4 G](#) The CIF-Embedded .res File Contains DFIX Records 8  
 Report

[PLAT860 ALERT 3 G](#) Number of Least-Squares Restraints ..... 8 Note  
[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  
[PLAT912 ALERT 4 G](#) Missing # of FCF Reflections Above STh/L= 0.600 39 Note  
[PLAT913 ALERT 3 G](#) Missing # of Very Strong Reflections in FCF .... 1 Note  
 -1 -3 1,

[PLAT933 ALERT 2 G](#) Number of HKL-OMIT Records in Embedded .res File 15 Note  
 -7 13 3, -5 12 1, -6 13 2, -3 12 0, 11 3 1, -2 13 0,  
 -3 14 1, -5 14 2, -6 10 1, -13 4 11, -1 -2 8, -1 -3 5,  
 -3 -2 2, -7 -6 4, -13 -6 13,

[PLAT941 ALERT 3 G](#) Average HKL Measurement Multiplicity ..... 2.5 Low  
[PLAT960 ALERT 3 G](#) Number of Intensities with I < - 2\*sig(I) ... 9 Check  
[PLAT965 ALERT 2 G](#) The SHELXL WEIGHT Optimisation has not Converged Please Check  
[PLAT967 ALERT 5 G](#) Note: Two-Theta Cutoff Value in Embedded .res .. 54.0  
 Degree

[PLAT969 ALERT 5 G](#) The 'Henn et al.' R-Factor-gap value ..... 2.844 Note  
 Predicted wR2: Based on SigI\*\*2 5.36 or SHELX Weight 14.33

[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density. 1 Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 1 **ALERT level B** = A potentially serious problem, consider carefully  
 7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 17 **ALERT level G** = General information/check it is not something unexpected
- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 7 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 8 ALERT type 3 Indicator that the structure quality may be low  
 3 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 TH41\_02fin - ellipsoid plot

