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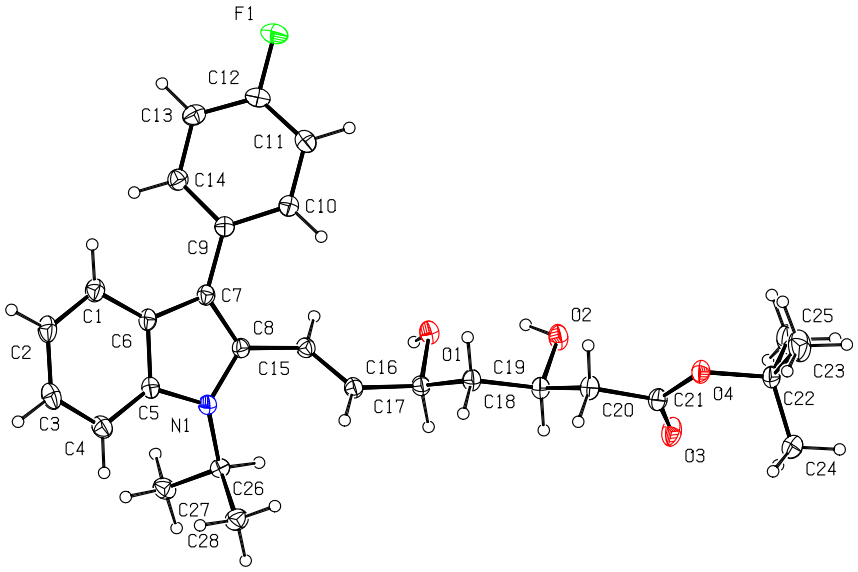
The crystal structure of t-butyl 7-[3-(4-fluorophenyl)-1-(propan-2-yl)-1*H*-indol-2-yl]-3,5-dihydroxyhept-6-enoate, $C_{28}H_{34}FNO_4$



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Abstract

$C_{28}H_{34}FNO_4$, monoclinic, *C*2/*c* (no. 15), a = 21.7795(12) Å, b = 5.9103(4) Å, c = 39.830(2) Å, β = 100.866(3)°, V = 5035.1(5) Å^3, Z = 8, $R_{gt}(F)$ = 0.0487, w$R_{ref}(F^2)$ = 0.1376, T = 170 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless needle
Size:	0.03 × 0.02 × 0.02 mm
Wavelength:	GaKα radiation (1.34139 Å)
μ:	0.45 mm^{-1}
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
θ_{max}, completeness:	60.9°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	75,706, 5827, 0.067
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4608
$N(param)_{refined}$:	314
Programs:	Bruker [1], Olex2 [2], Shelx [3, 4]

1 Source of materials

One hundred milligram t-butyl 7-[3-(4-fluorophenyl)-1-(propan-2-yl)-1*H*-indol-2-yl]-3,5-dihydroxyhept-6-enoate was dissolved in 2 mL of acetonitrile. The resulting mixture was stirred and dissolved at 50 °C to obtain a clear solution, which was filtered and placed in a 5 mL glass bottle, the film was covered with a puncture hole. The filtrate was slowly evaporated at room temperature. Crystals of the title compound were obtained after seven days.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
F1	0.64289 (4)	−0.51036 (17)	0.35067 (3)	0.0504 (3)
O1	0.50257 (4)	0.28335 (17)	0.44856 (2)	0.0316 (2)
H1	0.471613	0.213252	0.453123	0.047*
N1	0.37381 (5)	0.3815 (2)	0.32423 (3)	0.0279 (3)
C1	0.41353 (7)	0.0829 (3)	0.25274 (4)	0.0342 (3)
H1A	0.442906	−0.030037	0.249520	0.041*
O2	0.58523 (5)	0.52034 (18)	0.49588 (3)	0.0380 (3)
H2	0.565567	0.404490	0.487714	0.057*
C2	0.37292 (7)	0.1730 (3)	0.22512 (4)	0.0389 (4)
H2A	0.374388	0.120696	0.202735	0.047*
O3	0.59974 (5)	0.9597 (2)	0.53903 (3)	0.0439 (3)
C3	0.32995 (7)	0.3392 (3)	0.22958 (4)	0.0405 (4)
H3	0.303048	0.399305	0.210050	0.049*
O4	0.69288 (4)	1.02167 (18)	0.52420 (2)	0.0331 (2)
C4	0.32524 (7)	0.4195 (3)	0.26166 (4)	0.0358 (3)
H4	0.295405	0.531721	0.264492	0.043*
C5	0.36630 (6)	0.3284 (2)	0.28982 (3)	0.0289 (3)
C6	0.41053 (6)	0.1614 (2)	0.28568 (3)	0.0282 (3)
C7	0.44652 (6)	0.1144 (2)	0.31927 (3)	0.0269 (3)
C8	0.42327 (6)	0.2523 (2)	0.34179 (3)	0.0258 (3)
C9	0.49859 (6)	−0.0471 (2)	0.32759 (3)	0.0276 (3)
C10	0.55203 (6)	0.0003 (2)	0.35235 (4)	0.0296 (3)
H10	0.555192	0.141689	0.363891	0.036*
C11	0.60021 (7)	−0.1551 (3)	0.36029 (4)	0.0343 (3)
H11	0.635833	−0.122869	0.377386	0.041*
C12	0.59527 (7)	−0.3572 (3)	0.34284 (4)	0.0357 (3)
C13	0.54439 (7)	−0.4112 (3)	0.31815 (4)	0.0360 (3)
H13	0.542440	−0.551544	0.306365	0.043*
C14	0.49604 (7)	−0.2565 (2)	0.31082 (4)	0.0321 (3)
H14	0.460291	−0.293007	0.294056	0.038*
C15	0.44729 (6)	0.2759 (2)	0.37855 (3)	0.0275 (3)
H15	0.457977	0.141077	0.391312	0.033*
C16	0.45532 (6)	0.4708 (2)	0.39547 (3)	0.0292 (3)
H16	0.442960	0.605148	0.382908	0.035*
C17	0.48243 (6)	0.4956 (2)	0.43296 (3)	0.0281 (3)
H17	0.449509	0.559591	0.444659	0.034*
C18	0.53830 (6)	0.6559 (2)	0.43871 (3)	0.0299 (3)
H18A	0.572960	0.585332	0.429564	0.036*
H18B	0.526520	0.797363	0.425789	0.036*
C19	0.56116 (6)	0.7138 (2)	0.47628 (3)	0.0295 (3)
H19	0.525298	0.776066	0.485784	0.035*
C20	0.61312 (7)	0.8880 (3)	0.48109 (4)	0.0334 (3)
H20A	0.649454	0.824981	0.472602	0.040*
H20B	0.598609	1.023608	0.467255	0.040*
C21	0.63348 (7)	0.9571 (2)	0.51799 (4)	0.0308 (3)
C22	0.72419 (6)	1.1017 (2)	0.55847 (4)	0.0308 (3)
C23	0.78680 (8)	1.1825 (4)	0.55167 (5)	0.0584 (5)
H23A	0.807729	1.058110	0.542066	0.088*
H23B	0.812898	1.233092	0.573135	0.088*
H23C	0.780221	1.308591	0.535402	0.088*
C24	0.68906 (8)	1.2969 (3)	0.57044 (5)	0.0451 (4)
H24A	0.678061	1.406662	0.551834	0.068*
H24B	0.715474	1.370209	0.590062	0.068*
H24C	0.650840	1.240426	0.577174	0.068*
C25	0.73145 (10)	0.9051 (3)	0.58305 (5)	0.0551 (5)
H25A	0.756185	0.952532	0.605073	0.083*
H25B	0.752778	0.780429	0.573757	0.083*
H25C	0.690097	0.854602	0.586275	0.083*
C26	0.32656 (6)	0.4955 (2)	0.34036 (4)	0.0282 (3)
H26	0.339854	0.475027	0.365603	0.034*
C27	0.26227 (7)	0.3846 (3)	0.33028 (4)	0.0354 (3)
H27A	0.246340	0.408822	0.305846	0.053*
H27B	0.233375	0.452051	0.343558	0.053*
H27C	0.265916	0.221903	0.334967	0.053*
C28	0.32457 (7)	0.7488 (3)	0.33365 (4)	0.0386 (3)
H28A	0.365795	0.814467	0.342423	0.058*
H28B	0.293461	0.818941	0.345218	0.058*
H28C	0.313161	0.776443	0.309004	0.058*

2 Experimental details

Using Olex2 [2], the structure was solved with the Shelxt [3] structure solution program using Intrinsic Phasing and refined with the Shelxl [4] refinement package using least squares minimisation. The H atoms were fixed, fixed U_{iso} were set to 1.2 times of all C(H) groups, C(H,H) groups and N(H,H) groups; 1.5 times of C(H,H,H,H) groups, O(H) groups and O(H,H) groups.

3 Comment

Fluvastatin, a member of the group of drugs known as HMG-CoA reductase inhibitors, was the first statin available as an extended-release product [5]. The solid-state properties of Fluvastatin sodium salt crystallized from different solvents for comparison with crystalline forms of the commercially available raw material was reported [6]. The *t*-butyl 7-[3-(4-fluorophenyl)-1-(propan-2-yl)-1*H*-indol-2-yl]-3,5-dihydroxyhept-6-enoate is the final Fluvastatin precursor [7]. However, no single crystal structure is reported. The title crystal skeleton consists of two benzene rings and a nitrogen heterocyclic ring. Even though it has two hydroxyl groups, no hydrogen bonds exist in the structure of the molecule.

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