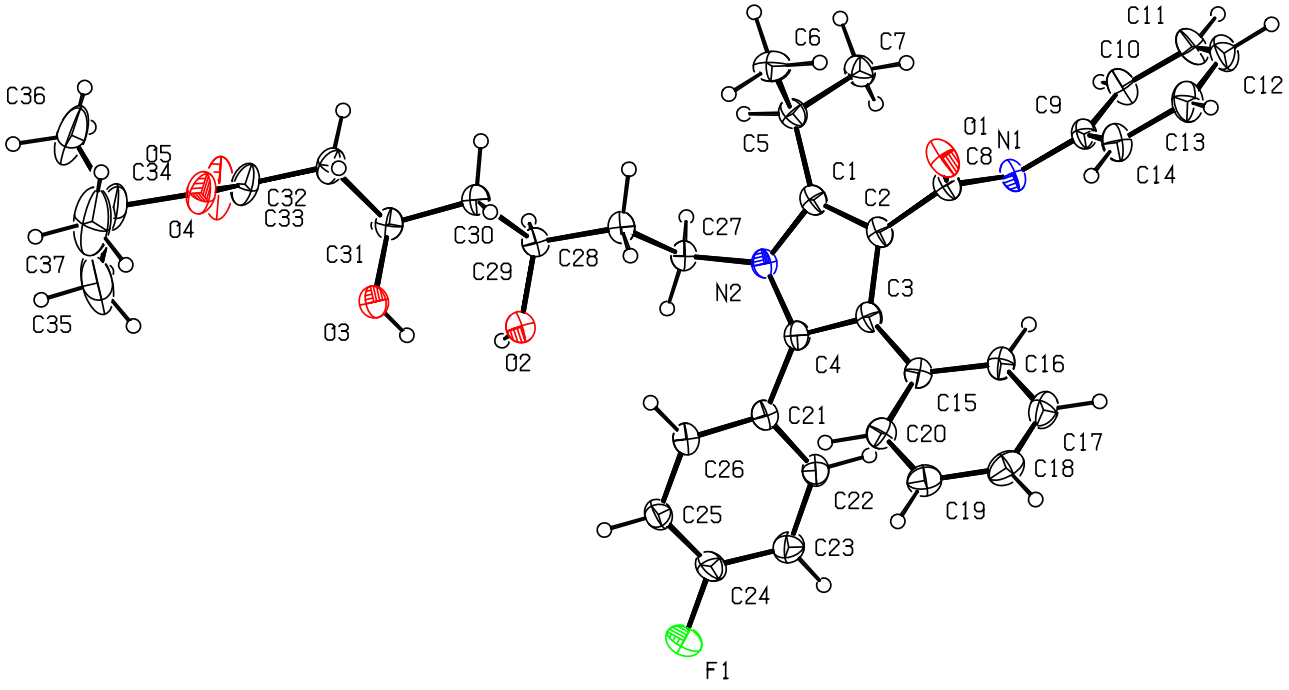
Wei-Jie Sun, Zhi-Chao Wang and Cheng-Jun Jiang*

The structure of *t*-butyl 7-[2-(4-fluorophenyl)-3-phenyl-4-(phenylcarbamoyl)-5-(propan-2-yl)-1*H*-pyrrol-1-yl]-3,5-dihydroxyheptanoate, $C_{37}H_{43}FN_2O_5$



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Abstract

$C_{37}H_{43}FN_2O_5$, monoclinic, $P2_1$ (no. 4), a = 13.8818(6) Å, b = 8.7373(4) Å, c = 15.6295(7) Å, β = 113.356(2)°, V = 1740.36(14) Å^3, Z = 2, $R_{gt}(F)$ = 0.0527, $wR_{ref}(F^2)$ = 0.1346, T = 170 K.

CCDC no.: 2389999

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:	0.09 × 0.02 × 0.01 mm
Wavelength:	Ga *K*α radiation (1.34139 Å)
μ:	0.42 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}:	50016, 8000, 0.083
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 5,498
N(param)$_{refined}$:	413
Programs:	Bruker,[1] Olex2,[2] SHELX[3,4]

1 Source of materials

t-Butyl 7-[2-(4-fluorophenyl)-3-phenyl-4-(phenylcarbamoyl)-5-(propan-2-yl)-1*H*-pyrrol-1-yl]-3,5-dihydroxyheptanoate (50.0 mg,

***Corresponding author: Cheng-Jun Jiang**, School of Biological and Chemical Engineering, Zhejiang University of Science and Technology, Liuhe Road 318#, Hangzhou, China, E-mail: jcj312@163.com. https://orcid.org/0000-0001-9297-9399
Wei-Jie Sun and Zhi-Chao Wang, School of Biological and Chemical Engineering, Zhejiang University of Science and Technology, Liuhe Road 318#, Hangzhou, China

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
F1	0.07836 (17)	0.1904 (3)	0.12580 (14)	0.0713 (7)
O1	0.4440 (2)	0.5604 (2)	0.76778 (16)	0.0518 (6)
N1	0.3879 (2)	0.3276 (3)	0.79197 (17)	0.0372 (6)
C1	0.4896 (2)	0.3120 (3)	0.6290 (2)	0.0350 (7)
O2	0.53474 (15)	0.3258 (2)	0.30643 (14)	0.0388 (5)
H2	0.534470	0.244264	0.277848	0.058*
N2	0.45066 (19)	0.2829 (3)	0.53462 (17)	0.0346 (6)
C2	0.4080 (2)	0.3729 (3)	0.6480 (2)	0.0346 (7)
O3	0.65180 (17)	0.4986 (3)	0.23343 (15)	0.0431 (5)
H3	0.594248	0.456156	0.224304	0.065*
C3	0.3180 (2)	0.3867 (3)	0.5623 (2)	0.0349 (7)
O4	0.8860 (3)	0.3814 (4)	0.2257 (3)	0.0985 (13)
C4	0.3460 (2)	0.3271 (3)	0.4927 (2)	0.0334 (6)
O5	0.8824 (2)	0.6378 (3)	0.2187 (2)	0.0626 (8)
C5	0.6023 (2)	0.2821 (4)	0.6933 (2)	0.0393 (7)
H5	0.635817	0.225621	0.656669	0.047*
C6	0.6637 (3)	0.4296 (4)	0.7280 (3)	0.0530 (9)
H6A	0.657951	0.493354	0.674558	0.080*
H6B	0.737664	0.405276	0.764553	0.080*
H6C	0.635117	0.485237	0.767100	0.080*
C7	0.6113 (3)	0.1809 (4)	0.7760 (2)	0.0454 (8)
H7A	0.587971	0.238431	0.818200	0.068*
H7B	0.684467	0.149428	0.809546	0.068*
H7C	0.567107	0.089924	0.753387	0.068*
C8	0.4154 (2)	0.4298 (4)	0.7408 (2)	0.0372 (7)
C9	0.3875 (2)	0.3590 (3)	0.8815 (2)	0.0361 (7)
C10	0.4208 (3)	0.2448 (4)	0.9477 (2)	0.0509 (9)
H10	0.444148	0.149881	0.933208	0.061*
C11	0.4203 (3)	0.2678 (5)	1.0346 (3)	0.0593 (10)
H11	0.443372	0.188634	1.079912	0.071*
C12	0.3868 (3)	0.4043 (5)	1.0562 (3)	0.0574 (10)
H12	0.388276	0.420965	1.116757	0.069*
C13	0.3511 (3)	0.5167 (5)	0.9898 (3)	0.0588 (10)
H13	0.325822	0.610071	1.004173	0.071*
C14	0.3515 (3)	0.4960 (4)	0.9018 (3)	0.0501 (9)
H14	0.327321	0.574713	0.856266	0.060*
C15	0.2195 (2)	0.4697 (3)	0.5482 (2)	0.0359 (7)
C16	0.1765 (3)	0.4718 (4)	0.6153 (2)	0.0444 (8)
H16	0.205378	0.407608	0.668495	0.053*
C17	0.0928 (3)	0.5656 (5)	0.6056 (3)	0.0557 (10)
H17	0.066079	0.566631	0.652886	0.067*
C18	0.0477 (3)	0.6573 (5)	0.5289 (3)	0.0569 (10)
H18	−0.009554	0.721894	0.523097	0.068*
C19	0.0865 (3)	0.6546 (4)	0.4601 (3)	0.0493 (8)
H19	0.055126	0.716292	0.406000	0.059*
C20	0.1715 (2)	0.5616 (4)	0.4700 (2)	0.0429 (8)
H20	0.197524	0.560682	0.422196	0.052*
C21	0.2779 (2)	0.2946 (3)	0.3952 (2)	0.0348 (7)
C22	0.1854 (2)	0.2125 (4)	0.3765 (2)	0.0424 (8)
H22	0.168817	0.178795	0.426832	0.051*
C23	0.1168 (3)	0.1791 (5)	0.2853 (2)	0.0509 (9)
H23	0.053140	0.125532	0.272868	0.061*
C24	0.1438 (3)	0.2254 (4)	0.2148 (2)	0.0485 (8)
C25	0.2336 (2)	0.3053 (4)	0.2290 (2)	0.0435 (8)
H25	0.249989	0.335433	0.177940	0.052*
C26	0.3000 (3)	0.3411 (4)	0.3197 (2)	0.0396 (7)
H26	0.361883	0.398541	0.330510	0.047*
C27	0.5135 (2)	0.2313 (3)	0.4835 (2)	0.0343 (7)
H27A	0.465956	0.192564	0.421533	0.041*
H27B	0.559112	0.145568	0.517780	0.041*
C28	0.5812 (3)	0.3582 (4)	0.4706 (2)	0.0379 (7)
H28A	0.539741	0.454008	0.454466	0.045*
H28B	0.641817	0.375184	0.530385	0.045*
C29	0.6214 (2)	0.3242 (4)	0.3955 (2)	0.0342 (6)
H29	0.653926	0.220063	0.406603	0.041*
C30	0.7037 (2)	0.4414 (4)	0.3973 (2)	0.0382 (7)
H30A	0.676711	0.545328	0.400099	0.046*
H30B	0.767737	0.426039	0.454609	0.046*
C31	0.7329 (2)	0.4323 (4)	0.3139 (2)	0.0386 (7)
H31	0.742641	0.322659	0.300830	0.046*
C32	0.8332 (3)	0.5208 (4)	0.3300 (3)	0.0514 (9)
H32A	0.821218	0.630714	0.337593	0.062*
H32B	0.889474	0.484734	0.388486	0.062*
C33	0.8685 (3)	0.5027 (5)	0.2521 (3)	0.0577 (10)
C34	0.9224 (4)	0.6507 (6)	0.1446 (4)	0.0776 (15)
C35	0.8502 (7)	0.5607 (11)	0.0595 (5)	0.146 (3)
H35A	0.861028	0.450795	0.072161	0.219*
H35B	0.866402	0.586855	0.005646	0.219*
H35C	0.777007	0.586770	0.046076	0.219*
C36	1.0332 (4)	0.5947 (9)	0.1794 (5)	0.135 (3)
H36A	1.076495	0.652699	0.235039	0.203*
H36B	1.060409	0.608927	0.130820	0.203*
H36C	1.035380	0.485783	0.195003	0.203*
C37	0.9136 (6)	0.8160 (7)	0.1226 (6)	0.133 (3)
H37A	0.841296	0.849745	0.107293	0.199*
H37B	0.932217	0.834464	0.069203	0.199*
H37C	0.961304	0.873341	0.176652	0.199*

0.08 mmol) was dissolved in the acetonitrile (3 ml) at 50 °C and water (1.5 ml) in 10 ml glass bottle. The glass bottle was covered with a porous film. Single crystal of the title compound were obtained after 7 days.

2 Experimental details

Absorption corrections were applied by using multi-scan program.[1] Using Olex2,[2] the structure was solved with the ShelXT[3] structure solution program and refined with the ShelXL[4] refinement package.

3 Comment

Atorvastatin (Lipitor, Pfizer) is a safe and effective 3-hydroxy-3-methyl-glutaryl–CoA (HMG–CoA) reductase inhibitor (statin). It is the most potent currently available statin.[5]

Structural mechanism for statin inhibition of HMG–CoA reductase was studied.[6] It is important to analyse the exact structure of the Atorvastatin and its intermediates. The *t*-butyl 7-[3-(4-fluorophenyl)-1-(propan-2-yl)-1H-indol-2-yl]-3,5-dihydroxyhept-6-enoate is the final Atorvastatin precursor.[7,8] However, no single crystal structure is reported. The title crystal skeleton consists of three benzene rings and a pyrrol ring. There are intermolecular hydrogen bonds, $H_3O_3\cdots N_1$, $H_2O_2\cdots O_1$, and intramolecular hydrogen bonds $H_3O_3\cdots O_2$. Bond lengths are al in the expected ranges.[9]

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Competing interests: The authors declare no conflicts of interest regarding this article.

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