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N-(*tert*-Butoxycarbonyl)-*O*-(hydroxyethyl)tyrosine methyl ester

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.060
wR factor = 0.168
Data-to-parameter ratio = 14.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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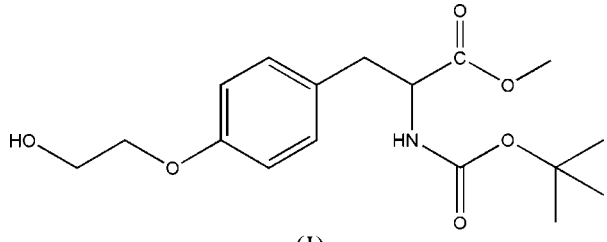
In the title compound (systematic name: *tert*-butyl *N*-{2-[4-(2-hydroxyethoxy)phenyl]-1-(methoxycarbonyl)ethyl}carbamate), $C_{17}H_{25}N_1O_6$, the crystal structure is stabilized by O—H···O and N—H···O hydrogen bonds.

Comment

The positron-labeled L-tyrosine analog *O*-(2-[18*F*]fluoroethyl)-L-tyrosine (FET) is becoming increasingly important as an amino acid positron emission tomography (PET) tracer for the detection and localization of tumors with a higher specificity than other available tracers, especially for brain tumors (Kaim *et al.*, 2002).

The structure of the title compound, (I), an intermediate in the synthesis of FET, is reported here (Fig. 1). A combination of intermolecular O—H···O and N—H···O hydrogen bonds (Table 1) helps to establish the crystal packing (Fig. 2).



(I)

Experimental

A solution of *N*-(*tert*-butoxycarbonyl)tyrosine methyl ester (1 g, 3.4 mmol) in dimethylformamide (25 ml) was added, with stirring, to potassium carbonate (1.17 g, 8.5 mmol), Bu_4NI (0.13 g, 0.34 mmol) and 18-C-6 crown ether (0.18 g, 0.68 mmol). The reaction mixture was heated at 398 K for 12 h, after which water (20 ml) was added and the layers were separated. The aqueous phase was extracted with dichloromethane, the combined organic layers were dried (Na_2SO_4) and the solvent evaporated. The residue was chromatographed on silica, with light petroleum–ethyl acetate (3:2 *v*/*v*) as eluant, to give the product (yield 0.47 g, 40.5%). Single crystals of (I) (m.p. 362–363 K) were obtained by slow evaporation of a light petroleum–ethyl acetate (1:2 *v*/*v*) solution.

Crystal data

$C_{17}H_{25}NO_6$
M_r = 339.38
Monoclinic, $C2/c$
a = 26.379 (6) Å
b = 9.706 (2) Å
c = 14.150 (3) Å
β = 98.327 (4)°
V = 3584.7 (14) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.30 × 0.28 × 0.24 mm

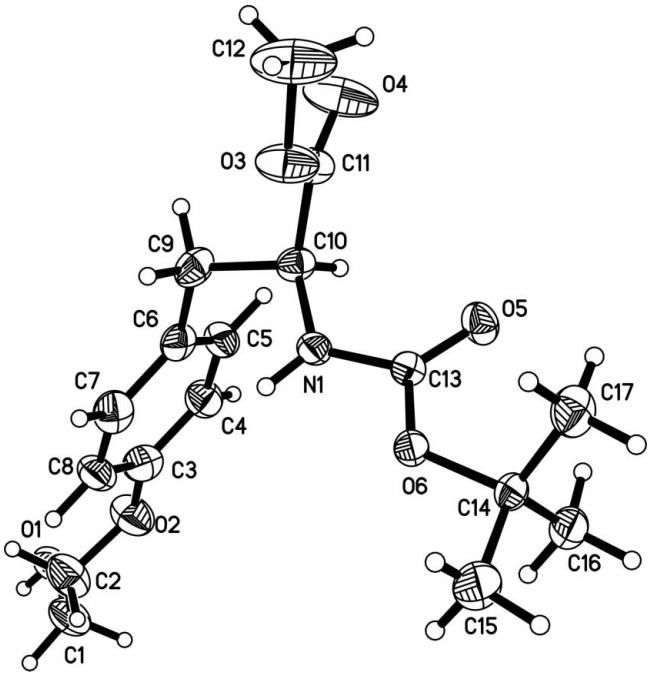


Figure 1
The molecular structure of (I) showing displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms).

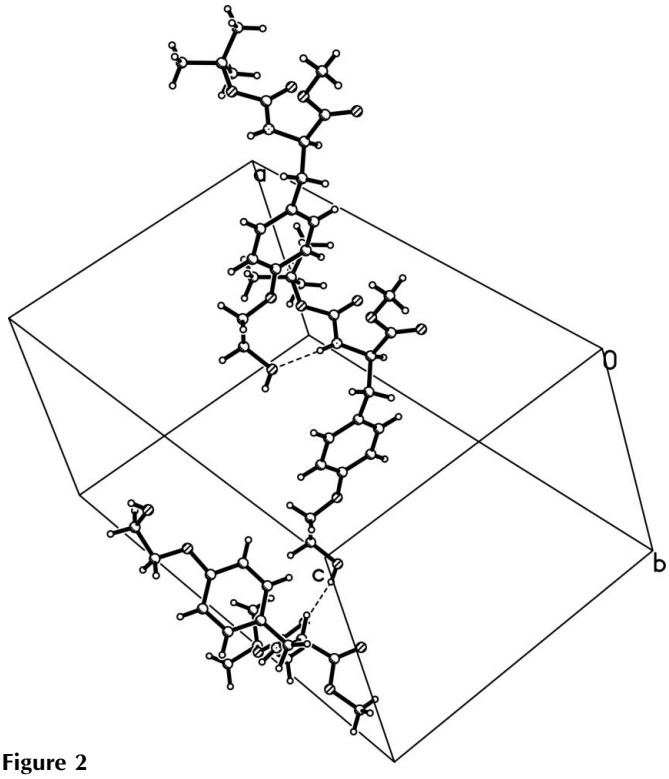


Figure 2
Part of the extended structure of (I). Dashed lines represent the hydrogen bonds

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.972, T_{max} = 0.978
8980 measured reflections
3172 independent reflections
1846 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.168
S = 1.02
3172 reflections
227 parameters
13 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.83 (3)	2.28 (3)	3.113 (4)	178 (3)
O1—H1···O5^{ii}	0.814 (10)	2.052 (14)	2.852 (3)	167 (4)

Symmetry codes: (i) $x, y+1, z$; (ii) $x, -y+1, z+\frac{1}{2}$.

The O- and N-bound H atoms were located in a difference map and their positions were freely refined with U_{iso}(H) = 1.2U_{eq}(N) or 1.5U_{eq}(O). The C-bound H atoms were geometrically placed (C—H = 0.93–0.98 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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