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N-(Boc-L-alanine)allylamine

Min Hong,[a] Liangfei Tian,[a] Yizhi Li[b] and Jin Zhu[a]*

[a]Department of Polymer Science and Engineering, School of Chemistry and Chemical Engineering, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of China, and [b]Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail: jinz@nju.edu.cn

The title compound {systematic name: *tert*-butyl *N*-[1-(allylaminocarbonyl)ethyl]carbamate}, $C_{11}H_{20}N_2O_3$, was prepared by the reaction of Boc-L-alanine (Boc = *tert*-butoxycarbonyl) with allylamine at room temperature. There are two independent molecules in the asymmetric unit, which have similar structures, except for slight differences in bond distances and angles. The molecules are connected by intermolecular N—H···O hydrogen bonds into a one-dimensional supramolecular chain.

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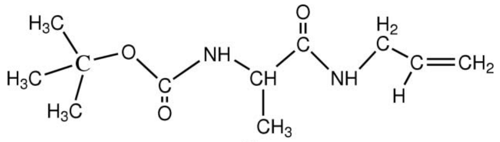
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.007 Å
R factor = 0.064
wR factor = 0.143
Data-to-parameter ratio = 9.9

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

Comment

Two components, one containing a free carboxyl function and the other a free amino group, couple directly and rapidly in high yield upon treatment with *N*,*N*′-dicyclohexylcarbodiimide at room temperature (Sheehan & Hess, 1955). The present work complements earlier structural studies of (*tert*-butoxycarbonyl)-protected amino acids (Semertzidis *et al.*, 1989; Van Meervelt *et al.*, 1995) and we report here the structure of the title compound, (I) (Fig. 1).



(I)

There are two independent molecules in the asymmetric unit of (I) (Fig. 1), which have similar structures except for

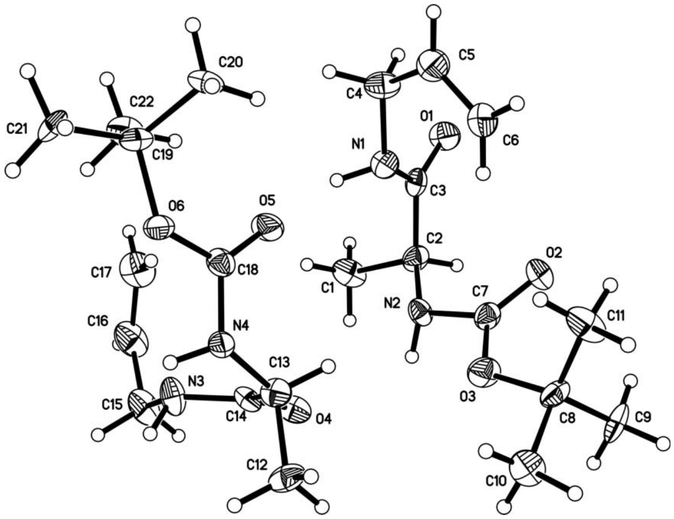


Figure 1
The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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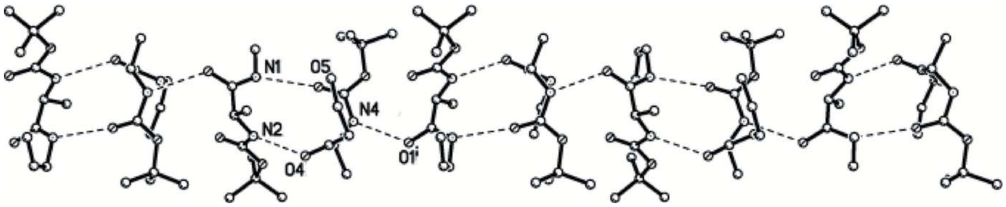

Figure 2
The one-dimensional chain arrangement of the title compound formed *via* intermolecular hydrogen bonds (shown as dashed lines). Symmetry codes are as in Table 2.

slight differences in bond distances and angles. The secondary urethane linkage has a *trans* conformation, with N2—C7—O3—C8 and N4—C18—O6—C19 torsion angles of 177.1 (3) and −169.9 (3)°, respectively. As a result of the electron-withdrawing effect of the amide group, the C5═C6 and C16═C17 bond distances are longer than normal (1.34 Å in propylene), whereas the neighbouring C—C bonds (Table 1) are slightly shorter than normal (1.50 Å).

The crystal structure is held together by intermolecular hydrogen bonds between the NH groups and carbonyl O atoms (Table 2 and Fig. 2). These hydrogen bonds contribute to the crystal stability and compactness, and result in a one-dimensional supramolecular chain arrangement (Fig. 2).

Table 1
Selected geometric parameters (Å, °).

C4—C5	1.490 (7)	C15—C16	1.490 (8)
C5—C6	1.390 (7)	C16—C17	1.390 (8)
N2—C7—O3—C8	177.1 (4)	N4—C18—O6—C19	−169.9 (4)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O5	0.88	2.15	2.899 (5)	144
N2—H2···O4	0.86	2.02	2.869 (5)	170
N3—H3*B*···O1^i	0.90	2.43	3.178 (5)	141
N4—H4*C*···O1^i	0.90	2.09	2.860 (5)	143

Symmetry code: (i) $-x+\frac{3}{2}, -y, z+\frac{1}{2}$.

Experimental

Compound (I) was prepared as described previously (Sheehan & Hess, 1955), using Boc-L-alanine, allylamine and *N*,*N*′-dicyclohexylcarbodiimide as starting materials (yield 75%; m.p. 370–371 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate solution at room temperature.

Crystal data

$C_{11}H_{20}N_2O_3$
M_r = 228.29
Orthorhombic, $P2_12_12_1$
a = 9.9639 (14) Å
b = 14.939 (2) Å
c = 17.998 (3) Å
V = 2678.9 (7) Å^3
Z = 8
Mo *Kα* radiation
μ = 0.08 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.97, T_{max} = 0.98
14763 measured reflections
2962 independent reflections
2229 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.143
S = 1.08
2962 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H and C—H distances of 0.86–0.90 and 0.93–0.97 Å, respectively, and with U_{iso}(H) = 1.2 or 1.5 times U_{eq} of the parent atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1996); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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