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L-Threonyl-L-alanine

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In the title compound, $C_7H_{14}N_2O_4$, peptide molecules are connected into *β*-sheet-like ribbons along the short tetragonal axis [4.7065 (4) Å] by one N—H···O and two C$^{\alpha}$;—H···O interactions.

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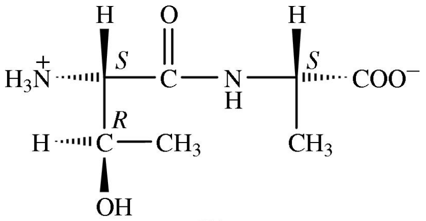
Key indicators

Single-crystal X-ray study
T = 105 K
Mean *σ*(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.074
Data-to-parameter ratio = 8.7

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

Comment

As part of a systematic survey of dipeptides with one hydrophobic and one hydrophilic residue (Netland *et al.*, 2004), the structure of L-threonyl-L-alanine, TA, has been determined. The molecular structure, with a rather extended peptide main chain (Table 1) is depicted in Fig. 1.



TA

Like L-threonyl-L-valine (TV) (Görbitz, 2005), which was investigated in parallel with TA, the TA crystallization experiments led to the formation of extremely thin needles. While the TV crystals share the hexagonal symmetry of numerous hydrophobic dipeptides (Görbitz, 2003, and references therein), the crystals of TA proved to be tetragonal, with space group $P4_2$. The crystal packing, shown in Fig. 2, is characterized by segregation of hydrophobic groups into two independent types of columns along the tetragonal axis. There are no regular peptides among only 31 $P4_2$ entries in the

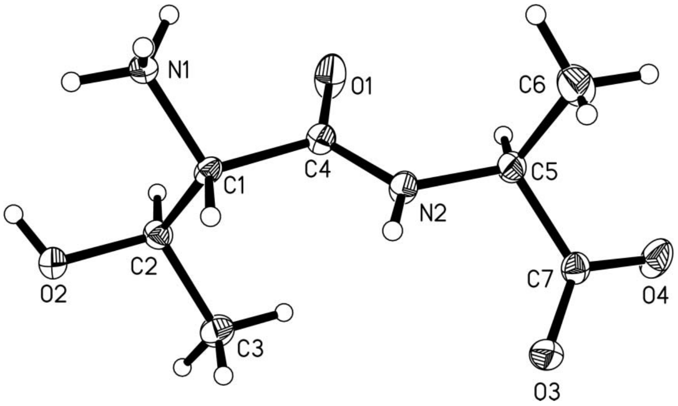


Figure 1
The molecular structure of TA. Displacement ellipsoids for the non-H atoms are shown at the 50% probability level. The H atoms are shown as spheres of arbitrary size.

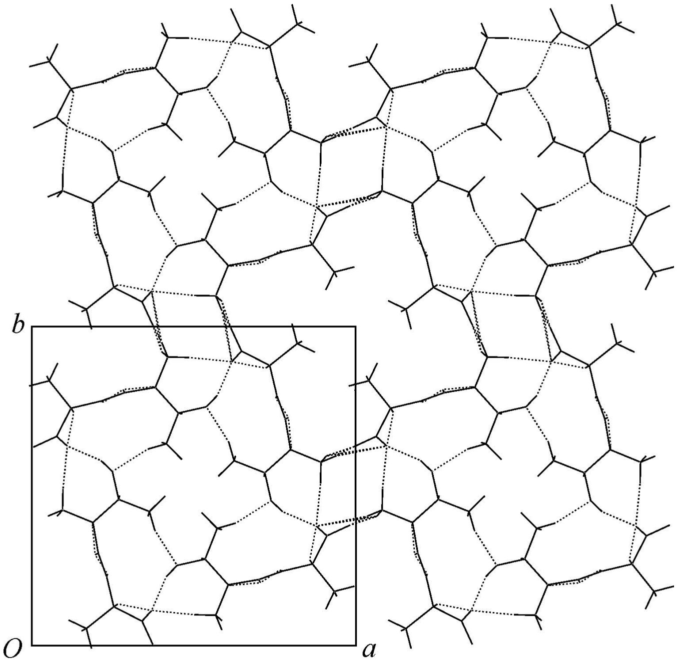


Figure 2
Molecular packing and unit-cell contents of TA viewed along the *c* axis. Hydrogen bonding is indicated by dashed lines.

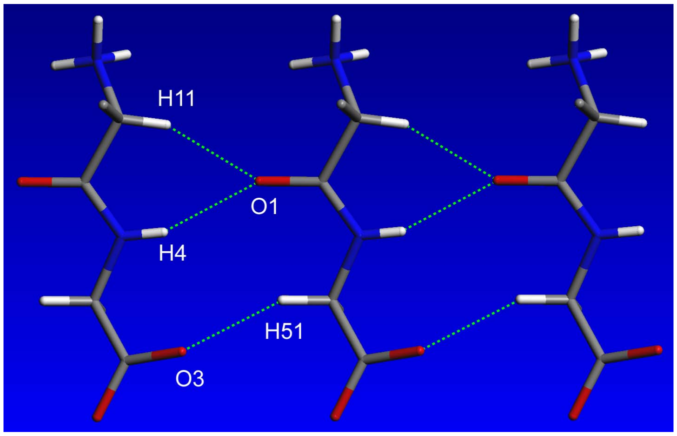


Figure 3
Detail of the hydrogen-bonding network, showing ribbons along the tetragonal axis with a 4.7 Å repeat unit. For clarity, side chains have been curtailed beyond Cβ.

Cambridge Structural Database (CSD; Version 5.26 of November 2004; Allen, 2002), but related structures in $I4$ with $Z = 8$, $a \sim 16.0$ Å and $c \sim 5.2$ Å were observed for L-alanyl-L-alanine (Fletterick *et al.*, 1971) and L-2-aminobutyryl-L-alanine (Görbitz, 2002). The retroanalogue of TA, L-alanyl-L-threonine (AT) (Netland *et al.*, 2004), has a completely different crystal packing pattern, in space group $P2_12_12_1$, but nevertheless incorporates the same N—H···O hydrogen bonds, except that the amide H atom is accepted by the threonine side-chain –OH in AT, but by the carbonyl group of the peptide bond in TA (Fig. 2 and Table 2). Together with two additional C$^{\alpha}$—H···O contacts, the latter interaction forms hydrogen-bonded ribbons parallel to the tetragonal axis, as shown in Fig. 3, a strong β-sheet-like synthon that occurs in 13 other dipeptide structures. The 4.7065 (4) Å *c* axis of TA represents a new lower limit for the repeat distance of this pattern; the previous range was 4.77–5.26 Å. The synthon was last seen in the structure of L-valyl-L-serine (VS) [$P2_1$; a = 4.7695 (2) Å; Johansen *et al.*, 2005], and it is interesting to note that the hydrogen-bonding pattern of TA in fact can be obtained directly from the rather unusual hydrogen-bonded sheets of VS by folding around the tetragonal axis.

The TA threonyl side-chain –OH also accepts an H atom, but with a methyl donor (Fig. 2 and Table 2). The –CH$_3$···OH– type of weak hydrogen bond has not received much attention in the literature, but a search of the CSD demonstrates a fairly high abundance in the crystal structures of organic compounds.

Experimental

L-Threonyl-L-alanine was obtained from Bachem. Needle-shaped crystals were grown by slow diffusion of acetonitrile into an aqueous solution (40 µl) containing about 1 mg of the peptide.

Crystal data

$C_7H_{14}N_2O_4$
$M_r = 190.20$
Tetragonal, $P4_2$
a = 13.9136 (7) Å
c = 4.7065 (4) Å
V = 911.12 (10) Å^3
$Z = 4$
D_x = 1.387 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3024 reflections
θ = 2.1–27.9°
μ = 0.11 mm^{-1}
T = 105 (2) K
Needle, colourless
0.45 × 0.05 × 0.05 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.905$, $T_{\max} = 0.994$
6059 measured reflections
1207 independent reflections
1097 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\max} = 27.9°$
$h = -10 \rightarrow 18$
$k = -17 \rightarrow 16$
$l = -6 \rightarrow 6$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.074$
$S = 1.09$
1207 reflections
138 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.119P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max}$ = 0.22 e Å^{-3}
$\Delta\rho_{\min}$ = −0.17 e Å^{-3}

Table 1
Selected torsion angles (°).

N1—C1—C4—N2	130.52 (16)	N1—C1—C2—O2	−59.93 (19)
C1—C4—N2—C5	177.03 (15)	N1—C1—C2—C3	−178.09 (16)
C4—N2—C5—C7	−137.75 (17)	C1—C2—O2—H5	87.2 (18)
N2—C5—C7—O3	−16.2 (2)		

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
N1—H1$\cdots$O4^{i}	0.91 (2)	1.94 (3)	2.798 (2)	156 (2)
N1—H2$\cdots$O3^{ii}	0.93 (2)	2.01 (2)	2.8822 (19)	156 (2)
N1—H3$\cdots$O4^{iii}	0.89 (3)	1.97 (3)	2.820 (2)	159 (2)
N2—H4$\cdots$O1^{iv}	0.82 (2)	2.16 (2)	2.928 (2)	156 (2)
O2—H5$\cdots$O3^{ii}	0.84 (3)	1.90 (3)	2.7163 (19)	163 (2)
C1—H11$\cdots$O1^{iv}	0.94 (3)	2.23 (2)	3.111 (2)	155 (2)
C3—H33$\cdots$O2^{v}	0.98	2.45	3.402 (3)	163
C5—H51$\cdots$O3^{vi}	1.00	2.50	3.405 (2)	151

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

Positional parameters were refined for H atoms involved in short hydrogen bonds. Other H atoms were positioned with idealized geometry and fixed C—H distances (0.98–1.00 Å). $U_{\rm iso}$ values were $1.2U_{\rm eq}$ of the carrier atom, or $1.5U_{\rm eq}$ for amino and methyl groups. In the absence of significant anomalous scattering effects, 918 Friedel pairs were merged. The absolute configuration was known for the purchased material.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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