

C7—C15	1.551 (15)	C20—O7	1.205 (13)
C8—C9	1.523 (14)	C20—O8	1.323 (13)
C8—C17	1.539 (15)	C21—O8	1.435 (16)
C8—C22	1.540 (13)	C22—O3	1.194 (13)
C9—C10	1.521 (13)	C22—O4	1.316 (13)
C10—C11	1.502 (14)	C23—O4	1.465 (13)
C2—C1—C14	112.7 (8)	C10—C11—O1	121.9 (9)
C2—C1—C18	112.8 (8)	C12—C11—O1	122.1 (10)
C2—C1—C20	107.5 (9)	C11—C12—C13	112.6 (9)
C14—C1—C18	108.4 (9)	C12—C13—C14	112.4 (9)
C14—C1—C20	110.2 (8)	C1—C14—C13	114.1 (8)
C18—C1—C20	105.0 (8)	C7—C15—C16	102.3 (8)
C1—C2—C3	113.4 (8)	C15—C16—C17	108.2 (10)
C2—C3—C4	125.7 (10)	C8—C17—C16	108.7 (9)
C3—C4—C5	124.4 (10)	C8—C17—O2	125.3 (10)
C4—C5—C6	126.5 (10)	C16—C17—O2	125.9 (11)
C5—C6—C7	128.2 (9)	C1—C18—O5	120.2 (10)
C6—C7—C8	113.9 (8)	C1—C18—O6	113.4 (10)
C8—C7—C15	105.7 (8)	O5—C18—O6	126.4 (10)
C7—C8—C9	116.0 (7)	C1—C20—O7	126.3 (9)
C7—C8—C17	102.9 (8)	C1—C20—O8	111.2 (9)
C7—C8—C22	111.1 (8)	O7—C20—O8	122.4 (10)
C9—C8—C17	112.6 (8)	C8—C22—O3	123.6 (9)
C9—C8—C22	107.8 (8)	C8—C22—O4	111.8 (9)
C17—C8—C22	105.9 (7)	O3—C22—O4	124.6 (9)
C8—C9—C10	116.3 (8)	C22—O4—C23	116.5 (9)
C9—C10—C11	112.3 (8)	C18—O6—C19	109.5 (10)
C10—C11—C12	116.0 (9)	C20—O8—C21	117.5 (9)
C15—C7—C8—C17	−30.8 (6)	C7—C15—C16—C17	−26.0 (6)
C8—C7—C15—C16	35.3 (6)	C15—C16—C17—C8	7.4 (5)
C7—C8—C17—C16	14.6 (6)	C15—C16—C17—O2	−176.1 (14)
C7—C8—C17—O2	−162.0 (12)		

For both compounds, data collection: *DATCOL NRCCAD* (Le Page, White & Gabe, 1986); cell refinement: *TRUANG NRCCAD*; data reduction: *DATRD2 NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989); program(s) used to solve structures: *SOLVER NRCVAX*. Program(s) used to refine structures: *SHELXL93* (Sheldrick, 1993) for (I); *LSTSQ NRCVAX* for (II). For both compounds, molecular graphics: *ORTEPII* (Johnson, 1976) *NRCVAX*. Software used to prepare material for publication: *SHELXL93* for (I); *TABLES NRCVAX* for (II).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: PT1020). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## Glycyl-L-Leucyl-L-Tyrosine Dihydrate 2-Propanol Solvate

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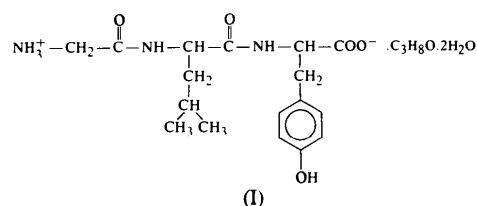
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## Abstract

The asymmetric unit ( $C_{17}H_{25}N_3O_5 \cdot C_3H_8O \cdot 2H_2O$ ) consists of two crystallographically independent peptide molecules, *A* and *B*, with different conformations,  $\chi_2^1$  being *trans* and *gauche*<sup>−</sup> for the Leu residues in molecules *A* and *B*, respectively. The backbone conformation of both peptide molecules resembles that of the  $\beta$ -pleated sheet arrangement found in proteins. Comparison with two other structures containing the tripeptide Gly-L-Leu-L-Tyr reveals almost identical molecular conformations, and in one instance also a common packing pattern.

## Comment

As part of a project dealing with the X-ray structures of tripeptides with non-Gly residues in the mid-position, we have crystallized Gly-L-Leu-L-Tyr as the dihydrate 2-propanol solvate (I). The structures of Gly-L-Leu-L-Tyr 2.5-hydrate dimethyl sulfoxide (DMSO) solvate (Wu, Tinant, Declercq & Van Meerssche, 1987; Subramanian & Parthasarathy, 1987) and the copper complex of the same peptide (Franks & van der Helm, 1970) have already been described.



The molecular conformations of the two independent tripeptide molecules in the asymmetric unit, with different side-chain conformations for the Leu residues, are essentially the same in all three structures (Table 4). Both molecules have an extended backbone conformation typical of the  $\beta$ -pleated sheet secondary structure observed in proteins, with  $\varphi_2$  in the range  $-123$  to  $-149^\circ$  and  $\psi_2$  in the range  $133$  to  $148^\circ$  (Table 4). The peptide and solvate 2-propanol molecules are depicted, together with atomic labelling, in Fig. 1, and the characteristic pleated conformations for the Leu residues are apparent.

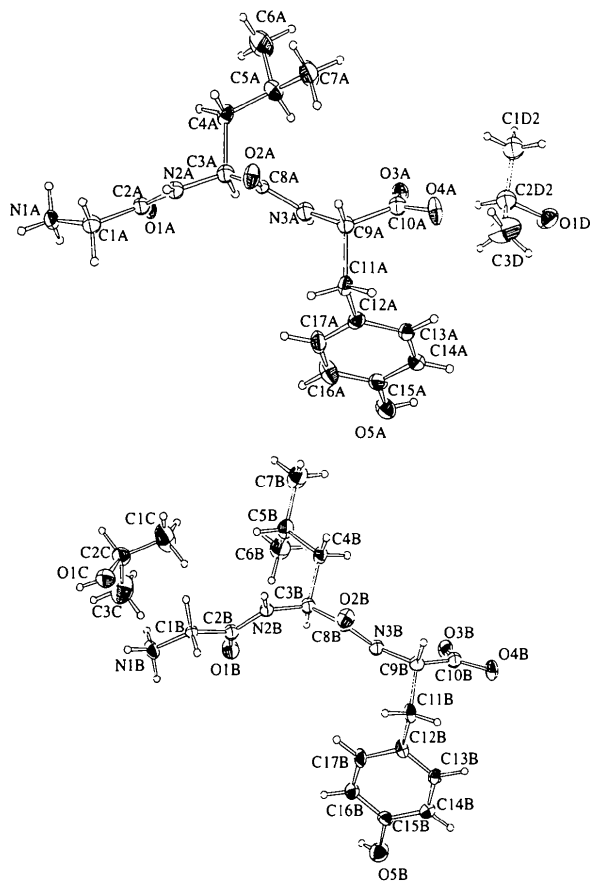


Fig. 1. Individual ORTEPII (Johnson, 1976) drawings with atom labelling of peptide molecules *A* and *B* together with 2-propanol molecules *C* and *D* showing molecular conformation. Only the most occupied positions of the disordered C atoms in molecule *D* are displayed. Displacement ellipsoids are drawn at the 50% probability level. Shaded atoms were refined anisotropically, unshaded isotropically. H atoms are arbitrarily scaled.

In contrast to the copper complex of the tripeptide, in which the peptide side-chain groups form hydrophobic columns, the crystal structures of both the DMSO and the 2-propanol solvate of Gly-L-Leu-L-Tyr can be divided into three layers parallel to the *ac* plane. The first layer is hydrophilic and contains the backbone of the peptide molecules (Fig. 2). Each

type of peptide molecule, *A* and *B*, forms a 'head-to-tail' hydrogen-bonded chain, the two chains running in opposite directions parallel to the *c* axis. The two chains are interconnected through hydrogen bonds of both amide...carbonyl and amino...carboxylate type. The second layer contains the phenol groups from the Tyr residues together with the water molecules *E* and *G*. The third layer is composed of the isopropyl groups from the Leu residues, the 2-propanol solvate molecules (*C* and *D*) and two additional water molecules (*F* and *H*). The solvent 2-propanol molecules are located in the same positions as the DMSO molecules in the DMSO solvate, with the hydroxyl O atoms in 2-propanol positioned where the O atoms in the O=S groups are found in the DMSO structures.

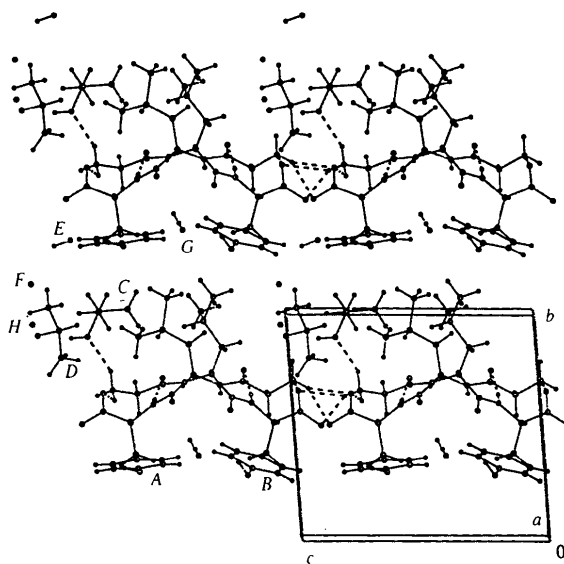


Fig. 2. Projection of the structure down the *a* axis showing molecular packing of tripeptide molecules (*A* and *B*), 2-propanol molecules (*C* and *D*) and solvent water molecules (*E-H*).

The four solvent water molecules in the 2-propanol structure (*E-H*) are found in approximately the same positions as four of the five water molecules in the DMSO structure. As only three out of eight water H atoms could be identified in the Fourier difference map, it is not possible to deduce a complete and unambiguous hydrogen-bond pattern for the 2-propanol solvate. Geometric parameters for hydrogen bonds formed by the H atoms included in the model are listed in Table 3.

In the DMSO structures, one of the DMSO molecules is disordered, and in the 2-propanol solvate the 2-propanol molecule occupying the corresponding position (molecule *D*) is also disordered.

## Experimental

Colourless crystals of the title compound were obtained by slow diffusion of 2-propanol into an aqueous solution of the

peptide at room temperature. The crystals are unstable upon exposure to air.

### Crystal data

$C_{17}H_{25}N_3O_5 \cdot C_3H_8O \cdot 2H_2O$

$M_r = 447.53$

Triclinic

$P1$

$a = 9.179(2) \text{ \AA}$

$b = 11.104(3) \text{ \AA}$

$c = 12.202(3) \text{ \AA}$

$\alpha = 84.08(2)^\circ$

$\beta = 83.98(2)^\circ$

$\gamma = 75.52(2)^\circ$

$V = 1193.7(5) \text{ \AA}^3$

$Z = 2$

$D_x = 1.245 \text{ Mg m}^{-3}$

$D_m$  not measured

### Data collection

Nicolet P3 diffractometer

$2\theta$  scans

Absorption correction:

none

4220 measured reflections

4220 independent reflections

3240 observed reflections

$[I > 2\sigma(I)]$

### Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.0789$

$wR(F^2) = 0.2492$

$S = 1.076$

4217 reflections

490 parameters

H-atom parameters not

refined

$w = 1/[\sigma^2(F_o^2) + (0.1300P)^2 + 2.2000P]$

where  $P = (F_o^2 + 2F_c^2)/3$

Mo  $K\alpha$  radiation

$\lambda = 0.71069 \text{ \AA}$

Cell parameters from 25

reflections

$\theta = 11.4\text{--}18.2^\circ$

$\mu = 0.096 \text{ mm}^{-1}$

$T = 120(2) \text{ K}$

Block

$0.40 \times 0.20 \times 0.10 \text{ mm}$

Colourless

$\theta_{\max} = 25.0^\circ$

$h = -10 \rightarrow 10$

$k = 0 \rightarrow 13$

$l = -14 \rightarrow 14$

3 standard reflections

monitored every 96

reflections

intensity decay:  $<1.8\%$

$(\Delta/\sigma)_{\max} = -0.303$

$\Delta\rho_{\max} = 0.562 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.348 \text{ e \AA}^{-3}$

Extinction correction: none

Atomic scattering factors

from *International Tables*

for *Crystallography* (1992,

Vol. C, Tables 4.2.6.8 and

6.1.1.4)

N1A	0.0615 (8)	0.6829 (7)	-0.0131 (6)	0.028 (2)
N2A	-0.0369 (8)	0.6592 (6)	0.2831 (6)	0.0208 (15)
N3A	0.0369 (8)	0.5739 (6)	0.5596 (6)	0.023 (2)
N1B	0.3937 (8)	0.6478 (7)	0.7216 (6)	0.026 (2)
N2B	0.5222 (7)	0.6866 (6)	0.4280 (5)	0.0171 (14)
N3B	0.4865 (8)	0.5950 (6)	0.1645 (6)	0.0210 (15)
C1A	0.0127 (10)	0.6200 (8)	0.0913 (7)	0.024 (2)
C2A	0.0488 (9)	0.6767 (8)	0.1904 (7)	0.021 (2)
C3A	-0.0128 (10)	0.7039 (8)	0.3868 (7)	0.022 (2)
C4A	-0.1069 (10)	0.8381 (8)	0.3966 (7)	0.023 (2)
C5A	-0.0959 (11)	0.9019 (9)	0.4993 (8)	0.030 (2)
C6A	-0.1301 (15)	1.0426 (11)	0.4719 (10)	0.050 (3)
C7A	-0.2014 (14)	0.8686 (10)	0.5972 (8)	0.042 (3)
C8A	-0.0565 (8)	0.6167 (7)	0.4794 (6)	0.013 (2)
C9A	0.0032 (9)	0.4935 (8)	0.6548 (7)	0.020 (2)
C10A	0.0258 (10)	0.5420 (8)	0.7638 (7)	0.023 (2)
C11A	0.0893 (9)	0.3550 (8)	0.6441 (7)	0.022 (2)
C12A	0.2578 (10)	0.3371 (8)	0.6426 (7)	0.022 (2)
C13A	0.3280 (10)	0.3173 (8)	0.7419 (7)	0.023 (2)
C14A	0.4838 (10)	0.3024 (8)	0.7414 (7)	0.027 (2)
C15A	0.5729 (10)	0.3046 (8)	0.6421 (7)	0.024 (2)
C16A	0.5032 (11)	0.3223 (10)	0.5423 (8)	0.034 (2)
C17A	0.3511 (11)	0.3374 (9)	0.5433 (7)	0.031 (2)
C1B	0.5069 (8)	0.6355 (7)	0.6233 (6)	0.015 (2)
C2B	0.4279 (9)	0.6753 (8)	0.5179 (7)	0.022 (2)
C3B	0.4760 (9)	0.7205 (7)	0.3167 (7)	0.019 (2)
C4B	0.5097 (10)	0.8438 (8)	0.2666 (7)	0.024 (2)
C5B	0.4430 (12)	0.9563 (8)	0.3358 (8)	0.033 (2)
C6B	0.2734 (14)	0.9933 (10)	0.3407 (9)	0.047 (3)
C7B	0.5104 (14)	1.0668 (10)	0.2879 (10)	0.047 (3)
C8B	0.5599 (8)	0.6209 (7)	0.2421 (6)	0.016 (2)
C9B	0.5576 (9)	0.5109 (8)	0.0789 (7)	0.021 (2)
C10B	0.4845 (9)	0.5568 (8)	-0.0287 (7)	0.021 (2)
C11B	0.5518 (9)	0.3766 (8)	0.1187 (7)	0.020 (2)
C12B	0.3934 (9)	0.3553 (8)	0.1370 (7)	0.021 (2)
C13B	0.3323 (10)	0.3060 (8)	0.0578 (7)	0.025 (2)
C14B	0.1938 (11)	0.2761 (9)	0.0774 (8)	0.031 (2)
C15B	0.1104 (11)	0.2955 (8)	0.1789 (8)	0.028 (2)
C16B	0.1678 (11)	0.3499 (8)	0.2585 (7)	0.027 (2)
C17B	0.3071 (10)	0.3756 (8)	0.2370 (7)	0.025 (2)
C1C	0.3132 (18)	1.0046 (11)	0.6365 (10)	0.065 (4)
C2C	0.2399 (12)	0.9935 (9)	0.7520 (8)	0.036 (2)
C3C	0.0792 (13)	0.9858 (14)	0.7540 (11)	0.058 (3)
C1D1†	0.643 (4)	1.019 (3)	0.890 (3)	0.043 (10)
C2D1†	0.692 (5)	0.910 (3)	0.972 (4)	0.046 (10)
C1D2‡	0.5841 (18)	1.0197 (15)	0.9564 (15)	0.040 (5)
C2D2‡	0.7206 (17)	0.9214 (14)	0.9217 (16)	0.034 (4)
C3D	0.6844 (15)	0.7981 (12)	0.9207 (14)	0.062 (4)

† Occupancy 0.34 (3). ‡ Occupancy 0.66 (3).

Table 2. Selected geometric parameters ( $\text{\AA}$ )

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{eq}}$
O1A	0.1524 (7)	0.7288 (6)	0.1843 (5)	0.0241 (13)
O2A	-0.1761 (6)	0.5798 (6)	0.4794 (5)	0.0277 (14)
O3A	0.0951 (7)	0.6260 (6)	0.7588 (5)	0.0242 (13)
O4A	-0.0157 (7)	0.4851 (6)	0.8511 (5)	0.032 (2)
O5A	0.7244 (7)	0.2955 (6)	0.6379 (6)	0.0327 (15)
O1B	0.2912 (7)	0.6979 (6)	0.5162 (5)	0.0313 (15)
O2B	0.6960 (6)	0.5681 (6)	0.2527 (5)	0.0267 (14)
O3B	0.3722 (7)	0.6457 (6)	-0.0287 (5)	0.0268 (14)
O4B	0.5406 (7)	0.4968 (6)	-0.1113 (5)	0.0247 (13)
O5B	-0.0224 (8)	0.2612 (7)	0.1975 (6)	0.038 (2)
O1C	0.3302 (8)	0.8828 (6)	0.8056 (6)	0.037 (2)
O1D	0.8318 (8)	0.9021 (7)	1.0089 (6)	0.040 (2)
O1E	0.8038 (7)	1.3257 (6)	0.8507 (6)	0.0302 (14)
O1F	0.9100 (8)	1.1330 (6)	1.0212 (6)	0.038 (2)
O1G	-0.1725 (12)	0.3424 (8)	0.3884 (9)	0.055 (3)
O1H	0.2037 (9)	0.9335 (8)	1.0228 (6)	0.051 (2)

	Molecule A	Molecule B
O1—C2	1.222 (10)	1.218 (10)
O2—C8	1.264 (9)	1.255 (10)
O3—C10	1.247 (10)	1.236 (10)
O4—C10	1.255 (11)	1.258 (10)
O5—C15	1.364 (11)	1.357 (11)
N1—C1	1.471 (11)	1.495 (10)
N2—C2	1.335 (11)	1.340 (11)
N2—C3	1.463 (11)	1.449 (10)
N3—C8	1.339 (10)	1.312 (10)
N3—C9	1.447 (11)	1.464 (11)
C1—C2	1.521 (12)	1.515 (11)
C3—C8	1.499 (11)	1.510 (11)
C3—C4	1.533 (12)	1.531 (12)
C4—C5	1.525 (12)	1.540 (12)
C5—C6	1.523 (14)	1.50 (2)
C5—C7	1.533 (14)	1.54 (2)
C9—C10	1.537 (11)	1.521 (11)
C9—C11	1.556 (12)	1.532 (12)
C11—C12	1.508 (12)	1.520 (12)
C12—C13	1.404 (12)	1.387 (12)
C12—C17	1.408 (13)	1.390 (12)

C13—C14	1.398 (13)	1.384 (13)
C14—C15	1.391 (13)	1.393 (13)
C15—C16	1.408 (13)	1.404 (13)
C16—C17	1.362 (14)	1.372 (13)
	Molecule C	Molecule D
C1—C2	1.50 (2)	1.50(2)*/1.49(3)†
C2—C3	1.50 (2)	1.49(2)/1.47(4)
C2—O1	1.44 (1)	1.51(2)/1.38(4)

\* Most occupied position. † Least occupied position.

Table 3. Hydrogen-bonding geometry (Å, °)

D—H...A	D—H	H...A	D...A	D—H...A
N1A—H1A...O3A <sup>i</sup>	0.91	2.11	2.89 (1)	143
N1A—H1A...O4A <sup>i</sup>	0.91	2.30	3.14 (1)	152
N1A—H2A...O3B	0.91	1.86	2.77 (1)	175
N1A—H3A...O1D <sup>ii</sup>	0.91	1.97	2.81 (1)	152
N2A—H6A...O2B <sup>iii</sup>	0.88	2.09	2.95 (1)	165
N3A—H17A...O1B	0.88	2.12	2.97 (1)	163
N1B—H1B...O3B <sup>iv</sup>	0.91	2.32	3.03 (1)	134
N1B—H1B...O4B <sup>iv</sup>	0.91	1.91	2.74 (1)	151
N1B—H2B...O3A	0.91	2.11	2.80 (1)	132
N1B—H3B...O1C	0.91	2.05	2.80 (1)	140
N2B—H6B...O2A <sup>i</sup>	0.88	2.00	2.84 (1)	159
N3B—H17B...O1A	0.88	2.18	3.05 (1)	172
O5A—H25A...O1E <sup>vi</sup>	0.84	2.01	2.84 (1)	171
O5B—H25B...O1G	0.84	2.02	2.70 (1)	137
O1C—H8C...O1H	0.84	2.04	2.83 (1)	157
O1E—H1E...O1F	1.05	2.11 (12)	2.89 (1)	128 (9)
O1G—H1G...O2A	0.97	2.34 (17)	2.96 (1)	121 (13)

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

Table 4. Molecular conformations (°) for Gly-L-Leu-L-Tyr in crystal structures

Torsion angle	2-Propanol solvate*		DMSO solvate†		Cu complex‡	
	A	B	A	B	A	B
<b>Backbones§</b>						
$\psi_1$	156.6 (7)	169.5 (7)	154	170	-176	180
$\omega_1$	177.7 (7)	178.5 (7)	-179	177	-177	-173
$\varphi_2$	-149.3 (7)	-123.5 (8)	-146	-132	-131	-130
$\psi_2$	132.7 (7)	143.6 (7)	135	148	142	139
$\omega_2$	177.5 (7)	173.1 (7)	176	174	177	-177
$\varphi_3$	-129.7 (8)	-145.5 (7)	-140	-146	-142	-149
$\psi_7$	-13.4 (10)	-6.7 (11)	-10	-10	-23	-20
<b>Side chains</b>						
$\chi_2^{1,1}$	-179.5 (7)	-55.0 (10)	-176	-60	176	-53
$\chi_2^{2,1}$	153.1 (9)	169.1 (8)	151	169	153	174
$\chi_2^{2,2}$	-83.8 (10)	-67.6 (10)	-86	-71	-92	-67
$\chi_3^1$	65.0 (9)	65.2 (9)	59	66	58	54
$\chi_3^{2,1}$	86.2 (9)	-86.8 (9)	88	-88	84	-79
$\chi_3^{2,2}$	-94.8 (9)	98.0 (9)	-89	99	-86	90

\* This work. † Subramanian & Parthasarathy (1987). ‡ Franks & van der Helm (1970). §  $\psi_1 = \text{N1-C1-C2-N2}$ ,  $\omega_1 = \text{C3-N2-C2-C1}$ ,  $\varphi_2 = \text{C2-N2-C3-C8}$ ,  $\psi_2 = \text{N2-C3-C8-N3}$ ,  $\omega_2 = \text{C9-N3-C8-C3}$ ,  $\varphi_3 = \text{C8-N3-C9-C10}$ ,  $\psi_7 = \text{N3-C9-C10-O3}$ ,  $\chi_2^1 = \text{N2-C3-C4-C5}$ ,  $\chi_2^{2,1} = \text{C3-C4-C5-C6}$ ,  $\chi_2^{2,2} = \text{C3-C4-C5-C7}$ ,  $\chi_3^1 = \text{N3-C9-C11-C12}$ ,  $\chi_3^{2,1} = \text{C9-C11-C12-C13}$ ,  $\chi_3^{2,2} = \text{C9-C11-C12-C17}$ .

The structure was solved by direct methods using *SIR92* (Altomare *et al.*, 1992) and refined with *SHELXL93* (Sheldrick, 1993). All heavy atoms, except C and amide N backbone atoms and the disordered 2-propanol C atoms, were refined anisotropically. H atoms with known geometry were added in theoretical positions. The coordinates for the H atoms

'ride' on the coordinates of the corresponding heavy atom. Isotropic temperature factors for amino, hydroxyl and methyl H atoms were fixed to 1.5 times  $U_{\text{eq}}$  of the bonded heavy atom. Isotropic temperature factors for the remaining H atoms were fixed to 1.2 times  $U_{\text{eq}}$  of the attached heavy atom. The coordinates of the hydroxyl H atoms for the two Tyr residues and the two 2-propanol molecules were refined using a 'rotating group refinement' constraint with O—H = 0.84 Å. Three of the H atoms in the water molecules were located from the difference Fourier map, and their positions refined. Two alternative positions have been refined for the C atoms C1D and C2D, with occupancy factors 0.66 (3) for the pair C1D2 and C2D2, and 0.34 (3) for C1D1 and C2D1.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1338). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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## 1-Phenyl-2-(propylamino)pentane, a Memory Enhancer

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## Abstract

The absolute configuration of [(*R*)-1-phenyl-2-pentyl]-propylammonium chloride, C<sub>14</sub>H<sub>24</sub>N<sup>+</sup>.Cl<sup>-</sup>, has been determined. The compound is a memory enhancer. Since the pharmacological effect of the related compound selegiline is highly dependent upon its configuration, the