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5-Ethyl L-glutamate

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.008 Å
R factor = 0.060
wR factor = 0.178
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.

In the title compound, $C_7H_{13}NO_4$, there are two independent molecules in the asymmetric unit. All bond lengths and angles in the molecules are in normal ranges. The ψ^1 and ψ^2 torsion angles are 159.9 (4) and −23.4 (5)°, respectively, in the first molecule, and the ψ^3 and ψ^4 torsion angles 157.7 (4) and −26.7 (5)°, respectively, in the second. Each of the independent molecules has a different comformation. The translationally and screw-related molecules are connected by N—H···O hydrogen bonds, forming a two-dimensional network parallel to the *ac* plane.

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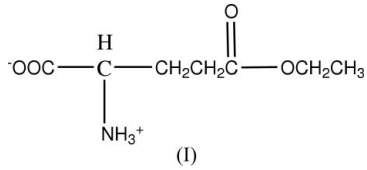
Comment

It has been reported that many esters of amino acids display a broad range of biological activities, *e.g.* as anti-oxidants, bactericides, food additives and cosmetics (Wang & Li, 1995); furthermore, these esters are useful ligands. As part of an ongoing study (Wu *et al.*, 2005), we report here the crystal structure of the title compound, (I).



(I)

In the crystal structure, (I) exists as a zwitterion (Fig. 1). All bond lengths and angles in the two independent molecules of (I) (Fig. 1) are normal. The N1—C2—C1—O1 (ψ^1), N1—C2—C1—O2 (ψ^2), N2—C9—C8—O5 (ψ^3) and N2—C9—C8—O6 (ψ^4) torsion angles are 159.9 (4), −23.4 (5), 157.7 (4) and −26.7 (5)°, respectively. In one independent molecule, atom

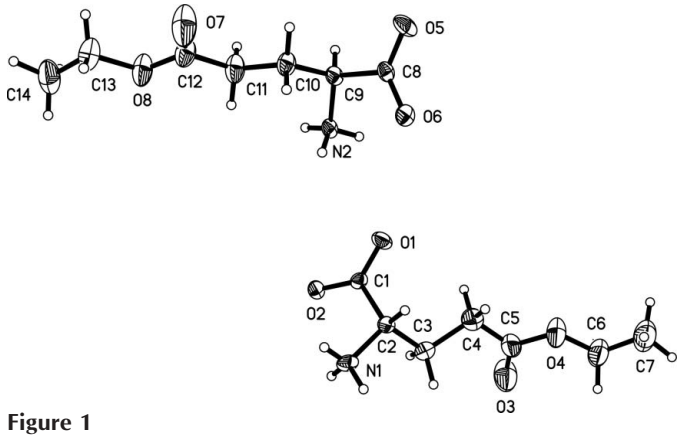


Figure 1
The structure of the asymmetric unit of (I), showing displacement ellipsoids at the 30% probability level (Bruker, 2001).

C^{γ} is intermediate between *trans* and *gauche* to N [N1—C2—C3—C4 (χ^1) = −159.8 (4)°], while atom C^{δ} is *trans* to C^{α} [C2—C3—C4—C5 (χ^2) = 170.5 (4)°]. In the second molecule, atom C^{γ} is *gauche* to N [N2—C9—C10—C11 (χ^3) = −57.3 (5)°] and atom C^{δ} is *trans* to C^{α} [C9—C10—C11—C12 (χ^4) = −175.8 (5)°]. The C—O lengths of the ionized carboxylate group are almost equal (Table 1). In L-glutamic acid (Lehmann & Nunes, 1980), the ψ^1 and ψ^2 torsion angles are −35 and 145° (no s.u. values available), and the bond lengths and angles are similar to those in the title compound.

In the crystal structure, translationally and screw-related molecules are connected by N—H···O hydrogen bonds to form a two-dimensional network parallel to the *ac* plane (Table 2 and Fig. 2).

Experimental

Compound (I) was synthesized according to the literature procedure of Li & Wang (1999). Colourless plate-like crystals were grown by slow evaporation of an aqueous solution at room temperature.

Crystal data

$C_7H_{13}NO_4$
M_r = 175.18
Monoclinic, $P2_1$
a = 9.691 (3) Å
b = 5.2631 (17) Å
c = 17.297 (6) Å
β = 90.752 (5)°
V = 882.2 (5) Å^3
Z = 4
D_x = 1.319 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1376 reflections
θ = 3.1–21.6°
μ = 0.11 mm^{-1}
T = 273 (2) K
Plate, colourless
0.50 × 0.49 × 0.02 mm

Data collection

Bruker SMART-APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.948, T_{max} = 0.998
5098 measured reflections
1927 independent reflections
1546 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.0°
$h = -8 \rightarrow 11$
$k = -6 \rightarrow 5$
$l = -21 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.178
S = 1.04
1927 reflections
221 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0984P)^2 + 0.2865P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.243 (5)	C8—O5	1.244 (6)
C1—O2	1.258 (5)	C8—O6	1.257 (5)
O1—C1—C2—N1	159.9 (4)	O5—C8—C9—N2	157.7 (4)
O2—C1—C2—N1	−23.4 (5)	O6—C8—C9—N2	−26.7 (5)
N1—C2—C3—C4	−159.6 (4)	N2—C9—C10—C11	−57.5 (5)
C2—C3—C4—C5	170.8 (4)	C9—C10—C11—C12	−175.5 (5)

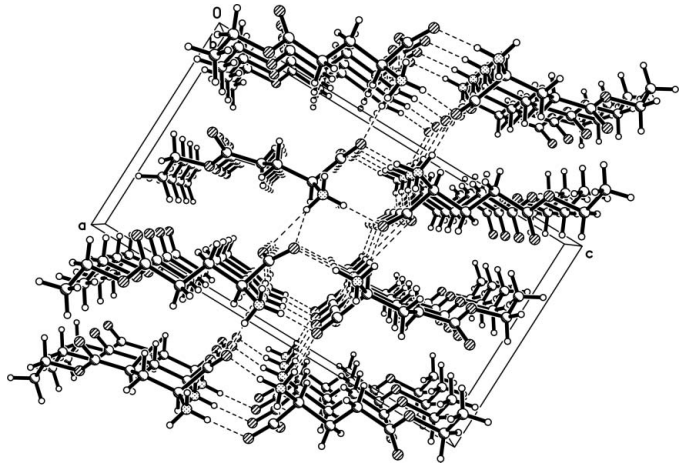


Figure 2
Packing diagram for (I). Hydrogen bonds are indicated by dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O5^{i}	0.89	1.96	2.840 (5)	170
N2—H2B···O2^{ii}	0.89	1.99	2.828 (4)	157
N2—H2C···O2^{iii}	0.89	1.93	2.807 (4)	170
N1—H1A···O1^{i}	0.89	1.98	2.813 (5)	155
N1—H1B···O6^{i}	0.89	1.88	2.741 (4)	161
N1—H1C···O6^{iv}	0.89	2.18	2.950 (4)	144
N1—H1C···O5^{iv}	0.89	2.35	3.178 (4)	154

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$; (iii) $-x+2, y+\frac{1}{2}, -z+1$; (iv) $-x+1, y-\frac{3}{2}, -z+1$.

All H atoms were placed in calculated positions, with N—H distances of 0.89 Å and C—H distances of 0.96 (CH_3), 0.97 (CH_2) and 0.98 Å (CH). They were included in the refinement in the riding-model approximation, with isotropic displacement parameters set to $1.2U_{eq}$ of the carrier atom ($1.5U_{eq}$ for CH_3 and NH_3 H atoms). In the absence of significant anomalous scattering, Friedel pairs were merged prior to the final refinement; the absolute configuration is known from the synthesis (Carey & Sundberg, 1984).

Data collection: *APEX* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Bruker, 2001); software used to prepare material for publication: *SHELXTL-NT*.

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