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# DL-Phenylglycinium chloride

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**Key indicators**

Single-crystal X-ray study
$T$ = 296 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.030
$wR$ factor = 0.116
Data-to-parameter ratio = 18.2

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

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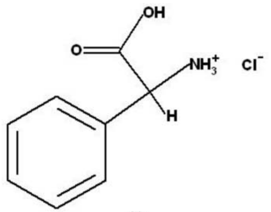
In the title compound, $C_8H_{10}NO_2^+\cdot Cl^-$, the asymmetric unit consists of a protonated DL-phenylglycine cation and a chloride anion. The crystal structure consists of alternating layers of hydrophobic and hydrophilic zones of phenylglycinium along the *c* axis. The chloride anions are located between hydrophobic zones, forming hydrogen bonds with N and O atoms of the cations, in hydrophilic zones. These ions are linked by cation–cation and cation–anion hydrogen bonds. This three-dimensional complex network of hydrogen bonds reinforces the cohesion of the ionic structure.

## Comment

D-Phenylglycine is an important starting material in the production of semisynthetic penicillins and cephalosporins and its derivatives are used in the synthesis of antitumor drugs and other pharmacological applications (Satyam *et al.*, 1996; Jayasinghe *et al.*, 1994). The crystal structures of D-phenylglycine hydrochloride (Ravichandran *et al.*, 1998), bis(D-phenylglycinium) sulfate monohydrate (Srinivasan *et al.*, 2001), D-phenylglycinium nitrate (Bouchouit *et al.*, 2004) and D-phenylglycinium perchlorate (Ramaswamy *et al.*, 2001) have been reported. In the present study, the structure of DL-phenylglycinium chloride, (I), has been investigated. The molecular geometry and the atom-numbering scheme of (I) are shown in Fig. 1.



(I)

The amino N atom is protonated. As in other amino acids (Bouacida *et al.*, 2005), in the phenylglycinium residue, the torsion angle O1—C8—C2—N1 is a measure of the relative orientation of the carboxyl group and the amino N atom; in (I) this is −23.3 (2)°, indicating that the orientation of the carboxyl group is influenced by the phenyl substituent at the $\alpha$-C atom. The corresponding angles in $\alpha$-glycine (Marsh, 1958) and diglycine hydrochloride (Natarajan *et al.*, 1992) are 19.1, 0.3 and 16.5°, respectively, and this angle is 18.9 ° in D-phenylglycine hydrochloride (Ravichandran *et al.*, 1998).

The branched-chain torsion angle C7—C2—C1—N1 is −118.51 (16)°, indicating a folded conformation. This angle varies according to the anion; in D-phenylglycine hydro-

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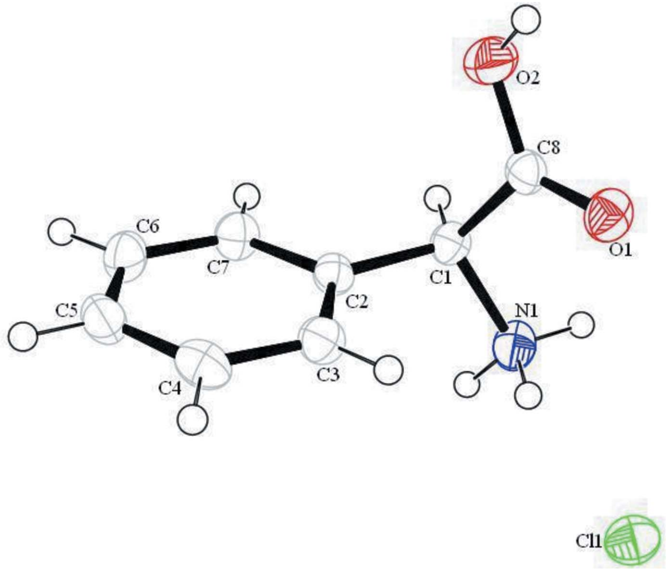

**Figure 1**
View of the structure of the title compound, showing the atomic labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

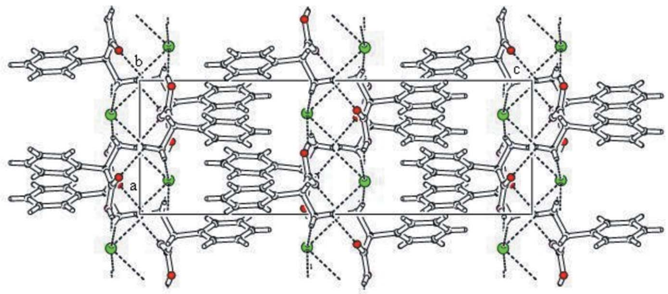

**Figure 2**
A diagram of the layered crystal packing in (I), viewed down the *b* axis.

chloride, D-phenylglycinium perchlorate, (*R*)-phenylglycine methyl ester (Goldberg, 1977) and (*R*)-(−)-1-phenylglycinium hydrogen squarate monohydrate (Angelova *et al.*, 1996) the angles are 129.2, 94.3, 137.6 and 119.9°, respectively.

The crystal structure can be described as alternating layers of hydrophobic and hydrophilic zones of phenylglycinium along the *c* axis. The molecular aggregation of the hydrophilic zone at $z = \frac{1}{2}$ is sandwiched between two hydrophobic zones (Fig. 2).

In this structure, two types of secondary interaction are observed, cation–cation and cation–anion (Fig. 3). The phenylglycinium cations and the chloride anions form hydrogen-bonded double layers at $z = 0$ and $z = \frac{1}{2}$, linked toegether by N—H⋯Cl, N—H⋯O and C—H⋯O hydrogen bonds. Additional hydrogen-bonding parameters are listed in Table 1.

## Experimental

The title compound was crystallized by slow evaporation of an aqueous solution of DL-phenylglycine, tin(II) chloride dihydrate and hydrochloric acid in a molar ratio of 5:5:1. Colourless prismatic transparent crystals were obtained after three weeks.

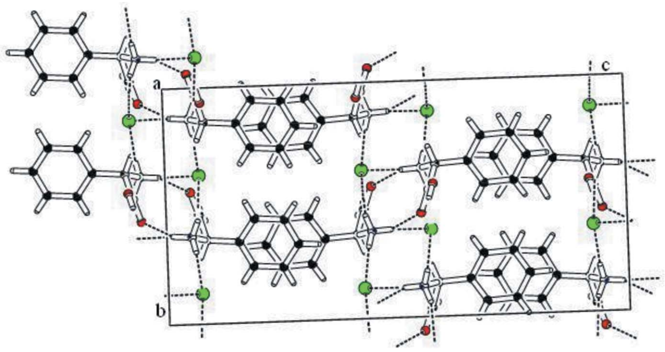

**Figure 3**
The hydrogen bonds (dashed lines) in (I), viewed down the *b* axis.

*Crystal data*

$C_8H_{10}NO_2^+ \cdot Cl^-$
$M_r = 187.62$
Orthorhombic, *Pbca*
$a = 7.303$ (2) Å
$b = 11.005$ (2) Å
$c = 21.447$ (4) Å
$V = 1723.7$ (7) Å$^3$
$Z = 8$
$D_x = 1.446$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 20517 reflections
$\theta = 1.9$–27.6°
$\mu = 0.4$ mm$^{-1}$
$T = 296$ (2) K
Prism, colourless
0.13 × 0.08 × 0.05 mm

*Data collection*

Nonius KappaCCD diffractometer
$\varphi$ scans, and $\omega$ scans with $\kappa$ offsets
Absorption correction: none
20517 measured reflections
1979 independent reflections
1563 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.030$
$\theta_{\max} = 27.6°$
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 11$
$l = -27 \rightarrow 27$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.116$
$S = 1.01$
1979 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 1.3984P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.24$ e Å$^{-3}$

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

| *D*—H⋯*A* | *D*—H | H⋯*A* | *D*⋯*A* | *D*—H⋯*A* |
|---|---|---|---|---|
| N1—H1*A*⋯Cl1$^{\rm i}$ | 0.89 | 2.58 | 3.3475 (18) | 145 |
| N1—H1*A*⋯O1$^{\rm i}$ | 0.89 | 2.31 | 2.879 (2) | 122 |
| N1—H1*B*⋯Cl1$^{\rm ii}$ | 0.89 | 2.31 | 3.1906 (17) | 173 |
| N1—H1*C*⋯Cl1 | 0.89 | 2.47 | 3.3375 (17) | 164 |
| O2—H2⋯Cl1$^{\rm iii}$ | 0.82 | 2.25 | 3.0332 (16) | 159 |
| C1—H1⋯O1$^{\rm iv}$ | 0.98 | 2.50 | 3.433 (2) | 159 |
| C5—H5⋯O2$^{\rm v}$ | 0.93 | 2.60 | 3.338 (2) | 137 |

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

All H atoms were located in difference Fourier maps but were placed in calculated positions and treated as riding on their parent C, N and O atoms, with C—H = 0.98 (C$sp^3$) and 0.93 Å (aromatic C), N—H = 0.89 Å and O—H = 0.82 Å, and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(NH$_3$ or OH or C$sp^3$) or 1.2$U_{\rm eq}$(aromatic C).

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction:

*SCALEPACK* and *DENZO* (Otwinowski & Minor 1997); program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia,1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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