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[(Isopropoxycarbonyl)phenylmethyl]ammonium chloride

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The title compound, $C_{11}H_{16}NO_2^+\cdot Cl^-$, was obtained as colorless crystals. The molecular packing is stabilized by strong N—H···Cl hydrogen-bonding interactions.

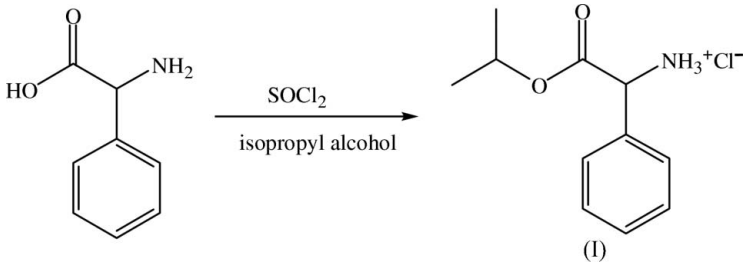
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.114
Data-to-parameter ratio = 15.3

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

Comment

To investigate the molecular recognition of ATP with proteins or structured peptide-based receptors is very important for understanding enzymatic mechanisms and drug design (Mao *et al.*, 2003; Butterfield & Waters, 2003).



(I)

The title compound, (I), an amino acid analog, was synthesized for investigation of the nature of its interaction with ATP. The bond lengths and angles in (I) are in agreement with values reported in the literature (Bouacida *et al.*, 2006).

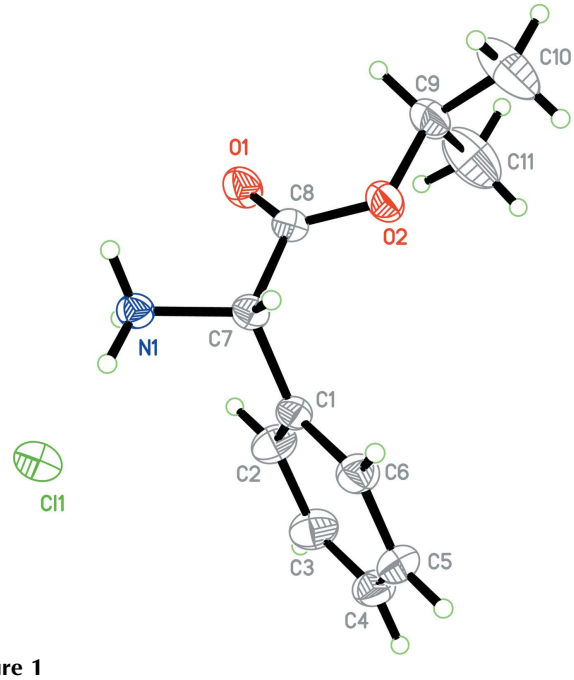


Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level. H atoms are drawn as spheres of arbitrary radius.

Experimental

The title compound was synthesised in a similar manner to that reported by (Kovalainen *et al.*, 1999). To a stirred solution of phenylglycine (1.51 g, 10 mmol) in isopropyl alcohol (50 ml) in an ice bath, thionyl chloride (1.45 mml, 20 mmol) was added dropwise, and stirring continued overnight at 353 K. The solvent was evaporated and the residue recrystallized from methanol and diethyl ester (2:1).

Crystal data

$C_{11}H_{16}NO_2^+\cdot Cl^-$
M_r = 229.70
Monoclinic, $P2_1/n$
a = 5.5811 (13) Å
b = 12.746 (3) Å
c = 16.886 (4) Å
β = 90.664 (4)°
V = 1201.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 295 (2) K
0.22 × 0.11 × 0.09 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.937, T_{max} = 0.974
5855 measured reflections
2086 independent reflections
1967 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.114
S = 1.02
2086 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl1	0.89	2.28	3.1192 (14)	158
N1—H1B···Cl1^{i}	0.89	2.36	3.2327 (15)	168
N1—H1C···Cl1^{ii}	0.89	2.29	3.1349 (15)	158
N1—H1C···O1^{iii}	0.89	2.66	3.1179 (19)	113

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

All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms, with C—H = 0.93 (aromatic), 0.98 (CH) or 0.96 Å (CH_3), N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(aromatic, CH or NH) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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: *SHELXL97*.

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