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4-[3-(4-Chlorobenzylideneamino)-2-oxooxazolidin-5-ylmethyl]morpholin-4-ium chloride monohydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.120
Data-to-parameter ratio = 17.5

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

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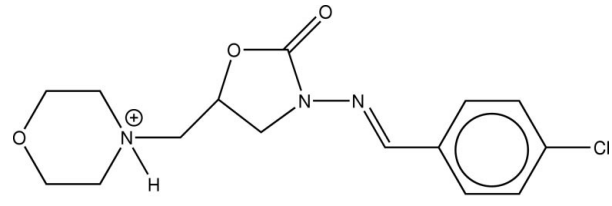
A series of derivatives of 3-amino-2-oxazolidinone have been prepared. The title derivative, $C_{15}H_{19}ClN_3O_3^+\cdot Cl^-\cdot H_2O$, is a potential psychotropic drug. The structure is assembled by strong and weak hydrogen bonds into a three-dimensional infinite framework. In the structure, intramolecular hydrogen bonds link C and O atoms to create a fused three-membered ring system.

Comment

In the Pharmaceutical Research Institute in Warsaw, a series of derivatives of 3-amino-2-oxazolidinone have been prepared (Chilmonczyk *et al.*, 1997). It has recently been found that the oxazolidinone derivative 5-morpholinomethyl-3-(4-chloride-benzylideneamino)-2-oxazolidinone is a potential psychotropic drug (Chilmonczyk, 1995). Preliminary clinical data show that the compound exhibits antidepressant activity in humans (Rybakowski & Araszkiewicz, 1999). It is generally accepted that a specific energetically preferred conformation of a compound (so-called bioactive conformation) determines the nature of interactions with its molecular target – pharmacological receptor. Therefore, it is of basic importance to get an insight into molecular parameters such as charge distribution, most preferred conformation or distances between specified points within a molecule (Krzywda *et al.*, 2000).

A perspective view of the title structure, (I), together with the atom-numbering scheme, is shown in Fig. 1. All interatomic distances are normal. The oxazolidinone ring exists in a conformation of an almost ideal half-chair, which can be deduced from the asymmetry parameters (Duax & Norton, 1975). Values and placement of asymmetry parameters are shown in Fig. 2.



H_2O

$Cl^{\ominus}$

(I)

The primary site of molecular interaction with an acid residue within a putative receptor site can be detected by hydrogen bonds. The structure of the title compound is

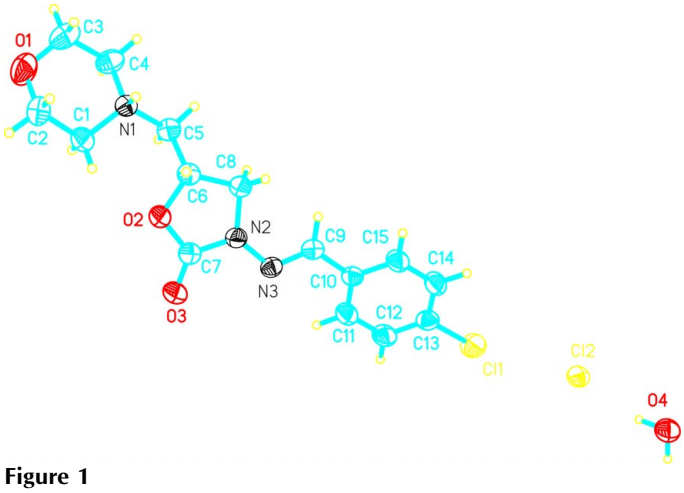


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

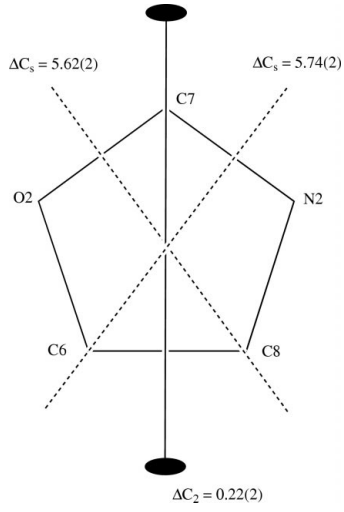


Figure 2
Values and placement of the asymmetry parameters for the oxazolidinone ring.

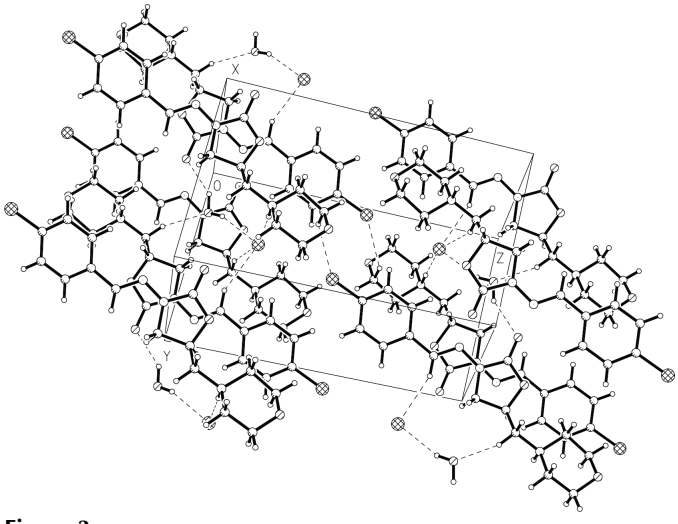


Figure 3
Part of the molecular packing of the title compound showing the intermolecular hydrogen bonds creating a three-dimensional net structure. Hydrogen bonds are indicated by dashed lines.

assembled by strong and weak hydrogen bonds to form a three-dimensional infinite framework (Fig. 3). The water O4 atom acts as a donor for one strong and three weak intermolecular hydrogen bonds. All these weak hydrogen bonds are created *via* the same H atom (H41); however, in the difference Fourier map there is no orientational disorder resulting from these. In addition, O4 acts as an acceptor for two intermolecular weak hydrogen bonds with C5 and Cl2. Also noteworthy is the fact that there is a proton transfer from hydrochloric acid to N1 which is stabilized by a weak N1—H1···Cl1 hydrogen bond. In addition, intramolecular hydrogen bonds exist linking C1 and O2 which provide additional stabilization of the molecule, creating a fused three-membered ring system.

Experimental

The title compound was prepared according to the method of Chilmonczyk *et al.* (1997).

Crystal data

$C_{15}H_{19}ClN_3O_3^+\cdot Cl^-\cdot H_2O$
M_r = 378.25
Triclinic, $P\overline{1}$
a = 7.122 (2) Å
b = 8.809 (2) Å
c = 15.178 (3) Å
α = 95.98 (2)°
β = 99.34 (2)°
γ = 107.43 (2)°
V = 884.6 (4) Å^3
Z = 2
D_x = 1.420 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 99 reflections
θ = 5–60°
μ = 0.39 mm^{-1}
T = 293 (2) K
Plate, colourless
0.49 × 0.42 × 0.04 mm

Data collection

Kuma KM-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.831, T_{max} = 0.985
4747 measured reflections
3858 independent reflections
3418 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 27.6°
$h = -1 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -19 \rightarrow 19$
3 standard reflections every 100 reflections
intensity decay: 1.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.120
S = 1.04
3858 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.3120P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (°).

C6—O2—C7—N2	−5.40 (19)	N2—C8—C6—O2	−15.35 (17)
O2—C7—N2—C8	−5.7 (2)	C8—C6—O2—C7	13.49 (18)
C7—N2—C8—C6	13.38 (19)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl2^{i}	0.91 (2)	2.13 (2)	3.0359 (17)	174 (2)
O4—H42···Cl2	0.92	2.36	3.217 (2)	154
O4—H41···O3^{ii}	0.93	2.06	2.873 (2)	146
O4—H41···N3^{ii}	0.93	2.72	3.506 (2)	143
O4—H41···O3^{iii}	0.93	3.36	3.807 (3)	112
C1—H1*B*···O2	0.96	2.46	2.989 (3)	115
C5—H5*B*···O4^{iv}	0.96	2.31	3.245 (3)	163
C9—H9···Cl2^{iv}	0.97	2.78	3.666 (2)	153

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

Data collection: *KM*-4 *Software* (Kuma, 1993); cell refinement: *KM*-4 *Software*; data reduction: *DATAPROC* (Kuma, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL*/*PC* (Sheldrick, 1990) and *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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