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4-[1-(4-Chlorophenyl)-3-oxobutylamino]-benzoic acid

B. Narayana,[a] K. Sunil,[a] B. K. Sarojini,[b] H. S. Yathirajan[c] and Michael Bolte[d]*

[a]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, [b]Department of Studies in Chemistry, P. A. College of Engineering, Mangalore University, Mangalagangotri 574 193, India, [c]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, and [d]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: bolte@chemie.uni-frankfurt.de

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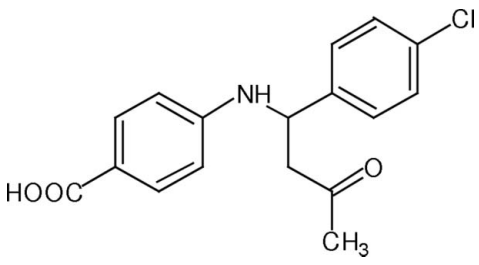
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.105; data-to-parameter ratio = 15.3.

Geometric parameters of the title compound, $C_{17}H_{16}ClNO_3$, are in the usual ranges. The two aromatic rings are almost perpendicular, with a dihedral angle of 89.26 (5)°. The carboxyl group is coplanar with the aromatic ring to which it is attached [dihedral angle = 1.70 (17)°]. The packing involves inversion-symmetric dimers bridged *via* hydrogen bonding of the carboxyl groups. In addition, there is an N—H···O hydrogen bond between the amino group and the carbonyl O atom.

Related literature

For related literature, see: Butcher *et al.* (2007); Desai *et al.* (2001); El-Masry *et al.* (2000); Hodnett & Dunn (1970); Kahwa *et al.* (1986); Misra *et al.* (1981); Narayana *et al.* (2007); Pandey *et al.* (1999); Saim *et al.* (2004); Santos *et al.* (2001); Sarojini *et al.* (2007); Singh & Dash (1988); Varma *et al.* (1986); Yathirajan *et al.* (2007).



Experimental

Crystal data

$C_{17}H_{16}ClNO_3$
M_r = 317.76
Monoclinic, $P2_1/n$
a = 6.0059 (5) Å
b = 34.018 (3) Å
c = 8.0271 (6) Å
β = 107.727 (6)°
V = 1562.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 173 (2) K
0.22 × 0.18 × 0.17 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.936, T_{max} = 0.948
10524 measured reflections
3176 independent reflections
2693 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.106
S = 1.05
3176 reflections
208 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2^{i}	0.95 (3)	1.68 (3)	2.6248 (15)	177 (2)
N1—H1···O1^{ii}	0.85 (2)	2.24 (2)	3.0543 (16)	160.5 (17)

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2438).

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supplementary materials

Acta Cryst. (2007). E**63**, o4420-o4421 [**doi:10.1107/S1600536807051471**]

4-[1-(4-Chlorophenyl)-3-oxobutylamino]benzoic acid

B. Narayana, K. Sunil, B. K. Sarojini, H. S. Yathirajan and M. Bolte

Comment

The synthesis and structure of Schiff bases have attracted much attention in biology and chemistry (Kahwa *et al.*, 1986). One of the aims of investigating the structural chemistry of Schiff bases is to develop protein and enzyme mimics (Santos *et al.*, 2001). Structural information is useful in investigating the coordination properties of Schiff bases functioning as ligands (Saim *et al.*, 2004). Some Schiff base derivatives were reported to possess antimicrobial, anti-inflammatory and central nervous system activities. Moreover, Schiff bases are also known to have biological activities such as antimicrobial (El-Masry *et al.*, 2000 & Pandey *et al.*, 1999), antifungal (Singh *et al.*, 1988 & Varma *et al.*, 1986), antitumor (Hodnett *et al.*, 1970. Misra *et al.*, 1981 & Desai *et al.*, 2001), and as herbicides.

The crystal structures of some schiff base compounds, *viz*., 2-bromo-*N*-[(*E*)-4-chlorobenzylidene]-5-methoxybenzohydrazide (Butcher *et al.*, 2007), 2-bromo-*N*'-[(*E*)-(4-fluorophenyl)methylene]-5-methoxybenzohydrazide monohydrate (Narayana *et al.*, 2007), bis{4-[(2-hydroxybenzylidine)hydrazino]-8-(trifluoromethyl)quinolinium} sulfate tetrahydrate (Yathirajan, *et al.*, 2007) and 2-Bromo-*N*'-[(1E)-(4-hydroxyphenyl)methylene]-5-methoxybenzohydrazide (Sarojini *et al.*, 2007) have been reported. A new Schiff base, $C_{14}H_{10}ClNO_2$ was synthesized and during crystallization it reacted with the solvent acetone to form a new compound, (I), $C_{17}H_{16}ClNO_3$ and its crystal structure is reported.

Geometric parameters of the title compound are in the usual ranges. The two aromatic rings are almost mutally perpendicular [dihedral angle 89.26 (5)°]. The carboxyl moiety is coplanar with the aromatic ring to which it is attached [dihedral angle 1.70 (17)°]. The packing involves inversion-symmetric dimers bridged *via* hydrogen bonding of the carboxyl groups. In addition, there is an N—H···O hydrogen bond between the amino group and the carbonyl O atom.

Experimental

The reaction is illustrated in scheme 2. A mixture of 4-aminobenzoic acid (1.37 g, 0.01 mol) and 4-chlorobenzaldehyde (1.4 g, 0.01 mol) in 15 ml of absolute ethanol containing 2 drops of 4 *M* sulfuric acid was refluxed for about 3 h. On cooling, the solid separated was filtered and recrystallized from acetone (m.p.: 441–443 K). During repeated crystallization, the Schiff base formed reacted with acetone and formed a new compound, (I). Analysis found: C: 64.18, H: 5.03, N: 4.37% for $C_{17}H_{16}ClNO_3$ requires: C: 64.26, H: 5.08, N: 4.41%.

Refinement

H atoms bonded to C were refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C) or U(H) = 1.5 $U_{eq}(C_{methyl})$] using a riding model with C—H ranging from 0.95Å to 1.00 Å. The methyl group was allowed to rotate but not to tip. The H atoms bonded to N and O were freely refined.

Figures

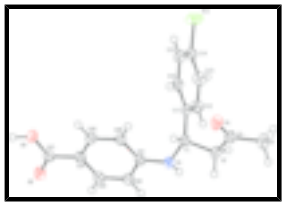

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

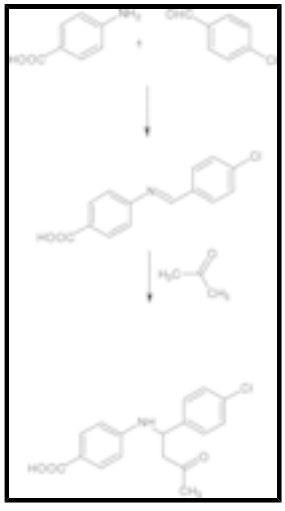

Fig. 2. The formation of the title compound.

4-[1-(4-Chlorophenyl)-3-oxobutylamino]benzoic acid

Crystal data

$C_{17}H_{16}ClNO_3$	F_{000} = 664
M_r = 317.76	D_x = 1.351 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 9512 reflections
a = 6.0059 (5) Å	θ = 4.4–26.5º
b = 34.018 (3) Å	μ = 0.26 mm^{-1}
c = 8.0271 (6) Å	T = 173 (2) K
β = 107.727 (6)º	Block, colourless
V = 1562.1 (2) Å^3	0.22 × 0.18 × 0.17 mm
Z = 4	

Data collection

Stoe IPDSII two-circle diffractometer	3176 independent reflections
Radiation source: fine-focus sealed tube	2693 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
T = 173(2) K	θ_{max} = 26.3º
ω scans	θ_{min} = 2.4º

Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$h = -7 \rightarrow 7$
$T_{min} = 0.936$, $T_{max} = 0.948$	$k = -41 \rightarrow 42$
10524 measured reflections	$l = -8 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.106$	$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.1867P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
3176 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
208 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.78406 (8)	0.233987 (12)	0.49552 (6)	0.04873 (16)
O1	1.40294 (18)	0.37231 (3)	1.05669 (14)	0.0351 (3)
O2	−0.00560 (18)	0.49116 (3)	0.19948 (14)	0.0360 (3)
O3	0.28629 (19)	0.47831 (3)	0.08845 (14)	0.0356 (3)
H3	0.186 (5)	0.4902 (8)	−0.014 (4)	0.076 (8)*
N1	0.7119 (2)	0.41099 (3)	0.86357 (16)	0.0266 (3)
H1	0.623 (3)	0.4061 (5)	0.925 (3)	0.037 (5)*
C1	0.9242 (2)	0.38766 (4)	0.89325 (18)	0.0238 (3)
H1A	1.0412	0.4038	0.8574	0.029*
C2	1.0228 (2)	0.37941 (4)	1.08945 (18)	0.0258 (3)
H2A	1.0076	0.4035	1.1545	0.031*
H2B	0.9278	0.3586	1.1211	0.031*
C3	1.2763 (2)	0.36668 (4)	1.14671 (18)	0.0268 (3)

C4	1.3646 (3)	0.34730 (5)	1.3232 (2)	0.0381 (4)
H4A	1.3032	0.3204	1.3159	0.057*
H4B	1.3122	0.3623	1.4085	0.057*
H4C	1.5358	0.3465	1.3602	0.057*
C11	0.8857 (2)	0.34943 (4)	0.78887 (17)	0.0235 (3)
C12	0.7091 (2)	0.32344 (4)	0.79678 (19)	0.0287 (3)
H12	0.6102	0.3301	0.8650	0.034*
C13	0.6762 (3)	0.28804 (4)	0.7062 (2)	0.0320 (3)
H13	0.5563	0.2704	0.7127	0.038*
C14	0.8206 (3)	0.27882 (4)	0.60664 (19)	0.0306 (3)
C15	0.9960 (3)	0.30408 (4)	0.59526 (19)	0.0315 (3)
H15	1.0936	0.2974	0.5260	0.038*
C16	1.0272 (2)	0.33933 (4)	0.68662 (19)	0.0271 (3)
H16	1.1470	0.3569	0.6792	0.032*
C21	0.5924 (2)	0.42668 (4)	0.70343 (17)	0.0227 (3)
C22	0.3689 (2)	0.44280 (4)	0.68004 (18)	0.0255 (3)
H22	0.3042	0.4425	0.7743	0.031*
C23	0.2432 (2)	0.45899 (4)	0.52246 (18)	0.0255 (3)
H23	0.0917	0.4693	0.5089	0.031*
C24	0.3347 (2)	0.46046 (4)	0.38183 (18)	0.0235 (3)
C25	0.5592 (2)	0.44553 (4)	0.40492 (18)	0.0248 (3)
H25	0.6255	0.4470	0.3117	0.030*
C26	0.6860 (2)	0.42854 (4)	0.56237 (18)	0.0252 (3)
H26	0.8370	0.4181	0.5753	0.030*
C27	0.1934 (2)	0.47808 (4)	0.21563 (18)	0.0254 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0599 (3)	0.0391 (2)	0.0479 (3)	−0.00685 (18)	0.0175 (2)	−0.01857 (18)
O1	0.0310 (5)	0.0445 (6)	0.0323 (6)	−0.0007 (4)	0.0131 (5)	0.0059 (5)
O2	0.0306 (5)	0.0475 (6)	0.0285 (6)	0.0121 (5)	0.0069 (4)	0.0052 (5)
O3	0.0385 (6)	0.0453 (6)	0.0243 (5)	0.0132 (5)	0.0113 (4)	0.0077 (5)
N1	0.0295 (6)	0.0288 (6)	0.0242 (6)	0.0054 (5)	0.0122 (5)	0.0051 (5)
C1	0.0251 (6)	0.0245 (6)	0.0225 (7)	0.0003 (5)	0.0085 (5)	0.0032 (5)
C2	0.0286 (7)	0.0273 (6)	0.0215 (7)	−0.0022 (5)	0.0078 (5)	0.0007 (5)
C3	0.0298 (7)	0.0257 (6)	0.0235 (7)	−0.0040 (5)	0.0060 (6)	0.0002 (5)
C4	0.0369 (8)	0.0458 (9)	0.0286 (8)	0.0006 (7)	0.0055 (6)	0.0104 (7)
C11	0.0246 (6)	0.0246 (6)	0.0195 (6)	0.0035 (5)	0.0042 (5)	0.0036 (5)
C12	0.0254 (6)	0.0323 (7)	0.0297 (7)	0.0001 (5)	0.0105 (5)	−0.0001 (6)
C13	0.0283 (7)	0.0320 (7)	0.0349 (8)	−0.0040 (5)	0.0082 (6)	−0.0005 (6)
C14	0.0336 (7)	0.0295 (7)	0.0255 (7)	0.0021 (6)	0.0043 (6)	−0.0034 (6)
C15	0.0344 (7)	0.0363 (7)	0.0258 (7)	0.0047 (6)	0.0120 (6)	−0.0001 (6)
C16	0.0276 (6)	0.0298 (7)	0.0249 (7)	0.0009 (5)	0.0097 (5)	0.0039 (5)
C21	0.0265 (6)	0.0187 (6)	0.0229 (7)	−0.0019 (5)	0.0077 (5)	0.0011 (5)
C22	0.0289 (7)	0.0241 (6)	0.0266 (7)	0.0003 (5)	0.0129 (5)	0.0023 (5)
C23	0.0245 (6)	0.0231 (6)	0.0298 (7)	0.0014 (5)	0.0094 (5)	0.0011 (5)
C24	0.0254 (6)	0.0204 (6)	0.0240 (7)	−0.0015 (5)	0.0064 (5)	0.0002 (5)

C25	0.0270 (6)	0.0260 (6)	0.0234 (7)	0.0002 (5)	0.0104 (5)	0.0018 (5)
C26	0.0232 (6)	0.0264 (6)	0.0269 (7)	0.0025 (5)	0.0089 (5)	0.0029 (5)
C27	0.0270 (6)	0.0236 (6)	0.0244 (7)	0.0010 (5)	0.0061 (5)	−0.0004 (5)

Geometric parameters (Å, °)

Cl1—C14	1.7465 (15)	C12—C13	1.389 (2)
O1—C3	1.2132 (18)	C12—H12	0.9500
O2—C27	1.2443 (17)	C13—C14	1.383 (2)
O3—C27	1.3041 (17)	C13—H13	0.9500
O3—H3	0.95 (3)	C14—C15	1.384 (2)
N1—C21	1.3750 (18)	C15—C16	1.388 (2)
N1—C1	1.4586 (17)	C15—H15	0.9500
N1—H1	0.85 (2)	C16—H16	0.9500
C1—C11	1.5261 (18)	C21—C22	1.4083 (18)
C1—C2	1.5304 (19)	C21—C26	1.4108 (18)
C1—H1A	1.0000	C22—C23	1.376 (2)
C2—C3	1.5133 (19)	C22—H22	0.9500
C2—H2A	0.9900	C23—C24	1.3991 (19)
C2—H2B	0.9900	C23—H23	0.9500
C3—C4	1.505 (2)	C24—C25	1.3990 (18)
C4—H4A	0.9800	C24—C27	1.4731 (19)
C4—H4B	0.9800	C25—C26	1.3876 (19)
C4—H4C	0.9800	C25—H25	0.9500
C11—C16	1.3922 (19)	C26—H26	0.9500
C11—C12	1.3971 (19)		
C27—O3—H3	111.9 (15)	C14—C13—H13	120.5
C21—N1—C1	123.05 (12)	C12—C13—H13	120.5
C21—N1—H1	112.3 (13)	C13—C14—C15	121.42 (13)
C1—N1—H1	118.1 (12)	C13—C14—Cl1	119.34 (11)
N1—C1—C11	113.28 (11)	C15—C14—Cl1	119.23 (11)
N1—C1—C2	108.25 (11)	C14—C15—C16	118.97 (13)
C11—C1—C2	110.80 (10)	C14—C15—H15	120.5
N1—C1—H1A	108.1	C16—C15—H15	120.5
C11—C1—H1A	108.1	C15—C16—C11	121.09 (13)
C2—C1—H1A	108.1	C15—C16—H16	119.5
C3—C2—C1	113.80 (11)	C11—C16—H16	119.5
C3—C2—H2A	108.8	N1—C21—C22	118.73 (12)
C1—C2—H2A	108.8	N1—C21—C26	123.07 (12)
C3—C2—H2B	108.8	C22—C21—C26	118.17 (12)
C1—C2—H2B	108.8	C23—C22—C21	120.84 (12)
H2A—C2—H2B	107.7	C23—C22—H22	119.6
O1—C3—C4	121.66 (13)	C21—C22—H22	119.6
O1—C3—C2	121.94 (13)	C22—C23—C24	121.04 (12)
C4—C3—C2	116.40 (12)	C22—C23—H23	119.5
C3—C4—H4A	109.5	C24—C23—H23	119.5
C3—C4—H4B	109.5	C23—C24—C25	118.66 (12)
H4A—C4—H4B	109.5	C23—C24—C27	119.05 (12)
C3—C4—H4C	109.5	C25—C24—C27	122.28 (12)

H4A—C4—H4C	109.5	C26—C25—C24	120.77 (12)
H4B—C4—H4C	109.5	C26—C25—H25	119.6
C16—C11—C12	118.59 (13)	C24—C25—H25	119.6
C16—C11—C1	121.09 (12)	C25—C26—C21	120.48 (12)
C12—C11—C1	120.31 (12)	C25—C26—H26	119.8
C13—C12—C11	120.93 (13)	C21—C26—H26	119.8
C13—C12—H12	119.5	O2—C27—O3	122.86 (13)
C11—C12—H12	119.5	O2—C27—C24	120.68 (13)
C14—C13—C12	119.00 (13)	O3—C27—C24	116.45 (12)
C21—N1—C1—C11	−63.24 (16)	C12—C11—C16—C15	−0.6 (2)
C21—N1—C1—C2	173.47 (12)	C1—C11—C16—C15	178.31 (12)
N1—C1—C2—C3	−162.23 (11)	C1—N1—C21—C22	169.04 (12)
C11—C1—C2—C3	72.99 (14)	C1—N1—C21—C26	−13.0 (2)
C1—C2—C3—O1	17.90 (19)	N1—C21—C22—C23	179.71 (12)
C1—C2—C3—C4	−163.22 (12)	C26—C21—C22—C23	1.64 (19)
N1—C1—C11—C16	128.90 (13)	C21—C22—C23—C24	−1.0 (2)
C2—C1—C11—C16	−109.22 (14)	C22—C23—C24—C25	−0.78 (19)
N1—C1—C11—C12	−52.24 (16)	C22—C23—C24—C27	179.97 (12)
C2—C1—C11—C12	69.65 (15)	C23—C24—C25—C26	1.86 (19)
C16—C11—C12—C13	0.7 (2)	C27—C24—C25—C26	−178.92 (12)
C1—C11—C12—C13	−178.23 (13)	C24—C25—C26—C21	−1.2 (2)
C11—C12—C13—C14	−0.3 (2)	N1—C21—C26—C25	−178.54 (12)
C12—C13—C14—C15	−0.1 (2)	C22—C21—C26—C25	−0.56 (19)
C12—C13—C14—Cl1	178.84 (11)	C23—C24—C27—O2	−0.66 (19)
C13—C14—C15—C16	0.2 (2)	C25—C24—C27—O2	−179.87 (13)
Cl1—C14—C15—C16	−178.76 (11)	C23—C24—C27—O3	−179.32 (12)
C14—C15—C16—C11	0.1 (2)	C25—C24—C27—O3	1.47 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2^{i}	0.95 (3)	1.68 (3)	2.6248 (15)	177 (2)
N1—H1···O1^{ii}	0.85 (2)	2.24 (2)	3.0543 (16)	160.5 (17)

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) *x*−1, *y*, *z*.

Fig. 1

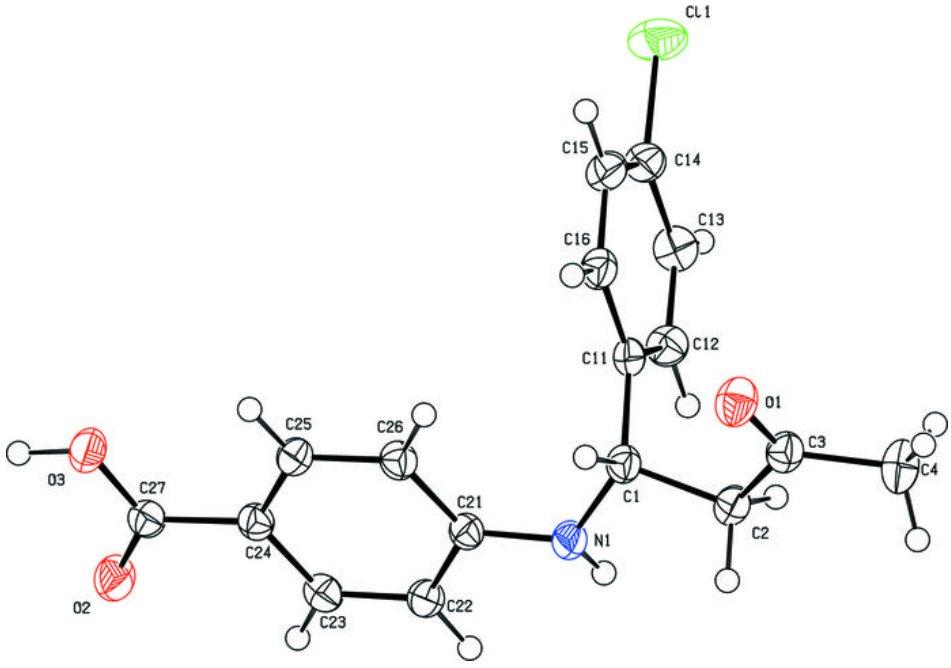
Cl1
C15
C14
C13
C16
C12
C11
O1
C3
C4
C25
C26
O3
C27
C21
C1
N1
C2
C24
O2
C23
C22

Fig. 2