IUCrData

ISSN 2414-3146

Tramadolium 2-chlorobenzoate

S. N. Sheshadri,[a] P. Nagendra,[b] B. P. Siddaraju,[c] K. Byrappa,[d] N. K. Lokanath[e] and S. Madan Kumar[f]*

[a]Department of Chemistry, GSSS Institute of Engineering Technology for Women, Mysuru 570016, India, [b]Department of Chemistry, BET Academy of Higher Education, Bharathi College, Bharthi Nagara, Mandya 571422, India, [c]Department of Engineering Chemistry, Cauvery Institute of Technology, Mandya 571402, India, [d]Department of Materials Science, Mangalagangotri, Mangalore University, Mangaluru 574 199, India, [e]Department of Studies in Physics, University of Mysore, Manasagangotri, Mysore 570006, India, and [f]PURSE Lab, Mangalagangotri, Mangalore University, Mangaluru 574 199, India. *Correspondence e-mail: madanmx@mangaloreuniversity.ac.in

Received 23 December 2015
Accepted 4 January 2016

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

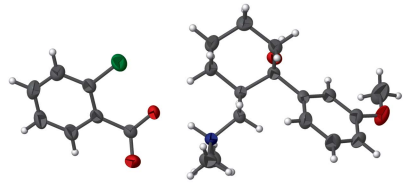
Keywords: Tramadol; cyclohexane; crystal structure.

CCDC reference: 1425992

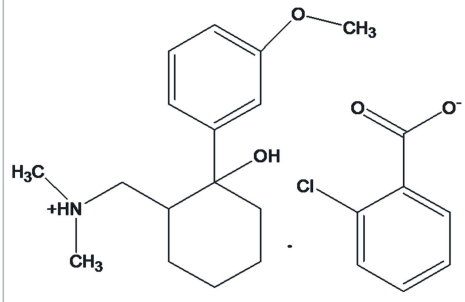
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecular salt, $C_{16}H_{26}NO_2^+\cdot C_7H_4ClO_2^-$, {systematic name: [2-hydroxy-2-(3-methoxyphenyl)cyclohexylmethyl]dimethylammonium 2-chlorobenzoate}, the cyclohexane ring of the cation exhibits a chair conformation with the aromatic and amine substituents in equatorial orientations and the hydroxyl group in an axial orientation. In the anion, the dihedral angle between the aromatic ring and the carboxylate group is 39.16 (13)°. In the crystal, the cations are linked to the anions by O—H···O, N—H···O and C—H···O hydrogen bonds, generating [010] chains. Further C—H···O and C—H···π interactions are also observed, which link the chains into a three-dimensional framework.

3D view



Chemical scheme



Structure description

A view of the title molecular salt is shown in Fig. 1. Details of the hydrogen bonds and C—H···π interactions are given in Table 1 and illustrated in Fig. 2. For a related structure, see: Sheshadri *et al.* (2015).

Synthesis and crystallization

Tramadol (3 g, 0.01 mol) and 2-chloro benzoic acid (1 g, 0.01 mol) were each dissolved in 10 ml of ethanol. The solutions were mixed and stirred in a beaker at 300 K for 30 min. The mixture was kept aside for three days at room temperature. Colourless blocks were formed and one was used for the data collection.

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O10—H10···O27^{i}	0.82	1.92	2.721 (3)	164
N17—H17···O28	0.98	1.66	2.619 (3)	164
C14—H14*B*···O28	0.97	2.50	3.305 (3)	140
C8—H8*B*···O28^{ii}	0.96	2.59	3.338 (4)	135
C18—H18*A*···O10^{ii}	0.96	2.58	3.428 (4)	148
C23—H23···*Cg*1^{iii}	0.93	2.66	3.546 (4)	160

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y+1, -z+2$; (iii) $x-1, y+1, z$.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank the DST–PURSE, Mangalore University, Mangaluru, for providing the single-crystal X-ray diffraction facility. PN thanks Bharthi College, Maddur, for research facilities.

References

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

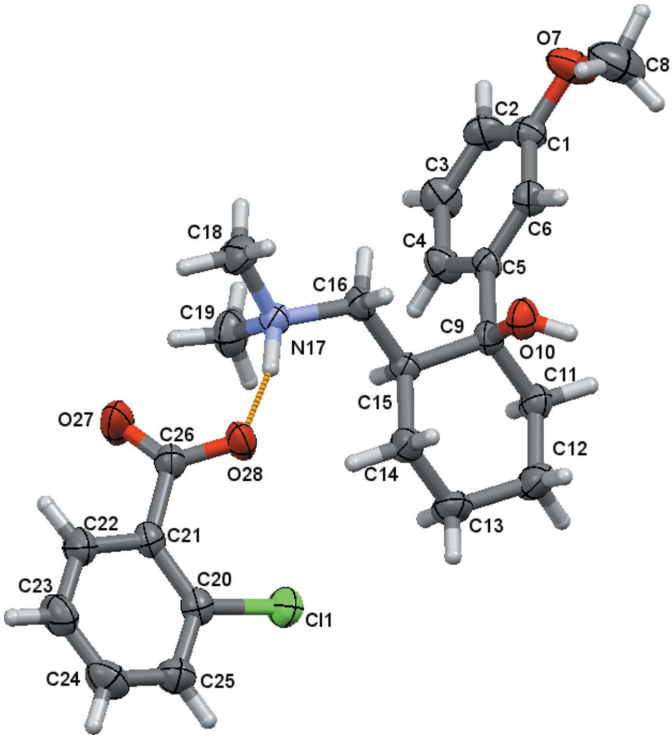


Figure 1
A view of the title compound with displacement ellipsoids drawn at the 50% probability level. The intramolecular hydrogen bond is drawn as a dashed line.

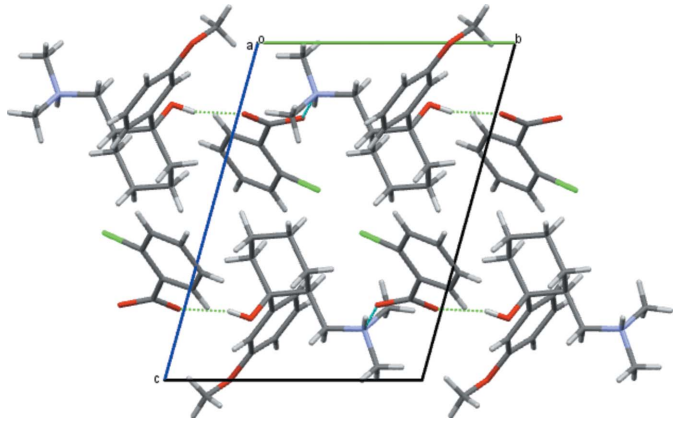


Figure 2
A view along the *a* axis of the packing of the title compound. Hydrogen bonds are drawn as a dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{26}NO_2^+ \cdot C_7H_4ClO_2^-$
M_r	419.93
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, *b*, *c* (Å)	9.205 (6), 9.688 (7), 12.943 (9)
α, β, γ (°)	104.871 (11), 91.465 (7), 100.983 (12)
V (Å^3)	1091.8 (13)
Z	2
Radiation type	Mo *Kα*
μ (mm^{-1})	0.20
Crystal size (mm)	0.47 × 0.46 × 0.23
Data collection	
Diffractometer	Rigaku Saturn724+ diffractometer
Absorption correction	Multi-scan (*NUMABS*; Rigaku 1999)
T_{min}, T_{max}	0.909, 0.954
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5644, 3759, 2737
R_{int}	0.021
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.601
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.047, 0.111, 1.03
No. of reflections	3759
No. of parameters	266
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.26

Computer programs: *CrystalClear SM Expert* (Rigaku, 2011), *SHELXS1997* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *OLEX2* (Dolomanov *et al.*, 2009).

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Rigaku. (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
Rigaku (2011). *CrystalClear SM Expert*. Rigaku Corporation, Tokyo, Japan
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Sheshadri, S. N., Nagendra, P., Siddaraju, B. P., Hemakumar, K. H., Byrappa, K., Lokanath, N. K. & Madan Kumar, S. (2015). *Acta Cryst.* E**71**, o864–o865.

full crystallographic data

IUCrData (2016). **1**, x160014 [doi:10.1107/S2414314616000146]

Tramadolium 2-chlorobenzoate

S. N. Sheshadri, P. Nagendra, B. P. Siddaraju, K. Byrappa, N. K. Lokanath and S. Madan Kumar

[2-Hydroxy-2-(3-methoxyphenyl)cyclohexylmethyl]dimethylammonium 2-chlorobenzoate

Crystal data

$C_{16}H_{26}NO_2^+ \cdot C_7H_4ClO_2^-$
M_r = 419.93
Triclinic, $P\overline{1}$
a = 9.205 (6) Å
b = 9.688 (7) Å
c = 12.943 (9) Å
α = 104.871 (11)°
β = 91.465 (7)°
γ = 100.983 (12)°
V = 1091.8 (13) Å^3
Z = 2
$F(000)$ = 448
D_x = 1.277 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 3759 reflections
θ = 3.1–25.3°
μ = 0.20 mm^{-1}
T = 293 K
Block, colourless
0.47 × 0.46 × 0.23 mm

Data collection

Rigaku Saturn724+ diffractometer
Radiation source: Sealed tube
Confocal monochromator
Detector resolution: 28.5714 pixels mm^{-1}
profile data from ω–scans
Absorption correction: multi-scan (*NUMABS*; Rigaku 1999)
T_{min} = 0.909, T_{max} = 0.954
5644 measured reflections
3759 independent reflections
2737 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.3°, θ_{min} = 3.1°
h = −11→11
k = −10→11
l = −13→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.111
S = 1.03
3759 reflections
266 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.271P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.18349 (7)	0.60882 (6)	0.56379 (5)	0.0535 (2)
O27	0.4450 (2)	0.97619 (19)	0.78882 (17)	0.0728 (6)
O28	0.34218 (16)	0.74702 (16)	0.77727 (13)	0.0451 (4)
C20	0.1255 (2)	0.7722 (2)	0.61387 (17)	0.0375 (5)
C21	0.2059 (2)	0.8822 (2)	0.69885 (16)	0.0357 (5)
C22	0.1524 (3)	1.0101 (3)	0.72920 (18)	0.0487 (6)
H22	0.2047	1.0868	0.7842	0.058*
C23	0.0248 (3)	1.0276 (3)	0.68102 (19)	0.0533 (7)
H23	−0.0095	1.1138	0.7047	0.064*
C24	−0.0514 (3)	0.9175 (3)	0.5981 (2)	0.0542 (7)
H24	−0.1377	0.9289	0.5652	0.065*
C25	−0.0009 (3)	0.7906 (3)	0.56338 (19)	0.0498 (6)
H25	−0.0516	0.7168	0.5059	0.060*
C26	0.3432 (3)	0.8682 (2)	0.75872 (17)	0.0398 (5)
O7	1.02381 (18)	0.2539 (2)	0.99917 (13)	0.0586 (5)
O10	0.54164 (16)	0.26798 (16)	0.81780 (12)	0.0416 (4)
H10	0.5134	0.1793	0.7962	0.062*
N17	0.60162 (19)	0.71995 (18)	0.84805 (13)	0.0347 (4)
H17	0.5020	0.7134	0.8162	0.042*
C1	0.9828 (2)	0.3083 (2)	0.91759 (17)	0.0388 (5)
C2	1.0957 (2)	0.3841 (3)	0.87499 (18)	0.0448 (6)
H2	1.1932	0.3986	0.9028	0.054*
C3	1.0643 (2)	0.4392 (3)	0.79062 (19)	0.0467 (6)
H3	1.1407	0.4914	0.7618	0.056*
C4	0.9191 (2)	0.4169 (3)	0.74858 (18)	0.0421 (6)
H4	0.8992	0.4520	0.6904	0.050*
C5	0.8031 (2)	0.3428 (2)	0.79229 (16)	0.0320 (5)
C6	0.8359 (2)	0.2882 (2)	0.87754 (16)	0.0356 (5)
H6	0.7598	0.2381	0.9080	0.043*
C8	0.9107 (3)	0.1785 (4)	1.0477 (2)	0.0814 (10)
H8A	0.8580	0.0929	0.9955	0.122*
H8B	0.8432	0.2408	1.0751	0.122*
H8C	0.9540	0.1505	1.1054	0.122*
C9	0.6417 (2)	0.3177 (2)	0.74684 (16)	0.0324 (5)
C11	0.6219 (2)	0.2069 (2)	0.63600 (17)	0.0422 (6)
H11A	0.6982	0.2398	0.5924	0.051*
H11B	0.6365	0.1139	0.6448	0.051*
C12	0.4703 (3)	0.1842 (3)	0.5766 (2)	0.0536 (7)
H12A	0.4688	0.1204	0.5051	0.064*
H12B	0.3943	0.1376	0.6142	0.064*
C13	0.4369 (3)	0.3285 (3)	0.56868 (19)	0.0517 (7)
H13A	0.3374	0.3125	0.5354	0.062*
H13B	0.5060	0.3695	0.5238	0.062*
C14	0.4494 (2)	0.4356 (2)	0.67874 (17)	0.0426 (6)
H14A	0.3752	0.3976	0.7218	0.051*

H14B	0.4295	0.5274	0.6711	0.051*
C15	0.6030 (2)	0.4623 (2)	0.73608 (15)	0.0317 (5)
H15	0.6758	0.5041	0.6927	0.038*
C16	0.6174 (2)	0.5690 (2)	0.84660 (16)	0.0364 (5)
H16A	0.5425	0.5303	0.8889	0.044*
H16B	0.7137	0.5743	0.8813	0.044*
C18	0.6123 (3)	0.8113 (3)	0.96057 (18)	0.0555 (7)
H18A	0.5395	0.7656	0.9997	0.083*
H18B	0.5947	0.9059	0.9610	0.083*
H18C	0.7097	0.8212	0.9936	0.083*
C19	0.7097 (3)	0.7899 (3)	0.7845 (2)	0.0543 (7)
H19A	0.8086	0.7877	0.8085	0.082*
H19B	0.7003	0.8892	0.7937	0.082*
H19C	0.6903	0.7379	0.7100	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0658 (4)	0.0412 (4)	0.0514 (4)	0.0202 (3)	−0.0058 (3)	0.0027 (3)
O27	0.0604 (12)	0.0367 (10)	0.1158 (16)	−0.0075 (9)	−0.0366 (11)	0.0273 (10)
O28	0.0375 (9)	0.0325 (9)	0.0685 (10)	0.0069 (7)	−0.0082 (8)	0.0202 (8)
C20	0.0386 (12)	0.0337 (12)	0.0425 (12)	0.0091 (10)	0.0056 (10)	0.0130 (10)
C21	0.0379 (12)	0.0309 (12)	0.0414 (12)	0.0080 (10)	0.0051 (10)	0.0144 (9)
C22	0.0600 (16)	0.0366 (14)	0.0492 (14)	0.0186 (12)	−0.0044 (12)	0.0055 (11)
C23	0.0600 (17)	0.0492 (16)	0.0585 (15)	0.0304 (13)	0.0031 (13)	0.0141 (13)
C24	0.0431 (14)	0.0646 (18)	0.0630 (16)	0.0217 (13)	−0.0018 (12)	0.0240 (14)
C25	0.0467 (15)	0.0476 (15)	0.0530 (14)	0.0104 (12)	−0.0094 (12)	0.0106 (11)
C26	0.0409 (13)	0.0300 (13)	0.0476 (13)	0.0067 (11)	−0.0025 (11)	0.0097 (10)
O7	0.0397 (10)	0.0873 (14)	0.0591 (10)	0.0111 (9)	−0.0044 (8)	0.0401 (10)
O10	0.0354 (9)	0.0330 (9)	0.0565 (9)	0.0024 (7)	0.0060 (7)	0.0151 (7)
N17	0.0313 (10)	0.0282 (10)	0.0420 (10)	0.0059 (8)	−0.0037 (8)	0.0056 (8)
C1	0.0382 (13)	0.0417 (13)	0.0384 (12)	0.0121 (10)	0.0003 (10)	0.0115 (10)
C2	0.0267 (11)	0.0532 (15)	0.0534 (14)	0.0064 (11)	−0.0023 (10)	0.0138 (11)
C3	0.0298 (12)	0.0554 (16)	0.0603 (15)	0.0089 (11)	0.0103 (11)	0.0243 (12)
C4	0.0348 (13)	0.0485 (15)	0.0496 (13)	0.0139 (11)	0.0042 (11)	0.0210 (11)
C5	0.0294 (11)	0.0278 (11)	0.0396 (12)	0.0110 (9)	0.0023 (9)	0.0067 (9)
C6	0.0302 (11)	0.0356 (13)	0.0418 (12)	0.0076 (9)	0.0049 (10)	0.0109 (10)
C8	0.0576 (18)	0.117 (3)	0.085 (2)	0.0026 (18)	−0.0068 (16)	0.067 (2)
C9	0.0275 (11)	0.0291 (12)	0.0419 (12)	0.0063 (9)	0.0036 (9)	0.0113 (9)
C11	0.0432 (13)	0.0329 (13)	0.0483 (13)	0.0134 (10)	−0.0031 (11)	0.0035 (10)
C12	0.0529 (15)	0.0395 (14)	0.0580 (15)	0.0116 (12)	−0.0144 (13)	−0.0053 (11)
C13	0.0447 (14)	0.0484 (15)	0.0557 (15)	0.0150 (12)	−0.0189 (12)	0.0009 (12)
C14	0.0369 (13)	0.0363 (13)	0.0532 (14)	0.0147 (10)	−0.0067 (11)	0.0049 (10)
C15	0.0285 (11)	0.0296 (11)	0.0363 (11)	0.0072 (9)	−0.0017 (9)	0.0073 (9)
C16	0.0371 (12)	0.0302 (12)	0.0437 (12)	0.0109 (10)	−0.0008 (10)	0.0105 (9)
C18	0.0679 (17)	0.0428 (15)	0.0488 (14)	0.0193 (13)	−0.0081 (13)	−0.0047 (11)
C19	0.0479 (15)	0.0417 (15)	0.0737 (17)	0.0018 (12)	0.0085 (13)	0.0209 (13)

Geometric parameters (Å, º)

Cl1—C20	1.739 (2)	C5—C6	1.390 (3)
O27—C26	1.234 (3)	C5—C9	1.535 (3)
O28—C26	1.255 (3)	C6—H6	0.9300
C20—C21	1.396 (3)	C8—H8A	0.9600
C20—C25	1.383 (3)	C8—H8B	0.9600
C21—C22	1.387 (3)	C8—H8C	0.9600
C21—C26	1.512 (3)	C9—C11	1.538 (3)
C22—H22	0.9300	C9—C15	1.548 (3)
C22—C23	1.375 (3)	C11—H11A	0.9700
C23—H23	0.9300	C11—H11B	0.9700
C23—C24	1.368 (4)	C11—C12	1.526 (3)
C24—H24	0.9300	C12—H12A	0.9700
C24—C25	1.369 (3)	C12—H12B	0.9700
C25—H25	0.9300	C12—C13	1.515 (3)
O7—C1	1.370 (3)	C13—H13A	0.9700
O7—C8	1.411 (3)	C13—H13B	0.9700
O10—H10	0.8200	C13—C14	1.519 (3)
O10—C9	1.423 (2)	C14—H14A	0.9700
N17—H17	0.9800	C14—H14B	0.9700
N17—C16	1.493 (3)	C14—C15	1.525 (3)
N17—C18	1.487 (3)	C15—H15	0.9800
N17—C19	1.482 (3)	C15—C16	1.520 (3)
C1—C2	1.367 (3)	C16—H16A	0.9700
C1—C6	1.395 (3)	C16—H16B	0.9700
C2—H2	0.9300	C18—H18A	0.9600
C2—C3	1.379 (3)	C18—H18B	0.9600
C3—H3	0.9300	C18—H18C	0.9600
C3—C4	1.386 (3)	C19—H19A	0.9600
C4—H4	0.9300	C19—H19B	0.9600
C4—C5	1.386 (3)	C19—H19C	0.9600
C21—C20—Cl1	121.50 (17)	O10—C9—C11	111.22 (17)
C25—C20—Cl1	117.08 (18)	O10—C9—C15	105.91 (16)
C25—C20—C21	121.4 (2)	C5—C9—C11	108.63 (16)
C20—C21—C26	124.04 (19)	C5—C9—C15	110.75 (16)
C22—C21—C20	116.4 (2)	C11—C9—C15	109.63 (17)
C22—C21—C26	119.52 (19)	C9—C11—H11A	108.8
C21—C22—H22	118.8	C9—C11—H11B	108.8
C23—C22—C21	122.4 (2)	H11A—C11—H11B	107.7
C23—C22—H22	118.8	C12—C11—C9	113.94 (18)
C22—C23—H23	120.2	C12—C11—H11A	108.8
C24—C23—C22	119.6 (2)	C12—C11—H11B	108.8
C24—C23—H23	120.2	C11—C12—H12A	109.5
C23—C24—H24	119.9	C11—C12—H12B	109.5
C23—C24—C25	120.2 (2)	H12A—C12—H12B	108.1
C25—C24—H24	119.9	C13—C12—C11	110.77 (19)

C20—C25—H25	120.0	C13—C12—H12A	109.5
C24—C25—C20	120.0 (2)	C13—C12—H12B	109.5
C24—C25—H25	120.0	C12—C13—H13A	109.4
O27—C26—O28	124.8 (2)	C12—C13—H13B	109.4
O27—C26—C21	118.5 (2)	C12—C13—C14	111.1 (2)
O28—C26—C21	116.63 (19)	H13A—C13—H13B	108.0
C1—O7—C8	118.02 (18)	C14—C13—H13A	109.4
C9—O10—H10	109.5	C14—C13—H13B	109.4
C16—N17—H17	107.5	C13—C14—H14A	109.3
C18—N17—H17	107.5	C13—C14—H14B	109.3
C18—N17—C16	109.97 (17)	C13—C14—C15	111.71 (18)
C19—N17—H17	107.5	H14A—C14—H14B	107.9
C19—N17—C16	113.29 (17)	C15—C14—H14A	109.3
C19—N17—C18	110.81 (19)	C15—C14—H14B	109.3
O7—C1—C6	123.4 (2)	C9—C15—H15	108.0
C2—C1—O7	116.1 (2)	C14—C15—C9	111.10 (17)
C2—C1—C6	120.5 (2)	C14—C15—H15	108.0
C1—C2—H2	120.1	C16—C15—C9	109.16 (16)
C1—C2—C3	119.7 (2)	C16—C15—C14	112.43 (17)
C3—C2—H2	120.1	C16—C15—H15	108.0
C2—C3—H3	119.9	N17—C16—C15	115.42 (17)
C2—C3—C4	120.2 (2)	N17—C16—H16A	108.4
C4—C3—H3	119.9	N17—C16—H16B	108.4
C3—C4—H4	119.6	C15—C16—H16A	108.4
C3—C4—C5	120.8 (2)	C15—C16—H16B	108.4
C5—C4—H4	119.6	H16A—C16—H16B	107.5
C4—C5—C6	118.54 (19)	N17—C18—H18A	109.5
C4—C5—C9	121.37 (19)	N17—C18—H18B	109.5
C6—C5—C9	120.08 (19)	N17—C18—H18C	109.5
C1—C6—H6	119.9	H18A—C18—H18B	109.5
C5—C6—C1	120.2 (2)	H18A—C18—H18C	109.5
C5—C6—H6	119.9	H18B—C18—H18C	109.5
O7—C8—H8A	109.5	N17—C19—H19A	109.5
O7—C8—H8B	109.5	N17—C19—H19B	109.5
O7—C8—H8C	109.5	N17—C19—H19C	109.5
H8A—C8—H8B	109.5	H19A—C19—H19B	109.5
H8A—C8—H8C	109.5	H19A—C19—H19C	109.5
H8B—C8—H8C	109.5	H19B—C19—H19C	109.5
O10—C9—C5	110.70 (17)		

Cl1—C20—C21—C22	177.46 (18)	C4—C5—C9—O10	−167.60 (18)
Cl1—C20—C21—C26	−3.5 (3)	C4—C5—C9—C11	70.0 (3)
Cl1—C20—C25—C24	−179.2 (2)	C4—C5—C9—C15	−50.4 (3)
C20—C21—C22—C23	1.8 (4)	C5—C9—C11—C12	−173.8 (2)
C20—C21—C26—O27	143.1 (2)	C5—C9—C15—C14	173.22 (17)
C20—C21—C26—O28	−39.3 (3)	C5—C9—C15—C16	−62.2 (2)
C21—C20—C25—C24	−1.4 (4)	C6—C1—C2—C3	−1.1 (3)
C21—C22—C23—C24	−1.8 (4)	C6—C5—C9—O10	13.8 (3)

C22—C21—C26—O27	−37.9 (3)	C6—C5—C9—C11	−108.6 (2)
C22—C21—C26—O28	139.7 (2)	C6—C5—C9—C15	130.95 (19)
C22—C23—C24—C25	0.1 (4)	C8—O7—C1—C2	178.2 (2)
C23—C24—C25—C20	1.5 (4)	C8—O7—C1—C6	−2.5 (3)
C25—C20—C21—C22	−0.2 (3)	C9—C5—C6—C1	178.68 (18)
C25—C20—C21—C26	178.8 (2)	C9—C11—C12—C13	53.9 (3)
C26—C21—C22—C23	−177.3 (2)	C9—C15—C16—N17	172.82 (16)
O7—C1—C2—C3	178.3 (2)	C11—C9—C15—C14	53.4 (2)
O7—C1—C6—C5	−178.0 (2)	C11—C9—C15—C16	177.90 (18)
O10—C9—C11—C12	64.1 (3)	C11—C12—C13—C14	−55.0 (3)
O10—C9—C15—C14	−66.7 (2)	C12—C13—C14—C15	57.8 (3)
O10—C9—C15—C16	57.8 (2)	C13—C14—C15—C9	−57.2 (3)
C1—C2—C3—C4	−0.5 (4)	C13—C14—C15—C16	−179.84 (19)
C2—C1—C6—C5	1.3 (3)	C14—C15—C16—N17	−63.4 (2)
C2—C3—C4—C5	1.8 (3)	C15—C9—C11—C12	−52.7 (3)
C3—C4—C5—C6	−1.6 (3)	C18—N17—C16—C15	177.93 (18)
C3—C4—C5—C9	179.80 (19)	C19—N17—C16—C15	−57.5 (2)
C4—C5—C6—C1	0.0 (3)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O10—H10···O27^{i}	0.82	1.92	2.721 (3)	164
N17—H17···O28	0.98	1.66	2.619 (3)	164
C14—H14*B*···O28	0.97	2.50	3.305 (3)	140
C8—H8*B*···O28^{ii}	0.96	2.59	3.338 (4)	135
C18—H18*A*···O10^{ii}	0.96	2.58	3.428 (4)	148
C23—H23···*Cg*1^{iii}	0.93	2.66	3.546 (4)	160

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) *x*−1, *y*+1, *z*.