Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-[(*S*)-1-(3,5-Dimethyl-2-hydroxyphenyl)ethyl]-*N*-[(*R*)-2-hydroxy-1-phenylethyl]ammonium chloride

Guangyou Zhang,[a] Xungang Gu,[a]* Xiangbo Wang,[a] Wanhui Wang[a] and Shuchun Li[b]‡

[a]School of Chemistry and Chemical Engineering, University of Jinan, Jinan 250022, People's Republic of China, and [b]Bureau of Education of Liaocheng, Liaocheng City, Shandong Province 252000, People's Republic of China
Correspondence e-mail: gu_505@163.com

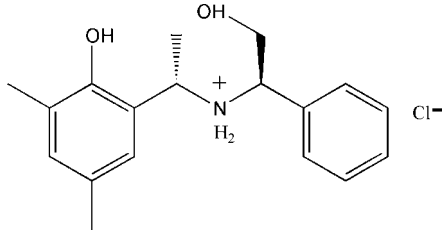
Received 24 October 2007; accepted 25 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.097; data-to-parameter ratio = 15.7.

In the title compound, $C_{18}H_{24}NO_2^+\cdot Cl^-$, the absolute configuration of the new stereogenic centre (the C atom with a CH_2OH substituent) was unambiguously determined to have an *R* configuration. The dihedral angle between the two aromatic rings is 30.82 (2)°. Intermolecular N—H···Cl and O—H···Cl hydrogen bonds and intramolecular N—H···O hydrogen bonds stabilize the crystal structure.

Related literature

For related literature, see: Cimarelli & Palmieri (1998, 2000); Cimarelli *et al.* (2002); Demir *et al.* (1999); Palmieri (1999, 2000); Rijnberg *et al.* (1997); Sola *et al.* (1998); Tümerdem *et al.* (2005); Tseng & Yang (2004); Xu *et al.* (2002); Zhang *et al.* (2006*a*,*b*).



Experimental

Crystal data

$C_{18}H_{24}NO_2^+\cdot Cl^-$
M_r = 321.83
Orthorhombic, $P2_12_12_1$
a = 7.6500 (15) Å
b = 13.764 (3) Å
c = 16.420 (3) Å
V = 1728.9 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 298 (2) K
0.44 × 0.32 × 0.21 mm

‡ Visting student from Liaocheng Bureau of Education of Liaocheng.

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.906, T_{max} = 0.955
8842 measured reflections
3202 independent reflections
2738 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.097
S = 1.02
3202 reflections
204 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Absolute structure: Flack (1983), with 1204 Friedel pairs
Flack parameter: −0.01 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···Cl1^{i}	0.82	2.44	3.249 (2)	169
O1—H1···Cl1^{ii}	0.82	2.28	3.0417 (18)	156
N1—H1*A*···Cl1^{iii}	0.90	2.25	3.125 (2)	165
N1—H1*B*···O1	0.90	2.07	2.732 (2)	129

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Natural Science Foundation of Shandong Province China (grant No. G0231) and the Foundation of the Education Ministry of China for Returned Students (grant No. G0220) for financial support. The X-ray data were collected at Shandong Normal University of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2080).

References

Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5.06a). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Cimarelli, C. & Palmieri, G. (1998). *Tetrahedron*, **54**, 15711–15720.
Cimarelli, C. & Palmieri, G. (2000). *Tetrahedron Asymmetry*, **11**, 2555–2563.
Cimarelli, C., Palmieri, G. & Volpini, E. (2002). *Tetrahedron Asymmetry*, **13**, 2011–2018.
Demir, A. S., Akhmedov, I. M. & Sesenoglu, O. (1999). *Turk. J. Chem.* **23**, 123–126.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Palmieri, G. (1999). *Eur. J. Org. Chem.* pp. 805–811.
Palmieri, G. (2000). *Tetrahedron Asymmetry*, **11**, 3361–3373.
Rijnberg, E., Hovestad, N. J., Kleij, A. W., Jastrzebski, J. T. B. H., Boersma, J., Janssen, M. D., Spek, A. L. & van Koten, G. (1997). *Organometallics*, **16**, 2847–2857.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sola, L., Reddy, K. S., Vidal-Ferran, A., Moyano, A., Pericas, M. A., Riera, A., Alvarez-Larena, A. & Piniella, J. F. (1998). *J. Org. Chem.* **63**, 7078–7082.
Tseng, S.-L. & Yang, T.-K. (2004). *Tetrahedron Asymmetry*, **15**, 3375–3380.

Tümerdem, R., Topal, G. & Turgut, Y. (2005). *Tetrahedron Asymmetry*, **16**, 865–868.
Xu, Q., Yang, H., Pan, X. & Chan, A. S. C. (2002). *Tetrahedron Asymmetry*, **13**, 945–951.
Zhang, G.-Y., Wang, X.-B., Zhao, J.-Y., Wang, W.-H. & Yang, X.-F. (2006*a*). *Acta Cryst.* E**62**, o2239–o2241.
Zhang, G.-Y., Wang, X.-B., Zhao, J.-Y., Wang, W.-H. & Yang, X.-F. (2006*b*). *Acta Cryst.* E**62**, o3035–o3037.

supporting information

Acta Cryst. (2008). E**64**, o240–o241 [https://doi.org/10.1107/S1600536807063106]

N-[(*S*)-1-(3,5-Dimethyl-2-hydroxyphenyl)ethyl]-*N*-[(*R*)-2-hydroxy-1-phenylethyl]ammonium chloride

Guangyou Zhang, Xungang Gu, Xiangbo Wang, Wanhui Wang and Shuchun Li

S1. Comment

The synthesis of new chiral ligands is widespread in asymmetric synthesis (Cimarelli & Palmieri, 1998, 2000; Tseng & Yang, 2004; Tümerdem *et al.*, 2005). Among them, enantiopure amino alcohols have recently found application in asymmetric synthesis as chiral bases, auxiliaries and ligands (Cimarelli *et al.*, 2002). Chiral amino phenols, which are similar to amino alcohols, are important building blocks in organic synthesis and have attracted increasing attention in recent years, owing to their effect in asymmetric synthesis and asymmetric induction (Palmieri, 1999, 2000; Cimarelli & Palmieri, 2000; Rijnberg *et al.*, 1997; Sola *et al.*, 1998; Xu *et al.*, 2002).

We previously reported the preparation and the structure of several chiral aminophenols including two chiral ligands, which derived from (*R*)-(-)2-phenylglycine (Zhang *et al.*, 2006*a*,b). As part of our continuing research on chiral aminophenols, we prepared a new aminoalkylphenol, namely, 2-[(*1S*)-1-{[(*1R*)-2-hydroxy-1-phenylethyl]amino}ethyl]-4,6-dimethylphenol. In order to determine its structure, the corresponding hydrochloride derivative, (I), was synthesized. Herein we report the crystal structure of (I), the title compound.

As shown in Fig. 1, the absolute configuration of (I) is (*R,S*), its geometric parameters are similar to those found in our previously reported relevant aminophenylphenols (Zhang *et al.*, 2006*a*,b), at the same time, selected bond lengths and angles of (I), including those of new stereogenic carbon center (C9), are reported in Table S1, so we can infer the absolute configuration of the aminoalkylphenol is also (*R,S*). The dihedral angle of the two aromatic rings (C1–C6 and C11–C18) is 30.82 (2)°.

The molecular strcture of compound is linked by intermolecular N—H···Cl and O—H···Cl (Fig.2) and intromolecular N—H···O hydrogen bonds, with N···O = 2.732 (2) Å (Table 2), which indicates a comparatively strong intramolecular hydrogen bond within the asymmetric unit.

S2. Experimental

The title compound was prepared according to the procedure of Zhang *et al.* *R*-(-)-2-Phenylglycinol was prepared by the reduction of *R*-(-)2-phenylglycine with $NaBH_4$ in tetrahydronfuran (THF) {80.2% yield, $[\alpha]_D^{24}$ = -25.5 (c_6, MeOH)} (Demir *et al.*, 1999). *R*-(-)-Phenylglycinol (0.27 g, 2 mmol) and 1-(2-hydroxy-3,5-dimethylphenyl)ethanone (0.33 g, 2 mmol) were dissolved in methanol (10 ml) and reacted at room temperature for 24 h. After removal of solvent, 10 ml THF was introduced and $NaBH_4$ (0.15 g, 4 mmol) was added at 273 K, the mixture was stirred at the temperature until the solution became colourless. The reaction was quenched with 5 *M* HCl and then neutralized with NaOH solution. The aqueous solution was extracted with chloroform, the organic layer was dried with anhydrous Na_2SO_4 and then filtered. The organic solvent was removed under reduced pressure. Further purification was carried out by thin-layer silica-gel chromatography [first run: chloroform/methanol (30:1 *v*/*v*); second run: hexane:ethyl acetate (3:1 *v*/*v*)] to give chiral aminophenylphenol [75.8% yield; $[\alpha]_D^{24}$ = -57.8($c_{0.5}$, $CHCl_3$)]. The compound (28.5 mg, 0.1 mmol) was dissolved in

methanol (10 ml) and concentrated HCl (0.1 ml) was added at room temperature, a white solid was precipitated. The corresponding HCl salt was crystallized from a 2-propanol/benzene mixture (1:20 *v*/*v*) (75% yield).

S3. Refinement

All H atoms were placed in idealized positions and treated as riding on their parent atoms, with N—H = 0.90 Å, O—H = 0.82 Å and *C*—*H*(methyl) = 0.96 Å, *C*—*H*(methylene) = 0.97 Å, C—H(methine) = 0.98 Å, C—H(aromatic) = 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C,*N*,*O*) or 1.5U_{eq}(CH_3).

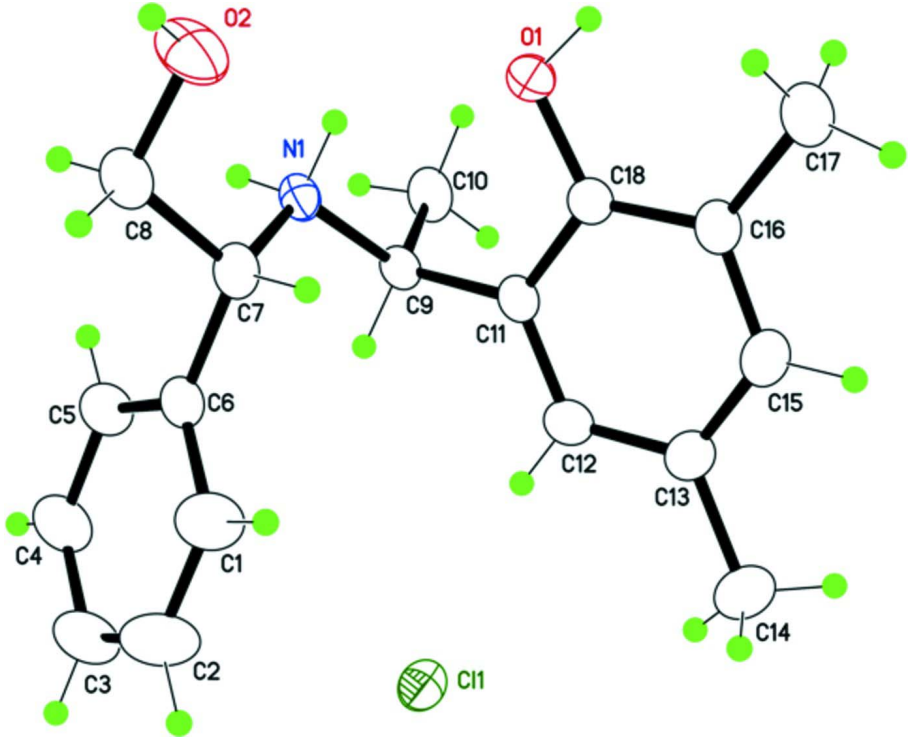


Figure 1

The asymmetric unit of (I), shown with 30% probability displacement ellipsoids.

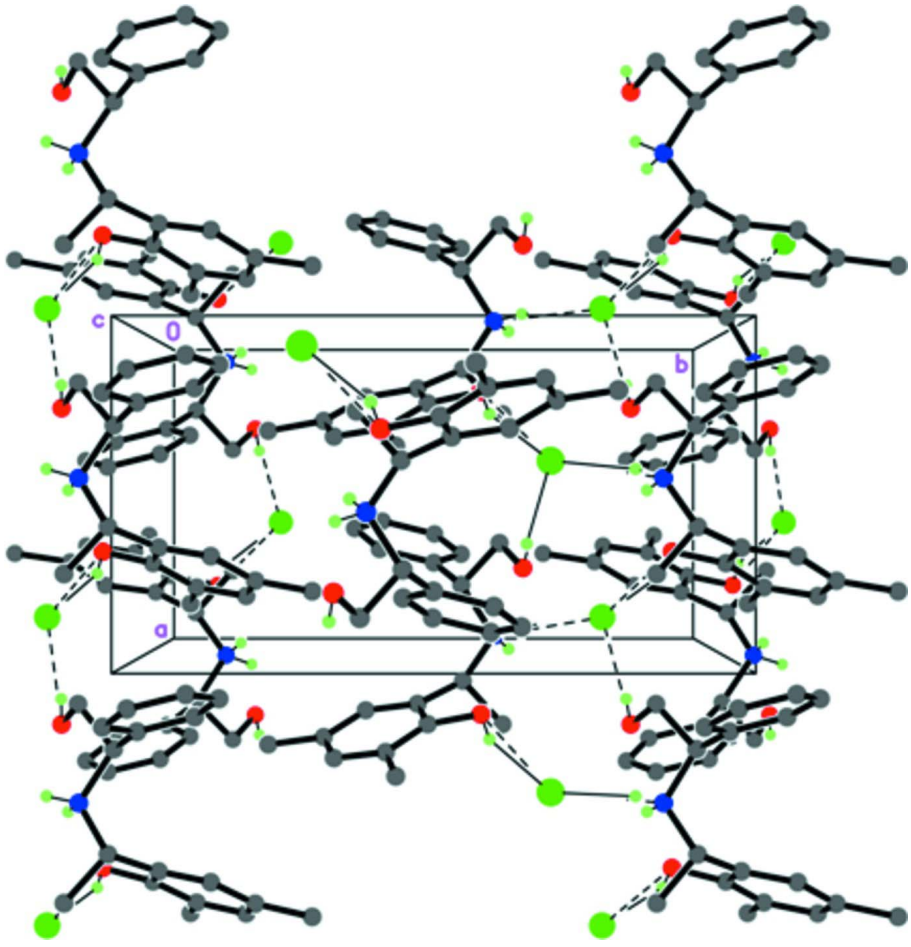


Figure 2

A packing view in (I), viewed down the *c* axis. All H atoms not involved in hydrogen bonding have been omitted.

N-[(S)-1-(3,5-Dimethyl-2-hydroxyphenyl)ethyl]-N-[(R)-2-hydroxy-1- phenylethyl]ammonium chloride

Crystal data

$C_{18}H_{24}NO_2^+ \cdot Cl^-$
$M_r = 321.83$
Orthorhombic, $P2_12_12_1$
Hall symbol: P2ac2ab
$a = 7.6500\ (15)$ Å
$b = 13.764\ (3)$ Å
$c = 16.420\ (3)$ Å
$V = 1728.9\ (6)$ Å^3
$Z = 4$
$F(000) = 688$
$D_x = 1.236$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2408 reflections
$\theta = 2.5–22.3°$
$\mu = 0.23$ mm^{-1}
$T = 298$ K
Block, colourless
0.44 × 0.32 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.906$, $T_{max} = 0.955$
8842 measured reflections
3202 independent reflections
2738 reflections with $I > 2\sigma(I)$

R_{int} = 0.034
θ_{max} = 25.5°, θ_{min} = 1.9°
h = −8→9
k = −16→16
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.097
S = 1.02
3202 reflections
204 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.1178P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Absolute structure: Flack (1983), with how many Friedel pairs?
Absolute structure parameter: −0.01 (7)

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 $F^2 > \sigma(F^2)$ 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}
C1	0.1767 (4)	0.09660 (19)	0.63609 (17)	0.0640 (8)
H1C	0.1916	0.1312	0.5879	0.077*
C2	0.1117 (5)	0.1430 (2)	0.7031 (2)	0.0778 (10)
H2A	0.0825	0.2085	0.6998	0.093*
C3	0.0893 (4)	0.0945 (2)	0.77455 (17)	0.0644 (8)
H3	0.0458	0.1263	0.8202	0.077*
C4	0.1318 (4)	−0.0016 (2)	0.77788 (15)	0.0597 (7)
H4	0.1172	−0.0354	0.8265	0.072*
C5	0.1958 (4)	−0.04971 (18)	0.71078 (14)	0.0507 (7)
H5	0.2225	−0.1155	0.7142	0.061*
C6	0.2206 (3)	−0.00047 (17)	0.63832 (13)	0.0393 (5)
C7	0.2868 (3)	−0.04882 (17)	0.56183 (13)	0.0417 (6)
H7	0.3156	0.0023	0.5226	0.050*
C8	0.1534 (3)	−0.1151 (2)	0.52276 (15)	0.0537 (7)
H8A	0.1227	−0.1673	0.5598	0.064*
H8B	0.0482	−0.0790	0.5098	0.064*
C9	0.5988 (3)	−0.05219 (16)	0.61594 (12)	0.0368 (5)
H9	0.5552	−0.0224	0.6662	0.044*
C10	0.7415 (3)	−0.1235 (2)	0.63911 (15)	0.0502 (6)
H10A	0.6954	−0.1706	0.6765	0.075*

H10B	0.8363	−0.0891	0.6644	0.075*
H10C	0.7831	−0.1559	0.5911	0.075*
C11	0.6644 (3)	0.02824 (16)	0.56161 (13)	0.0369 (5)
C12	0.6896 (3)	0.12039 (17)	0.59373 (15)	0.0442 (6)
H12	0.6527	0.1333	0.6466	0.053*
C13	0.7678 (3)	0.19304 (18)	0.54931 (15)	0.0467 (6)
C14	0.7978 (4)	0.29279 (19)	0.58643 (18)	0.0665 (8)
H14A	0.7111	0.3372	0.5664	0.100*
H14B	0.9120	0.3157	0.5717	0.100*
H14C	0.7892	0.2885	0.6446	0.100*
C15	0.8203 (4)	0.17215 (17)	0.47075 (15)	0.0491 (7)
H15	0.8747	0.2208	0.4407	0.059*
C16	0.7957 (3)	0.08221 (16)	0.43472 (13)	0.0423 (6)
C17	0.8537 (4)	0.0637 (2)	0.34898 (14)	0.0615 (8)
H17A	0.8875	0.1239	0.3241	0.092*
H17B	0.7592	0.0353	0.3187	0.092*
H17C	0.9514	0.0199	0.3492	0.092*
C18	0.7165 (3)	0.01038 (16)	0.48159 (13)	0.0389 (5)
Cl1	0.60116 (9)	0.19629 (5)	0.83115 (4)	0.0548 (2)
N1	0.4501 (2)	−0.10661 (13)	0.57750 (11)	0.0371 (4)
H1A	0.4225	−0.1570	0.6100	0.044*
H1B	0.4874	−0.1313	0.5298	0.044*
O1	0.6813 (2)	−0.08114 (12)	0.45252 (9)	0.0517 (5)
H1	0.7531	−0.0954	0.4174	0.078*
O2	0.2279 (3)	−0.15362 (19)	0.45100 (12)	0.0837 (7)
H2	0.1519	−0.1591	0.4160	0.125*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.084 (2)	0.0547 (16)	0.0531 (16)	0.0138 (16)	0.0037 (16)	0.0089 (13)
C2	0.103 (3)	0.0589 (17)	0.072 (2)	0.0279 (18)	−0.001 (2)	−0.0061 (16)
C3	0.0637 (18)	0.0781 (19)	0.0514 (16)	0.0197 (17)	−0.0026 (15)	−0.0144 (14)
C4	0.0643 (19)	0.0749 (18)	0.0398 (13)	0.0120 (16)	0.0072 (13)	0.0048 (13)
C5	0.0531 (17)	0.0521 (14)	0.0468 (14)	0.0073 (13)	0.0037 (13)	0.0062 (11)
C6	0.0308 (12)	0.0480 (13)	0.0391 (12)	0.0000 (11)	−0.0009 (10)	0.0018 (11)
C7	0.0373 (14)	0.0512 (14)	0.0367 (12)	−0.0033 (11)	−0.0014 (11)	0.0071 (10)
C8	0.0357 (15)	0.0822 (19)	0.0431 (14)	−0.0022 (13)	−0.0044 (11)	−0.0101 (13)
C9	0.0322 (12)	0.0499 (13)	0.0282 (10)	−0.0036 (11)	0.0016 (10)	−0.0064 (9)
C10	0.0377 (14)	0.0660 (15)	0.0470 (14)	−0.0032 (12)	−0.0022 (11)	0.0041 (12)
C11	0.0275 (12)	0.0459 (13)	0.0373 (12)	−0.0011 (9)	0.0012 (10)	−0.0018 (10)
C12	0.0403 (14)	0.0504 (14)	0.0419 (13)	0.0001 (12)	−0.0007 (11)	−0.0106 (11)
C13	0.0419 (14)	0.0435 (13)	0.0546 (15)	−0.0024 (12)	−0.0026 (12)	−0.0037 (12)
C14	0.073 (2)	0.0509 (16)	0.0755 (19)	−0.0086 (15)	−0.0006 (17)	−0.0123 (14)
C15	0.0480 (16)	0.0439 (15)	0.0554 (16)	−0.0025 (12)	0.0001 (13)	0.0095 (11)
C16	0.0401 (14)	0.0469 (13)	0.0400 (13)	−0.0018 (11)	0.0016 (12)	0.0057 (11)
C17	0.075 (2)	0.0663 (16)	0.0430 (14)	−0.0121 (14)	0.0128 (14)	0.0065 (12)
C18	0.0346 (13)	0.0432 (13)	0.0388 (12)	−0.0016 (11)	0.0004 (10)	−0.0041 (10)

Cl1	0.0623 (4)	0.0520 (4)	0.0501 (3)	0.0092 (3)	−0.0014 (3)	−0.0007 (3)
N1	0.0323 (11)	0.0466 (11)	0.0323 (9)	−0.0016 (8)	0.0035 (8)	−0.0002 (8)
O1	0.0625 (12)	0.0517 (10)	0.0410 (9)	−0.0134 (9)	0.0150 (9)	−0.0109 (8)
O2	0.0571 (14)	0.142 (2)	0.0522 (12)	0.0003 (13)	−0.0057 (11)	−0.0414 (12)

Geometric parameters (Å, º)

C1—C2	1.366 (4)	C10—H10B	0.9600
C1—C6	1.378 (3)	C10—H10C	0.9600
C1—H1C	0.9300	C11—C12	1.387 (3)
C2—C3	1.361 (4)	C11—C18	1.395 (3)
C2—H2A	0.9300	C12—C13	1.375 (3)
C3—C4	1.363 (4)	C12—H12	0.9300
C3—H3	0.9300	C13—C15	1.381 (3)
C4—C5	1.375 (3)	C13—C14	1.520 (3)
C4—H4	0.9300	C14—H14A	0.9600
C5—C6	1.382 (3)	C14—H14B	0.9600
C5—H5	0.9300	C14—H14C	0.9600
C6—C7	1.509 (3)	C15—C16	1.385 (3)
C7—N1	1.503 (3)	C15—H15	0.9300
C7—C8	1.512 (3)	C16—C18	1.392 (3)
C7—H7	0.9800	C16—C17	1.498 (3)
C8—O2	1.412 (3)	C17—H17A	0.9600
C8—H8A	0.9700	C17—H17B	0.9600
C8—H8B	0.9700	C17—H17C	0.9600
C9—N1	1.501 (3)	C18—O1	1.374 (3)
C9—C11	1.508 (3)	N1—H1A	0.9000
C9—C10	1.516 (3)	N1—H1B	0.9000
C9—H9	0.9800	O1—H1	0.8200
C10—H10A	0.9600	O2—H2	0.8200
C2—C1—C6	121.4 (3)	H10A—C10—H10C	109.5
C2—C1—H1C	119.3	H10B—C10—H10C	109.5
C6—C1—H1C	119.3	C12—C11—C18	118.7 (2)
C3—C2—C1	120.7 (3)	C12—C11—C9	119.52 (19)
C3—C2—H2A	119.6	C18—C11—C9	121.54 (19)
C1—C2—H2A	119.6	C13—C12—C11	121.6 (2)
C2—C3—C4	118.7 (3)	C13—C12—H12	119.2
C2—C3—H3	120.6	C11—C12—H12	119.2
C4—C3—H3	120.6	C12—C13—C15	118.1 (2)
C3—C4—C5	121.3 (2)	C12—C13—C14	120.7 (2)
C3—C4—H4	119.3	C15—C13—C14	121.2 (2)
C5—C4—H4	119.3	C13—C14—H14A	109.5
C4—C5—C6	120.2 (2)	C13—C14—H14B	109.5
C4—C5—H5	119.9	H14A—C14—H14B	109.5
C6—C5—H5	119.9	C13—C14—H14C	109.5
C1—C6—C5	117.7 (2)	H14A—C14—H14C	109.5
C1—C6—C7	119.2 (2)	H14B—C14—H14C	109.5

C5—C6—C7	123.1 (2)	C13—C15—C16	123.1 (2)
N1—C7—C6	111.72 (18)	C13—C15—H15	118.5
N1—C7—C8	108.31 (18)	C16—C15—H15	118.5
C6—C7—C8	113.11 (19)	C15—C16—C18	117.3 (2)
N1—C7—H7	107.8	C15—C16—C17	120.9 (2)
C6—C7—H7	107.8	C18—C16—C17	121.8 (2)
C8—C7—H7	107.8	C16—C17—H17A	109.5
O2—C8—C7	108.0 (2)	C16—C17—H17B	109.5
O2—C8—H8A	110.1	H17A—C17—H17B	109.5
C7—C8—H8A	110.1	C16—C17—H17C	109.5
O2—C8—H8B	110.1	H17A—C17—H17C	109.5
C7—C8—H8B	110.1	H17B—C17—H17C	109.5
H8A—C8—H8B	108.4	O1—C18—C16	123.0 (2)
N1—C9—C11	111.72 (17)	O1—C18—C11	115.65 (19)
N1—C9—C10	109.15 (18)	C16—C18—C11	121.3 (2)
C11—C9—C10	112.58 (19)	C9—N1—C7	115.96 (16)
N1—C9—H9	107.7	C9—N1—H1A	108.3
C11—C9—H9	107.7	C7—N1—H1A	108.3
C10—C9—H9	107.7	C9—N1—H1B	108.3
C9—C10—H10A	109.5	C7—N1—H1B	108.3
C9—C10—H10B	109.5	H1A—N1—H1B	107.4
H10A—C10—H10B	109.5	C18—O1—H1	109.5
C9—C10—H10C	109.5	C8—O2—H2	109.5

C6—C1—C2—C3	0.4 (6)	C9—C11—C12—C13	172.5 (2)
C1—C2—C3—C4	−0.4 (5)	C11—C12—C13—C15	0.4 (4)
C2—C3—C4—C5	−0.2 (5)	C11—C12—C13—C14	−178.6 (2)
C3—C4—C5—C6	0.9 (4)	C12—C13—C15—C16	0.9 (4)
C2—C1—C6—C5	0.3 (4)	C14—C13—C15—C16	179.9 (3)
C2—C1—C6—C7	178.2 (3)	C13—C15—C16—C18	−1.0 (4)
C4—C5—C6—C1	−0.9 (4)	C13—C15—C16—C17	179.4 (2)
C4—C5—C6—C7	−178.7 (2)	C15—C16—C18—O1	178.6 (2)
C1—C6—C7—N1	131.7 (2)	C17—C16—C18—O1	−1.8 (4)
C5—C6—C7—N1	−50.5 (3)	C15—C16—C18—C11	−0.2 (3)
C1—C6—C7—C8	−105.8 (3)	C17—C16—C18—C11	179.4 (2)
C5—C6—C7—C8	72.0 (3)	C12—C11—C18—O1	−177.4 (2)
N1—C7—C8—O2	−57.3 (3)	C9—C11—C18—O1	8.7 (3)
C6—C7—C8—O2	178.3 (2)	C12—C11—C18—C16	1.4 (3)
N1—C9—C11—C12	131.8 (2)	C9—C11—C18—C16	−172.5 (2)
C10—C9—C11—C12	−105.0 (2)	C11—C9—N1—C7	−63.3 (2)
N1—C9—C11—C18	−54.4 (3)	C10—C9—N1—C7	171.52 (17)
C10—C9—C11—C18	68.8 (3)	C6—C7—N1—C9	−55.1 (2)
C18—C11—C12—C13	−1.5 (3)	C8—C7—N1—C9	179.62 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···Cl1^{i}	0.82	2.44	3.249 (2)	169

O1—H1···Cl1^{ii}	0.82	2.28	3.0417 (18)	156
N1—H1*A*···Cl1^{iii}	0.90	2.25	3.125 (2)	165
N1—H1*B*···O1	0.90	2.07	2.732 (2)	129

Symmetry codes: (i) −*x*+1/2, −*y*, *z*−1/2; (ii) −*x*+3/2, −*y*, *z*−1/2; (iii) −*x*+1, *y*−1/2, −*z*+3/2.