Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,4-Diazoniabicyclo[2.2.2]octane bis(2-chlorobenzoate)

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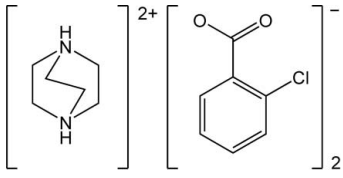
Received 25 June 2008; accepted 1 July 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.091; data-to-parameter ratio = 14.0.

The title compound, $C_6H_{14}N_2^{2+}\cdot 2C_7H_4ClO_2^-$, contains trimeric units linked by N—H···O hydrogen bonds. The carboxylate groups of the 2-chlorobenzoate anions form dihedral angles of 66.1 (1) and 76.1 (1)° with the respective chlorobenzene rings to which they are bound. The hydrogen-bonded trimers are arranged in layers in the (200) planes and the chlorobenzoate anions form edge-to-face interactions between layers, with dihedral angles of 61.9 (1) and 49.8 (1)° and centroid–centroid distances of 4.85 (1) and 4.65 (1) Å, respectively, for two crystallographically distinct interactions.

Related literature

For other co-crystals of 1,4-diazoniabicyclo[2.2.2]octane and carboxylic acids, see: Meehan *et al.* (1997); Burchell *et al.* (2000); Burchell, Glidewell *et al.* (2001); Burchell, Ferguson *et al.* (2001). For the crystal structure of 2-chlorobenzoic acid, see: Ferguson & Sim (1961).



Experimental

Crystal data

$C_6H_{14}N_2^{2+}\cdot 2C_7H_4ClO_2^-$
M_r = 425.30
Orthorhombic, $Pca2_1$
a = 19.7694 (12) Å
b = 11.3986 (6) Å
c = 8.9751 (5) Å
V = 2022.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker–Nonius X8 APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.844, T_{max} = 0.966
21779 measured reflections
3538 independent reflections
3251 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.06
3538 reflections
253 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1629 Friedel pairs
Flack parameter: −0.02 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.91	1.65	2.556 (2)	170
N2—H2A···O3	0.91	1.69	2.587 (2)	169

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We are grateful to the Danish Natural Science Research Council and the Carlsberg Foundation for provision of the X-ray equipment.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2155).

References

Bruker (2003). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker–Nonius BV, Delft, The Netherlands.
Burchell, C. J., Ferguson, G., Lough, A. J. & Glidewell, C. (2000). *Acta Cryst.* C**56**, 1126–1128.
Burchell, C. J., Ferguson, G., Lough, A. J., Gregson, R. M. & Glidewell, C. (2001). *Acta Cryst.* B**57**, 329–338.
Burchell, C. J., Glidewell, C., Lough, A. J. & Ferguson, G. (2001). *Acta Cryst.* B**57**, 201–212.
Ferguson, G. & Sim, G. A. (1961). *Acta Cryst.* **14**, 1262–1270.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Meehan, P. R., Ferguson, G., Glidewell, C. & Patterson, I. L. J. (1997). *Acta Cryst.* C**53**, 628–631.
Sheldrick, G. M. (2003). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o1416 [doi:10.1107/S1600536808020096]

1,4-Diazoniabicyclo[2.2.2]octane bis(2-chlorobenzoate)

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S1. Comment

The title compound, $(C_6H_{14}N_2)(C_7H_4ClO_2)_2$, was obtained by co-crystallization of diazabicylo[2.2.2]octane and 2-chlorobenzoic acid in methanol solution. The crystal structure of 2-chlorobenzoic acid (Ferguson & Sim, 1961) contains dimers formed by hydrogen bonds between the carboxyl groups. The purpose of the co-crystallization was to insert DABCO into the hydrogen-bonded dimer, to examine the influence on the intermolecular interactions between the 2-chlorobenzoic acid molecules.

The co-crystal contains the anticipated trimeric hydrogen-bond motif, with the trimers lying in layers parallel to the *bc* planes (Figs. 2 & 3). The Cl-substituents of the chlorobenzoate anions point into the centres of the layers, and the interlayer interactions comprise edge-to-face interactions involving H4A and H5A and their counterparts H11A and H12A, with dihedral angles 61.9 (1) and 49.8 (1)° and centroid-centroid distances 4.85 (1) and 4.65 (1) Å, for the two interactions respectively. The interactions are significantly different from the interlayer interactions in 2-chlorobenzoic acid itself, where adjacent rings form a dihedral angle of 49.3 (1)°, but the Cl-substituent points towards the adjacent ring centroid.

S2. Experimental

Separate saturated solutions of 2-chlorobenzoic acid (0.391 g, 0.0025 mmol) and diazabicyclo[2.2.2]octane (0.135 g, 0.0012 mmol) in warm methanol were combined and refluxed with stirring for 1 h. The solution was cooled slowly, giving colourless crystals of the title compound after *ca* 1 h.

S3. Refinement

H atoms bound to C atoms were placed geometrically and allowed to ride during refinement with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atoms bound to N1 and N2 were visible in a difference Fourier map, but were placed geometrically (N—H = 0.91 Å) and allowed to ride with U_{iso}(H) = 1.2U_{eq}(N). The assignment as a salt is consistent with expectations from pK_a values.

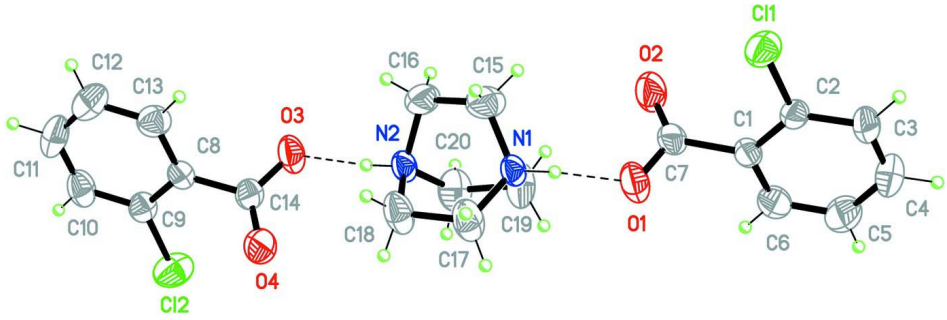

Figure 1

Molecular structure of the title compound showing displacement ellipsoids at the 50% probability level for non-H atoms. The dashed lines denote N^{+}—H···O^{-} hydrogen bonds.

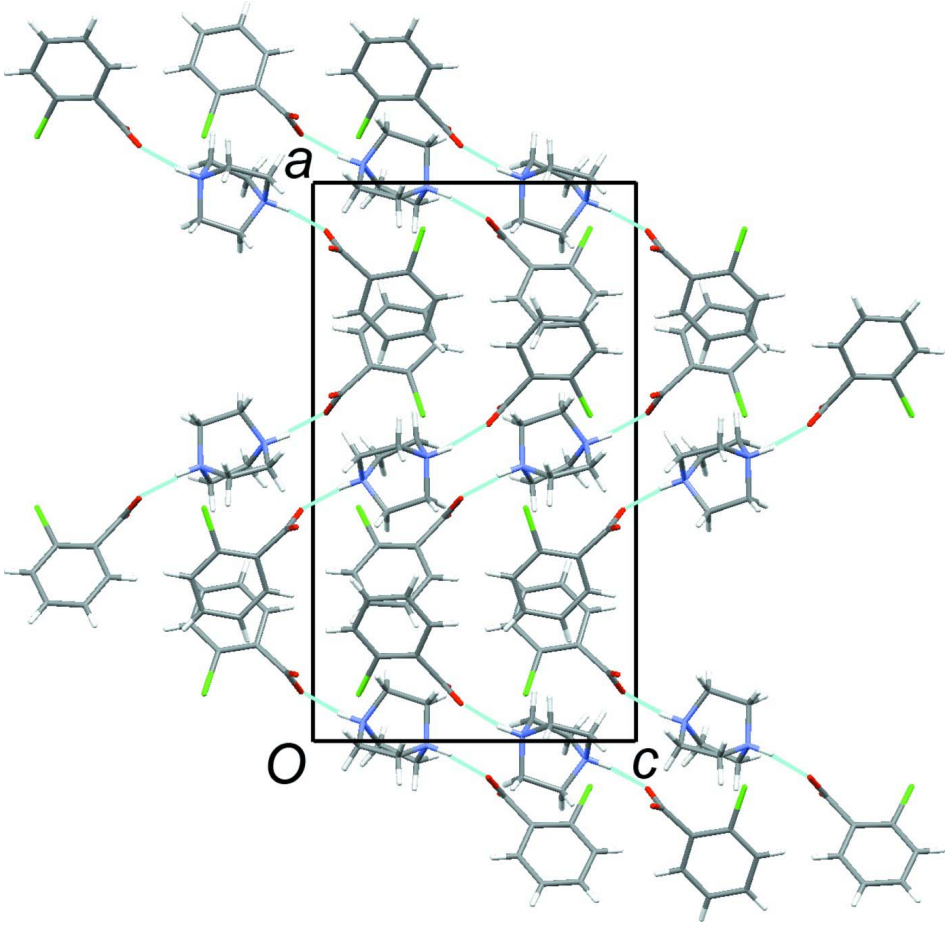

Figure 2

View along the *c* axis, showing the layered arrangement of hydrogen-bonded trimers. The light blue lines denote N^{+}—H···O^{-} hydrogen bonds.

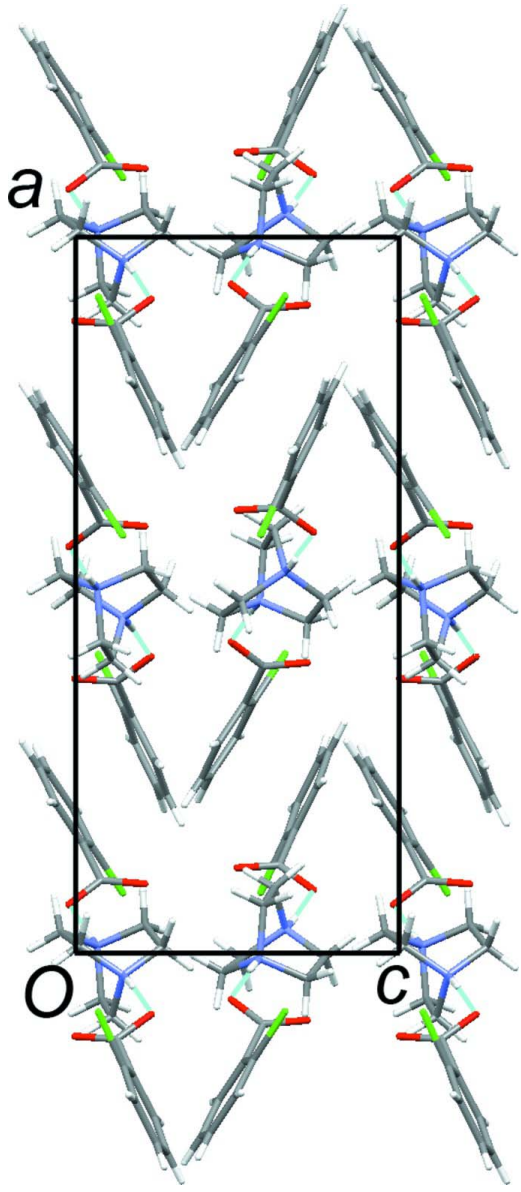

Figure 3

View along the *b* axis. The light blue lines denote N^+—H···O^- hydrogen bonds.

1,4-Diazoniabicyclo[2.2.2]octane bis(2-chlorobenzoate)

Crystal data

$C_6H_{14}N_2^{2+}\cdot 2C_7H_4ClO_2^-$
$M_r = 425.30$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 19.7694\ (12)$ Å
$b = 11.3986\ (6)$ Å
$c = 8.9751\ (5)$ Å
$V = 2022.5\ (2)$ Å^3
$Z = 4$
$F(000) = 888$
$D_x = 1.397$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9140 reflections
$\theta = 3.1–24.3°$
$\mu = 0.35$ mm^{-1}
$T = 298$ K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker–Nonius X8 APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Thin–slice ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.844, T_{max} = 0.966
21779 measured reflections
3538 independent reflections
3251 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.0°, θ_{min} = 3.6°
h = −23→23
k = −13→12
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.07
3538 reflections
253 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.354P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1629 Friedel pairs
Absolute structure parameter: −0.02 (5)

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}
Cl1	0.58385 (3)	1.34004 (5)	0.57363 (7)	0.05244 (17)
Cl2	0.41713 (4)	0.14065 (6)	0.64801 (8)	0.0658 (2)
O1	0.58704 (9)	1.03874 (14)	0.7359 (2)	0.0556 (5)
O2	0.61776 (12)	1.05458 (17)	0.5009 (2)	0.0716 (6)
O3	0.43357 (9)	0.45727 (15)	0.4822 (2)	0.0542 (4)
O4	0.40470 (10)	0.42055 (18)	0.7161 (2)	0.0653 (5)
N1	0.53241 (8)	0.84726 (14)	0.6495 (2)	0.0351 (4)
H1A	0.5474	0.9192	0.6783	0.042*
N2	0.49115 (9)	0.64905 (14)	0.5697 (2)	0.0383 (4)
H2A	0.4760	0.5771	0.5410	0.046*
C1	0.67102 (10)	1.17744 (18)	0.6779 (2)	0.0357 (4)
C2	0.66021 (10)	1.29512 (17)	0.6508 (2)	0.0353 (4)
C3	0.70790 (11)	1.3795 (2)	0.6867 (3)	0.0459 (5)
H3A	0.6996	1.4582	0.6666	0.055*
C4	0.76781 (12)	1.3457 (2)	0.7524 (3)	0.0574 (7)

H4A	0.8003	1.4019	0.7756	0.069*
C5	0.77993 (13)	1.2290 (3)	0.7838 (3)	0.0590 (7)
H5A	0.8200	1.2061	0.8299	0.071*
C6	0.73135 (12)	1.1464 (2)	0.7456 (3)	0.0503 (6)
H6A	0.7396	1.0677	0.7662	0.060*
C7	0.62150 (12)	1.08377 (18)	0.6306 (3)	0.0402 (5)
C8	0.34750 (10)	0.31988 (18)	0.5241 (2)	0.0349 (4)
C9	0.34941 (10)	0.20060 (18)	0.5500 (2)	0.0389 (5)
C10	0.30020 (12)	0.1256 (2)	0.4960 (3)	0.0506 (6)
H10A	0.3033	0.0453	0.5132	0.061*
C11	0.24651 (13)	0.1707 (2)	0.4167 (3)	0.0581 (7)
H11A	0.2130	0.1209	0.3808	0.070*
C12	0.24255 (13)	0.2890 (3)	0.3909 (3)	0.0582 (6)
H12A	0.2061	0.3197	0.3381	0.070*
C13	0.29285 (12)	0.3629 (2)	0.4434 (3)	0.0480 (6)
H13A	0.2900	0.4429	0.4243	0.058*
C14	0.39949 (10)	0.40479 (18)	0.5813 (3)	0.0390 (5)
C15	0.49080 (17)	0.8594 (2)	0.5144 (3)	0.0643 (7)
H15A	0.5158	0.9018	0.4387	0.077*
H15B	0.4501	0.9033	0.5372	0.077*
C16	0.47206 (16)	0.7375 (2)	0.4566 (3)	0.0635 (8)
H16A	0.4238	0.7335	0.4375	0.076*
H16B	0.4957	0.7219	0.3640	0.076*
C17	0.49289 (16)	0.7947 (2)	0.7703 (3)	0.0612 (7)
H17A	0.4571	0.8479	0.8003	0.073*
H17B	0.5218	0.7807	0.8557	0.073*
C18	0.46232 (14)	0.6791 (2)	0.7171 (3)	0.0584 (7)
H18A	0.4724	0.6173	0.7881	0.070*
H18B	0.4136	0.6865	0.7095	0.070*
C19	0.59035 (12)	0.7722 (2)	0.6143 (4)	0.0605 (7)
H19A	0.6217	0.7717	0.6974	0.073*
H19B	0.6139	0.8028	0.5278	0.073*
C20	0.56618 (12)	0.6470 (2)	0.5826 (4)	0.0594 (7)
H20A	0.5861	0.6185	0.4906	0.071*
H20B	0.5798	0.5951	0.6628	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0553 (3)	0.0404 (3)	0.0615 (4)	0.0067 (2)	−0.0201 (3)	−0.0033 (3)
Cl2	0.0831 (5)	0.0419 (3)	0.0725 (5)	0.0129 (3)	−0.0271 (4)	−0.0006 (3)
O1	0.0751 (11)	0.0435 (10)	0.0480 (10)	−0.0240 (8)	0.0158 (8)	−0.0078 (8)
O2	0.1056 (15)	0.0635 (12)	0.0456 (10)	−0.0416 (11)	0.0024 (10)	−0.0066 (9)
O3	0.0660 (10)	0.0450 (10)	0.0518 (10)	−0.0245 (8)	0.0108 (8)	−0.0083 (8)
O4	0.0916 (14)	0.0583 (12)	0.0459 (10)	−0.0319 (10)	−0.0071 (10)	−0.0053 (9)
N1	0.0452 (10)	0.0237 (9)	0.0365 (9)	−0.0071 (6)	0.0028 (8)	−0.0031 (8)
N2	0.0507 (10)	0.0275 (9)	0.0367 (9)	−0.0115 (7)	0.0034 (9)	−0.0037 (8)
C1	0.0422 (11)	0.0312 (10)	0.0339 (10)	−0.0038 (8)	0.0013 (8)	0.0011 (9)

C2	0.0407 (11)	0.0314 (11)	0.0339 (10)	−0.0006 (8)	−0.0050 (9)	−0.0029 (9)
C3	0.0535 (13)	0.0293 (11)	0.0548 (14)	−0.0077 (9)	−0.0042 (11)	−0.0029 (10)
C4	0.0486 (14)	0.0515 (16)	0.0722 (18)	−0.0153 (11)	−0.0054 (13)	−0.0106 (13)
C5	0.0471 (13)	0.0652 (18)	0.0646 (16)	0.0005 (12)	−0.0138 (12)	0.0029 (14)
C6	0.0558 (14)	0.0389 (13)	0.0563 (15)	0.0030 (10)	−0.0084 (12)	0.0079 (11)
C7	0.0549 (12)	0.0247 (11)	0.0410 (12)	−0.0012 (9)	−0.0017 (10)	−0.0003 (9)
C8	0.0369 (10)	0.0334 (11)	0.0344 (10)	−0.0019 (8)	0.0037 (8)	0.0010 (9)
C9	0.0423 (11)	0.0347 (11)	0.0397 (12)	−0.0015 (9)	0.0020 (9)	−0.0046 (10)
C10	0.0596 (15)	0.0373 (12)	0.0549 (14)	−0.0141 (11)	0.0100 (12)	−0.0085 (11)
C11	0.0412 (12)	0.0677 (17)	0.0655 (16)	−0.0144 (14)	−0.0008 (12)	−0.0238 (14)
C12	0.0422 (12)	0.0730 (18)	0.0593 (14)	0.0050 (14)	−0.0099 (11)	−0.0093 (15)
C13	0.0540 (13)	0.0431 (14)	0.0468 (13)	0.0025 (11)	−0.0040 (11)	0.0005 (10)
C14	0.0458 (11)	0.0274 (11)	0.0438 (12)	−0.0015 (9)	−0.0034 (11)	−0.0028 (10)
C15	0.101 (2)	0.0358 (14)	0.0562 (15)	0.0020 (14)	−0.0241 (15)	0.0025 (12)
C16	0.091 (2)	0.0486 (16)	0.0506 (13)	−0.0154 (14)	−0.0283 (14)	0.0028 (12)
C17	0.0835 (18)	0.0515 (15)	0.0488 (13)	−0.0258 (14)	0.0192 (13)	−0.0146 (12)
C18	0.0752 (18)	0.0469 (15)	0.0530 (14)	−0.0230 (13)	0.0240 (13)	−0.0150 (12)
C19	0.0451 (13)	0.0421 (14)	0.094 (2)	−0.0066 (10)	0.0046 (12)	−0.0102 (14)
C20	0.0556 (14)	0.0427 (14)	0.0798 (17)	0.0033 (11)	0.0064 (15)	−0.0115 (14)

Geometric parameters (Å, º)

Cl1—C2	1.738 (2)	C8—C13	1.390 (3)
Cl2—C9	1.742 (2)	C8—C14	1.502 (3)
O1—C7	1.273 (3)	C9—C10	1.383 (3)
O2—C7	1.213 (3)	C10—C11	1.378 (4)
O3—C14	1.266 (3)	C10—H10A	0.930
O4—C14	1.228 (3)	C11—C12	1.370 (4)
N1—C17	1.464 (3)	C11—H11A	0.930
N1—C19	1.465 (3)	C12—C13	1.386 (4)
N1—C15	1.472 (3)	C12—H12A	0.930
N1—H1A	0.910	C13—H13A	0.930
N2—C16	1.480 (3)	C15—C16	1.529 (4)
N2—C18	1.480 (3)	C15—H15A	0.970
N2—C20	1.488 (3)	C15—H15B	0.970
N2—H2A	0.910	C16—H16A	0.970
C1—C2	1.380 (3)	C16—H16B	0.970
C1—C6	1.385 (3)	C17—C18	1.526 (3)
C1—C7	1.509 (3)	C17—H17A	0.970
C2—C3	1.385 (3)	C17—H17B	0.970
C3—C4	1.378 (4)	C18—H18A	0.970
C3—H3A	0.930	C18—H18B	0.970
C4—C5	1.381 (4)	C19—C20	1.531 (3)
C4—H4A	0.930	C19—H19A	0.970
C5—C6	1.388 (4)	C19—H19B	0.970
C5—H5A	0.930	C20—H20A	0.970
C6—H6A	0.930	C20—H20B	0.970
C8—C9	1.380 (3)		

C17—N1—C19	109.7 (2)	C11—C12—C13	119.9 (2)
C17—N1—C15	110.5 (2)	C11—C12—H12A	120.0
C19—N1—C15	108.3 (2)	C13—C12—H12A	120.0
C17—N1—H1A	109.4	C12—C13—C8	121.4 (2)
C19—N1—H1A	109.4	C12—C13—H13A	119.3
C15—N1—H1A	109.4	C8—C13—H13A	119.3
C16—N2—C18	110.9 (2)	O4—C14—O3	125.4 (2)
C16—N2—C20	108.5 (2)	O4—C14—C8	119.2 (2)
C18—N2—C20	108.6 (2)	O3—C14—C8	115.4 (2)
C16—N2—H2A	109.6	N1—C15—C16	109.28 (19)
C18—N2—H2A	109.6	N1—C15—H15A	109.8
C20—N2—H2A	109.6	C16—C15—H15A	109.8
C2—C1—C6	117.32 (19)	N1—C15—H15B	109.8
C2—C1—C7	122.53 (19)	C16—C15—H15B	109.8
C6—C1—C7	120.10 (19)	H15A—C15—H15B	108.3
C1—C2—C3	121.9 (2)	N2—C16—C15	108.9 (2)
C1—C2—Cl1	119.41 (15)	N2—C16—H16A	109.9
C3—C2—Cl1	118.65 (16)	C15—C16—H16A	109.9
C4—C3—C2	119.4 (2)	N2—C16—H16B	109.9
C4—C3—H3A	120.3	C15—C16—H16B	109.9
C2—C3—H3A	120.3	H16A—C16—H16B	108.3
C3—C4—C5	120.4 (2)	N1—C17—C18	109.5 (2)
C3—C4—H4A	119.8	N1—C17—H17A	109.8
C5—C4—H4A	119.8	C18—C17—H17A	109.8
C4—C5—C6	118.9 (2)	N1—C17—H17B	109.8
C4—C5—H5A	120.6	C18—C17—H17B	109.8
C6—C5—H5A	120.6	H17A—C17—H17B	108.2
C1—C6—C5	122.1 (2)	N2—C18—C17	109.06 (19)
C1—C6—H6A	119.0	N2—C18—H18A	109.9
C5—C6—H6A	119.0	C17—C18—H18A	109.9
O2—C7—O1	124.7 (2)	N2—C18—H18B	109.9
O2—C7—C1	120.2 (2)	C17—C18—H18B	109.9
O1—C7—C1	115.07 (19)	H18A—C18—H18B	108.3
C9—C8—C13	117.1 (2)	N1—C19—C20	109.92 (18)
C9—C8—C14	123.97 (19)	N1—C19—H19A	109.7
C13—C8—C14	118.9 (2)	C20—C19—H19A	109.7
C8—C9—C10	122.1 (2)	N1—C19—H19B	109.7
C8—C9—Cl2	119.51 (16)	C20—C19—H19B	109.7
C10—C9—Cl2	118.36 (18)	H19A—C19—H19B	108.2
C11—C10—C9	119.5 (2)	N2—C20—C19	108.11 (18)
C11—C10—H10A	120.3	N2—C20—H20A	110.1
C9—C10—H10A	120.3	C19—C20—H20A	110.1
C12—C11—C10	119.9 (2)	N2—C20—H20B	110.1
C12—C11—H11A	120.0	C19—C20—H20B	110.1
C10—C11—H11A	120.0	H20A—C20—H20B	108.4
C6—C1—C2—C3	1.3 (3)	C11—C12—C13—C8	−0.7 (4)

C7—C1—C2—C3	−176.0 (2)	C9—C8—C13—C12	−0.2 (3)
C6—C1—C2—Cl1	−177.17 (17)	C14—C8—C13—C12	−178.5 (2)
C7—C1—C2—Cl1	5.6 (3)	C9—C8—C14—O4	−65.8 (3)
C1—C2—C3—C4	−0.5 (3)	C13—C8—C14—O4	112.4 (3)
Cl1—C2—C3—C4	177.9 (2)	C9—C8—C14—O3	116.1 (2)
C2—C3—C4—C5	−0.8 (4)	C13—C8—C14—O3	−65.7 (3)
C3—C4—C5—C6	1.2 (4)	C17—N1—C15—C16	−65.6 (3)
C2—C1—C6—C5	−0.8 (4)	C19—N1—C15—C16	54.6 (3)
C7—C1—C6—C5	176.6 (2)	C18—N2—C16—C15	52.6 (3)
C4—C5—C6—C1	−0.4 (4)	C20—N2—C16—C15	−66.6 (3)
C2—C1—C7—O2	75.5 (3)	N1—C15—C16—N2	10.2 (3)
C6—C1—C7—O2	−101.7 (3)	C19—N1—C17—C18	−65.0 (3)
C2—C1—C7—O1	−106.1 (2)	C15—N1—C17—C18	54.4 (3)
C6—C1—C7—O1	76.7 (3)	C16—N2—C18—C17	−63.8 (3)
C13—C8—C9—C10	1.3 (3)	C20—N2—C18—C17	55.4 (3)
C14—C8—C9—C10	179.6 (2)	N1—C17—C18—N2	8.7 (3)
C13—C8—C9—Cl2	179.07 (17)	C17—N1—C19—C20	53.6 (3)
C14—C8—C9—Cl2	−2.7 (3)	C15—N1—C19—C20	−67.1 (3)
C8—C9—C10—C11	−1.5 (4)	C16—N2—C20—C19	54.3 (3)
Cl2—C9—C10—C11	−179.29 (19)	C18—N2—C20—C19	−66.4 (3)
C9—C10—C11—C12	0.5 (4)	N1—C19—C20—N2	10.7 (3)
C10—C11—C12—C13	0.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1	0.91	1.65	2.556 (2)	170
N2—H2*A*···O3	0.91	1.69	2.587 (2)	169