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N-Benzoyl-*N*′,*N*″-diphenylguanidinium chloride

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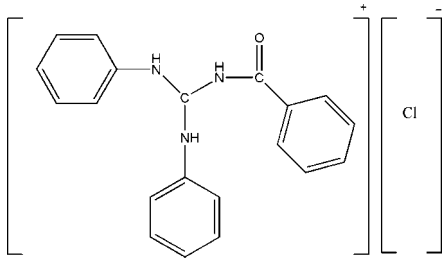
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.054; wR factor = 0.133; data-to-parameter ratio = 17.0.

In the title compound, $C_{20}H_{18}N_3O^+\cdot Cl^-$, the orientation of the aromatic rings around the planar CN_3^+ unit produces steric hindrance. As a consequence of this particular orientation of the guanidinium cation, hydrogen bonding is restricted to N—H···Cl and intramolecular N—H···O hydrogen bonds within the discrete unit. The guanidinium and carbonyl groups are coplanar as a result of the six-membered ring formed by the N—H···O intramolecular hydrogen bond. The dihedral angles between the guanidinium plane and the two phenyl rings are 62.31 (8) and 64.24 (8)°.

Related literature

For related structures, see: Said *et al.* (2006); Cunha *et al.* (2005). For related literature, see: Aldhaheri (1998); Cunha *et al.* (2002); Köhn *et al.* (2004); Moroni *et al.* (2001); Taniguchi *et al.* (1993); Yoshiizumi *et al.* (1998).



Experimental

Crystal data

$C_{20}H_{18}N_3O^+\cdot Cl^-$
M_r = 351.82
Triclinic, $P\overline{1}$
a = 8.586 (4) Å
b = 10.254 (5) Å
c = 10.966 (6) Å
α = 70.193 (10)°
β = 88.612 (19)°
γ = 84.524 (18)°
V = 904.2 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 296 (2) K
0.50 × 0.40 × 0.25 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: integration (Higashi, 1999)
T_{min} = 0.653, T_{max} = 0.803
7197 measured reflections
4050 independent reflections
3534 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.133
S = 1.13
4050 reflections
238 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1	0.86 (2)	2.32 (3)	3.143 (2)	159 (2)
N2—H2···Cl1	0.86 (2)	2.27 (2)	3.0977 (18)	162 (2)
N3—H3···O1	0.84 (3)	1.91 (3)	2.628 (2)	143 (2)

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* and *TEXSAN*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2109).

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supplementary materials

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N-Benzoyl-*N*',*N*''-diphenylguanidinium chloride

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Comment

Guanidines are used in medicine as analgesic, antihypertensive, antibacterial, cancerostatic and cytotoxic agents (Taniguchi *et al.*, 1993; Yoshiizumi *et al.*, 1998; Moroni *et al.*, 2001). They have potential applications in the fields of analytical and synthetic organic chemistry (Aldhaheri,1998; Köhn *et al.*, 2004). The title compound (I), Fig. 1, is a typical *N*,*N*′,*N*″-trisubstituted guanidinium halide salt with normal geometric parameters (Said *et al.*, 2006). The C(1)—O(1) bond shows the expected full double bond character while the short values for the C(1)—N(1), C(2)—N(1), C(2)—N(2), and C(2)—N(3) bond lengths indicate partial double bond character (Table 1). The dihedral angles between the guanidinium plane (C(2)/N(1)/N(2)/N(3)) and the two phenyl ring planes formed by C(15)—C(20) & C(9)—C(14) are 62.31 (8)° & 64.24 (8)° respectively, and that between the guanidinium plane and the aroyl group is 20.17 (10)°. The guanidinium and carbonyl groups are almost coplanar, as reflected by the torsion angles O(1)—C(1)—N(1)—C(2) = −7.5 (3)°, N(2)—C(2)— N(1)—C(1) = −174.26 (17))°, N(3)—C(2)—N(1)—C(1) = 7.2 (3)° and C(3)— C(1)—N(1)—C(2) = 175.92 (16)° (Table 1), this is associated with the intramolecular N—H···O hydrogen bond (Table 2), forming the six-membered ring commonly observed in this class of compounds (Cunha *et al.*, 2005).

Experimental

The guanidine was synthesized by a previously reported method (Cunha *et al.*, 2002), from *N*-benzoyl-*N*′-phenylthiourea and aniline. 0.315 g (1 mmol) of synthesized guanidine was added to a mixture of 20 ml e thanol and 1 ml of 37% *v*/*v* HCl with constant stirring at 323 K for 30 min. The reaction mixture was concentrated by evaporating 50% of the solvent under reduced pressure, and block like X-ray quality crystals were obtained by slow evaporation at room temperature.

Refinement

Hydrogen atoms bonded to C were included in calculated positions and refined as riding on their parent C atom with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atoms bonded to N were freely refined.

Figures

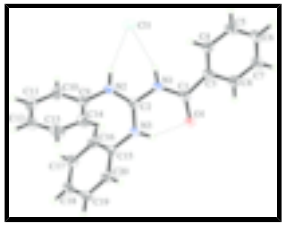


Fig. 1. Molecular structure of (I) showing atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown by dashed lines.

N-Benzoyl-*N*',*N*''-diphenylguanidinium chloride

Crystal data

$C_{20}H_{18}N_3O^+\cdot Cl^-$	$Z = 2$
$M_r = 351.82$	$F_{000} = 368$
Triclinic, $P\overline{1}$	$D_x = 1.292$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
$a = 8.586$ (4) Å	Cell parameters from 2693 reflections
$b = 10.254$ (5) Å	$\theta = 3.2$–27.5º
$c = 10.966$ (6) Å	$\mu = 0.22$ mm^{-1}
$\alpha = 70.193$ (10)º	$T = 296$ (2) K
$\beta = 88.612$ (19)º	Block, colourless
$\gamma = 84.524$ (18)º	0.50 × 0.40 × 0.25 mm
$V = 904.2$ (8) Å^3	

Data collection

Rigaku/MSC Mercury CCD diffractometer	4050 independent reflections
Radiation source: fine-focus sealed tube	3534 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
Detector resolution: 14.62 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 296(2)$ K	$\theta_{min} = 3.2$º
ω scans	$h = -8\rightarrow11$
Absorption correction: integration (Higashi, 1999)	$k = -13\rightarrow8$
$T_{min} = 0.653$, $T_{max} = 0.803$	$l = -14\rightarrow14$
7197 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.133$	$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.2415P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} < 0.001$
4050 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
238 parameters	$\Delta\rho_{min} = -0.32$ 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.46455 (19)	0.16051 (18)	0.64865 (17)	0.0414 (4)
O1	0.56362 (16)	0.06102 (15)	0.68532 (14)	0.0638 (4)
C2	0.57534 (18)	0.26054 (17)	0.43234 (16)	0.0373 (3)
N1	0.46189 (16)	0.25511 (16)	0.52470 (14)	0.0393 (3)
H1	0.396 (3)	0.328 (3)	0.505 (2)	0.061 (6)*
C3	0.33471 (18)	0.18014 (18)	0.73498 (16)	0.0395 (4)
C4	0.1942 (2)	0.2597 (2)	0.69126 (18)	0.0467 (4)
H4	0.1799	0.3114	0.6038	0.056*
C5	0.0754 (2)	0.2616 (2)	0.7787 (2)	0.0584 (5)
H5	−0.0194	0.3137	0.7493	0.070*
C6	0.0966 (3)	0.1873 (3)	0.9083 (2)	0.0649 (6)
H6	0.0164	0.1895	0.9663	0.078*
C7	0.2365 (3)	0.1096 (3)	0.9525 (2)	0.0705 (7)
H7	0.2516	0.0606	1.0404	0.085*
C8	0.3544 (2)	0.1046 (2)	0.86592 (19)	0.0581 (5)
H8	0.4477	0.0501	0.8956	0.070*
N2	0.55540 (18)	0.36772 (16)	0.32355 (14)	0.0440 (4)
H2	0.487 (3)	0.434 (3)	0.327 (2)	0.058 (6)*
C9	0.62383 (19)	0.37844 (19)	0.20058 (16)	0.0409 (4)
C10	0.6906 (3)	0.4978 (2)	0.1331 (2)	0.0624 (6)
H10	0.6949	0.5679	0.1685	0.075*
C11	0.7517 (4)	0.5130 (3)	0.0115 (2)	0.0777 (7)
H11	0.7984	0.5934	−0.0344	0.093*
C12	0.7439 (3)	0.4111 (3)	−0.0417 (2)	0.0725 (7)
H12	0.7847	0.4221	−0.1235	0.087*
C13	0.6759 (3)	0.2927 (3)	0.0261 (2)	0.0696 (6)
H13	0.6708	0.2233	−0.0101	0.084*
C14	0.6142 (2)	0.2750 (2)	0.1486 (2)	0.0557 (5)
H14	0.5675	0.1947	0.1943	0.067*
N3	0.69145 (16)	0.16005 (16)	0.45603 (16)	0.0432 (3)
H3	0.683 (3)	0.100 (3)	0.530 (2)	0.065 (7)*
C15	0.84141 (18)	0.17037 (17)	0.39319 (15)	0.0362 (3)
C16	0.9279 (2)	0.27925 (19)	0.38423 (18)	0.0447 (4)

H16	0.8881	0.3502	0.4143	0.054*
C17	1.0751 (2)	0.2818 (2)	0.3298 (2)	0.0543 (5)
H17	1.1341	0.3557	0.3221	0.065*
C18	1.1351 (2)	0.1753 (2)	0.28699 (19)	0.0545 (5)
H18	1.2342	0.1776	0.2506	0.065*
C19	1.0488 (2)	0.0662 (2)	0.2980 (2)	0.0538 (5)
H19	1.0896	−0.0057	0.2695	0.065*
C20	0.9007 (2)	0.0627 (2)	0.35154 (19)	0.0472 (4)
H20	0.8418	−0.0112	0.3593	0.057*
Cl1	0.28841 (5)	0.55341 (5)	0.39536 (5)	0.05030 (16)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0359 (8)	0.0424 (9)	0.0417 (9)	0.0028 (7)	0.0055 (7)	−0.0107 (7)
O1	0.0547 (8)	0.0564 (8)	0.0563 (8)	0.0208 (6)	0.0188 (6)	0.0039 (7)
C2	0.0352 (8)	0.0393 (8)	0.0386 (8)	0.0002 (6)	0.0047 (6)	−0.0161 (7)
N1	0.0340 (7)	0.0416 (8)	0.0395 (7)	0.0050 (6)	0.0055 (5)	−0.0125 (6)
C3	0.0341 (8)	0.0440 (9)	0.0396 (9)	0.0005 (6)	0.0047 (6)	−0.0144 (7)
C4	0.0396 (9)	0.0544 (11)	0.0423 (9)	0.0060 (7)	0.0012 (7)	−0.0144 (8)
C5	0.0384 (9)	0.0706 (14)	0.0621 (13)	0.0097 (9)	0.0065 (8)	−0.0213 (11)
C6	0.0529 (11)	0.0769 (15)	0.0576 (12)	0.0057 (10)	0.0225 (10)	−0.0179 (11)
C7	0.0669 (13)	0.0857 (17)	0.0422 (11)	0.0154 (12)	0.0141 (9)	−0.0065 (11)
C8	0.0480 (10)	0.0712 (13)	0.0422 (10)	0.0151 (9)	0.0035 (8)	−0.0078 (9)
N2	0.0470 (8)	0.0434 (8)	0.0373 (8)	0.0104 (6)	0.0062 (6)	−0.0124 (6)
C9	0.0390 (8)	0.0474 (9)	0.0326 (8)	0.0079 (7)	0.0002 (6)	−0.0119 (7)
C10	0.0884 (16)	0.0496 (11)	0.0458 (11)	−0.0048 (10)	0.0140 (10)	−0.0131 (9)
C11	0.1051 (19)	0.0655 (15)	0.0467 (12)	−0.0023 (13)	0.0217 (12)	−0.0014 (11)
C12	0.0776 (15)	0.0892 (18)	0.0357 (10)	0.0264 (13)	0.0086 (10)	−0.0114 (11)
C13	0.0798 (15)	0.0849 (17)	0.0535 (13)	0.0119 (13)	−0.0008 (11)	−0.0407 (13)
C14	0.0594 (12)	0.0614 (12)	0.0509 (11)	−0.0040 (9)	0.0045 (9)	−0.0257 (10)
N3	0.0373 (7)	0.0417 (8)	0.0443 (8)	0.0049 (6)	0.0100 (6)	−0.0092 (7)
C15	0.0327 (7)	0.0409 (8)	0.0334 (8)	0.0041 (6)	0.0033 (6)	−0.0128 (6)
C16	0.0467 (9)	0.0414 (9)	0.0474 (10)	0.0012 (7)	0.0027 (7)	−0.0184 (8)
C17	0.0442 (10)	0.0547 (11)	0.0598 (12)	−0.0093 (8)	0.0040 (8)	−0.0129 (9)
C18	0.0374 (9)	0.0683 (13)	0.0482 (11)	0.0048 (8)	0.0098 (8)	−0.0103 (9)
C19	0.0481 (10)	0.0619 (12)	0.0534 (11)	0.0141 (9)	0.0065 (8)	−0.0275 (10)
C20	0.0436 (9)	0.0475 (10)	0.0559 (11)	0.0013 (7)	0.0023 (8)	−0.0262 (9)
Cl1	0.0488 (3)	0.0513 (3)	0.0533 (3)	0.01300 (19)	−0.00668 (19)	−0.0253 (2)

Geometric parameters (Å, °)

C1—O1	1.224 (2)	C10—C11	1.385 (3)
C1—N1	1.376 (2)	C10—H10	0.9300
C1—C3	1.488 (2)	C11—C12	1.365 (4)
C2—N2	1.321 (2)	C11—H11	0.9300
C2—N3	1.326 (2)	C12—C13	1.367 (4)
C2—N1	1.379 (2)	C12—H12	0.9300
N1—H1	0.86 (2)	C13—C14	1.392 (3)

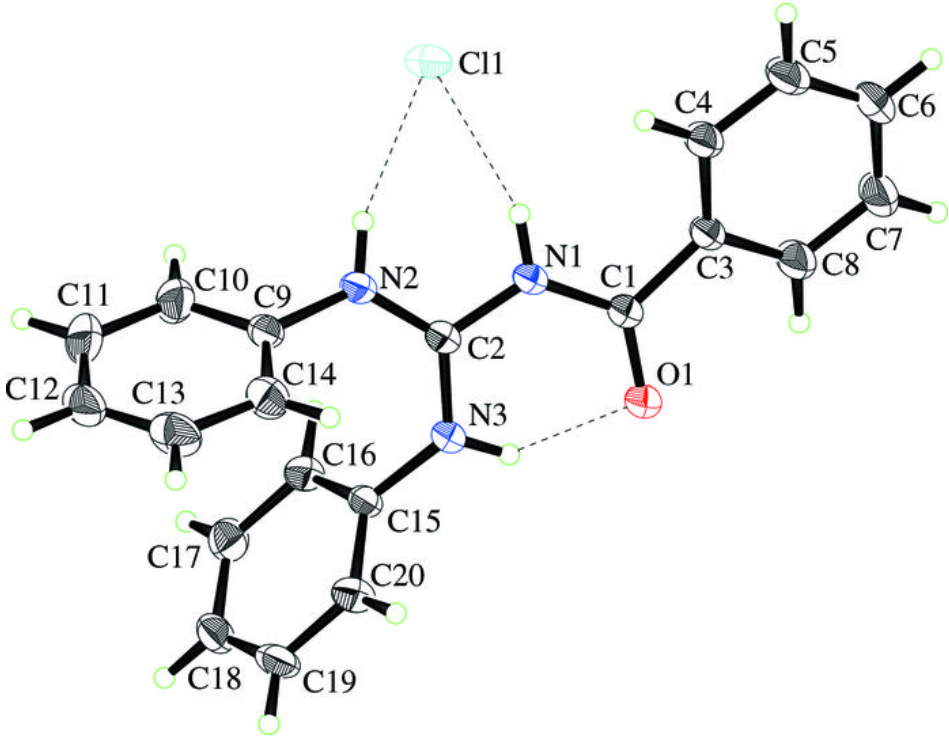
C3—C8	1.387 (3)	C13—H13	0.9300
C3—C4	1.387 (2)	C14—H14	0.9300
C4—C5	1.386 (3)	N3—C15	1.441 (2)
C4—H4	0.9300	N3—H3	0.84 (3)
C5—C6	1.373 (3)	C15—C16	1.374 (3)
C5—H5	0.9300	C15—C20	1.381 (2)
C6—C7	1.377 (3)	C16—C17	1.383 (3)
C6—H6	0.9300	C16—H16	0.9300
C7—C8	1.380 (3)	C17—C18	1.381 (3)
C7—H7	0.9300	C17—H17	0.9300
C8—H8	0.9300	C18—C19	1.371 (3)
N2—C9	1.432 (2)	C18—H18	0.9300
N2—H2	0.86 (2)	C19—C20	1.386 (3)
C9—C10	1.369 (3)	C19—H19	0.9300
C9—C14	1.374 (3)	C20—H20	0.9300
O1—C1—N1	122.33 (15)	C11—C10—H10	120.3
O1—C1—C3	121.03 (16)	C12—C11—C10	120.6 (2)
N1—C1—C3	116.55 (14)	C12—C11—H11	119.7
N2—C2—N3	125.14 (15)	C10—C11—H11	119.7
N2—C2—N1	115.35 (14)	C11—C12—C13	119.7 (2)
N3—C2—N1	119.49 (15)	C11—C12—H12	120.2
C1—N1—C2	125.74 (14)	C13—C12—H12	120.2
C1—N1—H1	119.5 (15)	C12—C13—C14	120.7 (2)
C2—N1—H1	113.5 (15)	C12—C13—H13	119.6
C8—C3—C4	119.34 (16)	C14—C13—H13	119.6
C8—C3—C1	116.33 (15)	C9—C14—C13	118.7 (2)
C4—C3—C1	124.15 (16)	C9—C14—H14	120.7
C5—C4—C3	119.63 (18)	C13—C14—H14	120.7
C5—C4—H4	120.2	C2—N3—C15	125.89 (15)
C3—C4—H4	120.2	C2—N3—H3	111.2 (17)
C6—C5—C4	120.55 (18)	C15—N3—H3	119.3 (17)
C6—C5—H5	119.7	C16—C15—C20	121.04 (16)
C4—C5—H5	119.7	C16—C15—N3	120.56 (15)
C5—C6—C7	120.06 (18)	C20—C15—N3	118.21 (16)
C5—C6—H6	120.0	C15—C16—C17	119.03 (17)
C7—C6—H6	120.0	C15—C16—H16	120.5
C6—C7—C8	119.8 (2)	C17—C16—H16	120.5
C6—C7—H7	120.1	C18—C17—C16	120.43 (19)
C8—C7—H7	120.1	C18—C17—H17	119.8
C7—C8—C3	120.55 (19)	C16—C17—H17	119.8
C7—C8—H8	119.7	C19—C18—C17	120.10 (17)
C3—C8—H8	119.7	C19—C18—H18	120.0
C2—N2—C9	126.71 (15)	C17—C18—H18	120.0
C2—N2—H2	115.2 (15)	C18—C19—C20	120.09 (18)
C9—N2—H2	117.8 (15)	C18—C19—H19	120.0
C10—C9—C14	120.97 (18)	C20—C19—H19	120.0
C10—C9—N2	118.28 (17)	C15—C20—C19	119.30 (18)
C14—C9—N2	120.63 (17)	C15—C20—H20	120.3
C9—C10—C11	119.3 (2)	C19—C20—H20	120.3

C9—C10—H10	120.3		
O1—C1—N1—C2	−7.5 (3)	C14—C9—C10—C11	−1.1 (3)
C3—C1—N1—C2	175.92 (16)	N2—C9—C10—C11	−177.3 (2)
N2—C2—N1—C1	−174.26 (17)	C9—C10—C11—C12	0.8 (4)
N3—C2—N1—C1	7.2 (3)	C10—C11—C12—C13	−0.3 (4)
O1—C1—C3—C8	16.6 (3)	C11—C12—C13—C14	0.1 (4)
N1—C1—C3—C8	−166.76 (18)	C10—C9—C14—C13	0.9 (3)
O1—C1—C3—C4	−158.4 (2)	N2—C9—C14—C13	176.99 (18)
N1—C1—C3—C4	18.2 (3)	C12—C13—C14—C9	−0.4 (3)
C8—C3—C4—C5	−0.5 (3)	N2—C2—N3—C15	23.2 (3)
C1—C3—C4—C5	174.43 (19)	N1—C2—N3—C15	−158.45 (16)
C3—C4—C5—C6	1.0 (3)	C2—N3—C15—C16	50.4 (3)
C4—C5—C6—C7	−0.2 (4)	C2—N3—C15—C20	−134.56 (19)
C5—C6—C7—C8	−1.2 (4)	C20—C15—C16—C17	1.5 (3)
C6—C7—C8—C3	1.7 (4)	N3—C15—C16—C17	176.39 (17)
C4—C3—C8—C7	−0.9 (3)	C15—C16—C17—C18	−1.0 (3)
C1—C3—C8—C7	−176.2 (2)	C16—C17—C18—C19	0.1 (3)
N3—C2—N2—C9	18.6 (3)	C17—C18—C19—C20	0.4 (3)
N1—C2—N2—C9	−159.87 (16)	C16—C15—C20—C19	−1.0 (3)
C2—N2—C9—C10	−133.2 (2)	N3—C15—C20—C19	−176.09 (17)
C2—N2—C9—C14	50.6 (3)	C18—C19—C20—C15	0.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1	0.86 (2)	2.32 (3)	3.143 (2)	159 (2)
N2—H2···Cl1	0.86 (2)	2.27 (2)	3.0977 (18)	162 (2)
N3—H3···O1	0.84 (3)	1.91 (3)	2.628 (2)	143 (2)

Fig. 1


Cl1
C5
C4
C6
C7
C3
C8
N1
C1
N2
C10
C9
C11
C2
O1
C14
C12
C13
N3
C16
C15
C17
C20
C18
C19