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2-(4-Nitrophenyl)-4,5-diphenyl-1*H*-imidazol-3-ium chloride

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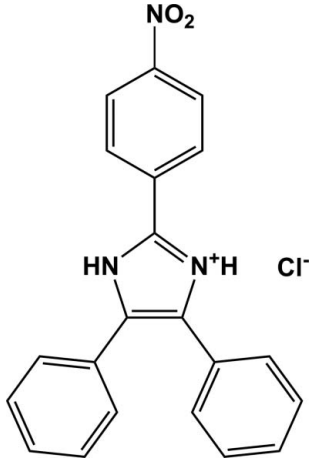
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.062; wR factor = 0.157; data-to-parameter ratio = 17.0.

In the cation of the title compound, $C_{21}H_{16}N_3O_2^+\cdot Cl^-$, the N atom in the 3-position of the imidazole ring is protonated. The three pendant aromatic rings are twisted from the plane of the imidazolium ring by dihedral angles of 31.69 (14)°, 31.09 (14)° and 34.77 (14)°. In the crystal structure, N—H···Cl hydrogen bonds link the molecules, forming a chain parallel to the b axis.

Related literature

For uses of imidazole derivatives, see: Dai & Fu (2008); Fu *et al.* (2008); Huang *et al.* (2008).



Experimental

Crystal data

$C_{21}H_{16}N_3O_2^+\cdot Cl^-$
M_r = 377.82
Monoclinic, $P2_1/c$
a = 15.106 (3) Å
b = 15.837 (3) Å
c = 7.8833 (16) Å
β = 105.10 (3)°
V = 1820.8 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 298 K
0.45 × 0.40 × 0.25 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.910, T_{max} = 1.000
(expected range = 0.859–0.944)
18591 measured reflections
4165 independent reflections
2393 reflections with $I > 2\sigma(I)$
R_{int} = 0.109

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.157
S = 1.03
4165 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl1	0.86	2.25	3.105 (2)	176
N2—H2A···Cl1^{i}	0.86	2.28	3.139 (2)	175

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2820).

References

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Huang, X.-F., Fu, D.-W. & Xiong, R.-G. (2008). *Cryst. Growth. Des.* **8**, 1795–1797.
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supporting information

Acta Cryst. (2009). E**65**, o1499 [doi:10.1107/S1600536809020807]

2-(4-Nitrophenyl)-4,5-diphenyl-1*H*-imidazol-3-ium chloride

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S1. Comment

Imidazole derivatives have found wide range of applications in coordination chemistry because of their multiple coordination modes as ligands to metal ions and for the construction of novel metal-organic frameworks (Huang *et al.* 2008; Fu *et al.* 2008; Dai & Fu 2008). We report herein the crystal structure of the title compound, 2-(4-nitrophenyl)-4,5-diphenyl-1*H*-imidazol-3-ium chloride.

The title compound contains an organic cation and a Cl^- anion in the asymmetric unit. The imidazole N atom in 3-position is protonated. The C1-C6, C8-C13 and C16-C21 benzene rings are twisted from the imidazolium ring an angle of 31.69 (14)°, 31.09 (14)° and 34.77 (14)°, respectively.

The crystal packing is stabilized by N—H···Cl hydrogen bonds to form a linear chain parallel to the *b* axis (Table 1 and Fig. 2).

S2. Experimental

Under nitrogen protection, 1,2-diphenyl-ethane-1,2-dione (20 mmol), 4-nitrobenzaldehyde (20 mmol) and amine acetate (50 mmol) were dissolved in 60 ml of HOAc. The mixture was stirred at 383 K for 20 h. The resulting solution was poured into ice water (200 ml) and after neutralizing the mixture with NaOH (6 mol/L) a white solid was obtained. After filtration and washing with distilled water the crude product was recrystallized from a ethanolic solution (150 ml) to which HCl (5 ml) was added to yield colourless block-shaped crystals of the title compound, suitable for X-ray analysis.

S3. Refinement

H atoms attached to C and N atoms were positioned geometrically and treated as riding, with C-H = 0.93 Å, N-H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N).

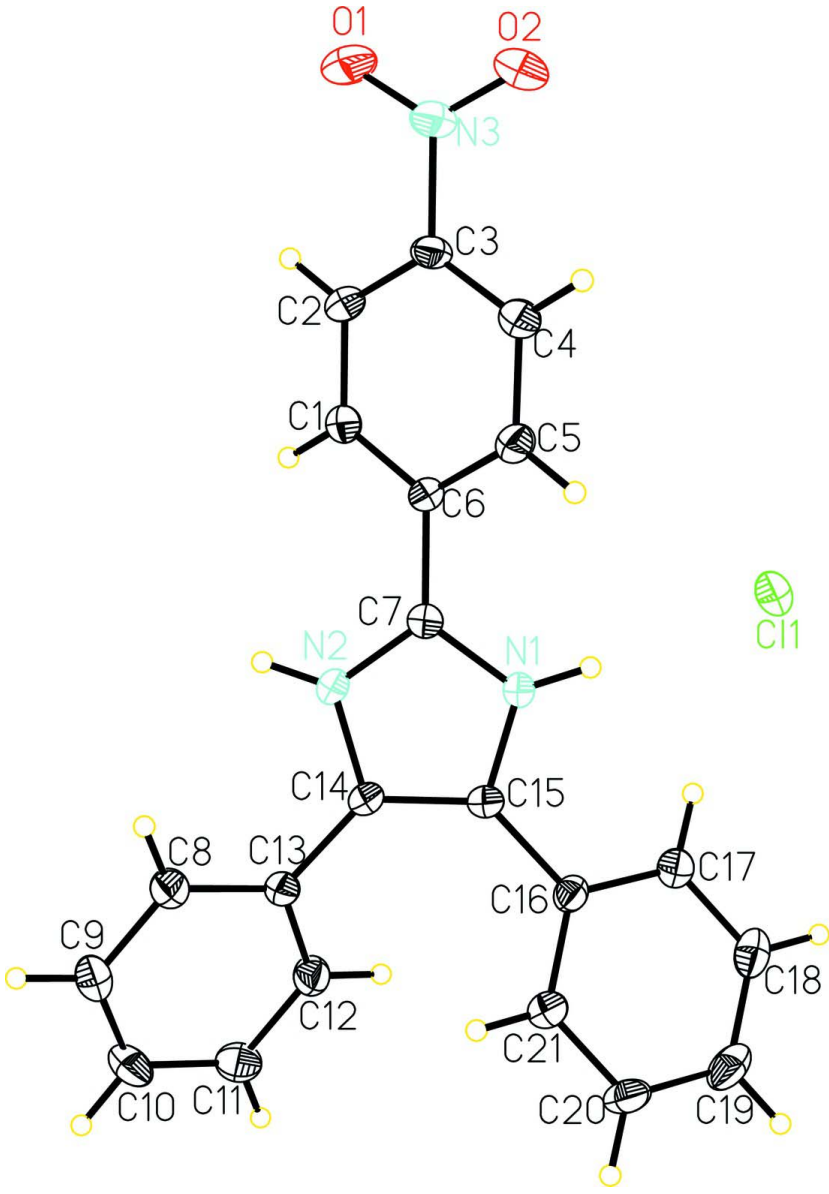

Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

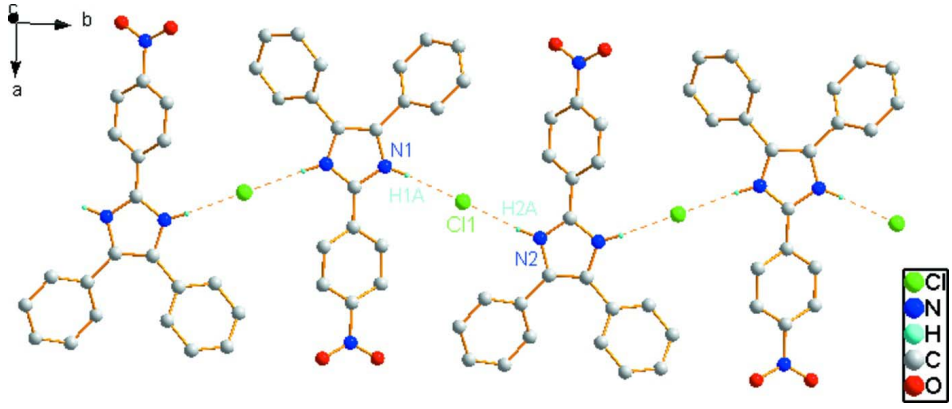

Figure 2

The crystal packing of the title compound viewed along the *c* axis, showing a hydrogen bonded chain. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

(I)

Crystal data

$C_{21}H_{16}N_3O_2^+\cdot Cl^-$
$M_r = 377.82$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 15.106$ (3) Å
$b = 15.837$ (3) Å
$c = 7.8833$ (16) Å
$\beta = 105.10$ (3)°
$V = 1820.8$ (7) Å^3
$Z = 4$
$F(000) = 784$
$D_x = 1.378$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4160 reflections
$\theta = 3.1$–$27.5°$
$\mu = 0.23$ mm^{-1}
$T = 298$ K
Block, colourless
0.45 × 0.40 × 0.25 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.910$, $T_{max} = 1.000$
18591 measured reflections
4165 independent reflections
2393 reflections with $I > 2\sigma(I)$
$R_{int} = 0.109$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -19\rightarrow19$
$k = -20\rightarrow20$
$l = -10\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.157$
$S = 1.03$
4165 reflections
245 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
$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.4461P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}
Extinction correction: *SHELXL97*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0053 (10)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.50431 (5)	0.90216 (4)	0.28931 (13)	0.0625 (3)
N1	0.57993 (14)	0.72042 (13)	0.2790 (3)	0.0325 (5)
H1A	0.5620	0.7717	0.2840	0.039*
C7	0.52567 (17)	0.65254 (16)	0.2629 (3)	0.0321 (6)
N2	0.57744 (14)	0.58548 (13)	0.2592 (3)	0.0339 (5)
H2A	0.5581	0.5342	0.2501	0.041*
N3	0.14392 (17)	0.65834 (17)	0.2081 (4)	0.0480 (7)
C6	0.42716 (17)	0.65341 (15)	0.2489 (3)	0.0323 (6)
C2	0.27691 (18)	0.59458 (17)	0.1358 (4)	0.0399 (7)
H2	0.2382	0.5540	0.0700	0.048*
C15	0.66881 (17)	0.69658 (16)	0.2865 (3)	0.0307 (6)
C13	0.73980 (17)	0.54725 (16)	0.2772 (3)	0.0320 (6)
C3	0.24275 (18)	0.65705 (17)	0.2217 (4)	0.0370 (7)
C1	0.37003 (18)	0.59320 (16)	0.1493 (4)	0.0389 (7)
H1	0.3944	0.5517	0.0912	0.047*
C14	0.66699 (17)	0.60935 (16)	0.2719 (3)	0.0308 (6)
C18	0.7947 (2)	0.89632 (18)	0.2438 (4)	0.0449 (8)
H18	0.7821	0.9490	0.1908	0.054*
C4	0.29746 (19)	0.71829 (17)	0.3209 (4)	0.0418 (7)
H4	0.2725	0.7601	0.3773	0.050*
O2	0.11287 (15)	0.71883 (15)	0.2695 (4)	0.0696 (7)
C5	0.39062 (19)	0.71577 (17)	0.3342 (4)	0.0404 (7)
H5	0.4291	0.7562	0.4008	0.049*
O1	0.09771 (15)	0.59864 (15)	0.1374 (4)	0.0740 (8)
C16	0.74249 (18)	0.75918 (15)	0.3069 (3)	0.0315 (6)
C17	0.7250 (2)	0.83847 (16)	0.2293 (4)	0.0374 (7)
H17	0.6657	0.8526	0.1671	0.045*
C9	0.8082 (2)	0.41135 (18)	0.3652 (4)	0.0455 (7)
H9	0.8052	0.3581	0.4132	0.055*
C21	0.83144 (18)	0.74111 (17)	0.4041 (4)	0.0387 (7)
H21	0.8441	0.6893	0.4608	0.046*
C12	0.81528 (19)	0.56718 (17)	0.2152 (4)	0.0390 (7)
H12	0.8172	0.6190	0.1606	0.047*
C8	0.73622 (19)	0.46743 (17)	0.3498 (4)	0.0399 (7)
H8	0.6853	0.4518	0.3881	0.048*

C11	0.8874 (2)	0.51169 (19)	0.2330 (4)	0.0497 (8)
H11	0.9381	0.5266	0.1934	0.060*
C20	0.9012 (2)	0.7994 (2)	0.4172 (4)	0.0480 (8)
H20	0.9605	0.7861	0.4812	0.058*
C19	0.8833 (2)	0.8769 (2)	0.3361 (4)	0.0501 (8)
H19	0.9303	0.9157	0.3435	0.060*
C10	0.8841 (2)	0.4339 (2)	0.3099 (4)	0.0517 (8)
H10	0.9331	0.3967	0.3243	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0444 (5)	0.0305 (4)	0.1135 (8)	0.0066 (3)	0.0224 (5)	0.0007 (4)
N1	0.0281 (13)	0.0225 (11)	0.0463 (14)	−0.0003 (9)	0.0087 (11)	−0.0024 (10)
C7	0.0270 (14)	0.0291 (14)	0.0390 (15)	0.0003 (12)	0.0064 (12)	−0.0005 (12)
N2	0.0293 (13)	0.0238 (11)	0.0482 (14)	−0.0043 (9)	0.0095 (10)	−0.0023 (10)
N3	0.0286 (14)	0.0472 (16)	0.0670 (17)	0.0050 (13)	0.0103 (13)	0.0089 (14)
C6	0.0252 (14)	0.0280 (13)	0.0437 (16)	−0.0024 (11)	0.0086 (12)	0.0015 (12)
C2	0.0272 (15)	0.0368 (16)	0.0520 (18)	−0.0064 (12)	0.0038 (13)	−0.0048 (14)
C15	0.0238 (15)	0.0315 (14)	0.0362 (15)	−0.0007 (11)	0.0068 (12)	−0.0010 (12)
C13	0.0274 (15)	0.0293 (14)	0.0388 (15)	0.0003 (11)	0.0076 (12)	−0.0029 (12)
C3	0.0225 (14)	0.0376 (15)	0.0494 (17)	0.0035 (12)	0.0066 (13)	0.0107 (14)
C1	0.0328 (16)	0.0290 (14)	0.0538 (18)	0.0004 (12)	0.0094 (13)	−0.0066 (13)
C14	0.0251 (14)	0.0293 (14)	0.0381 (15)	−0.0044 (11)	0.0084 (12)	−0.0005 (12)
C18	0.059 (2)	0.0314 (15)	0.0494 (18)	−0.0075 (15)	0.0227 (16)	−0.0027 (14)
C4	0.0341 (17)	0.0382 (16)	0.0564 (19)	0.0021 (13)	0.0175 (14)	−0.0052 (14)
O2	0.0399 (14)	0.0615 (15)	0.112 (2)	0.0115 (12)	0.0282 (14)	−0.0054 (14)
C5	0.0333 (17)	0.0343 (15)	0.0530 (18)	−0.0049 (12)	0.0102 (14)	−0.0111 (14)
O1	0.0313 (13)	0.0674 (16)	0.118 (2)	−0.0119 (12)	0.0094 (13)	−0.0165 (16)
C16	0.0311 (15)	0.0285 (13)	0.0371 (15)	−0.0045 (11)	0.0129 (12)	−0.0038 (12)
C17	0.0371 (17)	0.0324 (14)	0.0428 (16)	−0.0011 (12)	0.0109 (13)	−0.0009 (13)
C9	0.0491 (19)	0.0328 (15)	0.0538 (19)	0.0065 (14)	0.0122 (15)	0.0061 (14)
C21	0.0314 (16)	0.0374 (15)	0.0459 (17)	−0.0038 (13)	0.0072 (13)	−0.0037 (13)
C12	0.0386 (17)	0.0328 (15)	0.0484 (18)	−0.0005 (13)	0.0166 (14)	0.0022 (13)
C8	0.0364 (17)	0.0351 (15)	0.0496 (18)	0.0017 (13)	0.0139 (14)	0.0021 (13)
C11	0.0343 (17)	0.0530 (19)	0.067 (2)	0.0031 (15)	0.0235 (16)	−0.0019 (17)
C20	0.0266 (16)	0.054 (2)	0.060 (2)	−0.0079 (14)	0.0054 (14)	−0.0087 (16)
C19	0.047 (2)	0.0476 (18)	0.063 (2)	−0.0217 (15)	0.0264 (17)	−0.0146 (16)
C10	0.0420 (19)	0.0477 (19)	0.064 (2)	0.0179 (15)	0.0107 (16)	0.0036 (16)

Geometric parameters (Å, º)

N1—C7	1.338 (3)	C18—C19	1.380 (4)
N1—C15	1.381 (3)	C18—H18	0.93
N1—H1A	0.86	C4—C5	1.384 (4)
C7—N2	1.324 (3)	C4—H4	0.93
C7—C6	1.463 (4)	C5—H5	0.93
N2—C14	1.383 (3)	C16—C17	1.392 (3)

N2—H2A	0.86	C16—C21	1.392 (4)
N3—O1	1.220 (3)	C17—H17	0.9300
N3—O2	1.221 (3)	C9—C10	1.375 (4)
N3—C3	1.469 (4)	C9—C8	1.384 (4)
C6—C1	1.385 (4)	C9—H9	0.93
C6—C5	1.388 (4)	C21—C20	1.384 (4)
C2—C3	1.373 (4)	C21—H21	0.93
C2—C1	1.383 (4)	C12—C11	1.378 (4)
C2—H2	0.93	C12—H12	0.93
C15—C14	1.386 (3)	C8—H8	0.93
C15—C16	1.468 (3)	C11—C10	1.379 (4)
C13—C12	1.389 (4)	C11—H11	0.93
C13—C8	1.395 (4)	C20—C19	1.378 (4)
C13—C14	1.468 (3)	C20—H20	0.93
C3—C4	1.378 (4)	C19—H19	0.93
C1—H1	0.93	C10—H10	0.93
C18—C17	1.378 (4)		

C7—N1—C15	110.4 (2)	C3—C4—C5	118.1 (3)
C7—N1—H1A	124.8	C3—C4—H4	121.0
C15—N1—H1A	124.8	C5—C4—H4	121.0
N2—C7—N1	107.2 (2)	C4—C5—C6	120.6 (3)
N2—C7—C6	126.9 (2)	C4—C5—H5	119.7
N1—C7—C6	125.8 (2)	C6—C5—H5	119.7
C7—N2—C14	110.6 (2)	C17—C16—C21	118.2 (2)
C7—N2—H2A	124.7	C17—C16—C15	120.6 (2)
C14—N2—H2A	124.7	C21—C16—C15	121.1 (2)
O1—N3—O2	123.8 (3)	C18—C17—C16	120.6 (3)
O1—N3—C3	118.2 (3)	C18—C17—H17	119.7
O2—N3—C3	118.0 (3)	C16—C17—H17	119.7
C1—C6—C5	119.8 (2)	C10—C9—C8	120.4 (3)
C1—C6—C7	120.5 (2)	C10—C9—H9	119.8
C5—C6—C7	119.7 (2)	C8—C9—H9	119.8
C3—C2—C1	118.6 (2)	C20—C21—C16	120.7 (3)
C3—C2—H2	120.7	C20—C21—H21	119.6
C1—C2—H2	120.7	C16—C21—H21	119.6
N1—C15—C14	105.7 (2)	C11—C12—C13	121.2 (3)
N1—C15—C16	121.4 (2)	C11—C12—H12	119.4
C14—C15—C16	132.9 (2)	C13—C12—H12	119.4
C12—C13—C8	118.3 (2)	C9—C8—C13	120.3 (3)
C12—C13—C14	121.0 (2)	C9—C8—H8	119.9
C8—C13—C14	120.7 (2)	C13—C8—H8	119.9
C2—C3—C4	122.7 (3)	C12—C11—C10	119.8 (3)
C2—C3—N3	118.7 (3)	C12—C11—H11	120.1
C4—C3—N3	118.7 (3)	C10—C11—H11	120.1
C2—C1—C6	120.2 (3)	C19—C20—C21	120.4 (3)
C2—C1—H1	119.9	C19—C20—H20	119.8
C6—C1—H1	119.9	C21—C20—H20	119.8

N2—C14—C15	106.0 (2)	C20—C19—C18	119.3 (3)
N2—C14—C13	122.0 (2)	C20—C19—H19	120.3
C15—C14—C13	131.8 (2)	C18—C19—H19	120.3
C17—C18—C19	120.6 (3)	C9—C10—C11	120.0 (3)
C17—C18—H18	119.7	C9—C10—H10	120.0
C19—C18—H18	119.7	C11—C10—H10	120.0

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl1	0.86	2.25	3.105 (2)	176
N2—H2*A*···Cl1^{i}	0.86	2.28	3.139 (2)	175

Symmetry code: (i) −*x*+1, *y*−1/2, −*z*+1/2.