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# (2,4,6-Trimethylphenyl){2-[*N*-(2,4,6-trimethylphenyl)formamido]ethyl}-ammonium chloride

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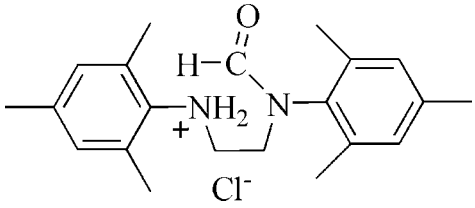
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.044; $wR$ factor = 0.107; data-to-parameter ratio = 20.9.

In the title salt, $C_{21}H_{29}N_2O^+\cdot Cl^-$, the benzene rings form a dihedral angle of 6.13 (1)°. In the crystal, N—H···Cl hydrogen bonds link the cations and anions into chains extending along the $c$ axis.

## Related literature

For closely related compounds, see: Kocher & Hermann (1997); Denk *et al.* (2001).




## Experimental

### Crystal data

$C_{21}H_{29}N_2O^+\cdot Cl^-$
$M_r$ = 360.91
Triclinic, $P\overline{1}$
$a$ = 8.2516 (2) Å
$b$ = 8.8822 (2) Å
$c$ = 14.7524 (4) Å
$\alpha$ = 74.857 (2)°
$\beta$ = 86.315 (2)°
$\gamma$ = 74.635 (2)°
$V$ = 1006.38 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.20 mm$^{-1}$
$T$ = 173 K
0.36 × 0.21 × 0.11 mm

### Data collection

Bruker APEXII CCD diffractometer
19610 measured reflections
4853 independent reflections
2975 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.062

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.107
$S$ = 0.90
4853 reflections
232 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···Cl1 | 0.92 | 2.23 | 3.0585 (14) | 149 |
| N2—H2$B$···Cl1$^{i}$ | 0.92 | 2.17 | 3.0531 (14) | 161 |

Symmetry code: (i) $-x, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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 thank Dr Manuel Fernandes for the data collection and the University of KwaZulu-Natal for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5637).

## References

Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Denk, M. K., Rodezno, J. M., Gupta, S. & Lough, A. J. (2001). *J. Organomet. Chem.* **617**, 242–253.
Kocher, C. & Hermann, W. A. (1997). *J. Organomet. Chem.* **532**, 261–265.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

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# (2,4,6-Trimethylphenyl){2-[*N*-(2,4,6-trimethylphenyl)formamido]ethyl}-ammonium chloride

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## S1. Comment

The title compound was isolated from the hydrolysis of an imidazolium based salt in a ring opening reaction. Stable *N*-heterocyclic carbene ligands are often prepared from imidazolium based salt precursors. However the reaction must be conducted under strict anaerobic conditions using Schlenk techniques, otherwise attack by moisture will lead to the isolation of products such as (I).

In (I) (Fig.1), the planes of the two phenyl rings (mean: C1–C6 and mean: C13–C18) form a dihedral angle of 6.13 (1)°. In the crystal, intermolecular N—H···Cl hydrogen bonds (Table 1) link the molecules into chains extending along the crystallographic *c* axis with a separation of 2.17–2.23 Å (Fig. 2).

## S2. Experimental

A mixture of 1,3–bis(2,4,6-trimethyl phenyl)imidazolinium chloride (0.101 g, 0.29 mmol) and potassium *tert*-butoxide (0.039 g, 0.35 mmol) were dissolved in 20 ml of tetrahydrofuran and stirred at room temperature for 30 min. After evaporating the solvent, the free carbene was extracted in warm toluene (2 *x* 20 ml). $FeCl_2$ (0.037 g, 0.29 mmol) was added to the toluene solution and refluxed for 24 h at 90 °C. Removal of the solvent gave a residue that was purified by recrystallization from $CH_2Cl_2$/hexane to yield orange crystals of (I). Yield: 0.05 g, 51%; m.p. 180 °C.

## S3. Refinement

H-atoms were refined using a riding model, with C—H = 0.95 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for aromatic and C—H = 0.98 Å and $U_{iso}$(H) = 1.5$U_{eq}$(C) for $CH_3$. The amino H atoms were placed in calculated positions with N—H = 0.92 Å and refined in a riding mode with $U_{iso}$(H) = 1.2$U_{eq}$(N).

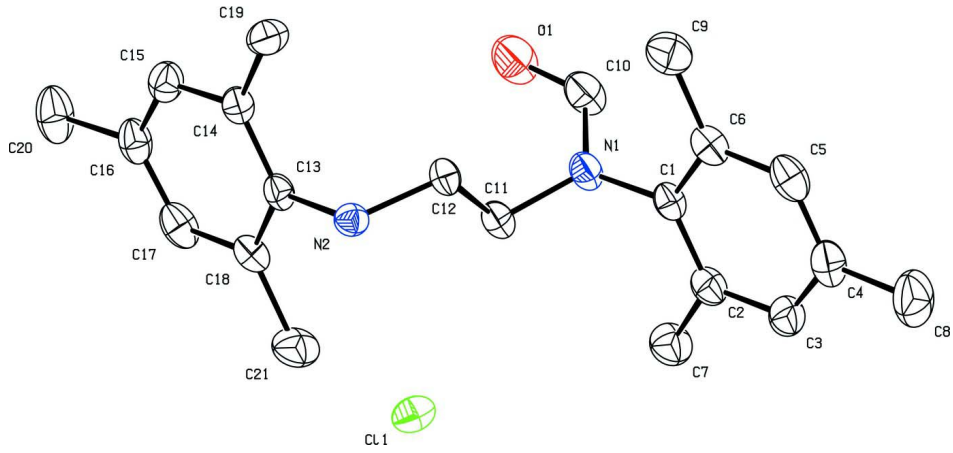


**Figure 1**

*ORTEP* diagram of compound (I). Thermal ellipsoids are represented at the 50% probability level. Hydrogen atoms are eliminated for clarity.

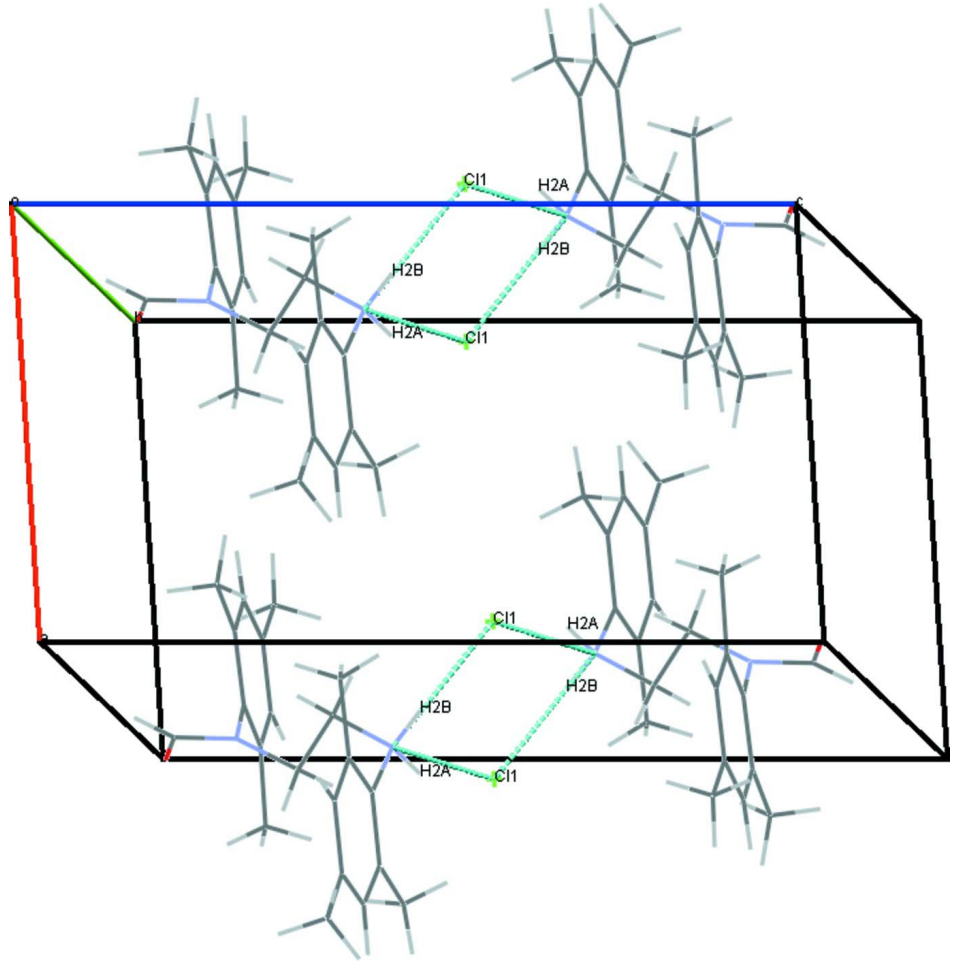


**Figure 2**

Packing in the title compound showing the N—H···Cl hydrogen bonds.

**(2,4,6-Trimethylphenyl){2-[*N*-(2,4,6- trimethylphenyl)formamido]ethyl}ammonium chloride**

*Crystal data*

$C_{21}H_{29}N_2O^+\cdot Cl^-$
$M_r = 360.91$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.2516$ (2) Å
$b = 8.8822$ (2) Å
$c = 14.7524$ (4) Å
$\alpha = 74.857$ (2)°
$\beta = 86.315$ (2)°
$\gamma = 74.635$ (2)°
$V = 1006.38$ (5) Å$^3$
$Z = 2$
$F(000) = 388$
$D_x = 1.191$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3132 reflections
$\theta = 2.5$–$24.0°$
$\mu = 0.20$ mm$^{-1}$
$T = 173$ K
Block, colourless
0.36 × 0.21 × 0.11 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
19610 measured reflections
4853 independent reflections
2975 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 28.0°$, $\theta_{min} = 1.4°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -19 \rightarrow 19$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.107$
$S = 0.90$
4853 reflections
232 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
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å$^{-3}$
$\Delta\rho_{min} = -0.25$ e Å$^{-3}$

*Special details*

**Experimental**. IR (ATR cm$^{-1}$): 2918, 2718, 2607, 1669, 1568, 1482, 1446, 1381, 1345, 1306, 1285, 1207, 1193, 1033, 850, 781, 705, 577, 477, 425; $\delta_H$ (400 MHz, $CDCl_3$): 1.60 (6*H*, s, $CH_3$), 2.16 (12*H*, m, $CH_3$), 2.58 (3*H*, s, $NH_2$), 3.76 (2*H*, s, $NCH_2NCHO$), 6.83 (3*H*, s, ArH), 6.88 (2*H*, s, ArH) and 7.89 p.p.m. (1*H*, s, NCHO); $\delta_C$ (100 MHz, $CDCl_3$): 18.09 ($C_6H_2(CH_3)_3$), 19.35 ($C_6H_2(CH_3)_3$), 21.15 ($C_6H_2(CH_3)_3$), 23.17 ($C_6H_2(CH_3)_3$), 51.12 ($NHCH_2$), 52.08 ($NCH_2$), 128.27, 130.18, 134.72, 135.91, 138.54, 140.21, 145.23 and 160.28 p.p.m. (NCHO); HRMS (ESI), Found, 325.22737 ($M^+$ - $Cl^-$) Calculated for $C_{21}H_{29}N_2O$ 325.22799 ($M^+$ - $Cl^-$).

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | −0.0762 (2) | 0.8248 (2) | 0.13320 (12) | 0.0263 (4) |
| C2 | −0.0175 (2) | 0.9590 (2) | 0.13117 (12) | 0.0298 (4) |
| C3 | −0.1346 (2) | 1.1060 (2) | 0.12548 (13) | 0.0347 (5) |
| H3 | −0.0958 | 1.1971 | 0.1266 | 0.042* |
| C4 | −0.3055 (2) | 1.1251 (2) | 0.11826 (13) | 0.0365 (5) |
| C5 | −0.3594 (2) | 0.9905 (2) | 0.11714 (13) | 0.0373 (5) |
| H5 | −0.4761 | 1.0021 | 0.1104 | 0.045* |
| C6 | −0.2486 (2) | 0.8385 (2) | 0.12561 (12) | 0.0318 (4) |
| C7 | 0.1675 (2) | 0.9497 (2) | 0.13254 (14) | 0.0390 (5) |
| H7A | 0.2107 | 0.9029 | 0.1969 | 0.058* |
| H7B | 0.1844 | 1.0584 | 0.1096 | 0.058* |
| H7C | 0.2277 | 0.8817 | 0.0920 | 0.058* |
| C8 | −0.4291 (3) | 1.2871 (3) | 0.11207 (17) | 0.0573 (6) |
| H8A | −0.4089 | 1.3296 | 0.1641 | 0.086* |
| H8B | −0.5439 | 1.2744 | 0.1159 | 0.086* |
| H8C | −0.4145 | 1.3622 | 0.0522 | 0.086* |
| C9 | −0.3162 (2) | 0.6959 (2) | 0.12768 (15) | 0.0441 (5) |
| H9A | −0.2934 | 0.6669 | 0.0676 | 0.066* |
| H9B | −0.4378 | 0.7239 | 0.1383 | 0.066* |
| H9C | −0.2616 | 0.6041 | 0.1786 | 0.066* |
| C10 | 0.0609 (2) | 0.5899 (2) | 0.07631 (14) | 0.0392 (5) |
| H10 | 0.0013 | 0.6435 | 0.0190 | 0.047* |
| C11 | 0.1348 (2) | 0.5881 (2) | 0.23205 (12) | 0.0288 (4) |
| H11A | 0.1508 | 0.6696 | 0.2630 | 0.035* |
| H11B | 0.2471 | 0.5234 | 0.2188 | 0.035* |
| C12 | 0.0402 (2) | 0.4789 (2) | 0.29708 (12) | 0.0277 (4) |
| H12A | −0.0680 | 0.5452 | 0.3143 | 0.033* |
| H12B | 0.0153 | 0.4042 | 0.2638 | 0.033* |
| C13 | 0.2789 (2) | 0.2444 (2) | 0.37526 (12) | 0.0249 (4) |
| C14 | 0.2386 (2) | 0.1044 (2) | 0.36930 (12) | 0.0265 (4) |
| C15 | 0.3711 (2) | −0.0292 (2) | 0.36709 (12) | 0.0320 (4) |
| H15 | 0.3467 | −0.1262 | 0.3634 | 0.038* |
| C16 | 0.5376 (2) | −0.0257 (2) | 0.37002 (12) | 0.0328 (4) |
| C17 | 0.5706 (2) | 0.1165 (2) | 0.37419 (13) | 0.0345 (5) |
| H17 | 0.6843 | 0.1205 | 0.3750 | 0.041* |
| C18 | 0.4440 (2) | 0.2546 (2) | 0.37721 (12) | 0.0280 (4) |
| C19 | 0.0599 (2) | 0.0917 (2) | 0.36649 (14) | 0.0345 (5) |
| H19A | −0.0098 | 0.1503 | 0.4090 | 0.052* |
| H19B | 0.0581 | −0.0221 | 0.3863 | 0.052* |
| H19C | 0.0155 | 0.1386 | 0.3024 | 0.052* |
| C20 | 0.6787 (2) | −0.1744 (2) | 0.36982 (15) | 0.0471 (6) |
| H20A | 0.6388 | −0.2712 | 0.3968 | 0.071* |
| H20B | 0.7730 | −0.1756 | 0.4074 | 0.071* |
| H20C | 0.7157 | −0.1727 | 0.3052 | 0.071* |
| C21 | 0.4916 (2) | 0.4051 (2) | 0.38237 (15) | 0.0409 (5) |

| | | | | |
|---|---|---|---|---|
| H21A | 0.6129 | 0.3795 | 0.3934 | 0.061* |
| H21B | 0.4309 | 0.4457 | 0.4340 | 0.061* |
| H21C | 0.4620 | 0.4877 | 0.3231 | 0.061* |
| N1 | 0.04243 (17) | 0.66963 (18) | 0.14387 (10) | 0.0289 (3) |
| N2 | 0.13837 (16) | 0.38311 (16) | 0.38442 (10) | 0.0246 (3) |
| H2A | 0.1811 | 0.4518 | 0.4072 | 0.030* |
| H2B | 0.0652 | 0.3452 | 0.4287 | 0.030* |
| O1 | 0.14983 (17) | 0.45239 (18) | 0.08378 (10) | 0.0544 (4) |
| Cl1 | 0.13717 (5) | 0.66160 (5) | 0.47043 (3) | 0.03312 (14) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0249 (9) | 0.0308 (10) | 0.0200 (9) | −0.0033 (8) | −0.0015 (7) | −0.0046 (8) |
| C2 | 0.0297 (10) | 0.0356 (11) | 0.0228 (9) | −0.0091 (9) | −0.0013 (8) | −0.0041 (8) |
| C3 | 0.0427 (11) | 0.0315 (11) | 0.0277 (10) | −0.0080 (9) | −0.0031 (9) | −0.0043 (9) |
| C4 | 0.0357 (11) | 0.0368 (12) | 0.0290 (10) | 0.0015 (9) | −0.0019 (9) | −0.0052 (9) |
| C5 | 0.0236 (9) | 0.0494 (13) | 0.0331 (11) | −0.0026 (9) | −0.0023 (8) | −0.0069 (10) |
| C6 | 0.0280 (10) | 0.0399 (12) | 0.0261 (10) | −0.0075 (9) | −0.0019 (8) | −0.0065 (9) |
| C7 | 0.0321 (10) | 0.0436 (12) | 0.0413 (12) | −0.0132 (9) | −0.0015 (9) | −0.0071 (10) |
| C8 | 0.0571 (14) | 0.0446 (14) | 0.0557 (15) | 0.0123 (11) | −0.0079 (12) | −0.0117 (12) |
| C9 | 0.0331 (11) | 0.0495 (13) | 0.0516 (14) | −0.0140 (10) | −0.0051 (10) | −0.0115 (11) |
| C10 | 0.0345 (11) | 0.0473 (13) | 0.0331 (11) | 0.0000 (10) | −0.0053 (9) | −0.0152 (10) |
| C11 | 0.0262 (9) | 0.0323 (10) | 0.0252 (9) | −0.0033 (8) | −0.0053 (7) | −0.0056 (8) |
| C12 | 0.0225 (9) | 0.0274 (10) | 0.0295 (10) | −0.0014 (8) | −0.0067 (7) | −0.0044 (8) |
| C13 | 0.0222 (9) | 0.0263 (10) | 0.0226 (9) | 0.0004 (7) | −0.0028 (7) | −0.0058 (8) |
| C14 | 0.0265 (9) | 0.0268 (10) | 0.0232 (9) | −0.0025 (8) | −0.0016 (7) | −0.0052 (8) |
| C15 | 0.0372 (11) | 0.0276 (10) | 0.0275 (10) | −0.0028 (8) | 0.0009 (8) | −0.0067 (8) |
| C16 | 0.0313 (10) | 0.0345 (11) | 0.0242 (10) | 0.0044 (9) | 0.0000 (8) | −0.0060 (8) |
| C17 | 0.0208 (9) | 0.0479 (12) | 0.0291 (10) | −0.0014 (9) | 0.0001 (8) | −0.0077 (9) |
| C18 | 0.0232 (9) | 0.0363 (11) | 0.0234 (9) | −0.0056 (8) | −0.0026 (7) | −0.0074 (8) |
| C19 | 0.0322 (10) | 0.0308 (11) | 0.0443 (12) | −0.0095 (9) | −0.0002 (9) | −0.0143 (9) |
| C20 | 0.0418 (12) | 0.0468 (13) | 0.0361 (12) | 0.0127 (10) | 0.0024 (9) | −0.0070 (10) |
| C21 | 0.0272 (10) | 0.0490 (13) | 0.0514 (13) | −0.0133 (9) | −0.0024 (9) | −0.0172 (11) |
| N1 | 0.0295 (8) | 0.0312 (9) | 0.0227 (8) | −0.0015 (7) | −0.0042 (6) | −0.0065 (7) |
| N2 | 0.0225 (7) | 0.0259 (8) | 0.0264 (8) | −0.0065 (6) | 0.0002 (6) | −0.0079 (6) |
| O1 | 0.0514 (9) | 0.0540 (10) | 0.0525 (10) | 0.0147 (8) | −0.0150 (8) | −0.0295 (8) |
| Cl1 | 0.0312 (3) | 0.0314 (3) | 0.0414 (3) | −0.0118 (2) | 0.0066 (2) | −0.0148 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.394 (2) | C11—H11B | 0.9900 |
| C1—C6 | 1.404 (2) | C12—N2 | 1.495 (2) |
| C1—N1 | 1.440 (2) | C12—H12A | 0.9900 |
| C2—C3 | 1.389 (2) | C12—H12B | 0.9900 |
| C2—C7 | 1.508 (2) | C13—C18 | 1.392 (2) |
| C3—C4 | 1.383 (3) | C13—C14 | 1.394 (2) |
| C3—H3 | 0.9500 | C13—N2 | 1.4802 (19) |

| | | | |
|---|---|---|---|
| C4—C5 | 1.385 (3) | C14—C15 | 1.391 (2) |
| C4—C8 | 1.511 (3) | C14—C19 | 1.513 (2) |
| C5—C6 | 1.396 (2) | C15—C16 | 1.386 (2) |
| C5—H5 | 0.9500 | C15—H15 | 0.9500 |
| C6—C9 | 1.506 (3) | C16—C17 | 1.378 (3) |
| C7—H7A | 0.9800 | C16—C20 | 1.512 (2) |
| C7—H7B | 0.9800 | C17—C18 | 1.393 (2) |
| C7—H7C | 0.9800 | C17—H17 | 0.9500 |
| C8—H8A | 0.9800 | C18—C21 | 1.511 (2) |
| C8—H8B | 0.9800 | C19—H19A | 0.9800 |
| C8—H8C | 0.9800 | C19—H19B | 0.9800 |
| C9—H9A | 0.9800 | C19—H19C | 0.9800 |
| C9—H9B | 0.9800 | C20—H20A | 0.9800 |
| C9—H9C | 0.9800 | C20—H20B | 0.9800 |
| C10—O1 | 1.227 (2) | C20—H20C | 0.9800 |
| C10—N1 | 1.345 (2) | C21—H21A | 0.9800 |
| C10—H10 | 0.9500 | C21—H21B | 0.9800 |
| C11—N1 | 1.463 (2) | C21—H21C | 0.9800 |
| C11—C12 | 1.513 (2) | N2—H2A | 0.9200 |
| C11—H11A | 0.9900 | N2—H2B | 0.9200 |

| | | | |
|---|---|---|---|
| C2—C1—C6 | 121.13 (16) | N2—C12—H12B | 109.2 |
| C2—C1—N1 | 119.19 (15) | C11—C12—H12B | 109.2 |
| C6—C1—N1 | 119.69 (15) | H12A—C12—H12B | 107.9 |
| C3—C2—C1 | 118.23 (16) | C18—C13—C14 | 122.59 (15) |
| C3—C2—C7 | 119.68 (16) | C18—C13—N2 | 119.86 (15) |
| C1—C2—C7 | 122.08 (16) | C14—C13—N2 | 117.49 (14) |
| C4—C3—C2 | 122.63 (18) | C15—C14—C13 | 117.36 (15) |
| C4—C3—H3 | 118.7 | C15—C14—C19 | 119.38 (16) |
| C2—C3—H3 | 118.7 | C13—C14—C19 | 123.25 (15) |
| C3—C4—C5 | 117.69 (17) | C16—C15—C14 | 122.21 (17) |
| C3—C4—C8 | 121.08 (19) | C16—C15—H15 | 118.9 |
| C5—C4—C8 | 121.24 (18) | C14—C15—H15 | 118.9 |
| C4—C5—C6 | 122.44 (17) | C17—C16—C15 | 118.06 (16) |
| C4—C5—H5 | 118.8 | C17—C16—C20 | 121.05 (17) |
| C6—C5—H5 | 118.8 | C15—C16—C20 | 120.88 (18) |
| C5—C6—C1 | 117.82 (17) | C16—C17—C18 | 122.75 (17) |
| C5—C6—C9 | 119.69 (16) | C16—C17—H17 | 118.6 |
| C1—C6—C9 | 122.49 (17) | C18—C17—H17 | 118.6 |
| C2—C7—H7A | 109.5 | C13—C18—C17 | 117.00 (16) |
| C2—C7—H7B | 109.5 | C13—C18—C21 | 123.79 (16) |
| H7A—C7—H7B | 109.5 | C17—C18—C21 | 119.21 (16) |
| C2—C7—H7C | 109.5 | C14—C19—H19A | 109.5 |
| H7A—C7—H7C | 109.5 | C14—C19—H19B | 109.5 |
| H7B—C7—H7C | 109.5 | H19A—C19—H19B | 109.5 |
| C4—C8—H8A | 109.5 | C14—C19—H19C | 109.5 |
| C4—C8—H8B | 109.5 | H19A—C19—H19C | 109.5 |
| H8A—C8—H8B | 109.5 | H19B—C19—H19C | 109.5 |

| | | | |
|---|---|---|---|
| C4—C8—H8C | 109.5 | C16—C20—H20A | 109.5 |
| H8A—C8—H8C | 109.5 | C16—C20—H20B | 109.5 |
| H8B—C8—H8C | 109.5 | H20A—C20—H20B | 109.5 |
| C6—C9—H9A | 109.5 | C16—C20—H20C | 109.5 |
| C6—C9—H9B | 109.5 | H20A—C20—H20C | 109.5 |
| H9A—C9—H9B | 109.5 | H20B—C20—H20C | 109.5 |
| C6—C9—H9C | 109.5 | C18—C21—H21A | 109.5 |
| H9A—C9—H9C | 109.5 | C18—C21—H21B | 109.5 |
| H9B—C9—H9C | 109.5 | H21A—C21—H21B | 109.5 |
| O1—C10—N1 | 124.35 (18) | C18—C21—H21C | 109.5 |
| O1—C10—H10 | 117.8 | H21A—C21—H21C | 109.5 |
| N1—C10—H10 | 117.8 | H21B—C21—H21C | 109.5 |
| N1—C11—C12 | 110.66 (14) | C10—N1—C1 | 121.01 (15) |
| N1—C11—H11A | 109.5 | C10—N1—C11 | 118.12 (15) |
| C12—C11—H11A | 109.5 | C1—N1—C11 | 120.64 (14) |
| N1—C11—H11B | 109.5 | C13—N2—C12 | 116.63 (13) |
| C12—C11—H11B | 109.5 | C13—N2—H2A | 108.1 |
| H11A—C11—H11B | 108.1 | C12—N2—H2A | 108.1 |
| N2—C12—C11 | 111.89 (13) | C13—N2—H2B | 108.1 |
| N2—C12—H12A | 109.2 | C12—N2—H2B | 108.1 |
| C11—C12—H12A | 109.2 | H2A—N2—H2B | 107.3 |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 2.7 (3) | C19—C14—C15—C16 | −179.61 (17) |
| N1—C1—C2—C3 | −176.89 (16) | C14—C15—C16—C17 | −0.8 (3) |
| C6—C1—C2—C7 | −175.73 (17) | C14—C15—C16—C20 | 178.54 (17) |
| N1—C1—C2—C7 | 4.6 (3) | C15—C16—C17—C18 | 1.2 (3) |
| C1—C2—C3—C4 | −2.5 (3) | C20—C16—C17—C18 | −178.12 (17) |
| C7—C2—C3—C4 | 176.02 (17) | C14—C13—C18—C17 | −0.8 (3) |
| C2—C3—C4—C5 | 0.3 (3) | N2—C13—C18—C17 | 176.08 (15) |
| C2—C3—C4—C8 | −179.90 (18) | C14—C13—C18—C21 | 179.17 (17) |
| C3—C4—C5—C6 | 1.8 (3) | N2—C13—C18—C21 | −3.9 (3) |
| C8—C4—C5—C6 | −178.02 (19) | C16—C17—C18—C13 | −0.4 (3) |
| C4—C5—C6—C1 | −1.6 (3) | C16—C17—C18—C21 | 179.60 (17) |
| C4—C5—C6—C9 | 177.59 (18) | O1—C10—N1—C1 | −174.15 (17) |
| C2—C1—C6—C5 | −0.8 (3) | O1—C10—N1—C11 | 0.4 (3) |
| N1—C1—C6—C5 | 178.83 (15) | C2—C1—N1—C10 | −117.52 (19) |
| C2—C1—C6—C9 | −179.92 (17) | C6—C1—N1—C10 | 62.9 (2) |
| N1—C1—C6—C9 | −0.3 (3) | C2—C1—N1—C11 | 68.1 (2) |
| N1—C11—C12—N2 | 175.09 (13) | C6—C1—N1—C11 | −111.52 (18) |
| C18—C13—C14—C15 | 1.2 (3) | C12—C11—N1—C10 | −83.4 (2) |
| N2—C13—C14—C15 | −175.77 (15) | C12—C11—N1—C1 | 91.09 (18) |
| C18—C13—C14—C19 | −179.60 (17) | C18—C13—N2—C12 | 106.18 (18) |
| N2—C13—C14—C19 | 3.4 (2) | C14—C13—N2—C12 | −76.74 (19) |
| C13—C14—C15—C16 | −0.4 (3) | C11—C12—N2—C13 | −75.89 (18) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···Cl1 | 0.92 | 2.23 | 3.0585 (14) | 149 |
| N2—H2*B*···Cl1$^{i}$ | 0.92 | 2.17 | 3.0531 (14) | 161 |

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