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2-Amino-5-(1*H*-tetrazol-5-yl)pyridinium chloride

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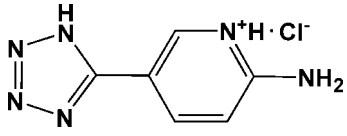
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.125; data-to-parameter ratio = 16.4.

In the title salt, $C_6H_7N_6^+\cdot Cl^-$, there are two organic cations with similar conformations and two chloride anions in the asymmetric unit. The pyridine and tetrazole rings are essentially coplanar in each cation, with dihedral angles of 4.94 (15) and 5.41 (14)°. The pyridine N atoms are protonated. The crystal packing is stabilized by N—H···N and N—H···Cl hydrogen bonds, forming an infinite sheets parallel to the (101).

Related literature

For uses of tetrazole derivatives, see: Dai & Fu (2008); Wang *et al.* (2005); Wen (2008); Xiong *et al.* (2002).



Experimental

Crystal data

$C_6H_7N_6^+\cdot Cl^-$
M_r = 198.63
Monoclinic, $P2_1/c$
a = 14.043 (3) Å
b = 13.238 (3) Å
c = 9.5766 (19) Å
β = 109.35 (3)°
V = 1679.7 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 298 (2) K
0.45 × 0.25 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.859, T_{max} = 0.920
16820 measured reflections
3855 independent reflections
3123 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.125
S = 1.11
3855 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N5^{i}	0.86	2.59	3.317 (2)	143
N1—H1···N6^{i}	0.86	2.04	2.894 (2)	171
N2—H2A···N5^{i}	0.86	2.15	2.972 (3)	160
N7—H7···N11^{ii}	0.86	2.57	3.304 (2)	144
N7—H7···N12^{ii}	0.86	2.06	2.913 (2)	169
N8—H8A···N11^{ii}	0.86	2.20	3.024 (3)	160
N2—H2B···Cl1^{iii}	0.86	2.36	3.2187 (18)	177
N3—H3A···Cl2^{i}	0.86	2.17	3.0047 (19)	165
N8—H8B···Cl2^{iv}	0.86	2.39	3.2432 (18)	172
N9—H9A···Cl1^{v}	0.86	2.18	3.0031 (18)	160

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

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: BH2196).

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supplementary materials

Acta Cryst. (2008). E**64**, o2232 [**doi:10.1107/S1600536808031164**]

2-Amino-5-(1*H*-tetrazol-5-yl)pyridinium chloride

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Comment

Tetrazole derivatives have found a 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 (Wang *et al.*, 2005; Xiong *et al.*, 2002; Wen, 2008; Dai & Fu, 2008). We report here the crystal structure of the title salt (Fig. 1).

The title compound contains two organic cations with similar conformation and two Cl^- ions in the asymmetric unit. The pyridine N atoms are protonated. The pyridine rings and tetrazole rings are nearly coplanar and are twisted from each other by a dihedral angle of only 4.94 (15) and 5.41 (14)°. The packing of ions is stabilized by N—H···N and N—H···Cl hydrogen bonds, to form an infinite two-dimensional layers parallel to the (1 0 1) plane in the crystal (Table 1 and Fig. 2).

Experimental

2-Amino-5-cyanopyridine (30 mmol), NaN_3 (45 mmol), NH_4Cl (33 mmol) and DMF (50 ml) were mixed in a flask under nitrogen atmosphere, and the mixture stirred at 383 K for 20 h. The resulting solution was then poured into ice-water (100 ml), and a white solid was obtained after adding hydrochloric acid (6 *M*) until pH=6. The precipitate was filtered and washed with distilled water. Colourless block-shaped crystals suitable for X-ray analysis were obtained from the crude product by slow evaporation of an ethanol/hydrochloric acid (50:1 *v*/*v*) solution.

Refinement

All H atoms were fixed geometrically and treated as riding to their carrier atoms, with C—H = 0.93 Å (aromatic) and N—H = 0.86 Å, and with $U_{iso}(H) = 1.2U_{eq}$(carrier atom).

Figures

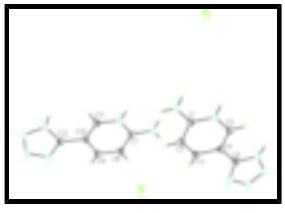

Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

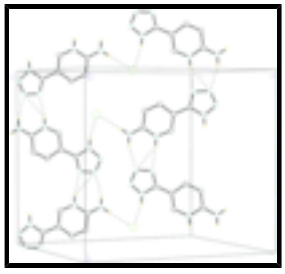

Fig. 2. The crystal packing of the title compound viewed along the *c* axis, showing the two-dimensional hydrogen bonds network. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

2-Amino-5-(1*H*-tetrazol-5-yl)pyridinium chloride

Crystal data

$C_6H_7N_6^+ \cdot Cl^-$	F_{000} = 816
M_r = 198.63	D_x = 1.571 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3690 reflections
a = 14.043 (3) Å	θ = 2.3–27.5º
b = 13.238 (3) Å	μ = 0.41 mm^{-1}
c = 9.5766 (19) Å	T = 298 (2) K
β = 109.35 (3)º	Block, colorless
V = 1679.7 (6) Å^3	0.45 × 0.25 × 0.20 mm
Z = 8	

Data collection

Rigaku Mercury2 diffractometer	3855 independent reflections
Radiation source: fine-focus sealed tube	3123 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 27.5º
T = 298(2) K	θ_{min} = 2.7º
ω scans	h = −18→18
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	k = −17→17
T_{min} = 0.859, T_{max} = 0.920	l = −12→12
16820 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
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.125	$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 0.4684P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.12	$(\Delta/\sigma)_{max} < 0.001$
3855 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
235 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.56207 (12)	0.65987 (12)	0.17350 (18)	0.0344 (4)
H1	0.5639	0.7245	0.1662	0.041*
N3	0.36346 (13)	0.52444 (13)	0.37792 (19)	0.0368 (4)
H3A	0.3600	0.5892	0.3818	0.044*
C1	0.62505 (14)	0.60404 (14)	0.1236 (2)	0.0313 (4)
N2	0.68458 (13)	0.64965 (13)	0.0611 (2)	0.0413 (4)
H2A	0.6831	0.7143	0.0523	0.050*
H2B	0.7247	0.6146	0.0292	0.050*
N6	0.40734 (13)	0.37577 (12)	0.33322 (19)	0.0382 (4)
N4	0.31050 (14)	0.45963 (13)	0.4305 (2)	0.0428 (4)
C6	0.42266 (14)	0.47298 (14)	0.3184 (2)	0.0310 (4)
N5	0.33724 (14)	0.37053 (13)	0.4030 (2)	0.0430 (4)
C4	0.49237 (14)	0.51714 (13)	0.2516 (2)	0.0304 (4)
C2	0.62316 (14)	0.49827 (14)	0.1406 (2)	0.0333 (4)
H2	0.6657	0.4574	0.1086	0.040*
C3	0.55896 (15)	0.45611 (14)	0.2039 (2)	0.0336 (4)
H3	0.5587	0.3864	0.2160	0.040*
C5	0.49636 (15)	0.61909 (14)	0.2344 (2)	0.0337 (4)
H5	0.4537	0.6610	0.2646	0.040*
N7	0.92034 (13)	0.39582 (12)	0.30105 (18)	0.0364 (4)
H7	0.9131	0.4604	0.2998	0.044*
N9	1.13591 (12)	0.26242 (13)	0.12521 (19)	0.0367 (4)
H9A	1.1409	0.3272	0.1246	0.044*
N8	0.80738 (13)	0.38416 (13)	0.4302 (2)	0.0422 (4)
H8A	0.8043	0.4490	0.4319	0.051*
H8B	0.7726	0.3485	0.4708	0.051*
C7	0.86565 (14)	0.33931 (15)	0.3650 (2)	0.0329 (4)
N10	1.19013 (14)	0.19768 (13)	0.0747 (2)	0.0425 (4)
N12	1.08698 (13)	0.11357 (12)	0.15986 (19)	0.0374 (4)
C12	1.07262 (14)	0.21051 (14)	0.1769 (2)	0.0311 (4)
N11	1.16049 (14)	0.10833 (13)	0.0959 (2)	0.0429 (4)
C10	1.00037 (14)	0.25408 (14)	0.2397 (2)	0.0304 (4)
C9	0.94263 (15)	0.19202 (14)	0.3023 (2)	0.0339 (4)
H9	0.9504	0.1222	0.3025	0.041*
C11	0.98593 (16)	0.35597 (14)	0.2389 (2)	0.0363 (4)
H11	1.0211	0.3983	0.1957	0.044*
C8	0.87624 (15)	0.23312 (15)	0.3618 (2)	0.0337 (4)
H8	0.8378	0.1915	0.4004	0.040*
Cl1	0.84188 (4)	0.97883 (4)	0.45292 (7)	0.04632 (17)

Cl2	0.65611 (4)	0.24380 (4)	0.05567 (6)	0.04478 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0407 (9)	0.0214 (8)	0.0500 (10)	0.0034 (7)	0.0270 (8)	0.0030 (7)
N3	0.0440 (10)	0.0261 (8)	0.0491 (10)	−0.0020 (7)	0.0273 (8)	−0.0008 (7)
C1	0.0332 (10)	0.0274 (9)	0.0362 (10)	0.0024 (7)	0.0157 (8)	0.0009 (7)
N2	0.0483 (11)	0.0305 (9)	0.0589 (11)	0.0027 (7)	0.0363 (9)	0.0028 (8)
N6	0.0456 (10)	0.0267 (8)	0.0507 (10)	−0.0021 (7)	0.0270 (8)	0.0009 (7)
N4	0.0518 (11)	0.0327 (9)	0.0561 (11)	−0.0061 (8)	0.0343 (9)	−0.0012 (8)
C6	0.0334 (10)	0.0265 (9)	0.0358 (10)	−0.0001 (7)	0.0152 (8)	−0.0004 (7)
N5	0.0529 (11)	0.0299 (9)	0.0581 (11)	−0.0034 (8)	0.0346 (9)	−0.0008 (8)
C4	0.0313 (9)	0.0259 (9)	0.0368 (10)	−0.0001 (7)	0.0149 (8)	0.0011 (7)
C2	0.0341 (10)	0.0284 (9)	0.0419 (11)	0.0044 (8)	0.0186 (8)	−0.0002 (8)
C3	0.0368 (10)	0.0238 (9)	0.0422 (11)	0.0017 (7)	0.0158 (8)	−0.0001 (8)
C5	0.0358 (10)	0.0281 (9)	0.0437 (11)	0.0035 (8)	0.0218 (8)	0.0018 (8)
N7	0.0468 (10)	0.0227 (8)	0.0486 (10)	0.0051 (7)	0.0279 (8)	0.0046 (7)
N9	0.0410 (10)	0.0264 (8)	0.0510 (10)	0.0036 (7)	0.0265 (8)	0.0027 (7)
N8	0.0473 (11)	0.0334 (9)	0.0586 (11)	0.0043 (8)	0.0345 (9)	0.0034 (8)
C7	0.0328 (10)	0.0327 (10)	0.0353 (10)	0.0024 (8)	0.0143 (8)	0.0018 (8)
N10	0.0473 (11)	0.0343 (9)	0.0569 (11)	0.0066 (8)	0.0320 (9)	0.0036 (8)
N12	0.0431 (10)	0.0293 (8)	0.0477 (10)	0.0038 (7)	0.0256 (8)	0.0015 (7)
C12	0.0348 (10)	0.0266 (9)	0.0339 (9)	0.0021 (7)	0.0142 (8)	0.0033 (7)
N11	0.0489 (11)	0.0344 (10)	0.0560 (11)	0.0059 (8)	0.0316 (9)	0.0010 (8)
C10	0.0328 (10)	0.0282 (9)	0.0325 (9)	0.0027 (7)	0.0139 (8)	0.0015 (7)
C9	0.0375 (10)	0.0236 (9)	0.0431 (11)	0.0009 (7)	0.0168 (9)	0.0031 (8)
C11	0.0427 (11)	0.0296 (10)	0.0446 (11)	0.0017 (8)	0.0253 (9)	0.0037 (8)
C8	0.0344 (10)	0.0298 (10)	0.0409 (10)	−0.0010 (8)	0.0178 (8)	0.0040 (8)
Cl1	0.0567 (3)	0.0300 (3)	0.0626 (4)	−0.0067 (2)	0.0336 (3)	−0.0052 (2)
Cl2	0.0502 (3)	0.0282 (3)	0.0624 (4)	0.0046 (2)	0.0273 (3)	0.0040 (2)

Geometric parameters (Å, °)

N1—C1	1.355 (2)	N7—C7	1.355 (2)
N1—C5	1.356 (2)	N7—C11	1.358 (2)
N1—H1	0.8600	N7—H7	0.8600
N3—N4	1.338 (2)	N9—N10	1.339 (2)
N3—C6	1.340 (2)	N9—C12	1.341 (2)
N3—H3A	0.8600	N9—H9A	0.8600
C1—N2	1.325 (2)	N8—C7	1.323 (2)
C1—C2	1.411 (3)	N8—H8A	0.8600
N2—H2A	0.8600	N8—H8B	0.8600
N2—H2B	0.8600	C7—C8	1.415 (3)
N6—C6	1.320 (2)	N10—N11	1.292 (2)
N6—N5	1.362 (2)	N12—C12	1.318 (2)
N4—N5	1.291 (2)	N12—N11	1.365 (2)
C6—C4	1.457 (2)	C12—C10	1.459 (2)
C4—C5	1.363 (3)	C10—C11	1.364 (3)

C4—C3	1.421 (3)	C10—C9	1.419 (3)
C2—C3	1.361 (3)	C9—C8	1.357 (3)
C2—H2	0.9300	C9—H9	0.9300
C3—H3	0.9300	C11—H11	0.9300
C5—H5	0.9300	C8—H8	0.9300
C1—N1—C5	123.42 (16)	C7—N7—C11	123.49 (17)
C1—N1—H1	118.3	C7—N7—H7	118.3
C5—N1—H1	118.3	C11—N7—H7	118.3
N4—N3—C6	109.55 (16)	N10—N9—C12	109.34 (16)
N4—N3—H3A	125.2	N10—N9—H9A	125.3
C6—N3—H3A	125.2	C12—N9—H9A	125.3
N2—C1—N1	119.62 (17)	C7—N8—H8A	120.0
N2—C1—C2	122.91 (17)	C7—N8—H8B	120.0
N1—C1—C2	117.47 (16)	H8A—N8—H8B	120.0
C1—N2—H2A	120.0	N8—C7—N7	119.82 (18)
C1—N2—H2B	120.0	N8—C7—C8	122.80 (18)
H2A—N2—H2B	120.0	N7—C7—C8	117.36 (17)
C6—N6—N5	105.81 (16)	N11—N10—N9	106.13 (15)
N5—N4—N3	105.89 (15)	C12—N12—N11	105.95 (16)
N6—C6—N3	107.67 (16)	N12—C12—N9	107.80 (16)
N6—C6—C4	126.56 (17)	N12—C12—C10	126.32 (17)
N3—C6—C4	125.76 (17)	N9—C12—C10	125.87 (17)
N4—N5—N6	111.08 (16)	N10—N11—N12	110.78 (16)
C5—C4—C3	117.77 (17)	C11—C10—C9	118.05 (17)
C5—C4—C6	120.74 (17)	C11—C10—C12	120.76 (17)
C3—C4—C6	121.49 (16)	C9—C10—C12	121.19 (17)
C3—C2—C1	119.91 (17)	C8—C9—C10	120.89 (17)
C3—C2—H2	120.0	C8—C9—H9	119.6
C1—C2—H2	120.0	C10—C9—H9	119.6
C2—C3—C4	120.90 (17)	N7—C11—C10	120.20 (17)
C2—C3—H3	119.5	N7—C11—H11	119.9
C4—C3—H3	119.5	C10—C11—H11	119.9
N1—C5—C4	120.49 (17)	C9—C8—C7	119.93 (17)
N1—C5—H5	119.8	C9—C8—H8	120.0
C4—C5—H5	119.8	C7—C8—H8	120.0
C5—N1—C1—N2	177.74 (19)	C11—N7—C7—N8	176.37 (19)
C5—N1—C1—C2	−1.8 (3)	C11—N7—C7—C8	−1.9 (3)
C6—N3—N4—N5	0.0 (2)	C12—N9—N10—N11	−0.2 (2)
N5—N6—C6—N3	0.1 (2)	N11—N12—C12—N9	−0.2 (2)
N5—N6—C6—C4	179.20 (18)	N11—N12—C12—C10	179.35 (18)
N4—N3—C6—N6	0.0 (2)	N10—N9—C12—N12	0.3 (2)
N4—N3—C6—C4	−179.15 (19)	N10—N9—C12—C10	−179.30 (18)
N3—N4—N5—N6	0.1 (2)	N9—N10—N11—N12	0.1 (2)
C6—N6—N5—N4	−0.1 (2)	C12—N12—N11—N10	0.1 (2)
N6—C6—C4—C5	175.7 (2)	N12—C12—C10—C11	−173.8 (2)
N3—C6—C4—C5	−5.4 (3)	N9—C12—C10—C11	5.6 (3)
N6—C6—C4—C3	−4.9 (3)	N12—C12—C10—C9	5.7 (3)
N3—C6—C4—C3	173.99 (19)	N9—C12—C10—C9	−174.82 (19)

N2—C1—C2—C3	−178.97 (19)	C11—C10—C9—C8	−1.1 (3)
N1—C1—C2—C3	0.6 (3)	C12—C10—C9—C8	179.35 (18)
C1—C2—C3—C4	0.9 (3)	C7—N7—C11—C10	−0.6 (3)
C5—C4—C3—C2	−1.2 (3)	C9—C10—C11—N7	2.1 (3)
C6—C4—C3—C2	179.48 (19)	C12—C10—C11—N7	−178.31 (18)
C1—N1—C5—C4	1.6 (3)	C10—C9—C8—C7	−1.4 (3)
C3—C4—C5—N1	0.0 (3)	N8—C7—C8—C9	−175.3 (2)
C6—C4—C5—N1	179.36 (18)	N7—C7—C8—C9	2.9 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N5^{i}	0.86	2.59	3.317 (2)	143
N1—H1···N6^{i}	0.86	2.04	2.894 (2)	171
N2—H2A···N5^{i}	0.86	2.15	2.972 (3)	160
N7—H7···N11^{ii}	0.86	2.57	3.304 (2)	144
N7—H7···N12^{ii}	0.86	2.06	2.913 (2)	169
N8—H8A···N11^{ii}	0.86	2.20	3.024 (3)	160
N2—H2B···Cl1^{iii}	0.86	2.36	3.2187 (18)	177
N3—H3A···Cl2^{i}	0.86	2.17	3.0047 (19)	165
N8—H8B···Cl2^{iv}	0.86	2.39	3.2432 (18)	172
N9—H9A···Cl1^{v}	0.86	2.18	3.0031 (18)	160

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

Fig. 1

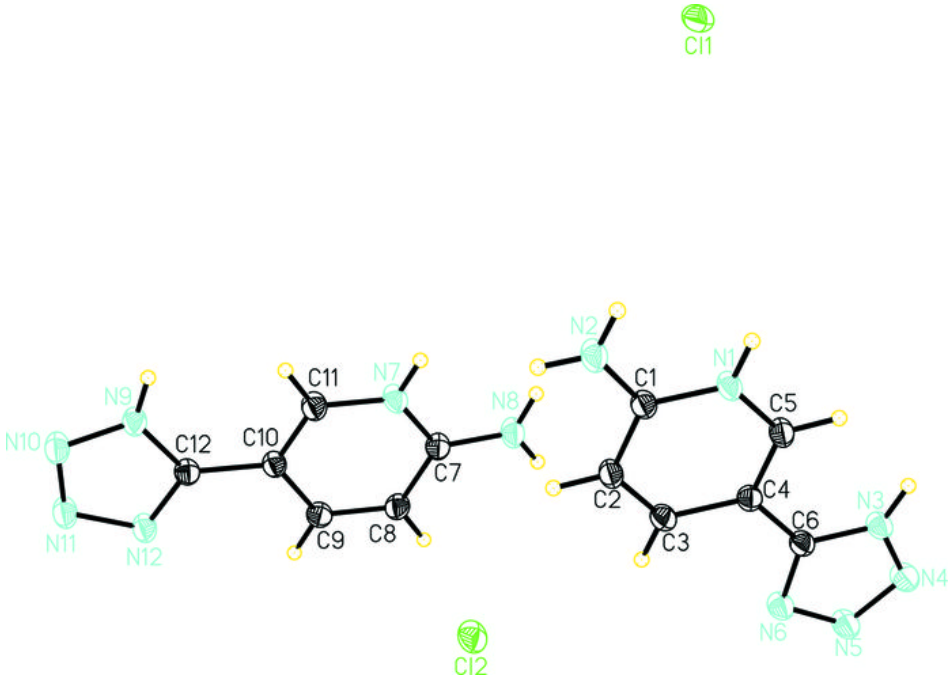
Cl1
N2
C1
N1
C5
N8
C11
N7
N9
C12
C10
C7
N10
C2
C4
N3
C6
C3
N11
N12
C9
C8
N4
N6
N5
Cl2

Fig. 2