2-Amino-3-hydroxy-4-phenylthiazolium chloride: π-stacked hydrogen-bonded chains of edge-fused $R_4^2(11)$ rings

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In the title compound, $C_9H_9N_2OS^+\cdot Cl^-$, the cations exhibit amidinium-type delocalization of the positive charge. The ions are linked by one O—H···Cl hydrogen bond and two N—H···Cl hydrogen bonds into chains of edge-fused $R_4^2(11)$ rings. The chains are linked into sheets by a π–π stacking interaction.

Comment

Masaki *et al.* (1966) reported the preparation of 3-hydroxy-4-phenyl-2(3*H*)-thiazolimine, from the condensation reaction of the oxime of bromomethyl phenyl ketone, BrCH₂C(Ph)=NOH, with barium thiocyanate, and these authors characterized the heterocycle as the picrate salt. The mass spectrum of the title compound, the hydrochloride salt (I), was reported by Entenmann (1975) as exhibiting a significant peak assigned to $[M - 16]^+$, corresponding to the loss of an O atom, which suggested that the O atom was not protonated. In solution, the picrate salt was reported to give a positive phenol test with iron(III) chloride. However, in neither report was the constitution of the cation definitively established; in particular, neither report gave any indication of the solid-state structure, and hence the determination now reported was undertaken.

Compound (I) consists of an ion pair containing a short O—H···Cl hydrogen bond (Fig. 1, and Tables 1 and 2). In the cation, the heterocyclic ring is planar, as expected, and the dihedral angle between this plane and the plane of the benzene ring is 41.9 (2)°. There are considerable differences between the corresponding pairs of exocyclic angles at atoms C2, N3 and C4. The very small interbond angle at atom S1 is also notable. The C2—N2 and C2—N3 bonds are similar in

length and both are significantly shorter than the N3—C4 bond. The bond orders, calculated using the recent recalibration by Kotelevskii & Prezhdo (2001) of the original equation relating bond order to bond length (Gordy, 1947), for the C2—N2, C2—N3 and C3—N4 bonds are 1.77, 1.72 and 1.33, respectively, suggesting amidinium-type delocalization of the positive charge between atoms N2 and N3, as indicated in the scheme below.

(I)
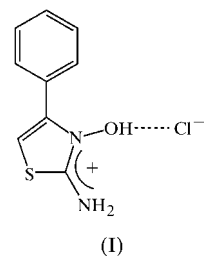
The amine group acts as a double donor in N—H···Cl hydrogen bonds involving two different anions (Table 2). In the shorter and more nearly linear of these two interactions, amine atom N2 acts as a hydrogen-bond donor, *via* atom H2*A*, to atom Cl1 at (*x*, *y* − 1, *z*), so generating by translation a $C_2^1(7)$ chain (Bernstein *et al.*, 1995) running parallel to the [010] direction (Fig. 2). Four chains of this type pass through each unit cell and these chains are linked into pairs by the second N—H···Cl hydrogen bond. In this interaction, atom N2 acts as a hydrogen-bond donor, this time *via* atom H2*B*, to atom Cl1 at ($\frac{1}{2} - x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$), so forming a $C_2^1(4)$ chain generated by the 2_1 screw axis along ($\frac{1}{4}$, *y*, $\frac{1}{4}$) (Fig. 2). The combination of the $C_2^1(4)$ and $C_2^1(7)$ motifs then produces a chain of edge-fused $R_4^2(11)$ rings. This chain of rings, containing the 2_1 axis along ($\frac{1}{4}$, *y*, $\frac{1}{4}$), lies within the domain $0 < x < \frac{1}{2}$, and a second chain, related to the first by inversion
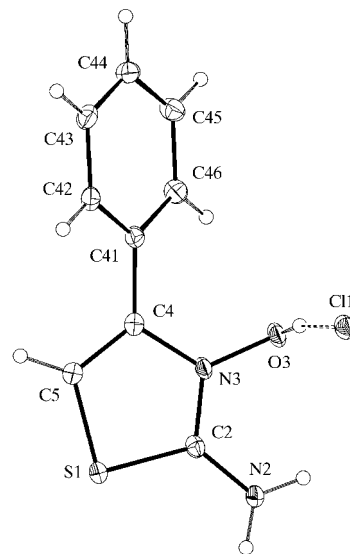
Figure 1
The independent ions in (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

organic compounds

and containing the 2_1 axis along $(\frac{3}{4}, y, \frac{3}{4})$, lies in the domain $\frac{1}{2} < x < 1$.

The only direction-specific interaction between adjacent chains of rings is a weak π–π stacking interaction between the heterocyclic rings of the cations related by a centre of symmetry. These rings are parallel, with an interplanar spacing of 3.631 (2) Å. The ring-centroid separation is 3.778 (2) Å, corresponding to a centroid offset of 1.044 (2) Å. These cations at (x, y, z) and $(1 - x, 1 - y, 1 - z)$ lie, respectively, in the chains of rings along $(\frac{1}{4}, y, \frac{1}{4})$ and $(\frac{3}{4}, -y, \frac{3}{4})$, so that propagation of this stacking interaction links the chain into a $(10\bar{1})$ sheet. However, there are no π–π stacking interactions involving the phenyl ring, nor are there any C—H$\cdots\pi$(arene) hydrogen bonds.

As well as acting as a threefold acceptor of hydrogen bonds, the anion at (x, y, z) also forms a short contact with the S atom of the molecule at $(1 - x, 1 - y, 1 - z)$. This S$\cdots$Cl distance is 3.3275 (7) Å, somewhat less than the sum of the van der Waals radii (3.50 Å; Bondi, 1964). The overall coordination polyhedron at atom Cl1, including the secondary bond (Alcock, 1972) involving the S atom, takes the form of a distorted trigonal bipyramid of VSEPR (valence-shell electron-pair repulsion) type MX_4E (Gillespie, 1972; Gillespie & Hargittai, 1991; Burdett, 1997), where X represents a bonding pair of electrons at the central atom M (here M = Cl) and E represents the equatorial lone pair of non-bonding electrons (Fig. 3). The angles at atom Cl1 are as follows: O3$\cdots$Cl1$\cdots$N2* = 110.79 (5)°, O3$\cdots$Cl1$\cdots$N2# = 78.64 (5)°, O3$\cdots$Cl1$\cdots$S1$ = 91.92 (3)°, N2*$\cdots$Cl1$\cdots$N2# = 92.69 (5)°,
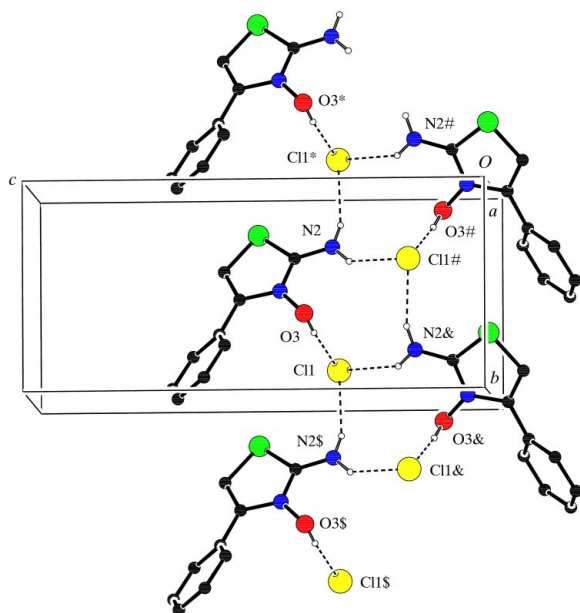

Figure 2
Part of the crystal structure of (I), showing the formation of a chain of edge-fused $R_4^2(11)$ rings along the b axis. For clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*), a hash (#), a dollar sign ($) or an ampersand (&) are at the symmetry positions $(x, y - 1, z)$, $(\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z)$, $(x, y + 1, z)$ and $(\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z)$, respectively.
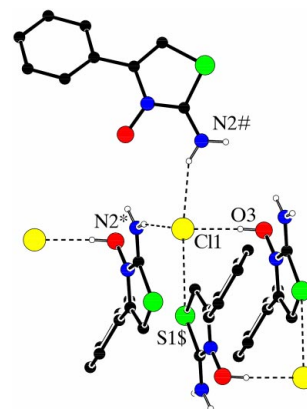

Figure 3
Part of the crystal structure of (I), showing the coordination at the anion. For clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (*), a hash (#) or a dollar sign ($) are at the symmetry positions $(x, y + 1, z)$, $(\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z)$ and $(1 - x, 1 - y, 1 - z)$, respectively.

N2*$\cdots$Cl1$\cdots$S1$ = 109.99 (4)° and N2#$\cdots$Cl1$\cdots$S1$ = 157.30 (4)°, where atoms marked with an asterisk (*), a hash (#) or a dollar sign ($) are at the symmetry positions $(x, y + 1, z)$, $(\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z)$ and $(1 - x, 1 - y, 1 - z)$, respectively.

Experimental

The neutral heterocycle 3-hydroxy-2-imino-4-phenylthiazole was prepared according to the method reported by Masaki *et al.* (1966). The hydrochloride salt, (I), was prepared by treating the neutral heterocycle in ethanol solution with aqueous HCl (6 mol dm^{-3}) and was recrystallized from ethanol. Compound (I) slowly darkened on heating and decomposed before melting.

Crystal data

$C_9H_9N_2OS^+\cdot Cl^-$	Mo $K\alpha$ radiation
$M_r = 228.69$	Cell parameters from 2247
Monoclinic, $P2_1/n$	reflections
$a = 9.2663 (5)$ Å	$\theta = 3.2$–$27.4°$
$b = 7.0716 (4)$ Å	$\mu = 0.55$ mm^{-1}
$c = 15.461 (1)$ Å	$T = 120 (2)$ K
$\beta = 90.194 (2)°$	Plate, colourless
$V = 1013.12 (10)$ Å^3	$0.32 \times 0.24 \times 0.12$ mm
$Z = 4$	
$D_x = 1.499$ Mg m^{-3}	

Data collection

Nonius KappaCCD diffractometer	1751 reflections with $I > 2\sigma(I)$
φ scans, and ω scans with κ offsets	$R_{int} = 0.067$
Absorption correction: multi-scan	$\theta_{max} = 27.4°$
(*SORTAV*; Blessing, 1995, 1997)	$h = -11 \rightarrow 11$
$T_{min} = 0.827$, $T_{max} = 0.934$	$k = -8 \rightarrow 9$
9736 measured reflections	$l = -19 \rightarrow 19$
2247 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.045$	$+ 0.159P]$
$wR(F^2) = 0.119$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
2247 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
128 parameters	$\Delta\rho_{min} = -0.41$ e Å^{-3}
H-atom parameters constrained	

organic compounds

Table 1
Selected geometric parameters (Å, °).

S1—C2	1.718 (2)	C5—S1	1.737 (2)
C2—N3	1.330 (3)	C2—N2	1.321 (3)
N3—C4	1.405 (3)	N3—O3	1.377 (2)
C4—C5	1.341 (3)	C4—C41	1.476 (3)
S1—C2—N3	110.64 (15)	N2—C2—N3	123.58 (19)
C2—N3—C4	116.04 (18)	C2—N3—O3	119.73 (17)
N3—C4—C5	110.03 (19)	O3—N3—C4	124.22 (17)
C4—C5—S1	113.00 (17)	N3—C4—C41	121.81 (19)
C5—S1—C2	90.29 (11)	C5—C4—C41	128.2 (2)
S1—C2—N2	125.72 (17)		
N3—C4—C41—C42	−139.2 (2)	N3—C4—C41—C46	43.1 (3)
C5—C4—C41—C42	40.7 (3)	C5—C4—C41—C46	−136.9 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O3—H3$\cdots$Cl1	0.84	2.11	2.929 (2)	167
N2—H2$A\cdots$Cl1[i]	0.88	2.30	3.131 (2)	157
N2—H2$B\cdots$Cl1[ii]	0.88	2.46	3.217 (2)	145

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

All H atoms were located from difference maps and subsequently treated as riding atoms, with C—H distances of 0.95 Å, N—H distances of 0.88 Å and an O—H distance of 0.84 Å.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PRPKAPPA* (Ferguson, 1999).

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2-Amino-3-hydroxy-4-phenylthiazolium chloride: *π*-stacked hydrogen-bonded chains of edge-fused *R*[_{\bf 4}^{\bf 2}](11) rings

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Computing details

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO*–SMN (Otwinowski & Minor, 1997); data reduction: *DENZO*–SMN; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

2-Amino-3-hydroxy-4-phenylthiazolium chloride

Crystal data

$C_9H_9N_2OS^+ \cdot Cl^-$	$F(000) = 472$
$M_r = 228.69$	$D_x = 1.499$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2247 reflections
$a = 9.2663$ (5) Å	$\theta = 3.2$–27.4°
$b = 7.0716$ (4) Å	$\mu = 0.55$ mm^{-1}
$c = 15.461$ (1) Å	$T = 120$ K
$\beta = 90.194$ (2)°	Plate, colourless
$V = 1013.12$ (10) Å^3	$0.32 \times 0.24 \times 0.12$ mm
$Z = 4$	

Data collection

KappaCCD diffractometer	9736 measured reflections
Radiation source: rotating anode	2247 independent reflections
Graphite monochromator	1751 reflections with $I > 2\sigma(I)$
φ scans, and ω scans with κ offsets	$R_{int} = 0.067$
Absorption correction: multi-scan (*SORTAV*; Blessing 1995, 1997)	$\theta_{max} = 27.4°$, $\theta_{min} = 3.2°$
	$h = -11 \rightarrow 11$
	$k = -8 \rightarrow 9$
$T_{min} = 0.827$, $T_{max} = 0.934$	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.045$	Secondary atom site location: difference Fourier map
$wR(F^2) = 0.119$	
$S = 1.04$	Hydrogen site location: inferred from neighbouring sites
2247 reflections	
128 parameters	H-atom parameters constrained
0 restraints	

$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 0.159P]$		$\Delta\rho_{max} = 0.53$ e Å^{-3}
where $P = (F_o^2 + 2F_c^2)/3$		$\Delta\rho_{min} = -0.41$ e Å^{-3}
$(\Delta/\sigma)_{max} = 0.001$		

Special details

Refinement. The space group $P2_1/n$ was uniquely assigned from the systematic absences.

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

	x	y	z	$U_{iso}*/U_{eq}$
S1	0.38910 (6)	0.22878 (8)	0.50432 (3)	0.02526 (19)
C2	0.3016 (2)	0.3484 (3)	0.42286 (13)	0.0216 (5)
N2	0.2959 (2)	0.2964 (3)	0.34083 (12)	0.0264 (4)
N3	0.24406 (19)	0.5079 (2)	0.45261 (11)	0.0217 (4)
O3	0.16664 (16)	0.6230 (2)	0.39757 (9)	0.0265 (4)
C4	0.2658 (2)	0.5452 (3)	0.54098 (13)	0.0229 (5)
C5	0.3437 (2)	0.4061 (3)	0.57711 (14)	0.0256 (5)
C41	0.2075 (2)	0.7165 (3)	0.58266 (14)	0.0221 (5)
C42	0.2927 (2)	0.8124 (3)	0.64260 (13)	0.0251 (5)
C43	0.2390 (2)	0.9687 (3)	0.68564 (14)	0.0274 (5)
C44	0.1001 (2)	1.0312 (3)	0.66872 (14)	0.0301 (6)
C45	0.0152 (3)	0.9379 (3)	0.60891 (15)	0.0307 (5)
C46	0.0680 (3)	0.7809 (3)	0.56603 (15)	0.0272 (5)
Cl1	0.39250 (6)	0.87277 (8)	0.33083 (3)	0.02775 (19)
H2A	0.3358	0.1893	0.3245	0.032*
H2B	0.2523	0.3689	0.3026	0.032*
H3	0.2207	0.7086	0.3785	0.040*
H5	0.3713	0.4046	0.6363	0.031*
H42	0.3882	0.7703	0.6540	0.030*
H43	0.2974	1.0331	0.7268	0.033*
H44	0.0632	1.1385	0.6983	0.036*
H45	−0.0798	0.9815	0.5972	0.037*
H46	0.0090	0.7169	0.5251	0.033*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0326 (3)	0.0234 (3)	0.0197 (3)	0.0063 (2)	−0.0034 (2)	0.0027 (2)
C2	0.0218 (11)	0.0206 (11)	0.0225 (11)	−0.0007 (9)	−0.0049 (8)	0.0026 (9)
N2	0.0360 (11)	0.0237 (10)	0.0195 (9)	0.0058 (9)	−0.0073 (8)	0.0002 (8)
N3	0.0254 (9)	0.0196 (10)	0.0201 (9)	0.0030 (8)	−0.0068 (7)	0.0033 (7)
O3	0.0310 (9)	0.0235 (9)	0.0247 (8)	0.0042 (7)	−0.0097 (7)	0.0051 (6)
C4	0.0243 (11)	0.0245 (12)	0.0199 (10)	−0.0007 (9)	−0.0013 (8)	0.0022 (9)
C5	0.0303 (12)	0.0262 (12)	0.0204 (11)	0.0038 (10)	−0.0012 (9)	0.0004 (9)
C41	0.0260 (11)	0.0199 (11)	0.0203 (10)	−0.0001 (9)	−0.0009 (8)	0.0022 (8)
C42	0.0273 (11)	0.0282 (12)	0.0196 (11)	0.0009 (10)	−0.0017 (9)	0.0041 (9)
C43	0.0336 (13)	0.0292 (13)	0.0196 (11)	−0.0032 (10)	−0.0022 (9)	−0.0013 (9)
C44	0.0398 (14)	0.0238 (13)	0.0267 (12)	0.0028 (10)	0.0052 (10)	−0.0012 (9)

C45	0.0296 (12)	0.0283 (13)	0.0342 (13)	0.0059 (11)	0.0001 (10)	0.0008 (10)
C46	0.0271 (12)	0.0257 (13)	0.0289 (12)	−0.0014 (10)	−0.0037 (10)	−0.0006 (10)
Cl1	0.0331 (3)	0.0245 (3)	0.0255 (3)	0.0016 (2)	−0.0097 (2)	0.0011 (2)

Geometric parameters (Å, º)

S1—C2	1.718 (2)	C41—C42	1.392 (3)
C2—N3	1.330 (3)	C41—C46	1.393 (3)
N3—C4	1.405 (3)	C42—C43	1.383 (3)
C4—C5	1.341 (3)	C42—H42	0.95
C5—S1	1.737 (2)	C43—C44	1.385 (3)
C2—N2	1.321 (3)	C43—H43	0.95
N3—O3	1.377 (2)	C44—C45	1.380 (3)
C4—C41	1.476 (3)	C44—H44	0.95
N2—H2A	0.88	C45—C46	1.383 (3)
N2—H2B	0.88	C45—H45	0.95
O3—H3	0.84	C46—H46	0.95
C5—H5	0.95		
S1—C2—N3	110.64 (15)	C42—C41—C4	118.9 (2)
C2—N3—C4	116.04 (18)	C46—C41—C4	121.9 (2)
N3—C4—C5	110.03 (19)	C43—C42—C41	120.4 (2)
C4—C5—S1	113.00 (17)	C43—C42—H42	119.8
C5—S1—C2	90.29 (11)	C41—C42—H42	119.8
S1—C2—N2	125.72 (17)	C42—C43—C44	120.0 (2)
N2—C2—N3	123.58 (19)	C42—C43—H43	120.0
C2—N3—O3	119.73 (17)	C44—C43—H43	120.0
O3—N3—C4	124.22 (17)	C45—C44—C43	120.1 (2)
N3—C4—C41	121.81 (19)	C45—C44—H44	120.0
C5—C4—C41	128.2 (2)	C43—C44—H44	120.0
C2—N2—H2A	120.0	C44—C45—C46	120.2 (2)
C2—N2—H2B	120.0	C44—C45—H45	119.9
H2A—N2—H2B	120.0	C46—C45—H45	119.9
N3—O3—H3	109.5	C45—C46—C41	120.2 (2)
C4—C5—H5	123.5	C45—C46—H46	119.9
S1—C5—H5	123.5	C41—C46—H46	119.9
C42—C41—C46	119.2 (2)		
C5—S1—C2—N2	176.8 (2)	N3—C4—C41—C42	−139.2 (2)
C5—S1—C2—N3	−0.42 (16)	C5—C4—C41—C42	40.7 (3)
N2—C2—N3—O3	3.9 (3)	N3—C4—C41—C46	43.1 (3)
S1—C2—N3—O3	−178.81 (14)	C5—C4—C41—C46	−136.9 (2)
N2—C2—N3—C4	−177.18 (19)	C46—C41—C42—C43	0.6 (3)
S1—C2—N3—C4	0.2 (2)	C4—C41—C42—C43	−177.19 (19)
C2—N3—C4—C5	0.3 (3)	C41—C42—C43—C44	−0.4 (3)
O3—N3—C4—C5	179.21 (18)	C42—C43—C44—C45	0.0 (3)
C2—N3—C4—C41	−179.73 (19)	C43—C44—C45—C46	0.4 (4)
O3—N3—C4—C41	−0.8 (3)	C44—C45—C46—C41	−0.2 (3)

N3—C4—C5—S1	−0.6 (2)	C42—C41—C46—C45	−0.2 (3)
C41—C4—C5—S1	179.41 (18)	C4—C41—C46—C45	177.46 (19)
C2—S1—C5—C4	0.61 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···Cl1	0.84	2.11	2.929 (2)	167
N2—H2*A*···Cl1[i]	0.88	2.30	3.131 (2)	157
N2—H2*B*···Cl1[ii]	0.88	2.46	3.217 (2)	145

Symmetry codes: (i) x, $y-1$, z; (ii) $-x+1/2$, $y-1/2$, $-z+1/2$.