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Pyrimethaminium nicotinate monohydrate

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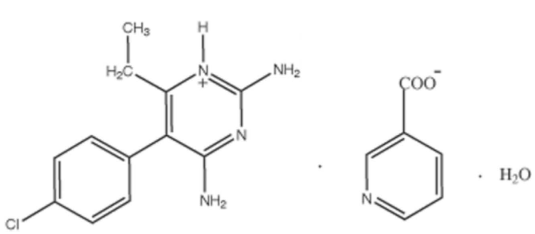
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.018 Å; R factor = 0.056; wR factor = 0.056; data-to-parameter ratio = 7.4.

In the title compound, $C_{12}H_{14}ClN_4^+\cdot C_6H_4NO_2^-\cdot H_2O$, the pyrimethamine molecule is protonated at one of the pyrimidine N atoms. The protonated N atom and 2-amino group of the cation interact with an adjacent nicotinate anion through a pair of N—H···O hydrogen bonds [graph set $R_2^2(8)$]. The cation, anion and water molecule form a hydrogen-bonded ring motif with graph-set notation $R_4^2(8)$. The crystal structure is further stabilized by N—H···O and O—H···O hydrogen bonds and π–π interactions [centroid–centroid distance = 3.637 (6) Å].

Related literature

For related literature, see: Bernstein *et al.* (1995); De *et al.* (1989); Devi *et al.* (2007); Olliaro (2001); Sansom *et al.* (1989); Sethuraman & Muthiah (2002).



Experimental

Crystal data

$C_{12}H_{14}ClN_4^+\cdot C_6H_4NO_2^-\cdot H_2O$
M_r = 389.84
Monoclinic, $P2_1$
a = 6.570 (2) Å
b = 16.055 (3) Å
c = 9.480 (2) Å
β = 99.19 (3)°
V = 987.1 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 120 (2) K
0.23 × 0.20 × 0.18 mm

Data collection

Philips PW1100 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.951, T_{max} = 0.961
1909 measured reflections
1807 independent reflections
617 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
1 standard reflections every 100 reflections intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.056
S = 0.85
1807 reflections
245 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), no Friedel pairs
Flack parameter: 0.12 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	1.83	2.686 (14)	175
N2—H2A···O1W	0.86	2.08	2.861 (15)	150
N2—H2B···O1	0.86	2.10	2.957 (13)	172
N4—H4A···O1^{i}	0.86	2.05	2.897 (14)	168
N4—H4B···O1W^{i}	0.86	2.26	3.031 (15)	150
O1W—H11W···N5^{i}	0.97 (9)	1.92 (9)	2.862 (16)	164 (10)
O1W—H12W···O2^{ii}	0.96 (10)	1.97 (10)	2.862 (14)	154 (9)

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

Data collection: *PW1100 Software* (Philips, 1978); cell refinement: *PW1100 Software*; data reduction: *PW1100 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2608).

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supplementary materials

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Pyrimethaminium nicotinate monohydrate

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Comment

Pyrimethamine [2,4-diamino-5-(*p*-chlorophenyl)-6-ethylpyrimidine] is an antifolate drug used in anti-malarial chemotherapy (Olliaro, 2001). The crystal structure of pyrimethamine (PMN) has been reported from our laboratory (Sethuraman & Muthiah, 2002) as have the structures of various protonated PMN salts (*e.g.* Devi *et al.*, 2007). As part of these ongoing studies, the synthesis and structure of the title compound, (I), is now described.

The asymmetric unit of (I) contains a protonated pyrimethaminium (PMN) cation, nicotinate anion and a water molecule (Fig. 1). The PMN is protonated at N1 as it is evident from the enhancement of the C—N—C from 116.3 (2)° in neutral PMN molecule A and 116.09 (18)° in molecule B (Sethuraman & Muthiah, 2002) to 119.9 (10)° in (I). The dihedral angle between the 2,4-diamino pyrimidine and *p*-chlorophenyl rings is 70.3 (6)°. The torsion angle C5—C6—C7—C8, which represents the deviation of the ethyl group from the pyrimidine ring is 77.6 (16)°. The values are close to the results of modeling studies of DHFR-PMN complexes (Sansom *et al.*, 1989). The C5—C9 bond length connecting the pyrimidine and phenyl ring in (I) is 1.472 (2) Å, in agreement with related structutres (De *et al.*, 1989). The protonated N1 cation interacts with the carboxylate group of the nicotinate ion *via* N—H···O hydrogen bonds forming cyclic hydrogen bonded ring motif represented by graph-set notation $R_2^2(8)$ (Bernstein *et al.*, 1995). The oxygen atom of the nicotinate anion bridges the 2-amino, 4-amino group of the PMN cation and water molecule forming a hydrogen bonded ring motif with graph-set notation $R_4^2(8)$. The frequently occurring $R_2^2(8)$ motif and $R_4^2(8)$ motif combine to form another motif, namely a DDA array (Fig. 2). Furthermore, the nicotinate anion and water molecule form a one dimensional supramolecular chain involving N—H···O and O—H···N hydrogen bonds (Fig. 3). π-π interactions between the aromatic rings are observed. The pyrimidine ring of PMN stacks with the nicotinate ring with a perpendicular separation of 3.551 Å, centroid-to-centroid distance of 3.637 (6)Å and a slip angle (the angle between the centroid-to-centroid vector and the normal to the plane) 19.05°.

Experimental

Hot methanolic solutions of pyrimethamine (62 mg) and nicotinic acid (31 mg) were mixed in a 1:1 ratio. The resultant mixture was warmed over a water bath for 15 minutes and kept at room temperature for crystallization. After a few days colourless blocks of (I) were obtained.

Refinement

The C– and N-bound hydrogen atoms were fixed geometrically (C—H = 0.93–0.96 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier). The water hydrogen atoms were located from a difference map and were refined with isotropic thermal parameters.

Figures

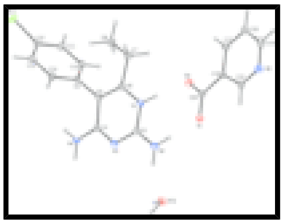

Fig. 1. View of the molecular structure of (I) with 10% probability displacement ellipsoids for the non-hydrogen atoms.

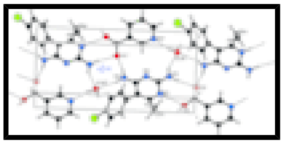

Fig. 2. A view of the hydrogen bonding network in (I). Symmetry code: (i) $-x + 1, y + 1/2, -z + 1$.

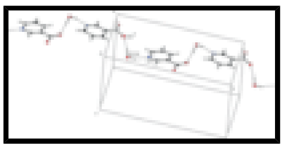

Fig. 3. One dimensional chain in (I) observed between the water molecules and nicotinate ion. Symmetry code: (ii) $x - 1, y, z$.

Pyrimethaminium nicotinate monohydrate

Crystal data

$C_{12}H_{14}ClN_4^+\cdot C_6H_4NO_2^-\cdot H_2O$	$F_{000} = 408$
$M_r = 389.84$	$D_x = 1.312$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
Hall symbol: P 2yb	Cell parameters from 25 reflections
$a = 6.570$ (2) Å	$\theta = 3.1–25.0$º
$b = 16.055$ (3) Å	$\mu = 0.22$ mm^{-1}
$c = 9.480$ (2) Å	$T = 120$ (2) K
$\beta = 99.19$ (3)º	Block, colourless
$V = 987.1$ (6) Å^3	0.23 × 0.20 × 0.18 mm
$Z = 2$	

Data collection

Philips PW1100 diffractometer	$R_{int} = 0.059$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.0$º
Monochromator: graphite	$\theta_{min} = 3.1$º
$T = 120(2)$ K	$h = -7\rightarrow7$
ω scans	$k = 0\rightarrow19$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = 0\rightarrow11$
$T_{min} = 0.951$, $T_{max} = 0.961$	1 standard reflections
1909 measured reflections	every 100 reflections
1807 independent reflections	intensity decay: none

617 reflections with $I > 2\sigma(I)$

Refinement

Refinement on F^2	Hydrogen site location: difmap and geom
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0004P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.056$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.85$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
1807 reflections	$\Delta\rho_{min} = -0.25$ e Å^{-3}
245 parameters	Extinction correction: none
4 restraints	Absolute structure: Flack (1983), no Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.12 (14)
Secondary atom site location: difference Fourier map	

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All e.s.d.'s are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating –*R*-factor-obs *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}
Cl1	1.3820 (6)	1.1235 (3)	1.0788 (4)	0.0826 (17)
N1	0.8723 (16)	0.7185 (6)	0.6563 (11)	0.045 (4)
N2	0.5768 (16)	0.6658 (6)	0.5248 (12)	0.068 (5)
N3	0.5978 (15)	0.8085 (6)	0.5670 (11)	0.048 (4)
N4	0.6373 (14)	0.9479 (6)	0.5999 (10)	0.043 (4)
C2	0.680 (2)	0.7323 (8)	0.5826 (14)	0.046 (5)
C4	0.7123 (18)	0.8716 (7)	0.6251 (12)	0.034 (5)
C5	0.9066 (17)	0.8607 (7)	0.7163 (12)	0.033 (4)
C6	0.9795 (18)	0.7822 (8)	0.7277 (12)	0.039 (5)
C7	1.181 (2)	0.7542 (8)	0.8174 (13)	0.059 (5)
C8	1.160 (2)	0.7484 (10)	0.9758 (14)	0.080 (6)
C9	1.0165 (17)	0.9297 (7)	0.7977 (13)	0.036 (4)
C10	1.2012 (18)	0.9616 (7)	0.7664 (13)	0.044 (5)
C11	1.309 (2)	1.0223 (8)	0.8517 (15)	0.058 (6)
C12	1.232 (2)	1.0511 (8)	0.9668 (16)	0.051 (5)

C13	1.052 (2)	1.0240 (8)	0.9967 (14)	0.055 (6)
C14	0.944 (2)	0.9633 (7)	0.9141 (13)	0.048 (5)
O1	0.7388 (16)	0.4955 (5)	0.5855 (10)	0.064 (4)
O2	1.0354 (14)	0.5657 (6)	0.6448 (10)	0.062 (4)
N5	1.042 (2)	0.2718 (7)	0.6972 (13)	0.069 (5)
C15	0.949 (2)	0.3422 (8)	0.6563 (14)	0.050 (5)
C16	1.0447 (18)	0.4212 (8)	0.6779 (11)	0.033 (4)
C17	1.252 (2)	0.4217 (9)	0.7387 (12)	0.051 (5)
C18	1.346 (2)	0.3473 (11)	0.7809 (14)	0.067 (6)
C19	1.235 (3)	0.2749 (9)	0.7587 (17)	0.071 (7)
C20	0.925 (2)	0.5006 (9)	0.6307 (14)	0.052 (6)
O1W	0.1720 (14)	0.6202 (7)	0.3881 (12)	0.068 (4)
H1	0.92590	0.66960	0.65760	0.0540*
H2A	0.45520	0.67150	0.47650	0.0810*
H2B	0.63200	0.61720	0.53600	0.0810*
H4A	0.51890	0.95490	0.54770	0.0510*
H4B	0.70710	0.99030	0.63570	0.0510*
H7A	1.28910	0.79350	0.80580	0.0710*
H7B	1.21960	0.70030	0.78420	0.0710*
H8A	1.05210	0.71010	0.98730	0.1190*
H8B	1.12810	0.80240	1.00990	0.1190*
H8C	1.28800	0.72920	1.02950	0.1190*
H10	1.25300	0.94190	0.68690	0.0520*
H11	1.43330	1.04290	0.83030	0.0690*
H13	0.99860	1.04630	1.07380	0.0660*
H14	0.81950	0.94450	0.93710	0.0570*
H15	0.81240	0.34010	0.61080	0.0600*
H17	1.32490	0.47140	0.75080	0.0620*
H18	1.48340	0.34620	0.82400	0.0810*
H19	1.30090	0.22520	0.78890	0.0850*
H11W	0.116 (17)	0.672 (5)	0.346 (13)	0.08 (5)*
H12W	0.086 (15)	0.604 (7)	0.456 (10)	0.09 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.086 (3)	0.073 (3)	0.080 (3)	−0.026 (3)	−0.014 (2)	−0.018 (3)
N1	0.052 (7)	0.025 (6)	0.053 (7)	0.011 (6)	−0.004 (6)	−0.003 (6)
N2	0.059 (8)	0.034 (7)	0.098 (10)	0.000 (6)	−0.024 (7)	−0.004 (7)
N3	0.049 (7)	0.031 (7)	0.061 (7)	−0.004 (6)	−0.002 (6)	0.002 (6)
N4	0.034 (6)	0.036 (6)	0.053 (7)	0.002 (5)	−0.008 (5)	−0.001 (5)
C2	0.056 (10)	0.032 (8)	0.047 (8)	−0.007 (7)	−0.005 (7)	0.008 (7)
C4	0.041 (8)	0.030 (8)	0.034 (8)	0.002 (6)	0.014 (6)	0.011 (6)
C5	0.035 (7)	0.019 (7)	0.044 (8)	−0.008 (6)	0.003 (6)	0.008 (6)
C6	0.041 (8)	0.043 (8)	0.033 (8)	−0.003 (7)	0.003 (6)	0.008 (7)
C7	0.069 (10)	0.053 (9)	0.051 (9)	0.002 (8)	−0.004 (7)	−0.001 (8)
C8	0.080 (11)	0.082 (11)	0.063 (10)	0.017 (9)	−0.031 (8)	−0.009 (9)
C9	0.030 (7)	0.033 (7)	0.043 (8)	0.004 (6)	0.003 (6)	0.009 (7)

C10	0.040 (8)	0.038 (8)	0.056 (9)	−0.003 (6)	0.017 (7)	−0.014 (7)
C11	0.043 (9)	0.058 (10)	0.077 (11)	−0.034 (7)	0.024 (8)	−0.018 (9)
C12	0.036 (9)	0.053 (9)	0.058 (10)	0.004 (7)	−0.013 (7)	−0.013 (8)
C13	0.059 (11)	0.066 (10)	0.038 (8)	0.008 (8)	0.006 (8)	−0.001 (8)
C14	0.059 (9)	0.037 (8)	0.050 (9)	−0.015 (7)	0.017 (7)	−0.009 (7)
O1	0.062 (7)	0.039 (6)	0.084 (7)	0.004 (5)	−0.011 (5)	−0.004 (6)
O2	0.061 (7)	0.036 (5)	0.083 (8)	−0.007 (5)	−0.004 (5)	−0.003 (6)
N5	0.082 (10)	0.048 (9)	0.073 (9)	−0.009 (8)	0.003 (7)	−0.002 (7)
C15	0.066 (9)	0.022 (7)	0.063 (9)	0.006 (7)	0.010 (7)	0.007 (8)
C16	0.044 (8)	0.031 (7)	0.027 (6)	0.006 (7)	0.017 (6)	0.006 (6)
C17	0.049 (9)	0.046 (9)	0.055 (9)	−0.003 (8)	−0.005 (7)	−0.001 (8)
C18	0.052 (9)	0.075 (11)	0.069 (10)	0.027 (10)	−0.005 (7)	−0.001 (10)
C19	0.104 (15)	0.036 (9)	0.076 (12)	0.010 (10)	0.025 (11)	0.007 (9)
C20	0.060 (11)	0.049 (9)	0.044 (9)	0.008 (9)	−0.004 (8)	−0.004 (8)
O1W	0.056 (6)	0.044 (6)	0.104 (9)	−0.005 (6)	0.013 (6)	0.000 (7)

Geometric parameters (Å, °)

Cl1—C12	1.765 (14)	C9—C14	1.380 (17)
O1—C20	1.233 (17)	C10—C11	1.386 (18)
O2—C20	1.267 (17)	C11—C12	1.36 (2)
O1W—H11W	0.97 (9)	C12—C13	1.332 (19)
O1W—H12W	0.96 (10)	C13—C14	1.374 (18)
N1—C6	1.359 (16)	C7—H7A	0.9693
N1—C2	1.361 (17)	C7—H7B	0.9684
N2—C2	1.335 (16)	C8—H8A	0.9577
N3—C4	1.328 (15)	C8—H8B	0.9601
N3—C2	1.336 (16)	C8—H8C	0.9616
N4—C4	1.328 (15)	C10—H10	0.9305
N1—H1	0.8597	C11—H11	0.9329
N2—H2B	0.8598	C13—H13	0.9313
N2—H2A	0.8599	C14—H14	0.9299
N4—H4A	0.8600	C15—C16	1.416 (18)
N4—H4B	0.8597	C16—C17	1.392 (17)
N5—C15	1.314 (17)	C16—C20	1.527 (19)
N5—C19	1.31 (2)	C17—C18	1.37 (2)
C4—C5	1.434 (16)	C18—C19	1.37 (2)
C5—C9	1.472 (16)	C15—H15	0.9322
C5—C6	1.346 (17)	C17—H17	0.9283
C6—C7	1.523 (18)	C18—H18	0.9297
C7—C8	1.533 (18)	C19—H19	0.9309
C9—C10	1.392 (16)		
H11W—O1W—H12W	106 (10)	C8—C7—H7B	109.47
C2—N1—C6	119.9 (10)	C6—C7—H7B	109.38
C2—N3—C4	117.4 (11)	H7A—C7—H7B	108.07
C2—N1—H1	120.04	C6—C7—H7A	109.39
C6—N1—H1	120.09	C7—C8—H8B	109.49
C2—N2—H2A	120.09	H8A—C8—H8B	109.64
C2—N2—H2B	119.91	H8A—C8—H8C	109.55

H2A—N2—H2B	120.00	H8B—C8—H8C	109.31
H4A—N4—H4B	120.00	C7—C8—H8A	109.55
C4—N4—H4B	120.02	C7—C8—H8C	109.28
C4—N4—H4A	119.98	C9—C10—H10	119.45
C15—N5—C19	118.1 (12)	C11—C10—H10	119.50
N2—C2—N3	121.1 (12)	C12—C11—H11	120.42
N1—C2—N3	122.1 (11)	C10—C11—H11	120.38
N1—C2—N2	116.7 (11)	C12—C13—H13	119.99
N3—C4—N4	117.4 (10)	C14—C13—H13	119.66
N4—C4—C5	119.4 (10)	C13—C14—H14	119.34
N3—C4—C5	123.2 (10)	C9—C14—H14	119.32
C4—C5—C9	122.6 (10)	N5—C15—C16	123.6 (12)
C4—C5—C6	115.7 (10)	C15—C16—C17	116.6 (12)
C6—C5—C9	121.6 (10)	C15—C16—C20	120.6 (11)
N1—C6—C7	113.0 (11)	C17—C16—C20	122.7 (12)
C5—C6—C7	126.0 (11)	C16—C17—C18	118.7 (13)
N1—C6—C5	121.0 (11)	C17—C18—C19	119.3 (13)
C6—C7—C8	111.0 (10)	N5—C19—C18	123.7 (14)
C5—C9—C14	120.7 (10)	O1—C20—O2	127.7 (13)
C5—C9—C10	122.4 (11)	O2—C20—C16	113.5 (11)
C10—C9—C14	116.8 (11)	O1—C20—C16	118.9 (12)
C9—C10—C11	121.0 (11)	N5—C15—H15	118.26
C10—C11—C12	119.2 (12)	C16—C15—H15	118.15
Cl1—C12—C11	117.7 (10)	C18—C17—H17	120.80
C11—C12—C13	121.2 (13)	C16—C17—H17	120.51
Cl1—C12—C13	121.1 (11)	C17—C18—H18	120.27
C12—C13—C14	120.4 (13)	C19—C18—H18	120.46
C9—C14—C13	121.3 (12)	N5—C19—H19	118.31
C8—C7—H7A	109.45	C18—C19—H19	118.02

C6—N1—C2—N2	−174.7 (11)	N1—C6—C7—C8	−102.2 (13)
C6—N1—C2—N3	6.0 (19)	C5—C6—C7—C8	77.6 (16)
C2—N1—C6—C5	−6.1 (17)	C5—C9—C14—C13	175.7 (11)
C2—N1—C6—C7	173.7 (11)	C5—C9—C10—C11	−175.1 (11)
C4—N3—C2—N1	0.8 (18)	C10—C9—C14—C13	−1.4 (18)
C2—N3—C4—C5	−7.5 (17)	C14—C9—C10—C11	2.0 (18)
C2—N3—C4—N4	174.7 (11)	C9—C10—C11—C12	−0.4 (19)
C4—N3—C2—N2	−178.5 (11)	C10—C11—C12—Cl1	176.1 (10)
C15—N5—C19—C18	−1(2)	C10—C11—C12—C13	−2(2)
C19—N5—C15—C16	−1(2)	C11—C12—C13—C14	3(2)
N3—C4—C5—C6	7.2 (17)	Cl1—C12—C13—C14	−175.4 (10)
N4—C4—C5—C9	7.5 (17)	C12—C13—C14—C9	−1(2)
N3—C4—C5—C9	−170.2 (11)	N5—C15—C16—C20	−178.5 (12)
N4—C4—C5—C6	−175.1 (11)	N5—C15—C16—C17	3.8 (18)
C4—C5—C9—C10	−111.4 (13)	C15—C16—C17—C18	−3.7 (17)
C4—C5—C9—C14	71.6 (16)	C15—C16—C20—O2	−173.8 (11)
C9—C5—C6—C7	−2.4 (19)	C17—C16—C20—O1	−175.8 (11)
C6—C5—C9—C10	71.3 (16)	C17—C16—C20—O2	3.8 (17)
C6—C5—C9—C14	−105.7 (14)	C20—C16—C17—C18	178.6 (11)
C4—C5—C6—C7	−179.9 (11)	C15—C16—C20—O1	6.6 (18)

C9—C5—C6—N1	177.3 (11)	C16—C17—C18—C19	1.7 (19)
C4—C5—C6—N1	−0.1 (17)	C17—C18—C19—N5	1(2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	1.83	2.686 (14)	175
N2—H2A···O1W	0.86	2.08	2.861 (15)	150
N2—H2B···O1	0.86	2.10	2.957 (13)	172
N4—H4A···O1^{i}	0.86	2.05	2.897 (14)	168
N4—H4B···O1W^{i}	0.86	2.26	3.031 (15)	150
O1W—H11W···N5^{i}	0.97 (9)	1.92 (9)	2.862 (16)	164 (10)
O1W—H12W···O2^{ii}	0.96 (10)	1.97 (10)	2.862 (14)	154 (9)

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

Fig. 1

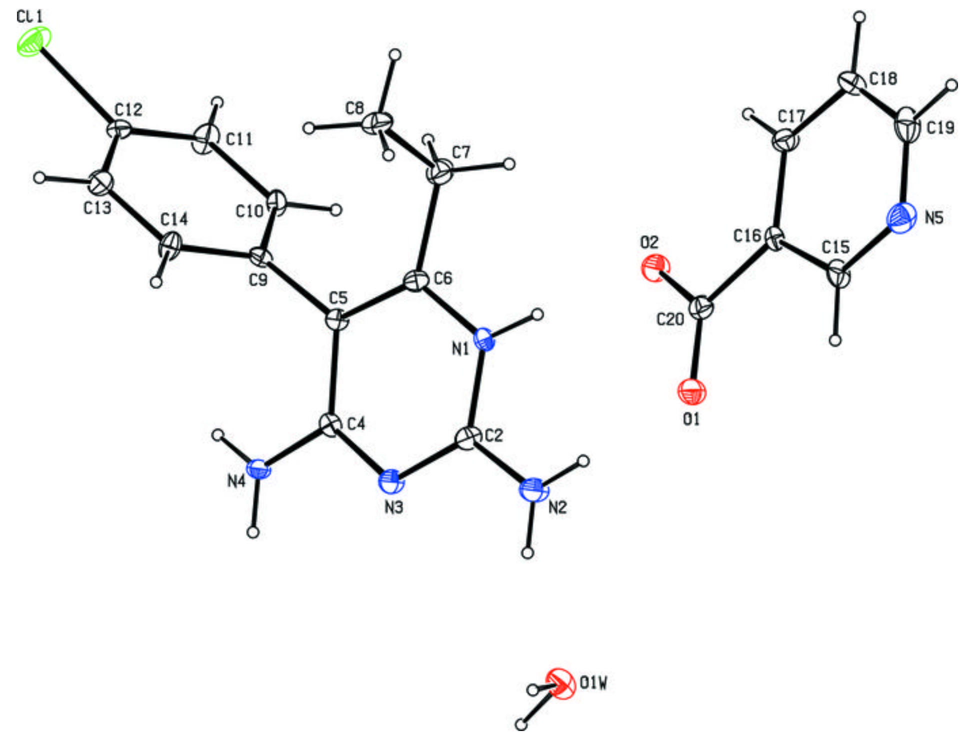
Cl1
C12
C11
C13
C14
C10
C9
C8
C7
C6
C5
N1
C4
C2
N4
N3
N2
O2
C16
C20
O1
C17
C18
C19
N5
C15
O1W

Fig. 2

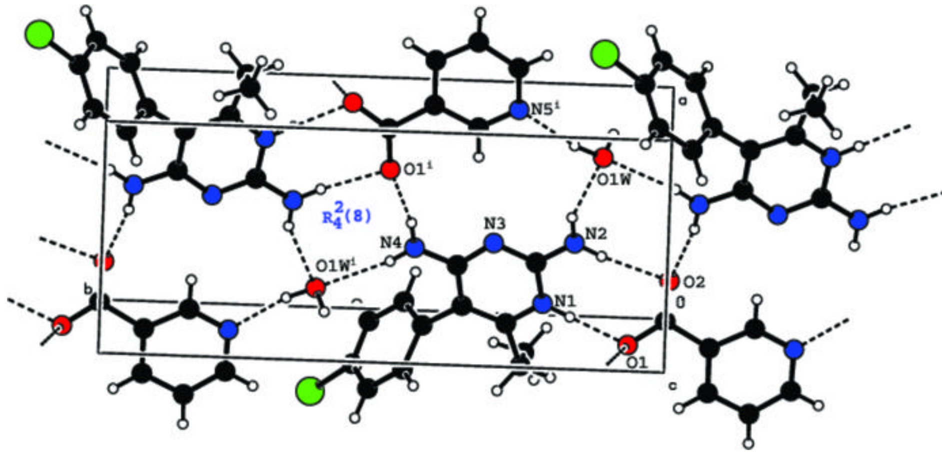

Fig. 3