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4-Methoxybenzamidineium chloride monohydrate

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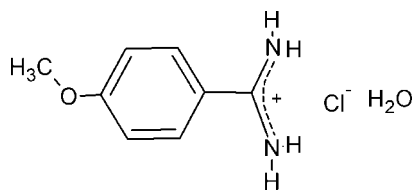
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.043; wR factor = 0.113; data-to-parameter ratio = 20.8.

In the cation of the title compound, $\text{C}_8\text{H}_{11}\text{N}_2\text{O}^+\cdot\text{Cl}^-\cdot\text{H}_2\text{O}$, the C–N bonds of the amidinium group are identical within experimental error [1.305 (2) and 1.304 (2) Å], and its plane forms a dihedral angle of 25.83 (8)° with the phenyl ring. The ionic components are associated in the crystal into polymeric hydrogen-bonded supramolecular tapes stabilized by N–H⁺···Cl[−] and N–H⁺···Ow intermolecular hydrogen bonds, and by Ow–H···Cl[−] interactions.

Related literature

For the biological and pharmacological relevance of benzamidine, see: Marquart *et al.* (1983); Sprang *et al.* (1987); Bode *et al.* (1990); Powers & Harper (1999); Grzesiak *et al.* (2000). For structural analysis of proton-transfer adducts containing molecules of biological interest, see: Portalone (2011a); Portalone & Irrera (2011). For the supramolecular association in proton-transfer adducts containing benzamidinium cations, see: Portalone (2010, 2011b, 2012). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

 $\text{C}_8\text{H}_{11}\text{N}_2\text{O}^+\cdot\text{Cl}^-\cdot\text{H}_2\text{O}$
 $M_r = 204.65$

 Monoclinic, $P2_1/c$
 $a = 11.3029$ (7) Å

 $b = 9.3142$ (5) Å

 $c = 9.9983$ (6) Å

 $\beta = 99.820$ (6)°

 $V = 1037.17$ (11) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 0.34$ mm^{−1}
 $T = 298$ K

 $0.30 \times 0.27 \times 0.25$ mm

Data collection

Oxford Diffraction Xcalibur S CCD diffractometer

Absorption correction: multi-scan

 (*CrysAlis RED*; Oxford

Diffraction, 2006)

 $T_{\min} = 0.905$, $T_{\max} = 0.968$

7158 measured reflections

2989 independent reflections

 1947 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.113$
 $S = 0.97$

2989 reflections

144 parameters

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\max} = 0.22$ e Å^{−3}
 $\Delta\rho_{\min} = -0.15$ e Å^{−3}
Table 1

Hydrogen-bond geometry (Å, °).

| D—H···A | D—H | H···A | D···A | D—H···A |
|------------------------------|----------|----------|-------------|------------|
| N1—H1A···Cl1 | 0.81 (2) | 2.85 (2) | 3.5523 (18) | 145 (2) |
| N1—H1B···O2W | 0.75 (2) | 2.06 (2) | 2.805 (2) | 168 (2) |
| N2—H2A···Cl1 | 0.96 (2) | 2.25 (2) | 3.1850 (16) | 164.4 (16) |
| N2—H2B···Cl1 ⁱ | 0.82 (2) | 2.43 (2) | 3.201 (2) | 157.5 (18) |
| O2W—HWA···Cl1 ⁱⁱ | 0.82 (3) | 2.36 (3) | 3.1731 (18) | 170 (3) |
| O2W—HWB···Cl1 ⁱⁱⁱ | 0.87 (2) | 2.29 (2) | 3.1603 (17) | 174.8 (19) |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2085).

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supporting information

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4-Methoxybenzamidine chloride monohydrate

Simona Irrera and Gustavo Portalone

S1. Comment

This Laboratory is currently engaged in systematic structural analysis of proton-transfer adducts containing molecules of biological interest (Portalone, 2011a; Portalone & Irrera, 2011). In this context benzamidine derivatives, which have shown strong biological and pharmacological activity (Powers & Harper, 1999; Grzesiak *et al.*, 2000), are being used in our group as bricks for supramolecular construction (Portalone, 2010, 2011b, 2012). Indeed, these molecules are strong Lewis bases and their cations can be easily anchored onto numerous inorganic and organic anions and polyanions, largely because of the presence of four potential donor sites for hydrogen-bonding. Benzamidine ions have also been included in a number of protein structures (Marquart *et al.*, 1983; Sprang *et al.*, 1987; Bode *et al.*, 1990).

The asymmetric unit of (I) comprises one non-planar 4-methoxybenzamidine cation, one chloride anion and one water molecule of crystallization (Fig. 1).

In the cation the amidinium group forms a dihedral angle of 25.83 (8)° with the mean plane of the phenyl ring, which agrees with the values observed in protonated benzamidine ions (23.2 - 30.4°, Portalone, 2010, 2012). The lack of planarity in all these systems is obviously caused by steric hindrances between the H atoms of the aromatic ring and the amidine moiety. This conformation is rather common in benzamidine-containing small-molecule crystal structures, with the exception of benzamidine diliturate, where the benzamidine cation is planar (Portalone, 2010). The pattern of bond lengths and bond angles of the 4-methoxybenzamidine cation agrees with that reported in previous structural investigations (Portalone, 2010, 2012). In particular the amidinium group, true to one's expectations, features similar C—N bonds [1.305 (2) and 1.304 (2) Å], evidencing the delocalization of the π electrons and their double-bond character.

Analysis of the crystal packing of (I), (Fig. 2), shows that the ions are associated in the crystal by six distinct N—H⁺⋯Cl⁻, N—H⁺⋯Ow and Ow—H⋯Cl⁻ intermolecular hydrogen bonds (Table 1). Each amidinium unit is bound to two chloride anions by three weak hydrogen bonds (N⁺⋯Cl⁻ = 3.185 (2) - 3.552 (2) Å) and to one water molecule by one N—H⁺⋯Ow interaction, just forming two $R^3_5(10)$ and one $R^1_2(6)$ supramolecular synthons (Bernstein *et al.*, 1995). Both of these $R^3_5(10)$ and $R^1_2(6)$ motifs lead to the formation of one dimensional polymeric hydrogen-bonded supramolecular tapes approximately along the crystallographic *b* axis. The water molecule, which plays a dual role as both donor and acceptor in hydrogen bonding interactions, acts as a bridge between tapes through the remaining two Ow—H⋯Cl⁻ intermolecular interactions.

S2. Experimental

4-methoxybenzamide (1 mmol, Fluka at 96% purity) was dissolved without further purification in 6 ml of hot water and heated under reflux for 3 h. While stirring, HCl (6 mol L⁻¹) was added dropwise until the pH reached 2. After cooling the solution to ambient temperature, colourless crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of the solvent over two weeks.

S3. Refinement

All H atoms were identified in difference Fourier maps, but for refinement all C-bound H atoms were placed in calculated positions, with C—H = 0.93 Å (phenyl) and 0.96 Å (methyl), and refined as riding on their carrier atoms. The U_{iso} values were kept equal to $1.2U_{eq}(C, \text{phenyl})$, and to $1.5U_{eq}(C, \text{methyl})$. Positional and thermal parameters of H atoms of the amidinium group and of water molecule were freely refined, giving N—H distances in the range 0.75 (2) - 0.96 (2) Å and O—H distances in the range 0.82 (3) - 0.87 (2) Å

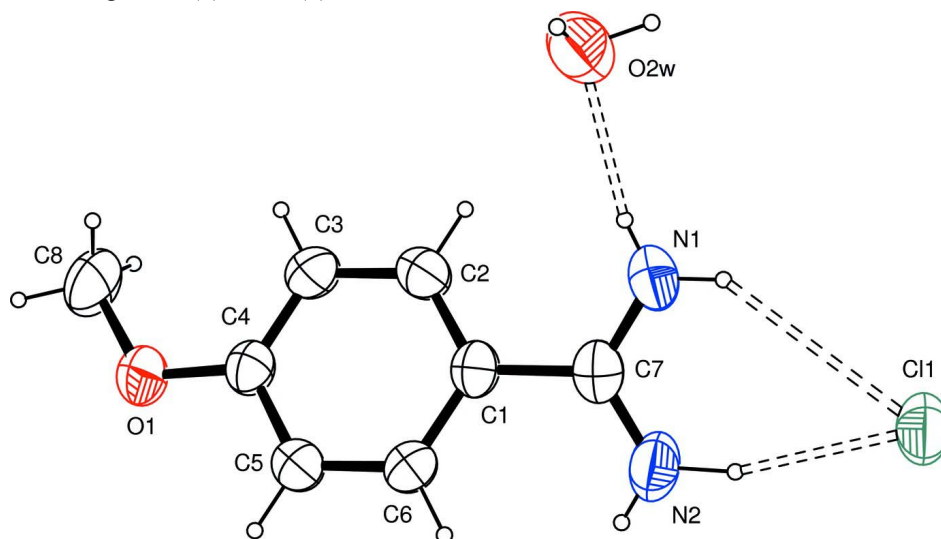
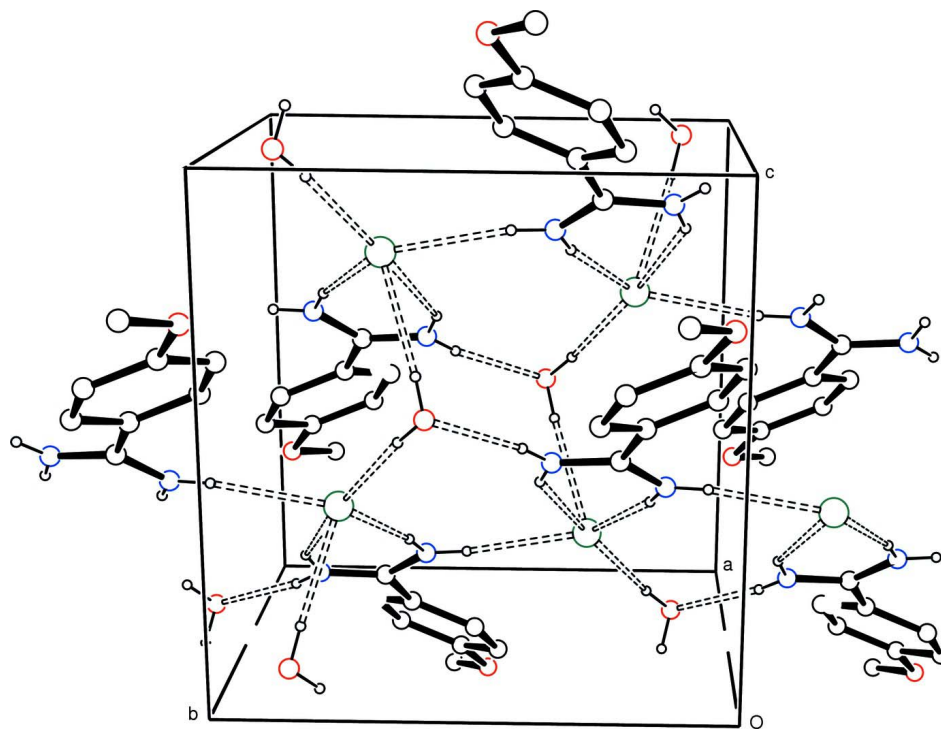


Figure 1

The asymmetric unit of (I), showing the atom-labelling scheme. Displacements ellipsoids are at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

**Figure 2**

Crystal packing diagram for (I), viewed approximately down *a*. Displacements ellipsoids are at the 50% probability level. H atoms are shown as small spheres of arbitrary radii. For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted. Hydrogen bonding is indicated by dashed lines.

4-Methoxybenzamidinium chloride monohydrate

Crystal data

$C_8H_{11}N_2O^+ \cdot Cl^- \cdot H_2O$

$M_r = 204.65$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 11.3029 (7) \text{ \AA}$

$b = 9.3142 (5) \text{ \AA}$

$c = 9.9983 (6) \text{ \AA}$

$\beta = 99.820 (6)^\circ$

$V = 1037.17 (11) \text{ \AA}^3$

$Z = 4$

$F(000) = 432$

$D_x = 1.311 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71069 \text{ \AA}$

Cell parameters from 3182 reflections

$\theta = 2.8\text{--}32.2^\circ$

$\mu = 0.34 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Tablets, colourless

$0.30 \times 0.27 \times 0.25 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur S CCD
diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: $16.0696 \text{ pixels mm}^{-1}$

ω and φ scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2006)

$T_{\min} = 0.905$, $T_{\max} = 0.968$

7158 measured reflections

2989 independent reflections

1947 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\max} = 30.0^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -15 \rightarrow 13$

$k = -13 \rightarrow 13$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.113$
 $S = 0.97$
 2989 reflections
 144 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 atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0667P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.15 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|---------------|--------------|----------------------------------|
| Cl1 | 0.59874 (3) | 0.29686 (5) | 0.19860 (4) | 0.06143 (17) |
| O1 | 0.02187 (9) | 0.02872 (12) | 0.72746 (11) | 0.0585 (3) |
| N1 | 0.37553 (14) | 0.36637 (18) | 0.40096 (17) | 0.0577 (4) |
| H1A | 0.4215 (18) | 0.391 (3) | 0.351 (2) | 0.087 (7)* |
| H1B | 0.3457 (16) | 0.424 (2) | 0.4357 (19) | 0.070 (7)* |
| N2 | 0.40806 (13) | 0.1372 (2) | 0.34687 (16) | 0.0609 (4) |
| H2A | 0.4716 (18) | 0.167 (2) | 0.300 (2) | 0.082 (6)* |
| H2B | 0.3898 (16) | 0.052 (3) | 0.3475 (19) | 0.077 (7)* |
| C1 | 0.26509 (11) | 0.18152 (15) | 0.49586 (13) | 0.0400 (3) |
| C2 | 0.17291 (12) | 0.26955 (17) | 0.52024 (16) | 0.0499 (4) |
| H2 | 0.1669 | 0.3620 | 0.4847 | 0.060* |
| C3 | 0.08913 (12) | 0.22277 (17) | 0.59666 (16) | 0.0497 (4) |
| H3 | 0.0273 | 0.2832 | 0.6120 | 0.060* |
| C4 | 0.09816 (11) | 0.08562 (16) | 0.64994 (14) | 0.0425 (3) |
| C5 | 0.19078 (12) | -0.00346 (17) | 0.62752 (15) | 0.0489 (4) |
| H5 | 0.1974 | -0.0953 | 0.6645 | 0.059* |
| C6 | 0.27322 (12) | 0.04365 (16) | 0.55054 (14) | 0.0460 (3) |
| H6 | 0.3348 | -0.0171 | 0.5350 | 0.055* |
| C7 | 0.35238 (11) | 0.22994 (17) | 0.41160 (14) | 0.0460 (4) |
| C8 | -0.07725 (14) | 0.1140 (2) | 0.75071 (19) | 0.0684 (5) |
| H8A | -0.0482 (3) | 0.2006 (11) | 0.7969 (13) | 0.103* |
| H8B | -0.1241 (9) | 0.0612 (8) | 0.8055 (12) | 0.103* |
| H8C | -0.1263 (8) | 0.1375 (12) | 0.6654 (9) | 0.103* |
| O2W | 0.27853 (14) | 0.61140 (16) | 0.50438 (18) | 0.0783 (4) |

| | | | | |
|-----|-------------|-----------|-----------|-------------|
| HWA | 0.319 (3) | 0.631 (4) | 0.579 (3) | 0.155 (14)* |
| HWB | 0.3124 (17) | 0.667 (2) | 0.452 (2) | 0.077 (6)* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|---------------|--------------|-------------|
| C11 | 0.0604 (3) | 0.0699 (3) | 0.0594 (3) | -0.00364 (19) | 0.02536 (19) | 0.0085 (2) |
| O1 | 0.0518 (6) | 0.0581 (7) | 0.0737 (7) | 0.0039 (5) | 0.0337 (5) | 0.0110 (6) |
| N1 | 0.0595 (8) | 0.0550 (9) | 0.0642 (9) | -0.0047 (7) | 0.0267 (7) | 0.0125 (8) |
| N2 | 0.0583 (8) | 0.0688 (11) | 0.0628 (9) | -0.0090 (8) | 0.0311 (7) | -0.0027 (8) |
| C1 | 0.0358 (6) | 0.0472 (8) | 0.0373 (7) | -0.0039 (6) | 0.0072 (5) | 0.0001 (6) |
| C2 | 0.0510 (8) | 0.0403 (8) | 0.0604 (9) | 0.0036 (6) | 0.0156 (7) | 0.0089 (7) |
| C3 | 0.0437 (7) | 0.0463 (9) | 0.0629 (9) | 0.0077 (6) | 0.0195 (6) | 0.0020 (7) |
| C4 | 0.0384 (6) | 0.0464 (8) | 0.0443 (7) | -0.0017 (6) | 0.0117 (5) | 0.0002 (6) |
| C5 | 0.0496 (7) | 0.0421 (8) | 0.0584 (9) | 0.0047 (7) | 0.0191 (6) | 0.0082 (7) |
| C6 | 0.0420 (7) | 0.0449 (8) | 0.0541 (8) | 0.0078 (6) | 0.0167 (6) | 0.0032 (7) |
| C7 | 0.0405 (7) | 0.0559 (10) | 0.0420 (7) | -0.0040 (6) | 0.0084 (6) | 0.0045 (7) |
| C8 | 0.0503 (8) | 0.0838 (13) | 0.0787 (12) | 0.0101 (8) | 0.0329 (8) | 0.0039 (10) |
| O2W | 0.1035 (11) | 0.0605 (8) | 0.0747 (10) | -0.0175 (8) | 0.0258 (9) | 0.0015 (7) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|------------|-------------|
| O1—C4 | 1.3613 (16) | C2—H2 | 0.9300 |
| O1—C8 | 1.4243 (18) | C3—C4 | 1.381 (2) |
| N1—C7 | 1.305 (2) | C3—H3 | 0.9300 |
| N1—H1A | 0.81 (2) | C4—C5 | 1.3837 (19) |
| N1—H1B | 0.75 (2) | C5—C6 | 1.3776 (19) |
| N2—C7 | 1.304 (2) | C5—H5 | 0.9300 |
| N2—H2A | 0.96 (2) | C6—H6 | 0.9300 |
| N2—H2B | 0.82 (2) | C8—H8A | 0.9596 |
| C1—C2 | 1.3798 (19) | C8—H8B | 0.9596 |
| C1—C6 | 1.3926 (19) | C8—H8C | 0.9596 |
| C1—C7 | 1.4731 (18) | O2W—HWA | 0.82 (3) |
| C2—C3 | 1.385 (2) | O2W—HWB | 0.87 (2) |
| C4—O1—C8 | 117.92 (13) | C3—C4—C5 | 120.02 (12) |
| C7—N1—H1A | 119.0 (17) | C6—C5—C4 | 120.14 (14) |
| C7—N1—H1B | 123.3 (15) | C6—C5—H5 | 119.9 |
| H1A—N1—H1B | 118 (2) | C4—C5—H5 | 119.9 |
| C7—N2—H2A | 120.7 (11) | C5—C6—C1 | 120.49 (12) |
| C7—N2—H2B | 119.6 (14) | C5—C6—H6 | 119.8 |
| H2A—N2—H2B | 119.7 (18) | C1—C6—H6 | 119.8 |
| C2—C1—C6 | 118.68 (12) | N2—C7—N1 | 118.95 (15) |
| C2—C1—C7 | 121.24 (13) | N2—C7—C1 | 120.53 (15) |
| C6—C1—C7 | 120.07 (12) | N1—C7—C1 | 120.52 (15) |
| C1—C2—C3 | 121.24 (14) | O1—C8—H8A | 109.5 |
| C1—C2—H2 | 119.4 | O1—C8—H8B | 109.5 |
| C3—C2—H2 | 119.4 | H8A—C8—H8B | 109.5 |

| | | | |
|-------------|--------------|-------------|--------------|
| C4—C3—C2 | 119.43 (13) | O1—C8—H8C | 109.5 |
| C4—C3—H3 | 120.3 | H8A—C8—H8C | 109.5 |
| C2—C3—H3 | 120.3 | H8B—C8—H8C | 109.5 |
| O1—C4—C3 | 124.57 (12) | HWA—O2W—HWB | 100 (3) |
| O1—C4—C5 | 115.41 (13) | | |
| C6—C1—C2—C3 | -0.4 (2) | C3—C4—C5—C6 | -0.9 (2) |
| C7—C1—C2—C3 | 178.39 (14) | C4—C5—C6—C1 | 0.7 (2) |
| C1—C2—C3—C4 | 0.2 (2) | C2—C1—C6—C5 | -0.1 (2) |
| C8—O1—C4—C3 | 2.8 (2) | C7—C1—C6—C5 | -178.88 (14) |
| C8—O1—C4—C5 | -178.22 (14) | C2—C1—C7—N2 | -153.81 (15) |
| C2—C3—C4—O1 | 179.33 (14) | C6—C1—C7—N2 | 25.0 (2) |
| C2—C3—C4—C5 | 0.4 (2) | C2—C1—C7—N1 | 26.4 (2) |
| O1—C4—C5—C6 | -179.90 (14) | C6—C1—C7—N1 | -154.78 (15) |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------------------|----------|-------------|-------------|---------------|
| N1—H1A \cdots C11 | 0.81 (2) | 2.85 (2) | 3.5523 (18) | 145 (2) |
| N1—H1B \cdots O2W | 0.75 (2) | 2.06 (2) | 2.805 (2) | 168 (2) |
| N2—H2A \cdots C11 | 0.96 (2) | 2.25 (2) | 3.1850 (16) | 164.4 (16) |
| N2—H2B \cdots C11 ⁱ | 0.82 (2) | 2.43 (2) | 3.201 (2) | 157.5 (18) |
| O2W—HWA \cdots C11 ⁱⁱ | 0.82 (3) | 2.36 (3) | 3.1731 (18) | 170 (3) |
| O2W—HWB \cdots C11 ⁱⁱⁱ | 0.87 (2) | 2.29 (2) | 3.1603 (17) | 174.8 (19) |

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