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3-Allyl-1-(3-cyanophenylmethylene)-2-methyl-1*H*-benzoimidazol-3-ium bromide monohydrate

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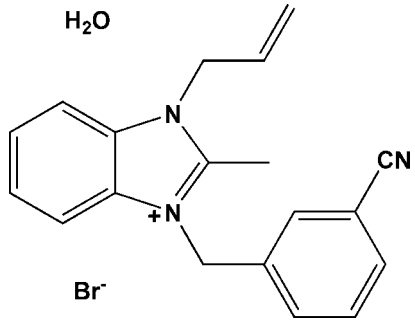
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.111; data-to-parameter ratio = 20.0.

In the title compound, $C_{19}H_{18}N_3^+\cdot Br^-\cdot H_2O$, the dihedral angle between the allyl group and the imidazole ring is 89.59 (14)°, while the dihedral angle between the cyanophenyl ring and the imidazole ring is 78.72 (7)°. O—H···Br hydrogen bonds form an infinite chain in the *c*-axis direction and C—H···Br and C—H···O interactions expand this chain into an infinite three-dimensional network.

Related literature

For related literature, see Aakeröy *et al.* (2005).



Experimental

Crystal data

$C_{19}H_{18}N_3^+\cdot Br^-\cdot H_2O$
M_r = 386.29
Monoclinic, $P2_1/c$
a = 13.4291 (18) Å
b = 15.6490 (17) Å
c = 9.0335 (14) Å
β = 104.048 (8)°
V = 1841.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.24 mm^{-1}
T = 293 (2) K
0.22 × 0.15 × 0.08 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.840, T_{max} = 1.000
(expected range = 0.702–0.836)
14149 measured reflections
4366 independent reflections
3365 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.111
S = 1.08
4366 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1···Br1	0.85	2.59	3.375 (2)	155
O1W—H2···Br1^{i}	0.85	2.78	3.422 (3)	134
C6—H6A···Br1^{ii}	0.93	3.21	3.939 (3)	137
C8—H8A···Br1^{iii}	0.96	2.94	3.767 (3)	145
C8—H8C···N3^{iv}	0.96	2.64	3.463 (4)	143
C13—H13A···O1W^{v}	0.93	2.50	3.359 (4)	154
C17—H17A···Br1^{vi}	0.97	2.89	3.843 (3)	168
C17—H17B···Br1^{iii}	0.97	2.91	3.862 (3)	167

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL*.

This work was supported by a Start-up Grant from SEU to YQ.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2074).

References

Aakeröy, C. B., Desper, J. & Urbina, J. F. (2005). *Cryst. Growth Des.* **5**, 1283–1293.
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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1999). *SHELXTL/PC*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

supporting information

Acta Cryst. (2008). E**64**, o109 [https://doi.org/10.1107/S1600536807061867]

3-Allyl-1-(3-cyanophenylmethylene)-2-methyl-1*H*-benzoimidazol-3-ium bromide monohydrate

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S1. Comment

The title compound (Figure 1) was obtained by refluxing 3-((2-methyl-1*H*-benzo[*d*]imidazol-1-yl)methyl)benzonitrile and allyl bromide in THF. The X-ray diffraction experiment certified the successful synthesis of the title compound. The dihedral angle between the allyl groups and the imidazole ring is 89.59 (14)°, while the dihedral angle between the cyano-benzene ring and the imidazole ring is 78.72 (7)°. The twist of the allyl group (torsion N3—C17—C18=C19) is 5.1 (5)°. The O—H···Br H-bonds form an infinite chain in the c-direction and the C—H···Br and C—H···O interactions expand this chain into an infinite three-dimensional network (Figure 2). The interaction distances and angles are shown in Table.

S2. Experimental

The synthesis of 3-((2-methyl-1*H*-benzo[*d*]imidazol-1-yl)methyl) benzonitrile has been reported by Aakeröy, *et al.* (2005). 2.48 g of this compound was dissolved in 30 ml THF and 3.7 g of allyl bromide (3-bromopropene) was added. The solution was stirred at 323 K for two days, after which a white solid appeared. This solid was filtered off and washed twice by acetone to get 1.90 g product (yield 64.7%). Colorless crystals of the title compound, suitable for X-ray diffraction, were obtained by evaporation of a solution in methanol and water.

S3. Refinement

H atoms of the crystal water were added at sites suitable for H-bonding. Positional parameters of other H atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with U_{iso}(H) = 1.2 or 1.5 U_{eq}. The methyl group was refined as a rigid rotor, allowing the group to rotate along the C—C bond.

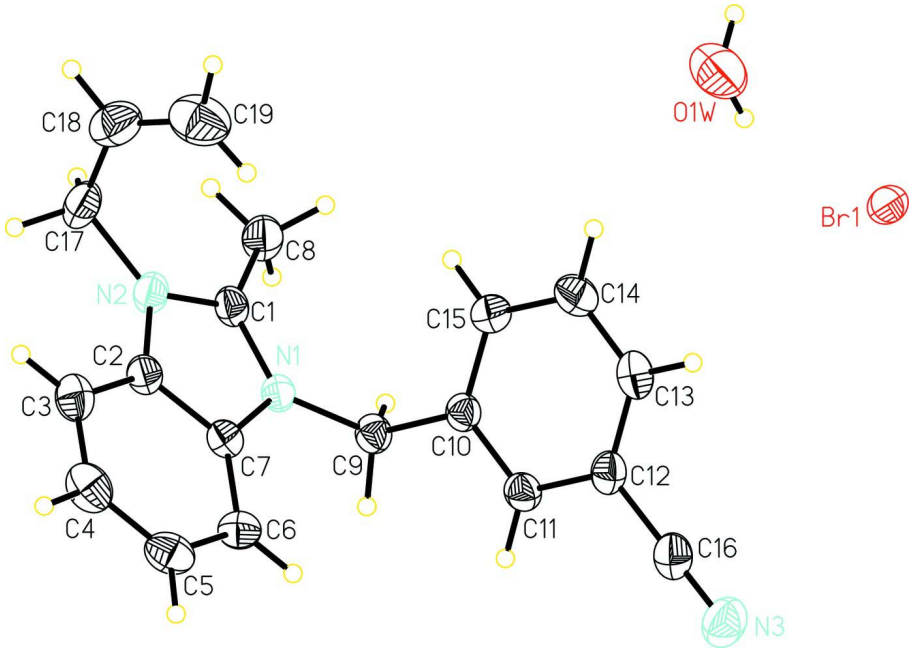

Figure 1

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

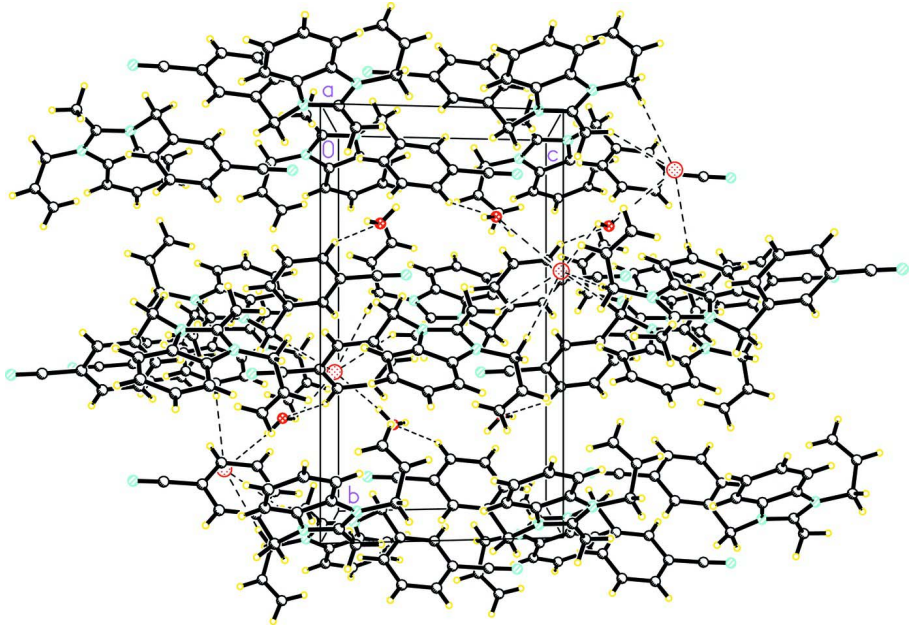

Figure 2

View of the crystal packing of the title compound down the *a* axis.

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Crystal data

$C_{19}H_{18}N_3^+ \cdot Br^- \cdot H_2O$
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Hall symbol: -P 2ybc
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$b = 15.6490\ (17)$ Å
$c = 9.0335\ (14)$ Å
$\beta = 104.048\ (8)°$
$V = 1841.6\ (4)$ Å^3
$Z = 4$
$F(000) = 792$
$D_x = 1.393$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4089 reflections
$\theta = 3.0–28.3°$
$\mu = 2.24$ mm^{-1}
$T = 293$ K
Prism, colorless
0.22 × 0.15 × 0.08 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.840$, $T_{max} = 1.000$
14149 measured reflections
4366 independent reflections
3365 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.7°$
$h = -17\rightarrow17$
$k = -20\rightarrow20$
$l = -8\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.111$
$S = 1.08$
4366 reflections
218 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
$w = 1/[\sigma^2(F_o^2) + (0.0552P)^2 + 0.1803P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.21740 (14)	0.01484 (13)	0.0889 (2)	0.0399 (4)
N2	0.13955 (16)	0.06050 (14)	−0.1380 (2)	0.0467 (5)
N3	0.4739 (2)	0.12165 (17)	0.8335 (3)	0.0710 (8)
C13	0.5074 (2)	0.1603 (2)	0.4691 (3)	0.0578 (7)

H13A	0.5544	0.1990	0.5246	0.069*
C16	0.4615 (2)	0.11908 (17)	0.7045 (4)	0.0553 (7)
C2	0.08324 (19)	0.09107 (16)	−0.0375 (3)	0.0441 (6)
C11	0.37725 (18)	0.05370 (16)	0.4585 (3)	0.0452 (6)
H11A	0.3372	0.0213	0.5081	0.054*
C7	0.13222 (18)	0.06166 (15)	0.1066 (3)	0.0419 (5)
C9	0.29401 (19)	−0.02289 (16)	0.2168 (3)	0.0441 (6)
H9A	0.3330	−0.0660	0.1779	0.053*
H9B	0.2591	−0.0507	0.2858	0.053*
C10	0.36673 (18)	0.04385 (15)	0.3033 (3)	0.0411 (5)
C6	0.0942 (2)	0.07708 (18)	0.2331 (3)	0.0513 (6)
H6A	0.1267	0.0566	0.3293	0.062*
C1	0.21926 (18)	0.01478 (16)	−0.0588 (3)	0.0432 (6)
C12	0.4477 (2)	0.11203 (16)	0.5407 (3)	0.0478 (6)
C3	−0.0059 (2)	0.13911 (17)	−0.0624 (4)	0.0560 (7)
H3A	−0.0386	0.1593	−0.1588	0.067*
C5	0.0052 (2)	0.12465 (17)	0.2082 (4)	0.0612 (8)
H5A	−0.0233	0.1367	0.2900	0.073*
C15	0.4277 (2)	0.09288 (18)	0.2320 (3)	0.0508 (6)
H15A	0.4216	0.0866	0.1279	0.061*
C8	0.2952 (2)	−0.0302 (2)	−0.1243 (3)	0.0585 (7)
H8A	0.2728	−0.0296	−0.2336	0.088*
H8B	0.3017	−0.0882	−0.0888	0.088*
H8C	0.3604	−0.0020	−0.0931	0.088*
C14	0.4973 (2)	0.1509 (2)	0.3143 (4)	0.0612 (8)
H14A	0.5374	0.1836	0.2652	0.073*
C4	−0.0434 (2)	0.15524 (19)	0.0631 (4)	0.0624 (8)
H4A	−0.1029	0.1875	0.0515	0.075*
C17	0.1160 (2)	0.0806 (2)	−0.3020 (3)	0.0597 (8)
H17A	0.0422	0.0852	−0.3401	0.072*
H17B	0.1394	0.0339	−0.3555	0.072*
C18	0.1641 (3)	0.1606 (3)	−0.3359 (4)	0.0743 (9)
H18A	0.1468	0.1784	−0.4372	0.089*
C19	0.2281 (3)	0.2095 (3)	−0.2405 (5)	0.0915 (12)
H19A	0.2481	0.1949	−0.1377	0.110*
H19B	0.2536	0.2588	−0.2753	0.110*
O1W	0.7083 (2)	0.25974 (19)	0.2290 (4)	0.1174 (12)
H1	0.7192	0.2206	0.2963	0.176*
H2	0.7528	0.2564	0.1764	0.176*
Br1	0.83295 (2)	0.126019 (17)	0.50549 (3)	0.04996 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0344 (10)	0.0447 (11)	0.0394 (12)	−0.0014 (8)	0.0065 (8)	−0.0018 (8)
N2	0.0428 (11)	0.0545 (13)	0.0395 (12)	0.0006 (10)	0.0034 (9)	−0.0039 (9)
N3	0.0726 (19)	0.085 (2)	0.0525 (17)	0.0022 (14)	0.0088 (14)	−0.0114 (13)
C13	0.0448 (14)	0.0614 (17)	0.0614 (19)	−0.0065 (14)	0.0014 (12)	−0.0066 (14)

C16	0.0478 (15)	0.0593 (17)	0.0553 (19)	0.0010 (13)	0.0058 (13)	−0.0084 (13)
C2	0.0380 (13)	0.0477 (14)	0.0454 (15)	−0.0015 (11)	0.0079 (10)	−0.0042 (11)
C11	0.0377 (12)	0.0482 (14)	0.0495 (15)	0.0033 (11)	0.0103 (11)	0.0050 (11)
C7	0.0376 (12)	0.0418 (13)	0.0463 (15)	−0.0028 (10)	0.0103 (10)	−0.0024 (10)
C9	0.0400 (12)	0.0416 (13)	0.0485 (15)	0.0012 (10)	0.0067 (11)	0.0047 (10)
C10	0.0365 (12)	0.0416 (13)	0.0434 (14)	0.0025 (10)	0.0062 (10)	0.0033 (10)
C6	0.0524 (15)	0.0555 (16)	0.0497 (16)	0.0002 (13)	0.0194 (12)	0.0003 (12)
C1	0.0359 (12)	0.0470 (14)	0.0446 (15)	−0.0051 (11)	0.0055 (10)	−0.0075 (11)
C12	0.0395 (13)	0.0525 (15)	0.0476 (16)	0.0054 (11)	0.0031 (11)	−0.0011 (11)
C3	0.0459 (15)	0.0548 (17)	0.0629 (19)	0.0037 (12)	0.0045 (13)	0.0010 (13)
C5	0.0600 (18)	0.0604 (18)	0.072 (2)	0.0020 (15)	0.0332 (16)	−0.0074 (14)
C15	0.0515 (15)	0.0549 (15)	0.0460 (16)	−0.0034 (13)	0.0116 (12)	0.0048 (12)
C8	0.0503 (15)	0.075 (2)	0.0502 (17)	0.0063 (14)	0.0124 (13)	−0.0138 (14)
C14	0.0550 (17)	0.0614 (17)	0.068 (2)	−0.0157 (15)	0.0154 (14)	0.0063 (15)
C4	0.0504 (16)	0.0529 (16)	0.086 (2)	0.0124 (14)	0.0196 (15)	−0.0016 (16)
C17	0.0580 (17)	0.077 (2)	0.0386 (16)	0.0116 (16)	0.0006 (12)	−0.0045 (13)
C18	0.084 (2)	0.080 (2)	0.062 (2)	0.016 (2)	0.0218 (18)	0.0164 (18)
C19	0.094 (3)	0.071 (2)	0.118 (3)	0.006 (2)	0.042 (3)	0.021 (2)
O1W	0.0692 (16)	0.126 (2)	0.153 (3)	0.0065 (16)	0.0181 (17)	0.084 (2)
Br1	0.05534 (19)	0.05266 (18)	0.04170 (18)	−0.00159 (12)	0.01142 (12)	0.00224 (11)

Geometric parameters (Å, º)

N1—C1	1.340 (3)	C6—H6A	0.9300
N1—C7	1.400 (3)	C1—C8	1.476 (4)
N1—C9	1.472 (3)	C3—C4	1.371 (4)
N2—C1	1.341 (3)	C3—H3A	0.9300
N2—C2	1.400 (3)	C5—C4	1.399 (5)
N2—C17	1.471 (3)	C5—H5A	0.9300
N3—C16	1.137 (4)	C15—C14	1.383 (4)
C13—C12	1.372 (4)	C15—H15A	0.9300
C13—C14	1.379 (4)	C8—H8A	0.9600
C13—H13A	0.9300	C8—H8B	0.9600
C16—C12	1.450 (4)	C8—H8C	0.9600
C2—C7	1.387 (4)	C14—H14A	0.9300
C2—C3	1.385 (4)	C4—H4A	0.9300
C11—C10	1.383 (3)	C17—C18	1.475 (5)
C11—C12	1.392 (4)	C17—H17A	0.9700
C11—H11A	0.9300	C17—H17B	0.9700
C7—C6	1.381 (3)	C18—C19	1.306 (5)
C9—C10	1.512 (3)	C18—H18A	0.9300
C9—H9A	0.9700	C19—H19A	0.9300
C9—H9B	0.9700	C19—H19B	0.9300
C10—C15	1.389 (4)	O1W—H1	0.8499
C6—C5	1.380 (4)	O1W—H2	0.8502
C1—N1—C7	109.1 (2)	C11—C12—C16	119.8 (3)
C1—N1—C9	127.1 (2)	C4—C3—C2	116.2 (3)

C7—N1—C9	123.7 (2)	C4—C3—H3A	121.9
C1—N2—C2	108.8 (2)	C2—C3—H3A	121.9
C1—N2—C17	126.9 (2)	C6—C5—C4	121.7 (3)
C2—N2—C17	124.2 (2)	C6—C5—H5A	119.1
C12—C13—C14	119.6 (3)	C4—C5—H5A	119.1
C12—C13—H13A	120.2	C14—C15—C10	120.7 (3)
C14—C13—H13A	120.2	C14—C15—H15A	119.6
N3—C16—C12	177.5 (3)	C10—C15—H15A	119.6
C7—C2—C3	121.8 (2)	C1—C8—H8A	109.5
C7—C2—N2	106.7 (2)	C1—C8—H8B	109.5
C3—C2—N2	131.5 (2)	H8A—C8—H8B	109.5
C10—C11—C12	120.2 (2)	C1—C8—H8C	109.5
C10—C11—H11A	119.9	H8A—C8—H8C	109.5
C12—C11—H11A	119.9	H8B—C8—H8C	109.5
C2—C7—C6	122.2 (2)	C15—C14—C13	120.1 (3)
C2—C7—N1	106.3 (2)	C15—C14—H14A	119.9
C6—C7—N1	131.5 (2)	C13—C14—H14A	119.9
N1—C9—C10	111.70 (19)	C3—C4—C5	122.1 (3)
N1—C9—H9A	109.3	C3—C4—H4A	119.0
C10—C9—H9A	109.3	C5—C4—H4A	119.0
N1—C9—H9B	109.3	N2—C17—C18	113.1 (3)
C10—C9—H9B	109.3	N2—C17—H17A	109.0
H9A—C9—H9B	107.9	C18—C17—H17A	109.0
C11—C10—C15	118.8 (2)	N2—C17—H17B	109.0
C11—C10—C9	119.7 (2)	C18—C17—H17B	109.0
C15—C10—C9	121.4 (2)	H17A—C17—H17B	107.8
C7—C6—C5	116.0 (3)	C19—C18—C17	127.6 (3)
C7—C6—H6A	122.0	C19—C18—H18A	116.2
C5—C6—H6A	122.0	C17—C18—H18A	116.2
N2—C1—N1	109.0 (2)	C18—C19—H19A	120.0
N2—C1—C8	125.4 (2)	C18—C19—H19B	120.0
N1—C1—C8	125.5 (2)	H19A—C19—H19B	120.0
C13—C12—C11	120.5 (3)	H1—O1W—H2	109.5
C13—C12—C16	119.6 (3)		

C1—N2—C2—C7	−0.1 (3)	C2—N2—C1—C8	178.2 (3)
C17—N2—C2—C7	−177.1 (2)	C17—N2—C1—C8	−5.0 (4)
C1—N2—C2—C3	−178.3 (3)	C7—N1—C1—N2	0.8 (3)
C17—N2—C2—C3	4.8 (4)	C9—N1—C1—N2	−175.9 (2)
C3—C2—C7—C6	1.2 (4)	C7—N1—C1—C8	−177.8 (2)
N2—C2—C7—C6	−177.2 (2)	C9—N1—C1—C8	5.6 (4)
C3—C2—C7—N1	178.9 (2)	C14—C13—C12—C11	0.1 (4)
N2—C2—C7—N1	0.6 (3)	C14—C13—C12—C16	177.2 (3)
C1—N1—C7—C2	−0.8 (3)	C10—C11—C12—C13	0.0 (4)
C9—N1—C7—C2	175.9 (2)	C10—C11—C12—C16	−177.2 (2)
C1—N1—C7—C6	176.6 (3)	C7—C2—C3—C4	−0.5 (4)
C9—N1—C7—C6	−6.6 (4)	N2—C2—C3—C4	177.4 (3)
C1—N1—C9—C10	99.8 (3)	C7—C6—C5—C4	0.0 (4)

C7—N1—C9—C10	−76.3 (3)	C11—C10—C15—C14	−0.3 (4)
C12—C11—C10—C15	0.2 (4)	C9—C10—C15—C14	−177.0 (3)
C12—C11—C10—C9	176.8 (2)	C10—C15—C14—C13	0.4 (5)
N1—C9—C10—C11	123.7 (2)	C12—C13—C14—C15	−0.3 (5)
N1—C9—C10—C15	−59.7 (3)	C2—C3—C4—C5	−0.4 (4)
C2—C7—C6—C5	−0.9 (4)	C6—C5—C4—C3	0.6 (5)
N1—C7—C6—C5	−178.0 (3)	C1—N2—C17—C18	−89.6 (3)
C2—N2—C1—N1	−0.4 (3)	C2—N2—C17—C18	86.7 (3)
C17—N2—C1—N1	176.5 (2)	N2—C17—C18—C19	5.1 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1···Br1	0.85	2.59	3.375 (2)	155
O1*W*—H2···Br1^{i}	0.85	2.78	3.422 (3)	134
C6—H6*A*···Br1^{ii}	0.93	3.21	3.939 (3)	137
C8—H8*A*···Br1^{iii}	0.96	2.94	3.767 (3)	145
C8—H8*C*···N3^{iv}	0.96	2.64	3.463 (4)	143
C13—H13*A*···O1*W*^{v}	0.93	2.50	3.359 (4)	154
C17—H17*A*···Br1^{vi}	0.97	2.89	3.843 (3)	168
C17—H17*B*···Br1^{iii}	0.97	2.91	3.862 (3)	167

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