Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(5-Ethenyl-1-azabicyclo[2.2.2]octan-2-yl)(6-methoxy-3-quinolyl)methanol methanol solvate

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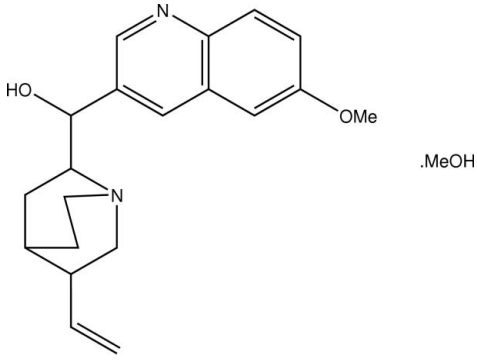
Received 27 October 2009; accepted 28 October 2009

Key indicators: single-crystal X-ray study; T = 98 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.108; data-to-parameter ratio = 10.5.

In the title methanol solvate, $C_{20}H_{24}N_2O_2\cdot CH_4O$, an L-shaped conformation is found as the two substituents at the central hydroxy group are almost orthogonal to each other [the C—C—C angle at the central sp^3-C atom is 110.12 (13)°]. The most notable feature of the crystal packing is the formation of supramolecular chains along the b direction mediated by O—H···N hydrogen bonds occurring between the hydroxy and quinoline N atoms; the methanol molecules are linked to these chains *via* O—H···N_{amine} hydrogen bonds. C—H···O interactions also occur.

Related literature

For background to pre-catalyst molecules for the Michael addition of acetone to *trans*-β-nitrostyrene, see: Mandal & Zhao (2008).



Experimental

Crystal data

$C_{20}H_{24}N_2O_2\cdot CH_4O$
M_r = 356.45
Orthorhombic, $P2_12_12_1$
a = 9.5374 (13) Å
b = 12.9842 (17) Å
c = 15.871 (2) Å
V = 1965.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 98 K
0.12 × 0.10 × 0.04 mm

Data collection

Rigaku AFC12K/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.788, T_{max} = 1.000
14410 measured reflections
2561 independent reflections
2501 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
S = 1.08
2561 reflections
243 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3o···N1	0.84	1.95	2.783 (2)	171
O1—H1o···N2^{i}	0.84	1.92	2.751 (2)	173
C20—H20b···O1^{ii}	0.98	2.33	3.298 (2)	171
C18—H18···O3^{iii}	0.95	2.58	3.471 (2)	155

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

Data collection: *CrystalClear* (Rigaku/MSC, 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: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

CGZ thanks the National Science Foundation (grant No. CHE-0909954) for financial support of this project.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5191).

References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Mandal, T. & Zhao, C.-G. (2008). *Angew. Chem. Int. Ed.* **47**, 7714–7717.
Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

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supporting information

Acta Cryst. (2009). E**65**, o2962 [https://doi.org/10.1107/S1600536809045073]

(5-Ethenyl-1-azabicyclo[2.2.2]octan-2-yl)(6-methoxy-3-quinolyl)methanol methanol solvate

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S1. Comment

Molecules related to and including the title compound, (I), have been evaluated as pre-catalysts for the Michael addition of acetone to *trans*-*β*-nitrostyrene, see: Mandal & Zhao (2008).

The molecule of (I), Fig. 1, adopts an `L′-shaped conformation whereby the substituted quinoline and dabco residues are linked at the central sp^3-C10 atom carrying the hydroxy group, the C1–C10–C11 angle is 110.12 (13)°. Viewed down the N1···C3 axis, the dabco molecule adopts an essentially eclipsed conformation. Both the hydroxy and vinyl groups are orientated towards the same side of the molecule.

In the crystal structure, molecules are connected into a supramolecular chain along the *b* axis *via* O—H···N2 hydrogen bonds formed between the O1-hydroxy group and the N2 atom of the quinoline residue, Table 1 and Fig. 2. The lattice methanol molecules associate with this chain *via* O—H···N1 hydrogen bonds. Chains are consolidated in the crystal packing by C–H···O interactions, Table 1.

S2. Experimental

Quinidine (TCI America Chemicals) and `L′-proline (Sigma Aldrich) were obtained commercially and used as received. A 1:1 molar ratio of quinidine (100 mg) and `L′-proline (35 mg) were taken in methanol (8 ml) and upon upon vapour diffusion of hexane, colourless crystals formed within 7 days.

S3. Refinement

The H atoms were geometrically placed (O—H = 0.84 Å and C—H = 0.95–1.00 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O, methyl-C). In the absence of significant anomalous scattering effects, 1951 Friedel pairs were averaged in the final refinement.

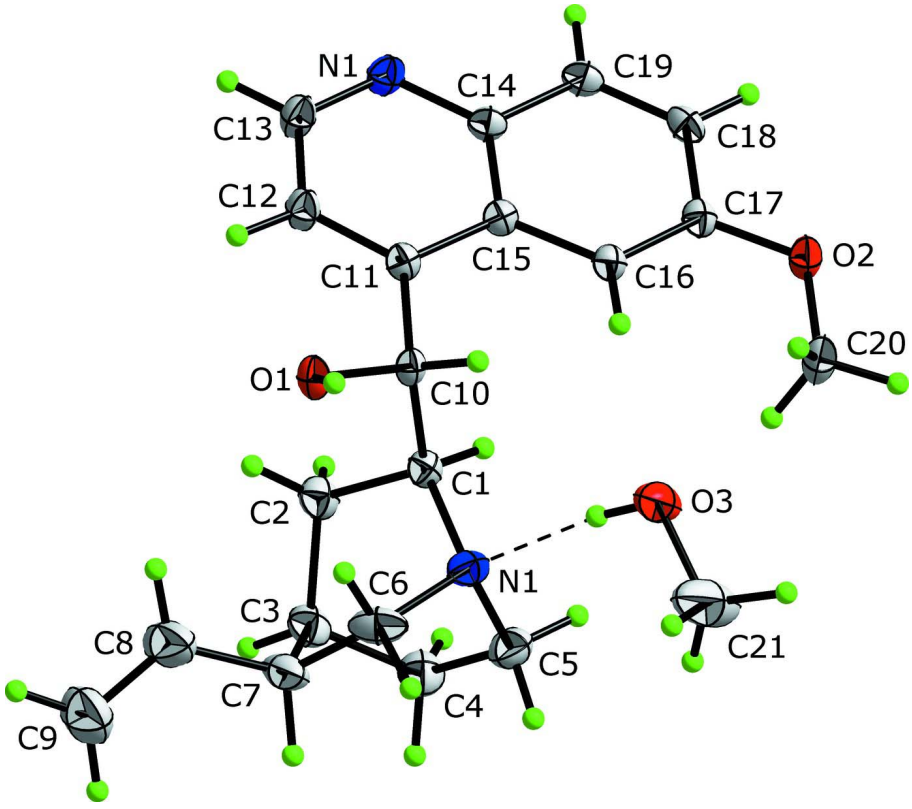

Figure 1

Molecular structure of the asymmetric unit in (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level. The O—H···N hydrogen bond is shown as a dashed line.

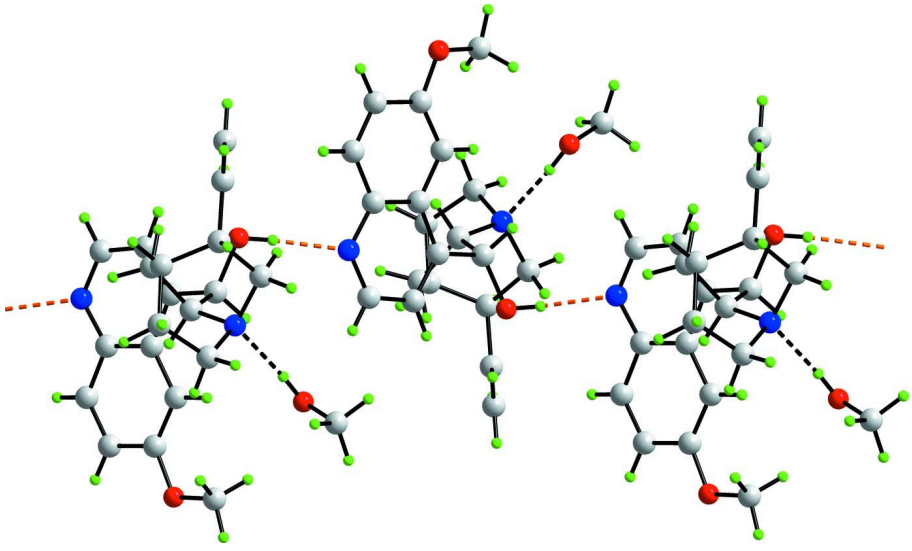

Figure 2

Supramolecular chain in (I) mediated by O–H···N hydrogen bonds (orange dashed lines). Methanol molecules are associated with this chain *via* O–H···N hydrogen bonds (black dashed lines).

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Crystal data

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Hall symbol: P 2ac 2ab
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b = 12.9842 (17) Å
c = 15.871 (2) Å
V = 1965.4 (4) Å^3
Z = 4
$F(000)$ = 768
D_x = 1.205 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7299 reflections
θ = 2.0–40.2°
μ = 0.08 mm^{-1}
T = 98 K
Platelet, colourless
0.12 × 0.10 × 0.04 mm

Data collection

Rigaku AFC12K/SATURN724 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.788, T_{max} = 1.000
14410 measured reflections
2561 independent reflections
2501 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.5°, θ_{min} = 2.0°
h = −12→12
k = −16→16
l = −18→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
S = 1.08
2561 reflections
243 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 0.3164P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: nd

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	−0.09211 (13)	0.48893 (9)	0.86000 (8)	0.0208 (3)
H1O	−0.0859	0.5528	0.8526	0.031*
O2	0.56486 (13)	0.36533 (10)	0.77309 (8)	0.0235 (3)
O3	0.32503 (17)	0.60866 (12)	0.92437 (9)	0.0349 (4)

H3O	0.2607	0.5712	0.9435	0.052*
N1	0.12984 (17)	0.48168 (12)	1.00313 (9)	0.0245 (3)
N2	0.05966 (17)	0.19494 (12)	0.67553 (10)	0.0228 (3)
C1	0.08927 (18)	0.39987 (13)	0.94193 (10)	0.0191 (3)
H1	0.1754	0.3580	0.9312	0.023*
C2	−0.0200 (2)	0.32607 (14)	0.98034 (12)	0.0250 (4)
H2A	−0.1135	0.3393	0.9556	0.030*
H2B	0.0061	0.2537	0.9684	0.030*
C3	−0.0236 (2)	0.34482 (17)	1.07595 (13)	0.0299 (4)
H3	−0.0827	0.2913	1.1041	0.036*
C4	0.1270 (2)	0.33999 (17)	1.10976 (13)	0.0324 (5)
H4A	0.1711	0.2738	1.0936	0.039*
H4B	0.1266	0.3449	1.1720	0.039*
C5	0.2101 (2)	0.43074 (17)	1.07174 (13)	0.0304 (4)
H5A	0.2310	0.4816	1.1165	0.036*
H5B	0.3004	0.4051	1.0491	0.036*
C6	0.0053 (2)	0.53057 (16)	1.04185 (12)	0.0327 (5)
H6A	−0.0539	0.5607	0.9970	0.039*
H6B	0.0362	0.5872	1.0792	0.039*
C7	−0.0833 (2)	0.45269 (18)	1.09371 (12)	0.0329 (5)
H7	−0.0694	0.4681	1.1549	0.039*
C8	−0.2379 (3)	0.4605 (2)	1.07452 (16)	0.0498 (7)
H8	−0.2650	0.4626	1.0170	0.060*
C9	−0.3375 (3)	0.4646 (2)	1.13121 (18)	0.0534 (7)
H9A	−0.3145	0.4626	1.1894	0.064*
H9B	−0.4327	0.4695	1.1141	0.064*
C10	0.04468 (16)	0.44563 (13)	0.85620 (11)	0.0175 (3)
H10	0.1126	0.5010	0.8402	0.021*
C11	0.04985 (18)	0.36143 (13)	0.78993 (10)	0.0182 (3)
C12	−0.07008 (19)	0.31535 (14)	0.76062 (12)	0.0227 (4)
H12	−0.1593	0.3392	0.7787	0.027*
C13	−0.06039 (19)	0.23226 (15)	0.70350 (12)	0.0249 (4)
H13	−0.1449	0.2015	0.6842	0.030*
C14	0.18062 (18)	0.24173 (13)	0.70160 (10)	0.0196 (3)
C15	0.18147 (17)	0.32619 (13)	0.75884 (10)	0.0172 (3)
C16	0.31191 (18)	0.37064 (13)	0.78240 (10)	0.0180 (3)
H16	0.3137	0.4283	0.8193	0.022*
C17	0.43522 (18)	0.33065 (13)	0.75211 (11)	0.0191 (3)
C18	0.43402 (19)	0.24588 (14)	0.69502 (11)	0.0213 (3)
H18	0.5199	0.2187	0.6743	0.026*
C19	0.31040 (19)	0.20397 (14)	0.67016 (11)	0.0216 (3)
H19	0.3106	0.1485	0.6311	0.026*
C20	0.57014 (19)	0.44156 (15)	0.83814 (14)	0.0288 (4)
H20A	0.5219	0.5040	0.8191	0.043*
H20B	0.6682	0.4579	0.8510	0.043*
H20C	0.5240	0.4150	0.8888	0.043*
C21	0.3789 (4)	0.6699 (3)	0.98995 (18)	0.0793 (13)
H21A	0.3187	0.7303	0.9979	0.119*

H21B	0.4740	0.6925	0.9755	0.119*
H21C	0.3816	0.6296	1.0421	0.119*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0171 (6)	0.0161 (5)	0.0292 (6)	0.0017 (5)	0.0012 (5)	−0.0008 (5)
O2	0.0157 (5)	0.0233 (6)	0.0314 (6)	−0.0006 (5)	0.0013 (5)	−0.0028 (5)
O3	0.0421 (9)	0.0361 (8)	0.0265 (6)	−0.0121 (7)	0.0075 (6)	−0.0059 (6)
N1	0.0303 (8)	0.0229 (7)	0.0203 (6)	−0.0048 (6)	−0.0025 (6)	−0.0006 (6)
N2	0.0230 (7)	0.0193 (7)	0.0262 (7)	−0.0012 (6)	−0.0012 (6)	−0.0032 (6)
C1	0.0206 (8)	0.0166 (7)	0.0202 (7)	−0.0011 (6)	0.0009 (6)	0.0007 (6)
C2	0.0281 (9)	0.0209 (8)	0.0259 (8)	−0.0048 (7)	0.0028 (7)	0.0031 (7)
C3	0.0292 (9)	0.0362 (11)	0.0242 (8)	−0.0031 (8)	0.0029 (8)	0.0098 (8)
C4	0.0322 (10)	0.0360 (11)	0.0291 (9)	0.0001 (9)	−0.0013 (8)	0.0110 (8)
C5	0.0320 (10)	0.0346 (10)	0.0244 (8)	−0.0049 (8)	−0.0060 (8)	0.0027 (8)
C6	0.0487 (12)	0.0262 (10)	0.0234 (8)	0.0091 (9)	−0.0014 (9)	−0.0047 (8)
C7	0.0318 (10)	0.0468 (12)	0.0201 (8)	0.0083 (10)	0.0039 (8)	−0.0020 (8)
C8	0.0360 (12)	0.080 (2)	0.0335 (11)	0.0157 (13)	−0.0006 (10)	−0.0086 (13)
C9	0.0388 (12)	0.0715 (19)	0.0500 (14)	0.0109 (13)	0.0095 (11)	0.0000 (14)
C10	0.0151 (7)	0.0161 (7)	0.0212 (7)	0.0002 (6)	0.0008 (6)	−0.0003 (6)
C11	0.0189 (7)	0.0155 (7)	0.0201 (7)	−0.0002 (6)	0.0010 (6)	0.0012 (6)
C12	0.0178 (7)	0.0216 (8)	0.0288 (8)	0.0019 (7)	0.0005 (7)	−0.0039 (7)
C13	0.0208 (8)	0.0230 (8)	0.0311 (9)	−0.0020 (7)	−0.0030 (7)	−0.0047 (7)
C14	0.0218 (8)	0.0175 (8)	0.0195 (7)	0.0009 (7)	0.0005 (6)	−0.0014 (6)
C15	0.0181 (7)	0.0151 (7)	0.0184 (7)	0.0002 (6)	0.0003 (6)	0.0009 (6)
C16	0.0190 (7)	0.0163 (7)	0.0186 (7)	−0.0009 (6)	0.0003 (6)	0.0007 (6)
C17	0.0186 (7)	0.0180 (8)	0.0207 (7)	−0.0003 (6)	0.0004 (6)	0.0033 (6)
C18	0.0210 (7)	0.0211 (8)	0.0217 (8)	0.0039 (7)	0.0046 (7)	0.0008 (7)
C19	0.0252 (8)	0.0183 (8)	0.0212 (7)	0.0025 (7)	0.0019 (7)	−0.0023 (6)
C20	0.0171 (7)	0.0270 (9)	0.0422 (10)	−0.0017 (7)	−0.0009 (8)	−0.0092 (8)
C21	0.106 (3)	0.092 (3)	0.0397 (14)	−0.069 (2)	0.0241 (16)	−0.0203 (15)

Geometric parameters (Å, º)

O1—C10	1.4218 (19)	C7—C8	1.509 (3)
O1—H1O	0.8400	C7—H7	1.0000
O2—C17	1.357 (2)	C8—C9	1.309 (4)
O2—C20	1.431 (2)	C8—H8	0.9500
O3—C21	1.407 (3)	C9—H9A	0.9500
O3—H3O	0.8401	C9—H9B	0.9500
N1—C6	1.480 (3)	C10—C11	1.518 (2)
N1—C5	1.487 (2)	C10—H10	1.0000
N1—C1	1.490 (2)	C11—C12	1.372 (2)
N2—C13	1.320 (2)	C11—C15	1.424 (2)
N2—C14	1.368 (2)	C12—C13	1.412 (2)
C1—C2	1.541 (2)	C12—H12	0.9500
C1—C10	1.544 (2)	C13—H13	0.9500

C1—H1	1.0000	C14—C19	1.422 (2)
C2—C3	1.537 (3)	C14—C15	1.424 (2)
C2—H2A	0.9900	C15—C16	1.421 (2)
C2—H2B	0.9900	C16—C17	1.373 (2)
C3—C4	1.534 (3)	C16—H16	0.9500
C3—C7	1.538 (3)	C17—C18	1.426 (2)
C3—H3	1.0000	C18—C19	1.357 (3)
C4—C5	1.543 (3)	C18—H18	0.9500
C4—H4A	0.9900	C19—H19	0.9500
C4—H4B	0.9900	C20—H20A	0.9800
C5—H5A	0.9900	C20—H20B	0.9800
C5—H5B	0.9900	C20—H20C	0.9800
C6—C7	1.553 (3)	C21—H21A	0.9800
C6—H6A	0.9900	C21—H21B	0.9800
C6—H6B	0.9900	C21—H21C	0.9800

C10—O1—H1O	108.6	C9—C8—H8	117.5
C17—O2—C20	116.01 (13)	C7—C8—H8	117.5
C21—O3—H3O	109.2	C8—C9—H9A	120.0
C6—N1—C5	107.46 (15)	C8—C9—H9B	120.0
C6—N1—C1	111.58 (15)	H9A—C9—H9B	120.0
C5—N1—C1	107.09 (15)	O1—C10—C11	110.12 (13)
C13—N2—C14	117.82 (15)	O1—C10—C1	111.56 (13)
N1—C1—C2	111.16 (14)	C11—C10—C1	108.93 (14)
N1—C1—C10	111.80 (14)	O1—C10—H10	108.7
C2—C1—C10	113.66 (14)	C11—C10—H10	108.7
N1—C1—H1	106.6	C1—C10—H10	108.7
C2—C1—H1	106.6	C12—C11—C15	118.50 (15)
C10—C1—H1	106.6	C12—C11—C10	121.46 (15)
C3—C2—C1	107.88 (15)	C15—C11—C10	120.01 (14)
C3—C2—H2A	110.1	C11—C12—C13	119.75 (16)
C1—C2—H2A	110.1	C11—C12—H12	120.1
C3—C2—H2B	110.1	C13—C12—H12	120.1
C1—C2—H2B	110.1	N2—C13—C12	123.58 (17)
H2A—C2—H2B	108.4	N2—C13—H13	118.2
C4—C3—C2	108.53 (17)	C12—C13—H13	118.2
C4—C3—C7	108.63 (18)	N2—C14—C19	118.35 (15)
C2—C3—C7	109.48 (16)	N2—C14—C15	122.68 (15)
C4—C3—H3	110.1	C19—C14—C15	118.98 (15)
C2—C3—H3	110.1	C16—C15—C14	119.04 (15)
C7—C3—H3	110.1	C16—C15—C11	123.35 (15)
C3—C4—C5	108.25 (16)	C14—C15—C11	117.60 (15)
C3—C4—H4A	110.0	C17—C16—C15	120.28 (15)
C5—C4—H4A	110.0	C17—C16—H16	119.9
C3—C4—H4B	110.0	C15—C16—H16	119.9
C5—C4—H4B	110.0	O2—C17—C16	124.69 (16)
H4A—C4—H4B	108.4	O2—C17—C18	114.79 (15)
N1—C5—C4	111.18 (16)	C16—C17—C18	120.52 (16)

N1—C5—H5A	109.4	C19—C18—C17	120.08 (16)
C4—C5—H5A	109.4	C19—C18—H18	120.0
N1—C5—H5B	109.4	C17—C18—H18	120.0
C4—C5—H5B	109.4	C18—C19—C14	121.07 (16)
H5A—C5—H5B	108.0	C18—C19—H19	119.5
N1—C6—C7	112.16 (16)	C14—C19—H19	119.5
N1—C6—H6A	109.2	O2—C20—H20A	109.5
C7—C6—H6A	109.2	O2—C20—H20B	109.5
N1—C6—H6B	109.2	H20A—C20—H20B	109.5
C7—C6—H6B	109.2	O2—C20—H20C	109.5
H6A—C6—H6B	107.9	H20A—C20—H20C	109.5
C8—C7—C3	112.7 (2)	H20B—C20—H20C	109.5
C8—C7—C6	112.37 (19)	O3—C21—H21A	109.5
C3—C7—C6	107.13 (15)	O3—C21—H21B	109.5
C8—C7—H7	108.2	H21A—C21—H21B	109.5
C3—C7—H7	108.2	O3—C21—H21C	109.5
C6—C7—H7	108.2	H21A—C21—H21C	109.5
C9—C8—C7	124.9 (2)	H21B—C21—H21C	109.5

C6—N1—C1—C2	−48.65 (19)	C1—C10—C11—C12	103.71 (18)
C5—N1—C1—C2	68.68 (19)	O1—C10—C11—C15	163.18 (14)
C6—N1—C1—C10	79.54 (17)	C1—C10—C11—C15	−74.18 (19)
C5—N1—C1—C10	−163.12 (14)	C15—C11—C12—C13	2.5 (3)
N1—C1—C2—C3	−14.0 (2)	C10—C11—C12—C13	−175.43 (16)
C10—C1—C2—C3	−141.20 (16)	C14—N2—C13—C12	−2.0 (3)
C1—C2—C3—C4	−51.1 (2)	C11—C12—C13—N2	−0.1 (3)
C1—C2—C3—C7	67.3 (2)	C13—N2—C14—C19	−178.37 (17)
C2—C3—C4—C5	65.3 (2)	C13—N2—C14—C15	1.8 (3)
C7—C3—C4—C5	−53.6 (2)	N2—C14—C15—C16	−179.73 (16)
C6—N1—C5—C4	66.4 (2)	C19—C14—C15—C16	0.4 (2)
C1—N1—C5—C4	−53.6 (2)	N2—C14—C15—C11	0.6 (2)
C3—C4—C5—N1	−10.8 (2)	C19—C14—C15—C11	−179.29 (15)
C5—N1—C6—C7	−54.7 (2)	C12—C11—C15—C16	177.65 (17)
C1—N1—C6—C7	62.44 (19)	C10—C11—C15—C16	−4.4 (2)
C4—C3—C7—C8	−171.49 (17)	C12—C11—C15—C14	−2.7 (2)
C2—C3—C7—C8	70.1 (2)	C10—C11—C15—C14	175.28 (15)
C4—C3—C7—C6	64.42 (19)	C14—C15—C16—C17	−1.8 (2)
C2—C3—C7—C6	−53.9 (2)	C11—C15—C16—C17	177.88 (16)
N1—C6—C7—C8	−133.14 (19)	C20—O2—C17—C16	6.9 (2)
N1—C6—C7—C3	−8.8 (2)	C20—O2—C17—C18	−172.46 (15)
C3—C7—C8—C9	106.1 (3)	C15—C16—C17—O2	−177.66 (16)
C6—C7—C8—C9	−132.7 (3)	C15—C16—C17—C18	1.6 (2)
N1—C1—C10—O1	−76.08 (17)	O2—C17—C18—C19	179.34 (16)
C2—C1—C10—O1	50.77 (19)	C16—C17—C18—C19	0.0 (3)
N1—C1—C10—C11	162.15 (14)	C17—C18—C19—C14	−1.4 (3)
C2—C1—C10—C11	−71.00 (17)	N2—C14—C19—C18	−178.68 (17)
O1—C10—C11—C12	−18.9 (2)	C15—C14—C19—C18	1.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3o···N1	0.84	1.95	2.783 (2)	171
O1—H1o···N2^{i}	0.84	1.92	2.751 (2)	173
C20—H20b···O1^{ii}	0.98	2.33	3.298 (2)	171
C18—H18···O3^{iii}	0.95	2.58	3.471 (2)	155

Symmetry codes: (i) $-x$, $y+1/2$, $-z+3/2$; (ii) $x+1$, y, z; (iii) $-x+1$, $y-1/2$, $-z+3/2$.