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#### Key indicators

Single-crystal X-ray study  
 T = 123 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
 R factor = 0.049  
 wR factor = 0.105  
 Data-to-parameter ratio = 9.7

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

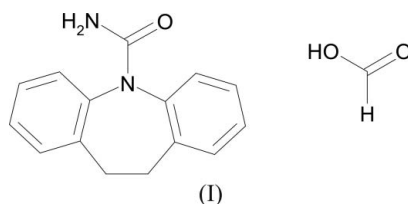
# 10,11-Dihydrocarbamazepine formic acid solvate

In the title compound [systematic name: 10,11-dihydro-5H-dibenz[*b,f*]azepine-5-carboxamide methanoic acid solvate],  $\text{C}_{15}\text{H}_{14}\text{N}_2\text{O} \cdot \text{CH}_2\text{O}_2$ , the dihydrocarbamazepine and formic acid molecules are hydrogen bonded to form an  $R_2^2(8)$  motif, which is further connected into a centrosymmetric double motif arrangement.

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#### Comment

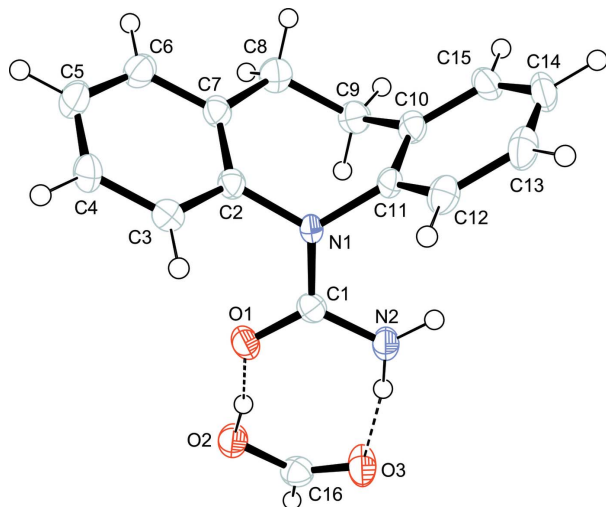
10,11-Dihydrocarbamazepine (DHC) is a recognized impurity in carbamazepine (CBZ), a dibenzazepine drug used to control seizures (Cyr *et al.*, 1987). DHC is known to crystallize in three polymorphic forms: monoclinic form I (Bandoli *et al.*, 1992), orthorhombic form II (Harrison *et al.*, 2006) and triclinic form III (Leech *et al.*, 2007a). The title compound, (I), was produced during an automated parallel crystallization search (Florence, Johnston, Fernandes *et al.*, 2006) on DHC as part of a wider study into the predicted and experimental structures of CBZ (Florence, Johnston, Price *et al.*, 2006; Florence, Leech *et al.*, 2006) and related molecules (Leech *et al.*, 2007b). The sample was identified as a new form using multi-sample foil transmission X-ray powder diffraction analysis (Florence *et al.*, 2003). Subsequent manual recrystallization from a saturated formic acid solution by slow evaporation at 298 K yielded samples of (I) suitable for single-crystal diffraction (Fig. 1).



The molecules in (I) adopt a hydrogen-bonded arrangement similar to that observed in the CBZ formic acid (1/1) solvate (Fleischman *et al.*, 2003). Specifically, the DHC and formic acid molecules are connected *via*  $\text{O}2-\text{H}2 \cdots \text{O}1$  and  $\text{N}2-\text{H}2\text{A} \cdots \text{O}3$  hydrogen bonds to form an  $R_2^2(8)$  (Etter, 1990) dimer motif (Table 1). A third hydrogen bond,  $\text{N}2-\text{H}2\text{B} \cdots \text{O}3^i$  [symmetry code: (i)  $-x + 1, -y + 1, -z$ ] joins adjacent dimers to form a centrosymmetric double motif arrangement (Fig. 2).

#### Experimental

DHC was used as received from Sigma–Aldrich and a single-crystal sample of the title compound was obtained by slow evaporation of a saturated formic acid solution at 298 K.


**Figure 1**

The asymmetric unit of (I), showing the atomic numbering used. Displacement ellipsoids are drawn at the 50% probability level; H atoms are shown as circles of arbitrary radius and hydrogen bonds as dashed lines.

#### Crystal data

|                                  |   |
|----------------------------------|---|
| $C_{15}H_{14}N_2O \cdot CH_2O_2$ | $\gamma = 88.221 (7)^\circ$               |
| $M_r = 284.31$                   | $V = 706.28 (14) \text{ \AA}^3$           |
| Triclinic, $P\bar{1}$            | $Z = 2$                                   |
| $a = 5.2298 (4) \text{ \AA}$     | Mo $K\alpha$ radiation                    |
| $b = 9.3849 (12) \text{ \AA}$    | $\mu = 0.09 \text{ mm}^{-1}$              |
| $c = 14.4858 (18) \text{ \AA}$   | $T = 123 (2) \text{ K}$                   |
| $\alpha = 83.853 (5)^\circ$      | $0.40 \times 0.10 \times 0.04 \text{ mm}$ |
| $\beta = 88.230 (7)^\circ$       |   |

#### Data collection

|                                |  |
|--------------------------------|--|
| Nonius KappaCCD diffractometer | 1260 reflections with $I > 2\sigma(I)$ |
| Absorption correction: none    | $R_{\text{int}} = 0.075$               |
| 9817 measured reflections      | $\theta_{\text{max}} = 23.0^\circ$     |
| 1956 independent reflections   |  |

#### Refinement

|                                 |  |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.049$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.105$               | $\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$                    |
| $S = 1.10$                      | $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$                   |
| 1956 reflections                |  |
| 202 parameters                  |  |

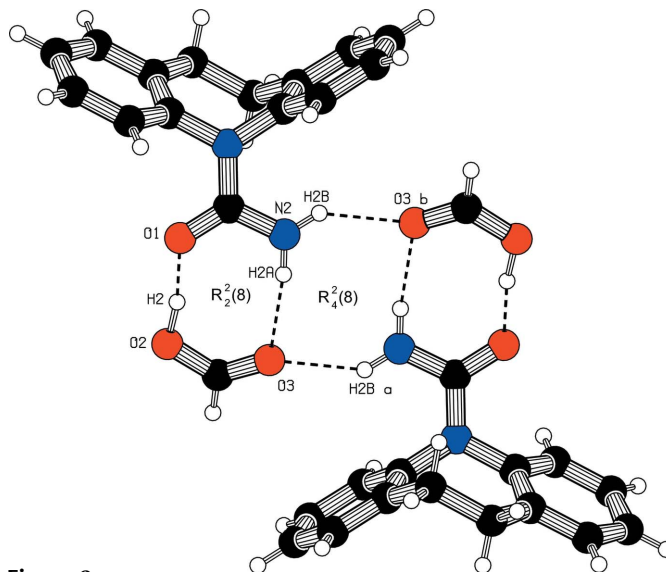
**Table 1**

Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

| $D-H \cdots A$       | $D-H$    | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|----------------------|----------|--------------|--------------|----------------|
| $O2-H2 \cdots O1$    | 1.04 (4) | 1.52 (4)     | 2.552 (3)    | 170 (4)        |
| $N2-H2A \cdots O3$   | 0.88 (3) | 2.08 (3)     | 2.933 (4)    | 163 (3)        |
| $N2-H2B \cdots O3^i$ | 0.89 (3) | 2.13 (3)     | 2.873 (4)    | 141 (2)        |

Symmetry code: (i)  $-x + 1, -y + 1, -z$ .

The three H-atoms attached to N2 and O2 were located in a difference map and refined isotropically [ $N-H = 0.88 (3)$  and  $0.89 (3) \text{ \AA}$ ;  $O-H = 1.04 (4) \text{ \AA}$ ]. All other H atoms were constrained to idealized geometries and included in the refinement using the riding-model approximation:  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  and  $C-H = 0.95$  or  $0.99 \text{ \AA}$ .


**Figure 2**

Plot showing the hydrogen-bonded dimer arrangement in (I) with two  $R_2^2(8)$  dimers joined in a centrosymmetric arrangement via an  $R_4^2(8)$  motif.

Data collection: *COLLECT* (Hooft, 1988) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*; 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: *SHELXL97*.

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## supporting information

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10,11-dihydro-5*H*-dibenz[*b,f*]azepine-5-carboxamide–methanoic acid (1/1)*Crystal data*

$C_{15}H_{14}N_2O \cdot CH_2O_2$   
 $M_r = 284.31$   
 Triclinic,  $P\bar{1}$   
 $a = 5.2298$  (4) Å  
 $b = 9.3849$  (12) Å  
 $c = 14.4858$  (18) Å  
 $\alpha = 83.853$  (5)°  
 $\beta = 88.230$  (7)°  
 $\gamma = 88.221$  (7)°  
 $V = 706.28$  (14) Å<sup>3</sup>

$Z = 2$   
 $F(000) = 300$   
 $D_x = 1.337$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å  
 Cell parameters from 1893 reflections  
 $\theta = 2.9$ – $23.0$ °  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 123$  K  
 Cut needle, colourless  
 $0.40 \times 0.10 \times 0.04$  mm

*Data collection*

Nonius KappaCCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 9817 measured reflections  
 1956 independent reflections

1260 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.075$   
 $\theta_{max} = 23.0$ °,  $\theta_{min} = 3.4$ °  
 $h = -5 \rightarrow 5$   
 $k = -10 \rightarrow 10$   
 $l = -15 \rightarrow 15$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.049$   
 $wR(F^2) = 0.105$   
 $S = 1.10$   
 1956 reflections  
 202 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.1228P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.21$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.22$  e Å<sup>-3</sup>

*Special details*

**Experimental.** Sample crystals twinned. "Single" small piece cut out from a larger, twinned sample.

**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 ( $\text{\AA}^2$ )*

|     | <i>x</i>   | <i>y</i>   | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|------------|---------------|----------------------------------|
| O1  | 0.8138 (3) | 0.2089 (2) | 0.16182 (13)  | 0.0296 (5)                       |
| O2  | 0.4587 (4) | 0.0846 (2) | 0.08699 (14)  | 0.0334 (6)                       |
| O3  | 0.3740 (4) | 0.2814 (2) | -0.01018 (15) | 0.0396 (6)                       |
| N1  | 0.9571 (4) | 0.4012 (2) | 0.22662 (16)  | 0.0210 (6)                       |
| N2  | 0.7533 (5) | 0.4307 (3) | 0.08607 (19)  | 0.0303 (7)                       |
| C1  | 0.8391 (5) | 0.3413 (3) | 0.1576 (2)    | 0.0240 (7)                       |
| C2  | 1.0350 (5) | 0.3108 (3) | 0.3085 (2)    | 0.0228 (7)                       |
| C3  | 1.2318 (5) | 0.2098 (3) | 0.2976 (2)    | 0.0287 (8)                       |
| H3  | 1.3057     | 0.2014     | 0.2376        | 0.034*                           |
| C4  | 1.3197 (5) | 0.1222 (3) | 0.3728 (2)    | 0.0346 (8)                       |
| H4  | 1.4536     | 0.0535     | 0.3649        | 0.042*                           |
| C5  | 1.2126 (6) | 0.1347 (3) | 0.4601 (2)    | 0.0375 (8)                       |
| H5  | 1.2707     | 0.0737     | 0.5123        | 0.045*                           |
| C6  | 1.0202 (5) | 0.2364 (3) | 0.4710 (2)    | 0.0316 (8)                       |
| H6  | 0.9502     | 0.2454     | 0.5314        | 0.038*                           |
| C7  | 0.9255 (5) | 0.3262 (3) | 0.3960 (2)    | 0.0251 (7)                       |
| C8  | 0.7116 (5) | 0.4311 (3) | 0.4178 (2)    | 0.0316 (8)                       |
| H8A | 0.7784     | 0.4946     | 0.4612        | 0.038*                           |
| H8B | 0.5737     | 0.3753     | 0.4516        | 0.038*                           |
| C9  | 0.5902 (5) | 0.5259 (3) | 0.3387 (2)    | 0.0302 (8)                       |
| H9A | 0.5071     | 0.4645     | 0.2976        | 0.036*                           |
| H9B | 0.4552     | 0.5877     | 0.3646        | 0.036*                           |
| C10 | 0.7779 (5) | 0.6198 (3) | 0.2814 (2)    | 0.0260 (7)                       |
| C11 | 0.9627 (5) | 0.5542 (3) | 0.22754 (19)  | 0.0222 (7)                       |
| C12 | 1.1457 (5) | 0.6342 (3) | 0.1759 (2)    | 0.0292 (8)                       |
| H12 | 1.2713     | 0.5880     | 0.1398        | 0.035*                           |
| C13 | 1.1451 (5) | 0.7815 (3) | 0.1770 (2)    | 0.0351 (8)                       |
| H13 | 1.2703     | 0.8366     | 0.1416        | 0.042*                           |
| C14 | 0.9616 (6) | 0.8484 (3) | 0.2297 (2)    | 0.0379 (9)                       |
| H14 | 0.9604     | 0.9495     | 0.2305        | 0.046*                           |
| C15 | 0.7796 (6) | 0.7672 (3) | 0.2813 (2)    | 0.0330 (8)                       |
| H15 | 0.6540     | 0.8136     | 0.3173        | 0.040*                           |
| C16 | 0.3294 (5) | 0.1610 (4) | 0.0221 (2)    | 0.0313 (8)                       |
| H16 | 0.1873     | 0.1172     | -0.0015       | 0.038*                           |

|     |           |           |             |             |
|-----|-----------|-----------|-------------|-------------|
| H2  | 0.603 (7) | 0.143 (4) | 0.112 (3)   | 0.095 (13)* |
| H2A | 0.661 (6) | 0.390 (3) | 0.047 (2)   | 0.051 (11)* |
| H2B | 0.772 (5) | 0.525 (3) | 0.0820 (19) | 0.030 (9)*  |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| O1  | 0.0344 (11) | 0.0196 (13) | 0.0353 (14) | 0.0023 (9)   | -0.0079 (9)  | -0.0045 (10) |
| O2  | 0.0402 (13) | 0.0269 (13) | 0.0332 (14) | -0.0025 (10) | -0.0093 (10) | -0.0005 (11) |
| O3  | 0.0433 (13) | 0.0257 (14) | 0.0488 (15) | -0.0036 (10) | -0.0159 (11) | 0.0054 (12)  |
| N1  | 0.0267 (12) | 0.0143 (14) | 0.0217 (15) | 0.0005 (10)  | -0.0032 (11) | 0.0006 (12)  |
| N2  | 0.0413 (17) | 0.0199 (18) | 0.0294 (18) | -0.0020 (13) | -0.0108 (13) | 0.0013 (15)  |
| C1  | 0.0231 (16) | 0.024 (2)   | 0.025 (2)   | 0.0050 (13)  | 0.0009 (14)  | -0.0047 (17) |
| C2  | 0.0234 (15) | 0.0192 (17) | 0.026 (2)   | -0.0019 (13) | -0.0043 (13) | -0.0014 (15) |
| C3  | 0.0330 (17) | 0.0253 (18) | 0.028 (2)   | 0.0018 (14)  | -0.0029 (14) | -0.0052 (16) |
| C4  | 0.0389 (18) | 0.0260 (19) | 0.038 (2)   | 0.0112 (15)  | -0.0112 (17) | -0.0015 (17) |
| C5  | 0.0461 (19) | 0.031 (2)   | 0.034 (2)   | 0.0018 (16)  | -0.0160 (16) | 0.0034 (17)  |
| C6  | 0.0371 (18) | 0.0312 (19) | 0.026 (2)   | -0.0037 (15) | -0.0027 (14) | 0.0011 (16)  |
| C7  | 0.0271 (16) | 0.0203 (17) | 0.028 (2)   | -0.0037 (13) | -0.0025 (14) | -0.0009 (15) |
| C8  | 0.0298 (17) | 0.0327 (19) | 0.031 (2)   | -0.0003 (14) | 0.0045 (14)  | -0.0014 (16) |
| C9  | 0.0268 (16) | 0.0319 (19) | 0.032 (2)   | 0.0054 (14)  | -0.0015 (14) | -0.0052 (16) |
| C10 | 0.0243 (16) | 0.0237 (19) | 0.030 (2)   | 0.0013 (14)  | -0.0091 (14) | -0.0003 (16) |
| C11 | 0.0244 (16) | 0.0190 (18) | 0.0226 (18) | 0.0025 (13)  | -0.0055 (13) | 0.0009 (14)  |
| C12 | 0.0249 (17) | 0.031 (2)   | 0.031 (2)   | -0.0007 (14) | -0.0043 (14) | 0.0036 (16)  |
| C13 | 0.0354 (19) | 0.028 (2)   | 0.039 (2)   | -0.0085 (15) | -0.0083 (15) | 0.0097 (17)  |
| C14 | 0.050 (2)   | 0.0170 (18) | 0.047 (2)   | -0.0040 (17) | -0.0233 (18) | 0.0026 (18)  |
| C15 | 0.0417 (19) | 0.021 (2)   | 0.037 (2)   | 0.0062 (15)  | -0.0113 (16) | -0.0072 (16) |
| C16 | 0.0299 (17) | 0.034 (2)   | 0.031 (2)   | 0.0000 (16)  | -0.0053 (15) | -0.0073 (18) |

*Geometric parameters (Å, °)*

|        |           |         |           |
|--------|-----------|---------|-----------|
| O1—C1  | 1.249 (3) | C6—H6   | 0.9500    |
| O2—C16 | 1.311 (3) | C7—C8   | 1.515 (4) |
| O2—H2  | 1.04 (4)  | C8—C9   | 1.517 (4) |
| O3—C16 | 1.203 (3) | C8—H8A  | 0.9900    |
| N1—C1  | 1.370 (3) | C8—H8B  | 0.9900    |
| N1—C11 | 1.439 (3) | C9—C10  | 1.509 (4) |
| N1—C2  | 1.444 (3) | C9—H9A  | 0.9900    |
| N2—C1  | 1.341 (4) | C9—H9B  | 0.9900    |
| N2—H2A | 0.88 (3)  | C10—C15 | 1.384 (4) |
| N2—H2B | 0.89 (3)  | C10—C11 | 1.393 (4) |
| C2—C7  | 1.393 (4) | C11—C12 | 1.385 (4) |
| C2—C3  | 1.394 (4) | C12—C13 | 1.384 (4) |
| C3—C4  | 1.375 (4) | C12—H12 | 0.9500    |
| C3—H3  | 0.9500    | C13—C14 | 1.385 (4) |
| C4—C5  | 1.382 (4) | C13—H13 | 0.9500    |
| C4—H4  | 0.9500    | C14—C15 | 1.387 (4) |
| C5—C6  | 1.383 (4) | C14—H14 | 0.9500    |

|              |            |                 |            |
|--------------|------------|-----------------|------------|
| C5—H5        | 0.9500     | C15—H15         | 0.9500     |
| C6—C7        | 1.396 (4)  | C16—H16         | 0.9500     |
| C16—O2—H2    | 112 (2)    | C7—C8—H8B       | 107.6      |
| C1—N1—C11    | 121.2 (2)  | C9—C8—H8B       | 107.6      |
| C1—N1—C2     | 119.3 (2)  | H8A—C8—H8B      | 107.0      |
| C11—N1—C2    | 118.4 (2)  | C10—C9—C8       | 113.6 (2)  |
| C1—N2—H2A    | 114 (2)    | C10—C9—H9A      | 108.8      |
| C1—N2—H2B    | 122.6 (18) | C8—C9—H9A       | 108.8      |
| H2A—N2—H2B   | 123 (3)    | C10—C9—H9B      | 108.8      |
| O1—C1—N2     | 121.9 (3)  | C8—C9—H9B       | 108.8      |
| O1—C1—N1     | 120.8 (3)  | H9A—C9—H9B      | 107.7      |
| N2—C1—N1     | 117.2 (3)  | C15—C10—C11     | 118.4 (3)  |
| C7—C2—C3     | 120.7 (3)  | C15—C10—C9      | 123.3 (3)  |
| C7—C2—N1     | 121.9 (2)  | C11—C10—C9      | 118.2 (2)  |
| C3—C2—N1     | 117.4 (3)  | C12—C11—C10     | 120.9 (3)  |
| C4—C3—C2     | 120.6 (3)  | C12—C11—N1      | 121.0 (2)  |
| C4—C3—H3     | 119.7      | C10—C11—N1      | 118.1 (2)  |
| C2—C3—H3     | 119.7      | C13—C12—C11     | 119.9 (3)  |
| C3—C4—C5     | 119.7 (3)  | C13—C12—H12     | 120.1      |
| C3—C4—H4     | 120.1      | C11—C12—H12     | 120.1      |
| C5—C4—H4     | 120.1      | C12—C13—C14     | 119.9 (3)  |
| C4—C5—C6     | 119.6 (3)  | C12—C13—H13     | 120.1      |
| C4—C5—H5     | 120.2      | C14—C13—H13     | 120.1      |
| C6—C5—H5     | 120.2      | C13—C14—C15     | 119.8 (3)  |
| C5—C6—C7     | 122.1 (3)  | C13—C14—H14     | 120.1      |
| C5—C6—H6     | 118.9      | C15—C14—H14     | 120.1      |
| C7—C6—H6     | 118.9      | C10—C15—C14     | 121.1 (3)  |
| C2—C7—C6     | 117.2 (3)  | C10—C15—H15     | 119.4      |
| C2—C7—C8     | 126.3 (3)  | C14—C15—H15     | 119.4      |
| C6—C7—C8     | 116.5 (3)  | O3—C16—O2       | 126.0 (3)  |
| C7—C8—C9     | 119.1 (3)  | O3—C16—H16      | 117.0      |
| C7—C8—H8A    | 107.6      | O2—C16—H16      | 117.0      |
| C9—C8—H8A    | 107.6      |                 |            |
| C11—N1—C1—O1 | -173.2 (2) | C6—C7—C8—C9     | -176.6 (2) |
| C2—N1—C1—O1  | -4.9 (4)   | C7—C8—C9—C10    | -58.4 (3)  |
| C11—N1—C1—N2 | 6.9 (4)    | C8—C9—C10—C15   | -110.7 (3) |
| C2—N1—C1—N2  | 175.2 (2)  | C8—C9—C10—C11   | 67.7 (3)   |
| C1—N1—C2—C7  | -114.7 (3) | C15—C10—C11—C12 | 0.6 (4)    |
| C11—N1—C2—C7 | 53.9 (3)   | C9—C10—C11—C12  | -177.8 (2) |
| C1—N1—C2—C3  | 67.4 (3)   | C15—C10—C11—N1  | -178.9 (2) |
| C11—N1—C2—C3 | -124.0 (3) | C9—C10—C11—N1   | 2.6 (4)    |
| C7—C2—C3—C4  | 0.7 (4)    | C1—N1—C11—C12   | -83.4 (3)  |
| N1—C2—C3—C4  | 178.6 (2)  | C2—N1—C11—C12   | 108.2 (3)  |
| C2—C3—C4—C5  | -0.1 (4)   | C1—N1—C11—C10   | 96.2 (3)   |
| C3—C4—C5—C6  | -0.8 (4)   | C2—N1—C11—C10   | -72.2 (3)  |
| C4—C5—C6—C7  | 1.3 (4)    | C10—C11—C12—C13 | -0.4 (4)   |

|             |            |                 |           |
|-------------|------------|-----------------|-----------|
| C3—C2—C7—C6 | -0.3 (4)   | N1—C11—C12—C13  | 179.2 (2) |
| N1—C2—C7—C6 | -178.1 (2) | C11—C12—C13—C14 | 0.0 (4)   |
| C3—C2—C7—C8 | 180.0 (2)  | C12—C13—C14—C15 | 0.1 (4)   |
| N1—C2—C7—C8 | 2.2 (4)    | C11—C10—C15—C14 | -0.5 (4)  |
| C5—C6—C7—C2 | -0.7 (4)   | C9—C10—C15—C14  | 177.9 (3) |
| C5—C6—C7—C8 | 179.0 (3)  | C13—C14—C15—C10 | 0.1 (4)   |
| C2—C7—C8—C9 | 3.1 (4)    |                 |           |

*Hydrogen-bond geometry (Å, °)*

| <i>D</i> —H $\cdots$ <i>A</i>           | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|---|-------------|---------------------|----------------------------|-------------------------------|
| O2—H2 $\cdots$ O1                       | 1.04 (4)    | 1.52 (4)            | 2.552 (3)                  | 170 (4)                       |
| N2—H2 <i>A</i> $\cdots$ O3              | 0.88 (3)    | 2.08 (3)            | 2.933 (4)                  | 163 (3)                       |
| N2—H2 <i>B</i> $\cdots$ O3 <sup>i</sup> | 0.89 (3)    | 2.13 (3)            | 2.873 (4)                  | 141 (2)                       |

Symmetry code: (i)  $-x+1, -y+1, -z$ .