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# 3-(2-Aminoethyl)-2-anilinoquinazolin-4(3*H*)-one methanol hemisolvate

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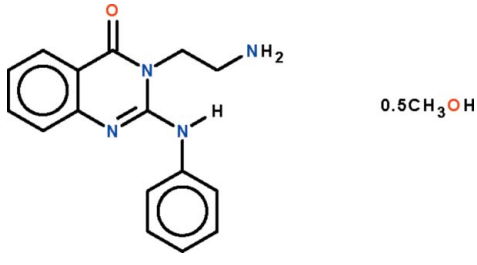
Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.003 Å; disorder in solvent or counterion; $R$ factor = 0.062; $wR$ factor = 0.186; data-to-parameter ratio = 16.2.

The title methanol hemisolvated quinazolin-(3*H*)-one, $C_{16}H_{16}N_4O{\cdot}0.5CH_3OH$, has an anilino substituent in the 2-position and an aminoethyl substituent in the 3-position of the planar fused-ring system (r.m.s. deviation = 0.019 Å). The anilino N atom donates an intramolecular hydrogen bond to the aminoethyl N atom. The molecule and the solvent methanol molecule are linked by N—H···N, N—H···O and O—H···O hydrogen bonds. The methanol molecule is disordered over two equally occupied positions about a twofold rotation axis.

## Related literature

For the synthesis of this class of compounds, see: Yang *et al.* (2008). For the crystal structure of a chlorine-substituted derivative, see: Yang *et al.* (2009).




## Experimental

### Crystal data

$C_{16}H_{16}N_4O{\cdot}0.5CH_4O$
$M_r$ = 296.35
Monoclinic, $C2/c$
$a$ = 19.5972 (11) Å
$b$ = 12.2035 (7) Å
$c$ = 12.8681 (8) Å
$\beta$ = 103.301 (1)°
$V$ = 2994.9 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 295 K
0.30 × 0.20 × 0.10 mm

### Data collection

Bruker APEXII diffractometer
Absorption correction: none
14007 measured reflections
3399 independent reflections
2377 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.073

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.186
$S$ = 1.09
3399 reflections
210 parameters
13 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H31···N4 | 0.88 | 2.04 | 2.811 (3) | 146 |
| N4—H41···O2$^{i}$ | 0.88 | 2.13 | 2.990 (6) | 168 |
| O2—H2*O*···O1 | 0.84 | 2.01 | 2.755 (6) | 147 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5121).

## References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.
Yang, X.-H., Chen, X.-B. & Zhou, S.-X. (2009). *Acta Cryst.* E**65**, o185–o186.
Yang, X.-H., Wu, M.-H., Sun, S.-F., Ding, M.-W., Xie, J.-L. & Xia, Q.-H. (2008). *J. Heterocycl. Chem.* **45**, 1365–1369.

# supplementary materials

*Acta Cryst.* (2009). E**65**, o2989 [ **doi:10.1107/S1600536809045516** ]

# 3-(2-Aminoethyl)-2-anilinoquinazolin-4(3*H*)-one methanol hemisolvate

**T. Gao, Y.-H. Jiao and S. W. Ng**

## Experimental

To a THF (10 ml) solution of 2-ethoxycarbonyliminophosphorane (1.27 g, 3.0 mmol) was added phenylisocyanate (0.36 g, 3.0 mmol). The solution was set aside undisturbed for 6 h at 273 K. To this solution was added ethanolamine (0.18 g, 3 mmol) in THF (5 ml). The mixture was stirred overnight. The solvent was removed and the solid recrystallized from a chloroform/methanol (1/1) mixture to give colorless crystals in 80% yield; m.p. 433–434 K.

## Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.97 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5*U*(C). The amino and hydroxy H atoms were similarly generated.

The methanol molecule is disordered over two equally occupied positions about a two-fold rotation axis. The C–O distance was restrained to 1.500±0.002 Å. The anisotropic displacemnt parameters of the methanolic O and C atoms were restrained to be nearly isotropic.

## Figures

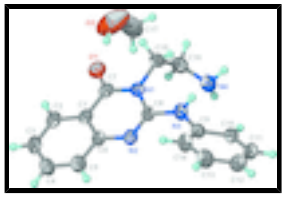


Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of the title compound at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

## 3-(2-Aminoethyl)-2-anilinoquinazolin-4(3*H*)-one methanol hemisolvate

*Crystal data*

| | |
|---|---|
| $C_{16}H_{16}N_4O·0.5CH_4O$ | $F_{000}$ = 1256 |
| $M_r$ = 296.35 | $D_x$ = 1.314 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 3816 reflections |
| *a* = 19.5972 (11) Å | θ = 2.4–25.9º |
| *b* = 12.2035 (7) Å | μ = 0.09 mm$^{-1}$ |
| *c* = 12.8681 (8) Å | *T* = 295 K |
| β = 103.301 (1)º | Block, colorless |
| *V* = 2994.9 (3) Å$^3$ | 0.30 × 0.20 × 0.10 mm |
| *Z* = 8 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII diffractometer | 2377 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.073$ |
| Monochromator: graphite | $\theta_{max} = 27.5^o$ |
| $T = 295$ K | $\theta_{min} = 2.0^o$ |
| ω scans | $h = -17\rightarrow25$ |
| Absorption correction: None | $k = -15\rightarrow14$ |
| 14007 measured reflections | $l = -16\rightarrow16$ |
| 3399 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.062$ | H-atom parameters constrained |
| $wR(F^2) = 0.186$ | $w = 1/[\sigma^2(F_o^2) + (0.1044P)^2 + 0.1504P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.09$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3399 reflections | $\Delta\rho_{max} = 0.55$ e Å$^{-3}$ |
| 210 parameters | $\Delta\rho_{min} = -0.29$ e Å$^{-3}$ |
| 13 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1 | 0.68958 (7) | 0.41303 (12) | 0.81309 (11) | 0.0573 (4) | |
| N1 | 0.73674 (8) | 0.41620 (12) | 0.66714 (11) | 0.0424 (4) | |
| N2 | 0.84958 (8) | 0.34284 (13) | 0.67038 (11) | 0.0458 (4) | |
| N3 | 0.77752 (9) | 0.40366 (13) | 0.51241 (12) | 0.0498 (4) | |
| H31 | 0.7345 | 0.4239 | 0.4817 | 0.060* | |
| N4 | 0.63136 (9) | 0.37965 (16) | 0.44490 (14) | 0.0632 (5) | |
| H41 | 0.6131 | 0.4263 | 0.3939 | 0.076* | |
| H42 | 0.6131 | 0.3143 | 0.4284 | 0.076* | |
| C1 | 0.80430 (10) | 0.34133 (14) | 0.83148 (13) | 0.0414 (4) | |
| C2 | 0.81360 (11) | 0.31401 (16) | 0.93932 (14) | 0.0503 (5) | |
| H2 | 0.7782 | 0.3290 | 0.9746 | 0.060* | |
| C3 | 0.87449 (12) | 0.26533 (18) | 0.99341 (15) | 0.0576 (6) | |
| H3 | 0.8804 | 0.2465 | 1.0650 | 0.069* | |
| C4 | 0.92707 (11) | 0.24457 (19) | 0.94030 (15) | 0.0589 (6) | |
| H4 | 0.9684 | 0.2115 | 0.9767 | 0.071* | |
| C5 | 0.91908 (11) | 0.27202 (19) | 0.83510 (16) | 0.0573 (6) | |
| H5 | 0.9552 | 0.2579 | 0.8011 | 0.069* | |

| | | | | | |
|---|---|---|---|---|---|
| C6 | 0.85720 (10) | 0.32115 (15) | 0.77791 (13) | 0.0427 (5) | |
| C7 | 0.73916 (10) | 0.39143 (15) | 0.77321 (14) | 0.0437 (5) | |
| C8 | 0.79099 (10) | 0.38642 (15) | 0.61962 (14) | 0.0414 (4) | |
| C9 | 0.82431 (10) | 0.39287 (14) | 0.44502 (14) | 0.0426 (5) | |
| C10 | 0.79487 (10) | 0.36669 (15) | 0.33875 (14) | 0.0462 (5) | |
| H10 | 0.7472 | 0.3515 | 0.3175 | 0.055* | |
| C11 | 0.83579 (12) | 0.36311 (17) | 0.26507 (15) | 0.0530 (5) | |
| H11 | 0.8154 | 0.3462 | 0.1942 | 0.064* | |
| C12 | 0.90627 (13) | 0.38417 (19) | 0.29508 (18) | 0.0614 (6) | |
| H12 | 0.9338 | 0.3820 | 0.2451 | 0.074* | |
| C13 | 0.93592 (12) | 0.40868 (19) | 0.40098 (18) | 0.0616 (6) | |
| H13 | 0.9838 | 0.4225 | 0.4220 | 0.074* | |
| C14 | 0.89551 (11) | 0.41293 (17) | 0.47595 (16) | 0.0534 (5) | |
| H14 | 0.9161 | 0.4292 | 0.5468 | 0.064* | |
| C15 | 0.67613 (10) | 0.48235 (17) | 0.61029 (15) | 0.0516 (5) | |
| H15A | 0.6922 | 0.5335 | 0.5634 | 0.062* | |
| H15B | 0.6587 | 0.5248 | 0.6624 | 0.062* | |
| C16 | 0.61626 (11) | 0.41579 (18) | 0.54480 (17) | 0.0586 (6) | |
| H16A | 0.6080 | 0.3524 | 0.5857 | 0.070* | |
| H16B | 0.5739 | 0.4599 | 0.5298 | 0.070* | |
| O2 | 0.5495 (3) | 0.4637 (6) | 0.7850 (7) | 0.176 (3) | 0.50 |
| H2O | 0.5856 | 0.4244 | 0.8006 | 0.211* | 0.50 |
| C17 | 0.4883 (4) | 0.3949 (6) | 0.7344 (11) | 0.101 (3) | 0.50 |
| H17A | 0.4553 | 0.3937 | 0.7792 | 0.152* | 0.50 |
| H17B | 0.5037 | 0.3216 | 0.7254 | 0.152* | 0.50 |
| H17C | 0.4662 | 0.4250 | 0.6660 | 0.152* | 0.50 |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0468 (8) | 0.0701 (10) | 0.0607 (8) | 0.0019 (7) | 0.0243 (7) | −0.0043 (6) |
| N1 | 0.0402 (9) | 0.0437 (9) | 0.0438 (8) | 0.0002 (7) | 0.0110 (7) | −0.0028 (6) |
| N2 | 0.0417 (9) | 0.0570 (10) | 0.0402 (8) | 0.0011 (7) | 0.0130 (7) | −0.0002 (6) |
| N3 | 0.0430 (9) | 0.0665 (11) | 0.0405 (8) | 0.0019 (8) | 0.0107 (7) | 0.0053 (7) |
| N4 | 0.0614 (12) | 0.0661 (12) | 0.0558 (10) | 0.0053 (9) | 0.0006 (9) | −0.0015 (8) |
| C1 | 0.0435 (10) | 0.0412 (10) | 0.0411 (9) | −0.0070 (8) | 0.0128 (8) | −0.0050 (7) |
| C2 | 0.0578 (13) | 0.0540 (12) | 0.0437 (10) | −0.0063 (10) | 0.0214 (9) | −0.0038 (8) |
| C3 | 0.0697 (14) | 0.0649 (13) | 0.0384 (9) | −0.0019 (11) | 0.0128 (10) | 0.0028 (9) |
| C4 | 0.0490 (12) | 0.0744 (15) | 0.0494 (11) | 0.0035 (11) | 0.0035 (10) | 0.0062 (9) |
| C5 | 0.0446 (12) | 0.0782 (15) | 0.0510 (11) | 0.0058 (10) | 0.0152 (9) | 0.0035 (10) |
| C6 | 0.0424 (10) | 0.0490 (11) | 0.0378 (9) | −0.0038 (8) | 0.0112 (8) | −0.0014 (7) |
| C7 | 0.0443 (11) | 0.0438 (10) | 0.0459 (10) | −0.0063 (8) | 0.0164 (8) | −0.0070 (7) |
| C8 | 0.0413 (10) | 0.0424 (10) | 0.0415 (9) | −0.0040 (8) | 0.0112 (8) | −0.0027 (7) |
| C9 | 0.0445 (11) | 0.0432 (10) | 0.0411 (9) | −0.0007 (8) | 0.0122 (8) | 0.0067 (7) |
| C10 | 0.0482 (11) | 0.0448 (11) | 0.0440 (9) | −0.0001 (8) | 0.0072 (8) | 0.0011 (7) |
| C11 | 0.0636 (14) | 0.0570 (12) | 0.0404 (9) | 0.0007 (10) | 0.0159 (9) | −0.0006 (8) |
| C12 | 0.0654 (15) | 0.0711 (15) | 0.0554 (12) | 0.0043 (11) | 0.0293 (11) | 0.0041 (10) |
| C13 | 0.0466 (12) | 0.0792 (16) | 0.0620 (13) | −0.0042 (10) | 0.0187 (10) | 0.0085 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.0490 (12) | 0.0683 (14) | 0.0423 (10) | −0.0097 (10) | 0.0091 (9) | 0.0032 (9) |
| C15 | 0.0507 (12) | 0.0492 (12) | 0.0548 (11) | 0.0090 (9) | 0.0119 (9) | −0.0007 (8) |
| C16 | 0.0445 (12) | 0.0671 (14) | 0.0618 (13) | 0.0074 (10) | 0.0071 (10) | 0.0025 (10) |
| O2 | 0.109 (4) | 0.189 (6) | 0.231 (6) | −0.017 (4) | 0.043 (4) | −0.115 (5) |
| C17 | 0.044 (6) | 0.143 (5) | 0.117 (8) | 0.021 (4) | 0.017 (5) | 0.021 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.227 (2) | C5—H5 | 0.9300 |
| N1—C7 | 1.388 (2) | C9—C14 | 1.382 (3) |
| N1—C8 | 1.391 (2) | C9—C10 | 1.394 (2) |
| N1—C15 | 1.482 (2) | C10—C11 | 1.376 (3) |
| N2—C8 | 1.297 (2) | C10—H10 | 0.9300 |
| N2—C6 | 1.383 (2) | C11—C12 | 1.370 (3) |
| N3—C8 | 1.360 (2) | C11—H11 | 0.9300 |
| N3—C9 | 1.406 (2) | C12—C13 | 1.386 (3) |
| N3—H31 | 0.8800 | C12—H12 | 0.9300 |
| N4—C16 | 1.453 (3) | C13—C14 | 1.383 (3) |
| N4—H41 | 0.8800 | C13—H13 | 0.9300 |
| N4—H42 | 0.8800 | C14—H14 | 0.9300 |
| C1—C6 | 1.393 (3) | C15—C16 | 1.514 (3) |
| C1—C2 | 1.398 (2) | C15—H15A | 0.9700 |
| C1—C7 | 1.458 (3) | C15—H15B | 0.9700 |
| C2—C3 | 1.371 (3) | C16—H16A | 0.9700 |
| C2—H2 | 0.9300 | C16—H16B | 0.9700 |
| C3—C4 | 1.385 (3) | O2—C17 | 1.486 (2) |
| C3—H3 | 0.9300 | O2—H2O | 0.8400 |
| C4—C5 | 1.368 (3) | C17—H17A | 0.9600 |
| C4—H4 | 0.9300 | C17—H17B | 0.9600 |
| C5—C6 | 1.400 (3) | C17—H17C | 0.9600 |
| C7—N1—C8 | 121.23 (15) | N2—C8—N1 | 124.28 (16) |
| C7—N1—C15 | 116.50 (15) | N3—C8—N1 | 114.57 (16) |
| C8—N1—C15 | 122.13 (15) | C14—C9—C10 | 119.07 (18) |
| C8—N2—C6 | 117.49 (16) | C14—C9—N3 | 124.37 (17) |
| C8—N3—C9 | 127.54 (17) | C10—C9—N3 | 116.44 (17) |
| C8—N3—H31 | 116.2 | C11—C10—C9 | 120.53 (19) |
| C9—N3—H31 | 116.2 | C11—C10—H10 | 119.7 |
| C16—N4—H41 | 109.5 | C9—C10—H10 | 119.7 |
| C16—N4—H42 | 109.5 | C12—C11—C10 | 120.61 (19) |
| H41—N4—H42 | 109.5 | C12—C11—H11 | 119.7 |
| C6—C1—C2 | 120.49 (17) | C10—C11—H11 | 119.7 |
| C6—C1—C7 | 118.89 (16) | C11—C12—C13 | 119.0 (2) |
| C2—C1—C7 | 120.62 (18) | C11—C12—H12 | 120.5 |
| C3—C2—C1 | 120.45 (19) | C13—C12—H12 | 120.5 |
| C3—C2—H2 | 119.8 | C14—C13—C12 | 121.1 (2) |
| C1—C2—H2 | 119.8 | C14—C13—H13 | 119.5 |
| C2—C3—C4 | 119.24 (17) | C12—C13—H13 | 119.5 |
| C2—C3—H3 | 120.4 | C9—C14—C13 | 119.66 (19) |
| C4—C3—H3 | 120.4 | C9—C14—H14 | 120.2 |

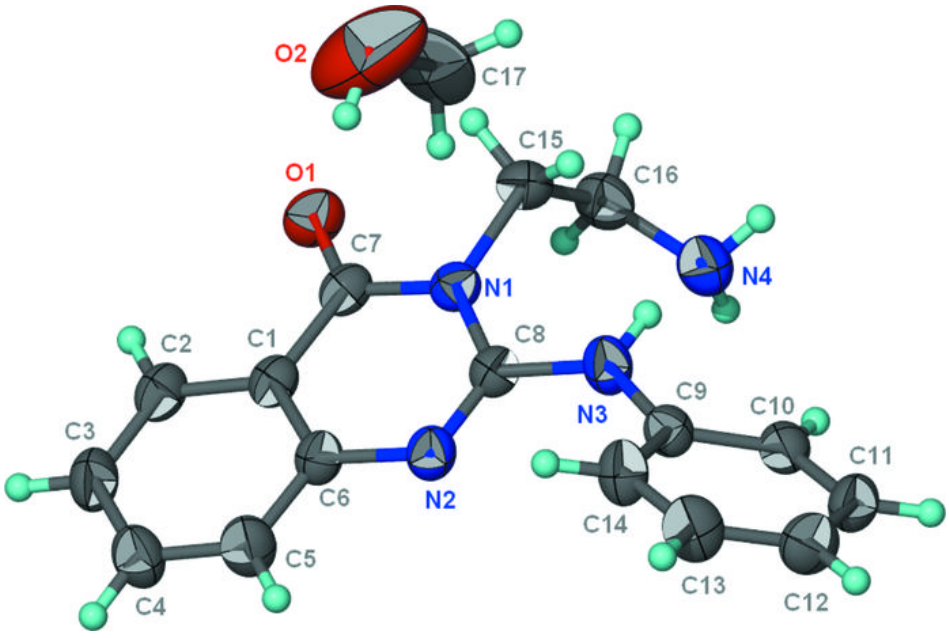
| | | | |
|---|---|---|---|
| C5—C4—C3 | 120.99 (19) | C13—C14—H14 | 120.2 |
| C5—C4—H4 | 119.5 | N1—C15—C16 | 114.39 (17) |
| C3—C4—H4 | 119.5 | N1—C15—H15A | 108.7 |
| C4—C5—C6 | 120.9 (2) | C16—C15—H15A | 108.7 |
| C4—C5—H5 | 119.6 | N1—C15—H15B | 108.7 |
| C6—C5—H5 | 119.6 | C16—C15—H15B | 108.7 |
| N2—C6—C1 | 122.70 (17) | H15A—C15—H15B | 107.6 |
| N2—C6—C5 | 119.27 (17) | N4—C16—C15 | 111.46 (19) |
| C1—C6—C5 | 117.96 (16) | N4—C16—H16A | 109.3 |
| O1—C7—N1 | 120.87 (17) | C15—C16—H16A | 109.3 |
| O1—C7—C1 | 123.97 (17) | N4—C16—H16B | 109.3 |
| N1—C7—C1 | 115.15 (16) | C15—C16—H16B | 109.3 |
| N2—C8—N3 | 121.13 (18) | H16A—C16—H16B | 108.0 |
| C6—C1—C2—C3 | −1.1 (3) | C6—N2—C8—N3 | −175.64 (16) |
| C7—C1—C2—C3 | 178.97 (17) | C6—N2—C8—N1 | 2.5 (3) |
| C1—C2—C3—C4 | 0.7 (3) | C9—N3—C8—N2 | −9.1 (3) |
| C2—C3—C4—C5 | 0.1 (3) | C9—N3—C8—N1 | 172.63 (16) |
| C3—C4—C5—C6 | −0.5 (4) | C7—N1—C8—N2 | −6.1 (3) |
| C8—N2—C6—C1 | 1.8 (3) | C15—N1—C8—N2 | 169.49 (18) |
| C8—N2—C6—C5 | 178.68 (18) | C7—N1—C8—N3 | 172.12 (15) |
| C2—C1—C6—N2 | 177.50 (16) | C15—N1—C8—N3 | −12.3 (2) |
| C7—C1—C6—N2 | −2.5 (3) | C8—N3—C9—C14 | −31.8 (3) |
| C2—C1—C6—C5 | 0.6 (3) | C8—N3—C9—C10 | 152.29 (18) |
| C7—C1—C6—C5 | −179.41 (17) | C14—C9—C10—C11 | −1.4 (3) |
| C4—C5—C6—N2 | −176.84 (19) | N3—C9—C10—C11 | 174.75 (17) |
| C4—C5—C6—C1 | 0.2 (3) | C9—C10—C11—C12 | 0.6 (3) |
| C8—N1—C7—O1 | −176.29 (16) | C10—C11—C12—C13 | 0.3 (3) |
| C15—N1—C7—O1 | 7.9 (3) | C11—C12—C13—C14 | −0.5 (3) |
| C8—N1—C7—C1 | 4.9 (2) | C10—C9—C14—C13 | 1.2 (3) |
| C15—N1—C7—C1 | −170.91 (15) | N3—C9—C14—C13 | −174.6 (2) |
| C6—C1—C7—O1 | −179.64 (17) | C12—C13—C14—C9 | −0.3 (3) |
| C2—C1—C7—O1 | 0.3 (3) | C7—N1—C15—C16 | −96.6 (2) |
| C6—C1—C7—N1 | −0.9 (2) | C8—N1—C15—C16 | 87.6 (2) |
| C2—C1—C7—N1 | 179.07 (16) | N1—C15—C16—N4 | −77.5 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H31···N4 | 0.88 | 2.04 | 2.811 (3) | 146 |
| N4—H41···O2$^{i}$ | 0.88 | 2.13 | 2.990 (6) | 168 |
| O2—H2O···O1 | 0.84 | 2.01 | 2.755 (6) | 147 |

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

**Fig. 1**


O2
C17
C15
C16
O1
C7
N1
N4
C2
C1
C8
N3
C9
C10
C3
C11
C6
N2
C14
C5
C13
C4
C12