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# 4-[(7-Fluoroquinazolin-4-yl)oxy]aniline

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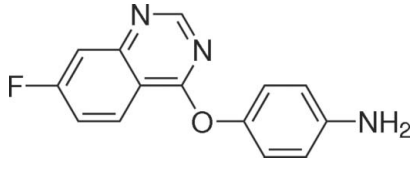
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.045; $wR$ factor = 0.110; data-to-parameter ratio = 7.3.

In the molecule of the title compound, $C_{14}H_{10}FN_3O$, the bicyclic quinazoline system is effectively planar, with a mean deviation from planarity of 0.0140 (3) Å. The quinazoline heterocyclic system and the adjacent benzene ring make a dihedral angle of 85.73 (9)°. Two intermolecular N—H···N hydrogen bonds contribute to the stability of the crystal structure. In addition, a weak $\pi$–$\pi$ stacking interaction [centroid–centroid distance = 3.902 (2) Å] is observed.

## Related literature

For general background to quinazolines, see: Labuda *et al.* (2009). Graves *et al.* (2002); For the preparation of the title compound, see: Zhang *et al.* (2010). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{14}H_{10}FN_3O$
$M_r$ = 255.25
Orthorhombic, $P2_12_12_1$
$a$ = 8.0210 (16) Å
$b$ = 8.3370 (17) Å
$c$ = 17.562 (4) Å
$V$ = 1174.4 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.969, $T_{max}$ = 0.990
2351 measured reflections
1256 independent reflections
883 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.082
3 standard reflections every 200 reflections
intensity decay: 1%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.110
$S$ = 1.02
1256 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 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—H1$A$···N2$^{i}$ | 0.89 | 2.67 | 3.408 (4) | 142 |
| N1—H1$B$···N3$^{ii}$ | 0.89 | 2.38 | 3.205 (4) | 154 |

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

The authors thank the Center of Testing and Analysis, Nanjing University, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2317).

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# supporting information

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## 4-[(7-Fluoroquinazolin-4-yl)oxy]aniline

**Jing Jia, Guibin Wang and Dingqiang Lu**

### S1. Comment

Quinazoline and its derivatives have been a research hotspot for a long time, owing to their significant role in the synthesis of some tyrosine protein kinase inhibitors and their potential anti-cancer activities (Labuda *et al.*, 2009; Graves *et al.*, 2002). As part of our studies into the synthesis of quinazoline derivatives, the title compound 4-[(4-benzenamine)-yloxy]-7-fluoroquinazoline, which may be used as an intermediate towards some quinazoline derivatives, was synthesised. We report herein the crystal structure of the title compound.

In the molecule of the title compound, (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The bicyclic quinazoline system is effectively planar with a mean deviation of only 0.0140 (3)Å. The dihedral angle between the benzene ring C1-C6 and the quinazoline ring system is 85.73 (9)°.

Two intermolecular N-H···N hydrogen bonds contribute to the stability of the molecular configuration and the packing of the molecules (Fig. 2 and Table 1). The crystal structure (Fig. 2) is also stabilized by a weak $\pi$–$\pi$ stacking interaction with centroid–centroid separation of 3.902 (2) Å for Cg1···Cg2$^{i}$ , where Cg1, Cg2 are the centroids of the rings N2/C7/C14/C9/N3/C8 and C1–C6, respectively [symmetry code: (i) -1/2+x, 1/2-y, 1-z].

### S2. Experimental

The title compound was prepared by following a reported procedure (Zhang *et al.*, 2010). 4-Chloro-7-fluoroquinazoline (10 g, 54.77 mmol) was added to a mixture of dimethylformamide (100 ml), potassium tert-butoxide (6.15 g, 54.77 mmol) and 4-aminophenol (5.98 g, 54.77 mmol), and then heated to 343 K for 8 h. After cooling to room temperature, the reaction mixture was added to water (250 ml) and ethyl acetate (250 ml). The organic phase was collected and the water phase was extracted with ethyl acetate (250 ml). All the organic phases were combined and washed with brine (2× 250 ml). The organic phase was dried with anhydrous sodium sulfate for 6 h and then distilled (b.p. 313 K at 0.1 Mpa) and recrystallized from ethyl acetate, to give a total yield of 4-[(4-benzenamine)yloxy]-7-fluoroquinazoline of 81.0 % (11.32 g, 44.35 mmol). M.p. 353-355 K. ESI-MS(m/z): 256.1$[M+H]^+$, 278.1$[M+Na]^+$. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$: 8.72 (s, 1 H, 8-H), 8.40 (dd, $J_{H-F}$ = 6.0 Hz, J = 9.0 Hz, 1 H, 13-H), 7.7 (dd, J = 2.5 Hz, $J_{H-F}$ = 10.0 Hz, 1 H, 10-H), 7.61 (td, J = 2.5, 9.0 Hz, $J_{H-F}$ = 9.0 Hz, 1H, 12-H), 7.00 (d, J = 9.0 Hz, 1H, C1-H), 7.00 (d, J = 9.0 Hz, 1H, C5-H), 6.71 (d, J = 8.5 Hz, 1H, C2-H), 6.71 (d, J = 8.5 Hz, 1H, C4-H), 5.10(s, 2H, N1-H). $^{13}$C NMR(500 MHz, DMSO-$d_6$) $\delta$: 166.58 (C-7), 165.12 (d, $J_{C-F}$ = 251.3 Hz, C-11), 155.17 (C-8), 152.64 (d, $J_{C-F}$ = 13.8 Hz, C-9), 146.47 (C-6), 142.05 (C-3), 126.55 (d, $J_{C-F}$ = 11.3 Hz, C-13), 121.89 (C-1), 121.89 (C-5), 117.38 (d, $J_{C-F}$ = 25.0 Hz, C-12), 114.18 (C-2), 114.18 (C-4), 112.82 (C-14), 111.38 (d, $J_{C-F}$ = 21.3 Hz, C-10). IR(KBr)(cm$^{-1}$): $\nu_{N-H}$ (3420.80, 3327.69), $\nu_{C=C-H}$ (3077.53), $\nu_{C=N}$ (1628.11), $\delta_{C=C-H}$ (1609.25, 1575.87, 1509.07, 1459.02), $\nu_{C-N}$ (1286.23), $\nu_{Ar-O}$ (1248.06). UV-vis: $\lambda_{max}$($CH_3OH$) nm ($\varepsilon$): 217.5 (40174), $\lambda_{max}$ (0.1M HCl) nm ($\varepsilon$): 230.2 (30173), $\lambda_{max}$(0.1M NaOH) nm ($\varepsilon$): 216.4 (16773).

Crystals of the title compound suitable for X-ray diffraction were grown from ethyl acetate.

### S3. Refinement

The H atoms of the $NH_2$ group were initially located from a Difference-Fourier map, but were then constrained to ride on their parent atom N1, with N-H = 0.89 Å, and $U_{iso}$(H) = 1.2 $U_{eq}$(N1) in the final stages of the refinement. The remaining H atoms were positioned geometrically with C-H = 0.93 and 0.98 Å for aromatic and methine H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}$(H) = 1.2 $U_{eq}$(C). In the absence of any significant anomalous scattering, Friedel pairs were merged before the final refinement and the absolute structure was assigned arbitrarily.

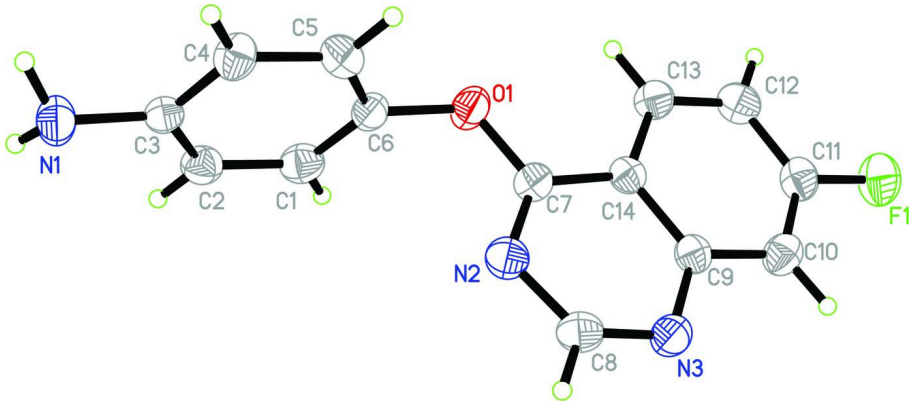


**Figure 1**

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level

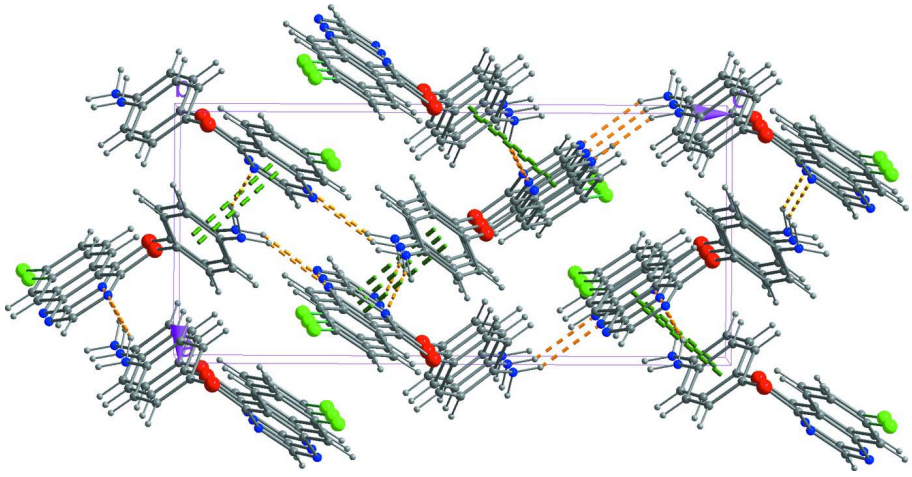

**Figure 2**

A partial packing diagram. Hydrogen bonds and weak $\pi$–$\pi$ stacking interactions are shown as dashed lines.

### 4-[(7-Fluoroquinazolin-4-yl)oxy]aniline

*Crystal data*

$C_{14}H_{10}FN_3O$
$M_r$ = 255.25
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a$ = 8.0210 (16) Å
$b$ = 8.3370 (17) Å
$c$ = 17.562 (4) Å
$V$ = 1174.4 (4) Å$^3$
$Z$ = 4
$F$(000) = 528
$D_x$ = 1.444 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 25 reflections
$\theta$ = 9.0–12.0°

$\mu$ = 0.11 mm$^{-1}$
$T$ = 293 K

Block, colorless
0.30 × 0.20 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.969, $T_{max}$ = 0.990
2351 measured reflections

1256 independent reflections
883 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.082
$\theta_{max}$ = 25.3°, $\theta_{min}$ = 2.3°
$h$ = −9→0
$k$ = −10→10
$l$ = −21→0
3 standard reflections every 200 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.110
$S$ = 1.02
1256 reflections
172 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
$w = 1/[\sigma^2(F_o^2) + (0.046P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

*Special details*

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 0.3205 (3) | 0.8351 (3) | 0.76958 (14) | 0.0778 (8) |
| O1 | 0.4564 (4) | 0.2636 (3) | 0.54742 (14) | 0.0600 (8) |
| N1 | 0.5255 (5) | −0.3210 (3) | 0.39680 (17) | 0.0613 (9) |
| H1A | 0.6191 | −0.3749 | 0.4060 | 0.074* |
| H1B | 0.5050 | −0.3230 | 0.3470 | 0.074* |
| N2 | 0.2795 (4) | 0.1426 (3) | 0.63318 (17) | 0.0543 (9) |
| N3 | 0.1694 (4) | 0.2924 (4) | 0.73803 (17) | 0.0558 (9) |
| C1 | 0.5944 (5) | 0.0096 (4) | 0.5327 (2) | 0.0557 (10) |
| H1C | 0.6622 | 0.0345 | 0.5740 | 0.067* |
| C2 | 0.6148 (5) | −0.1334 (4) | 0.49402 (19) | 0.0522 (9) |
| H2B | 0.6978 | −0.2042 | 0.5093 | 0.063* |
| C3 | 0.5145 (5) | −0.1730 (4) | 0.43328 (19) | 0.0449 (9) |
| C4 | 0.3965 (5) | −0.0629 (4) | 0.41001 (19) | 0.0527 (10) |

| | | | | |
|---|---|---|---|---|
| H4A | 0.3302 | −0.0854 | 0.3679 | 0.063* |
| C5 | 0.3757 (5) | 0.0809 (4) | 0.4487 (2) | 0.0564 (10) |
| H5A | 0.2952 | 0.1540 | 0.4329 | 0.068* |
| C6 | 0.4732 (5) | 0.1138 (4) | 0.50944 (18) | 0.0472 (9) |
| C7 | 0.3580 (5) | 0.2687 (4) | 0.60919 (19) | 0.0467 (9) |
| C8 | 0.1880 (5) | 0.1638 (5) | 0.6966 (2) | 0.0593 (11) |
| H8A | 0.1297 | 0.0739 | 0.7132 | 0.071* |
| C9 | 0.2538 (4) | 0.4244 (4) | 0.71251 (19) | 0.0444 (8) |
| C10 | 0.2435 (5) | 0.5671 (4) | 0.7550 (2) | 0.0552 (10) |
| H10A | 0.1805 | 0.5725 | 0.7994 | 0.066* |
| C11 | 0.3285 (6) | 0.6964 (4) | 0.7291 (2) | 0.0540 (10) |
| C12 | 0.4236 (5) | 0.6976 (4) | 0.6636 (2) | 0.0580 (10) |
| H12A | 0.4787 | 0.7902 | 0.6481 | 0.070* |
| C13 | 0.4348 (5) | 0.5598 (4) | 0.6223 (2) | 0.0520 (10) |
| H13A | 0.4979 | 0.5577 | 0.5779 | 0.062* |
| C14 | 0.3511 (4) | 0.4204 (4) | 0.64658 (18) | 0.0420 (8) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.0938 (19) | 0.0589 (13) | 0.0808 (16) | −0.0023 (15) | −0.0035 (15) | −0.0267 (12) |
| O1 | 0.0754 (19) | 0.0483 (14) | 0.0565 (14) | −0.0111 (16) | 0.0223 (15) | −0.0100 (12) |
| N1 | 0.070 (2) | 0.0483 (17) | 0.0654 (19) | 0.0034 (18) | 0.0088 (19) | −0.0101 (15) |
| N2 | 0.0546 (19) | 0.0488 (19) | 0.059 (2) | −0.0069 (17) | 0.0063 (18) | 0.0018 (15) |
| N3 | 0.062 (2) | 0.0521 (18) | 0.0539 (18) | −0.0034 (18) | 0.0099 (18) | −0.0034 (16) |
| C1 | 0.057 (2) | 0.061 (2) | 0.049 (2) | −0.007 (2) | −0.004 (2) | 0.0017 (19) |
| C2 | 0.051 (2) | 0.057 (2) | 0.049 (2) | 0.005 (2) | −0.0010 (19) | 0.0061 (18) |
| C3 | 0.048 (2) | 0.0434 (19) | 0.0432 (19) | −0.0021 (19) | 0.0097 (18) | 0.0039 (16) |
| C4 | 0.050 (2) | 0.059 (2) | 0.049 (2) | −0.002 (2) | −0.008 (2) | −0.0106 (19) |
| C5 | 0.059 (2) | 0.051 (2) | 0.059 (2) | 0.007 (2) | −0.003 (2) | 0.005 (2) |
| C6 | 0.057 (2) | 0.0423 (19) | 0.0429 (19) | −0.0055 (19) | 0.009 (2) | −0.0038 (17) |
| C7 | 0.047 (2) | 0.049 (2) | 0.0441 (19) | −0.002 (2) | 0.0011 (19) | −0.0011 (17) |
| C8 | 0.059 (2) | 0.055 (2) | 0.064 (2) | −0.010 (2) | 0.012 (2) | 0.009 (2) |
| C9 | 0.0401 (19) | 0.046 (2) | 0.0473 (19) | 0.0028 (18) | −0.0046 (18) | 0.0004 (18) |
| C10 | 0.052 (2) | 0.065 (2) | 0.048 (2) | 0.002 (2) | 0.000 (2) | −0.0055 (19) |
| C11 | 0.057 (2) | 0.050 (2) | 0.054 (2) | 0.001 (2) | −0.011 (2) | −0.0116 (19) |
| C12 | 0.058 (2) | 0.050 (2) | 0.066 (2) | −0.012 (2) | −0.004 (2) | 0.002 (2) |
| C13 | 0.057 (2) | 0.050 (2) | 0.049 (2) | −0.007 (2) | −0.0003 (19) | −0.0032 (18) |
| C14 | 0.0399 (19) | 0.0430 (18) | 0.0431 (18) | 0.0008 (17) | −0.0055 (17) | 0.0003 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F1—C11 | 1.359 (4) | C4—C5 | 1.388 (4) |
| O1—C7 | 1.342 (4) | C4—H4A | 0.9300 |
| O1—C6 | 1.422 (4) | C5—C6 | 1.352 (5) |
| N1—C3 | 1.394 (4) | C5—H5A | 0.9300 |
| N1—H1A | 0.8900 | C7—C14 | 1.427 (4) |
| N1—H1B | 0.8901 | C8—H8A | 0.9300 |

| | | | |
|---|---|---|---|
| N2—C7 | 1.295 (4) | C9—C14 | 1.397 (5) |
| N2—C8 | 1.346 (4) | C9—C10 | 1.407 (5) |
| N3—C8 | 1.305 (5) | C10—C11 | 1.354 (5) |
| N3—C9 | 1.368 (4) | C10—H10A | 0.9300 |
| C1—C6 | 1.366 (5) | C11—C12 | 1.380 (5) |
| C1—C2 | 1.381 (5) | C12—C13 | 1.362 (5) |
| C1—H1C | 0.9300 | C12—H12A | 0.9300 |
| C2—C3 | 1.376 (5) | C13—C14 | 1.408 (4) |
| C2—H2B | 0.9300 | C13—H13A | 0.9300 |
| C3—C4 | 1.380 (5) | | |

| | | | |
|---|---|---|---|
| C7—O1—C6 | 117.6 (3) | N2—C7—O1 | 121.5 (3) |
| C3—N1—H1A | 114.6 | N2—C7—C14 | 123.4 (3) |
| C3—N1—H1B | 117.1 | O1—C7—C14 | 115.0 (3) |
| H1A—N1—H1B | 109.0 | N3—C8—N2 | 129.2 (4) |
| C7—N2—C8 | 115.3 (3) | N3—C8—H8A | 115.4 |
| C8—N3—C9 | 115.0 (3) | N2—C8—H8A | 115.4 |
| C6—C1—C2 | 119.1 (4) | N3—C9—C14 | 121.9 (3) |
| C6—C1—H1C | 120.5 | N3—C9—C10 | 118.5 (3) |
| C2—C1—H1C | 120.5 | C14—C9—C10 | 119.6 (3) |
| C3—C2—C1 | 121.3 (4) | C11—C10—C9 | 117.7 (3) |
| C3—C2—H2B | 119.4 | C11—C10—H10A | 121.2 |
| C1—C2—H2B | 119.4 | C9—C10—H10A | 121.2 |
| C2—C3—C4 | 118.1 (3) | C10—C11—F1 | 118.5 (4) |
| C2—C3—N1 | 122.2 (4) | C10—C11—C12 | 124.4 (3) |
| C4—C3—N1 | 119.7 (3) | F1—C11—C12 | 117.1 (3) |
| C3—C4—C5 | 120.8 (3) | C13—C12—C11 | 118.3 (3) |
| C3—C4—H4A | 119.6 | C13—C12—H12A | 120.9 |
| C5—C4—H4A | 119.6 | C11—C12—H12A | 120.9 |
| C6—C5—C4 | 119.5 (4) | C12—C13—C14 | 120.2 (3) |
| C6—C5—H5A | 120.3 | C12—C13—H13A | 119.9 |
| C4—C5—H5A | 120.3 | C14—C13—H13A | 119.9 |
| C5—C6—C1 | 121.2 (3) | C9—C14—C13 | 119.8 (3) |
| C5—C6—O1 | 119.6 (3) | C9—C14—C7 | 115.1 (3) |
| C1—C6—O1 | 119.1 (3) | C13—C14—C7 | 125.0 (3) |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.6 (6) | C8—N3—C9—C10 | −178.5 (4) |
| C1—C2—C3—C4 | 2.4 (5) | N3—C9—C10—C11 | 179.7 (3) |
| C1—C2—C3—N1 | −175.6 (4) | C14—C9—C10—C11 | 0.7 (5) |
| C2—C3—C4—C5 | −2.4 (5) | C9—C10—C11—F1 | −179.8 (4) |
| N1—C3—C4—C5 | 175.6 (4) | C9—C10—C11—C12 | 0.4 (6) |
| C3—C4—C5—C6 | 0.6 (6) | C10—C11—C12—C13 | −0.6 (6) |
| C4—C5—C6—C1 | 1.3 (5) | F1—C11—C12—C13 | 179.5 (4) |
| C4—C5—C6—O1 | 177.7 (3) | C11—C12—C13—C14 | −0.2 (6) |
| C2—C1—C6—C5 | −1.3 (5) | N3—C9—C14—C13 | 179.5 (3) |
| C2—C1—C6—O1 | −177.7 (3) | C10—C9—C14—C13 | −1.5 (5) |
| C7—O1—C6—C5 | 95.7 (4) | N3—C9—C14—C7 | −1.2 (5) |
| C7—O1—C6—C1 | −87.9 (4) | C10—C9—C14—C7 | 177.8 (3) |

| | | | |
|---|---|---|---|
| C8—N2—C7—O1 | 178.7 (3) | C12—C13—C14—C9 | 1.2 (5) |
| C8—N2—C7—C14 | 0.5 (5) | C12—C13—C14—C7 | −178.0 (4) |
| C6—O1—C7—N2 | −0.7 (5) | N2—C7—C14—C9 | 0.7 (5) |
| C6—O1—C7—C14 | 177.7 (3) | O1—C7—C14—C9 | −177.7 (3) |
| C9—N3—C8—N2 | 0.8 (6) | N2—C7—C14—C13 | 179.9 (3) |
| C7—N2—C8—N3 | −1.3 (6) | O1—C7—C14—C13 | 1.5 (5) |
| C8—N3—C9—C14 | 0.5 (5) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···N2$^{i}$ | 0.89 | 2.67 | 3.408 (4) | 142 |
| N1—H1*B*···N3$^{ii}$ | 0.89 | 2.38 | 3.205 (4) | 154 |

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