# organic compounds

# [2-Cyclopropyl-4-(4-fluorophenyl)-quinolin-3-yl]methanol

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The title compound, $C_{19}H_{16}FNO$, crystallizes with two independent molecules in the asymmetric unit. In the two molecules, the dihedral angles between the benzene and quinoline rings are 72.6 (5) and 76.2 (5)°, between the cyclopropane and quinoline rings they are 65.2 (5) and 66.0 (5)°, and between the benzene and cyclopropane rings they are 25.9 (5) and 33.9 (5)°. There are intermolecular O—H···O, O—H···N and C—H···O hydrogen bonds, as well as intramolecular C—H···O hydrogen bonds, which may be effective in stabilizing the crystal structure.

## Related literature

For a related structure, see: Prasath et al. (2010).
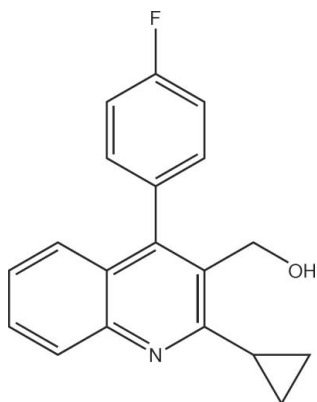
## Experimental

### Crystal data

| | |
|---|---|
| $C_{19}H_{16}FNO$ | Monoclinic, $P2_1/c$ |
| $M_r = 293.33$ | $a = 10.069$ (2) Å |
| $b = 24.683$ (5) Å | Mo $K\alpha$ radiation |
| $c = 13.275$ (3) Å | $\mu = 0.09$ mm$^{-1}$ |
| $\beta = 111.97$ (3)° | $T = 293$ K |
| $V = 3059.7$ (13) Å$^3$ | $0.30 \times 0.20 \times 0.20$ mm |
| $Z = 8$ | |

### Data collection

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | 5536 independent reflections |
| Absorption correction: empirical (using intensity measurements) via $\psi$ scan (North et al., 1968) $T_{min} = 0.974$, $T_{max} = 0.983$ | 3098 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.031$ |
| | 3 standard reflections every 200 reflections |
| 5865 measured reflections | intensity decay: 1% |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.058$ | 398 parameters |
| $wR(F^2) = 0.166$ | H-atom parameters constrained |
| $S = 1.00$ | $\Delta\rho_{max} = 0.20$ e Å$^{-3}$ |
| 5536 reflections | $\Delta\rho_{min} = -0.18$ e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···N2$^i$ | 0.85 | 2.04 | 2.849 (3) | 159 |
| O2—H2$B$···O1$^{ii}$ | 0.82 | 2.10 | 2.909 (3) | 170 |
| C30—H30$A$···O1$^i$ | 0.93 | 2.57 | 3.307 (3) | 136 |
| C37—H37$B$···O1$^i$ | 0.97 | 2.59 | 3.372 (4) | 138 |
| C36—H36$A$···O2 | 0.98 | 2.49 | 3.117 (4) | 121 |
| C17—H17$A$···O1 | 0.98 | 2.55 | 3.168 (4) | 121 |
| C12—H12$A$···O2$^{iii}$ | 0.93 | 2.42 | 3.318 (5) | 161 |

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *CAD-4 EXPRESS*; 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: *SHELXTL*.

## References

Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Prasath, R., Sarveswari, S., Vijayakumar, V., Narasimhamurthy, T. & Tiekink, E. R. T. (2010). *Acta Cryst.* E**66**, o1110.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

## [2-Cyclopropyl-4-(4-fluorophenyl)quinolin-3-yl]methanol

### Hongshun Sun, Hong Xu and Yu-Long Li

### S1. Comment

Derivatives of quinoline are important chemical materials. We report here the crystal structure of the title compound which has been prepared in our laboratory.

The title compound crystallizes with two independent but closely similar molecules per asymmetric unit (Fig. 1 and Fig. 2). In the two molecules, the dihedral angles between benzene and quinoline rings are 72.6 (5) and 76.2 (5)°, between cyclopropane and quinoline rings are 65.2 (5) and 66.0 (5)° and between benzene and cyclopropane rings are 25.9 (5) and 33.9 (5)°. The molecular packing (Fig. 3) is stabilized by intermolecular O—H···O, O—H···N and C—H···O hydrogen bonds (Table 1). In addition, intramolecular C—H···O hydrogen bonds are also present in the crystal structure.

The crystal structure of a closely related compound has been reported (Prasath *et al.*, 2010).

### S2. Experimental

A dry, 250-ml three-neck flask was charged with 100 ml of THF, 3.27 g (57.47 mmol) of $KBH_4$, and 5.46 g (57.47 mmol) of $MgCl_2$. The reaction mixture was heated under reflux for 2 h, then 10.0 g (57.47 mmol) of methyl 2-cyclopropyl-4-(4-fluorophenyl)quinoline-3-carboxylate was added dropwise over 5 min and refluxed for an additional 40 min. After cooling, methanol (15 ml) was carefully added dropwise to quench the reaction and the white inorganic solid was filtered and washed with 80 ml of THF/MeOH (10:1). The combined filtrate was concentrated to dryness, MeOH (40 ml) was added to the residue and concentrated to dryness again. The resulting residue was dissolved in 300 ml of ethyl acetate and washed with brine, dried over $MgSO_4$ and concentrated to dryness to provide 7.58 g (yield 90.3%) of the title compound as colourless crystals.

### S3. Refinement

All H atoms bonded to the C atoms were placed geometrically at the distances of 0.93 or 0.97 Å, and included in the refinement in riding motion approximation with $U_{iso}(H) = 1.2U_{eq}(C/O)$ of the carrier atom.
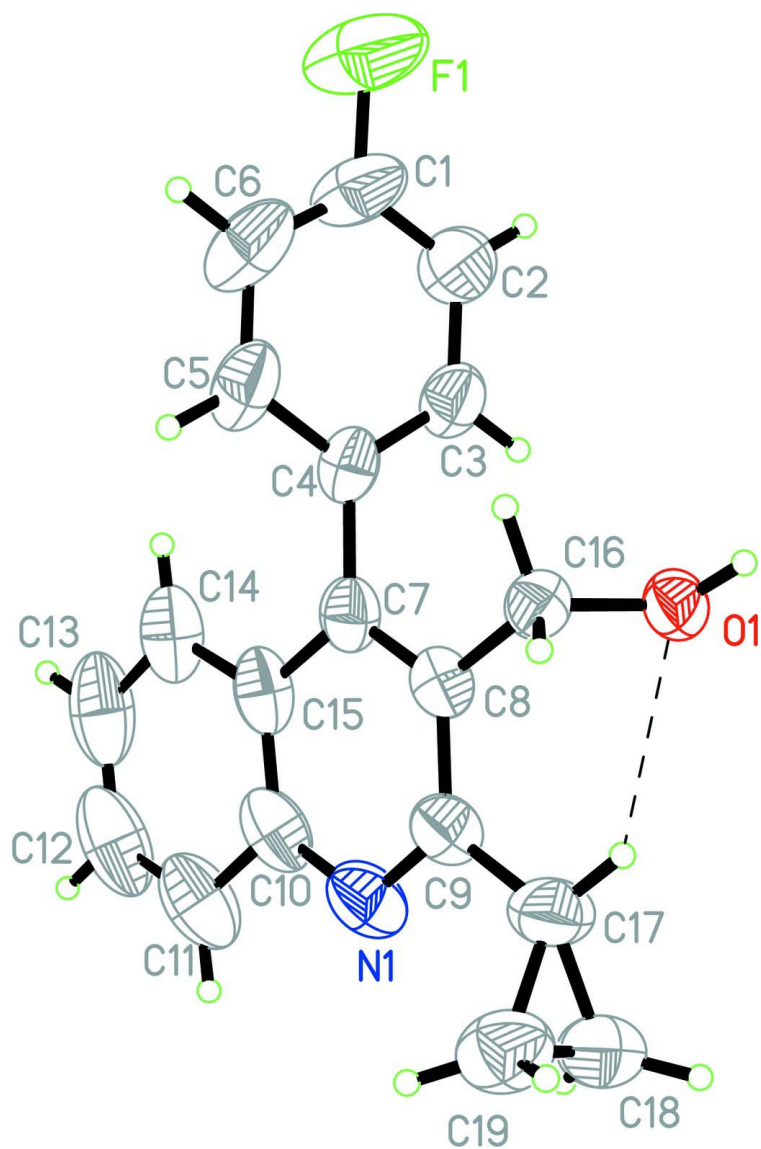
**Figure 1**

The presentation of a molecule of (I), showing the atom-numbering scheme; displacement ellipsoids have been plotted at the 50% probability level.
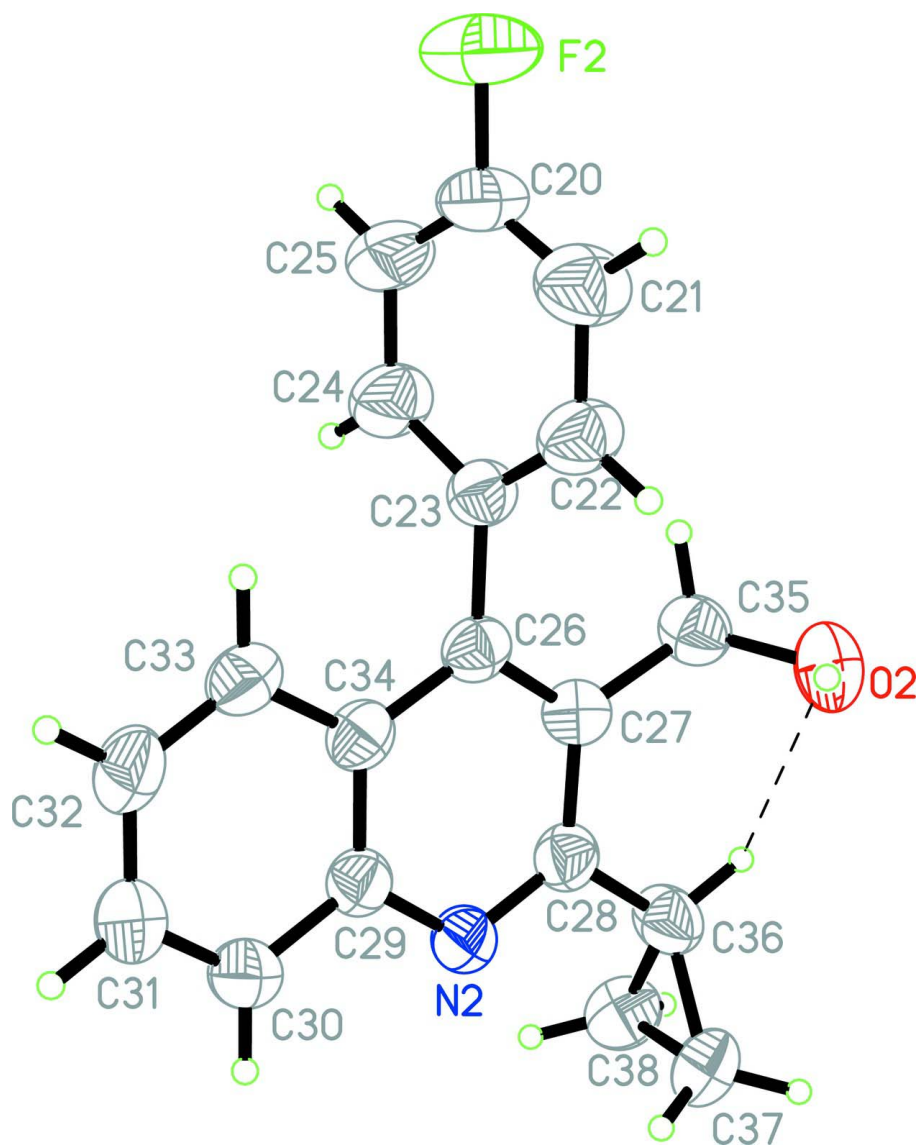
**Figure 2**

The presentation of the second molecule of (I), showing the atom-numbering scheme; displacement ellipsoids have been plotted at the 50% probability level.
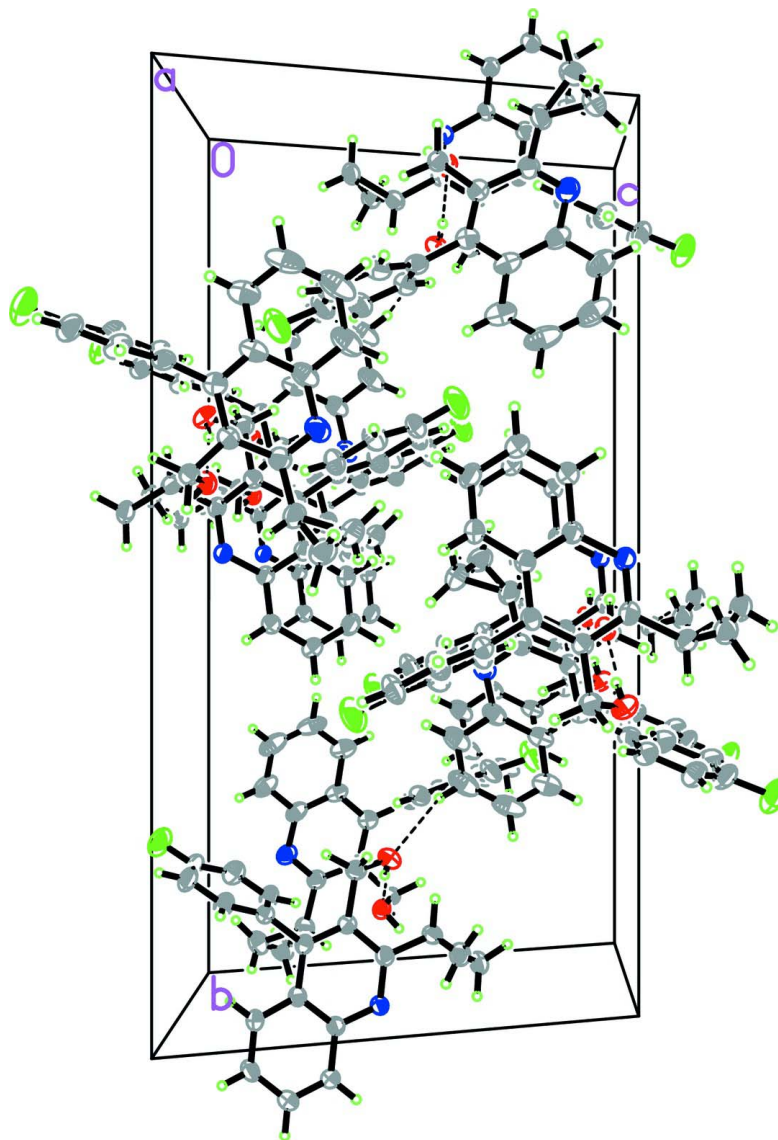
**Figure 3**

The crystal packing of (I) viewed down the *a* axis.

**[2-Cyclopropyl-4-(4-fluorophenyl)quinolin-3-yl]methanol**

*Crystal data*

| | |
|---|---|
| $C_{19}H_{16}FNO$ | $F(000) = 1232$ |
| $M_r = 293.33$ | $D_x = 1.274$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 25 reflections |
| $a = 10.069$ (2) Å | $\theta = 10–13°$ |
| $b = 24.683$ (5) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 13.275$ (3) Å | $T = 293$ K |
| $\beta = 111.97$ (3)° | Block, colourless |
| $V = 3059.7$ (13) Å$^3$ | $0.30 \times 0.20 \times 0.20$ mm |
| $Z = 8$ | |

*Data collection*

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | 5536 independent reflections |
| Radiation source: fine-focus sealed tube | 3098 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.031$ |
| $\omega/2\theta$ scans | $\theta_{max} = 25.3°$, $\theta_{min} = 1.7°$ |
| Absorption correction: empirical (using intensity measurements) | $h = 0 \rightarrow 12$ |
| | $k = 0 \rightarrow 29$ |
| via $\psi$ scan (North *et al.*, 1968) | $l = -15 \rightarrow 14$ |
| $T_{min} = 0.974$, $T_{max} = 0.983$ | 3 standard reflections every 200 reflections |
| 5865 measured reflections | intensity decay: 1% |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.058$ | $w = 1/[\sigma^2(F_o^2) + (0.070P)^2 + 1.0P]$ |
| $wR(F^2) = 0.166$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.00$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 5536 reflections | $\Delta\rho_{max} = 0.20$ e Å$^{-3}$ |
| 398 parameters | $\Delta\rho_{min} = -0.18$ e Å$^{-3}$ |
| 0 restraints | Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2$\theta$)]$^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0222 (15) |
| Secondary atom site location: difference Fourier map | |

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 0.2535 (3) | 0.75467 (12) | 1.27963 (19) | 0.1195 (10) |
| O1 | 0.1866 (2) | 0.57598 (8) | 0.91629 (15) | 0.0484 (5) |
| H1A | 0.2535 | 0.5566 | 0.9596 | 0.058* |
| N1 | −0.2147 (3) | 0.62400 (12) | 0.6641 (2) | 0.0629 (8) |
| C1 | 0.1723 (5) | 0.73584 (16) | 1.1794 (3) | 0.0755 (11) |
| C2 | 0.2351 (4) | 0.72914 (15) | 1.1055 (3) | 0.0669 (10) |
| H2A | 0.3308 | 0.7382 | 1.1227 | 0.080* |
| C3 | 0.1544 (3) | 0.70875 (13) | 1.0056 (3) | 0.0555 (8) |
| H3A | 0.1963 | 0.7036 | 0.9547 | 0.067* |
| C4 | 0.0109 (3) | 0.69557 (12) | 0.9784 (2) | 0.0481 (8) |
| C5 | −0.0491 (4) | 0.70487 (14) | 1.0557 (3) | 0.0662 (10) |
| H5A | −0.1456 | 0.6974 | 1.0386 | 0.079* |
| C6 | 0.0312 (5) | 0.72479 (15) | 1.1564 (3) | 0.0795 (12) |

| | | | | |
|---|---|---|---|---|
| H6A | −0.0094 | 0.7306 | 1.2079 | 0.095* |
| C7 | −0.0722 (3) | 0.67043 (13) | 0.8715 (2) | 0.0484 (8) |
| C8 | −0.0453 (3) | 0.61787 (12) | 0.8492 (2) | 0.0458 (7) |
| C9 | −0.1199 (3) | 0.59642 (13) | 0.7432 (2) | 0.0517 (8) |
| C10 | −0.2455 (3) | 0.67573 (14) | 0.6860 (3) | 0.0586 (9) |
| C11 | −0.3457 (4) | 0.70551 (17) | 0.6010 (3) | 0.0779 (12) |
| H11A | −0.3882 | 0.6897 | 0.5328 | 0.093* |
| C12 | −0.3812 (4) | 0.7570 (2) | 0.6169 (4) | 0.0897 (14) |
| H12A | −0.4492 | 0.7758 | 0.5603 | 0.108* |
| C13 | −0.3157 (4) | 0.78179 (17) | 0.7183 (4) | 0.0858 (13) |
| H13A | −0.3399 | 0.8172 | 0.7283 | 0.103* |
| C14 | −0.2163 (4) | 0.75455 (15) | 0.8030 (3) | 0.0696 (10) |
| H14A | −0.1738 | 0.7714 | 0.8702 | 0.083* |
| C15 | −0.1780 (3) | 0.70061 (13) | 0.7883 (3) | 0.0544 (9) |
| C16 | 0.0571 (3) | 0.58239 (12) | 0.9353 (2) | 0.0442 (7) |
| H16A | 0.0780 | 0.5986 | 1.0062 | 0.053* |
| H16B | 0.0138 | 0.5472 | 0.9346 | 0.053* |
| C17 | −0.0908 (4) | 0.54001 (14) | 0.7175 (3) | 0.0656 (10) |
| H17A | −0.0118 | 0.5217 | 0.7745 | 0.079* |
| C18 | −0.1149 (4) | 0.52291 (16) | 0.6044 (3) | 0.0720 (11) |
| H18A | −0.1488 | 0.5501 | 0.5476 | 0.086* |
| H18B | −0.0495 | 0.4965 | 0.5945 | 0.086* |
| C19 | −0.2152 (4) | 0.50415 (16) | 0.6537 (3) | 0.0748 (11) |
| H19A | −0.2110 | 0.4663 | 0.6745 | 0.090* |
| H19B | −0.3103 | 0.5200 | 0.6277 | 0.090* |
| F2 | −0.9501 (3) | 0.66225 (11) | 0.39541 (17) | 0.1052 (8) |
| O2 | −0.5786 (2) | 0.65058 (9) | 0.94408 (17) | 0.0597 (6) |
| H2B | −0.6423 | 0.6278 | 0.9302 | 0.090* |
| N2 | −0.3504 (2) | 0.50285 (10) | 0.93101 (18) | 0.0451 (6) |
| C20 | −0.8499 (4) | 0.63914 (14) | 0.4840 (3) | 0.0646 (10) |
| C21 | −0.8889 (4) | 0.62502 (15) | 0.5687 (3) | 0.0680 (10) |
| H21A | −0.9808 | 0.6318 | 0.5664 | 0.082* |
| C22 | −0.7874 (3) | 0.60039 (14) | 0.6577 (3) | 0.0584 (9) |
| H22A | −0.8115 | 0.5904 | 0.7162 | 0.070* |
| C23 | −0.6507 (3) | 0.59032 (12) | 0.6613 (2) | 0.0432 (7) |
| C24 | −0.6163 (4) | 0.60645 (14) | 0.5742 (3) | 0.0620 (9) |
| H24A | −0.5242 | 0.6006 | 0.5760 | 0.074* |
| C25 | −0.7164 (4) | 0.63104 (15) | 0.4851 (3) | 0.0719 (11) |
| H25A | −0.6928 | 0.6419 | 0.4268 | 0.086* |
| C26 | −0.5441 (3) | 0.56122 (12) | 0.7552 (2) | 0.0415 (7) |
| C27 | −0.4757 (3) | 0.58558 (11) | 0.8541 (2) | 0.0417 (7) |
| C28 | −0.3783 (3) | 0.55476 (12) | 0.9413 (2) | 0.0439 (7) |
| C29 | −0.4175 (3) | 0.47784 (12) | 0.8325 (2) | 0.0419 (7) |
| C30 | −0.3911 (3) | 0.42248 (12) | 0.8223 (2) | 0.0517 (8) |
| H30A | −0.3277 | 0.4038 | 0.8817 | 0.062* |
| C31 | −0.4569 (3) | 0.39590 (14) | 0.7268 (3) | 0.0565 (9) |
| H31A | −0.4373 | 0.3594 | 0.7212 | 0.068* |
| C32 | −0.5536 (4) | 0.42303 (14) | 0.6370 (3) | 0.0567 (9) |

| | | | |
|---|---|---|---|
| H32A | −0.5986 | 0.4046 | 0.5719 | 0.068* |
| C33 | −0.5820 (3) | 0.47647 (13) | 0.6448 (2) | 0.0505 (8) |
| H33A | −0.6470 | 0.4942 | 0.5847 | 0.061* |
| C34 | −0.5145 (3) | 0.50553 (12) | 0.7426 (2) | 0.0423 (7) |
| C35 | −0.5051 (3) | 0.64418 (12) | 0.8719 (2) | 0.0501 (8) |
| H35A | −0.4149 | 0.6636 | 0.9008 | 0.060* |
| H35B | −0.5619 | 0.6603 | 0.8025 | 0.060* |
| C36 | −0.3029 (3) | 0.58073 (13) | 1.0480 (2) | 0.0537 (8) |
| H36A | −0.3322 | 0.6181 | 1.0535 | 0.064* |
| C37 | −0.2562 (3) | 0.54946 (14) | 1.1518 (2) | 0.0580 (9) |
| H37A | −0.2621 | 0.5673 | 1.2151 | 0.070* |
| H37B | −0.2758 | 0.5109 | 1.1474 | 0.070* |
| C38 | −0.1478 (3) | 0.56916 (14) | 1.1108 (2) | 0.0567 (9) |
| H38A | −0.1012 | 0.5427 | 1.0812 | 0.068* |
| H38B | −0.0874 | 0.5991 | 1.1490 | 0.068* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.144 (2) | 0.140 (2) | 0.0805 (16) | −0.0509 (19) | 0.0496 (16) | −0.0475 (16) |
| O1 | 0.0440 (12) | 0.0567 (13) | 0.0429 (11) | 0.0092 (10) | 0.0144 (9) | 0.0049 (10) |
| N1 | 0.0524 (17) | 0.062 (2) | 0.0595 (18) | 0.0048 (14) | 0.0040 (14) | 0.0106 (15) |
| C1 | 0.098 (3) | 0.073 (3) | 0.064 (2) | −0.026 (2) | 0.040 (2) | −0.029 (2) |
| C2 | 0.060 (2) | 0.073 (3) | 0.072 (2) | −0.0147 (19) | 0.031 (2) | −0.014 (2) |
| C3 | 0.055 (2) | 0.058 (2) | 0.063 (2) | −0.0011 (16) | 0.0326 (17) | −0.0075 (17) |
| C4 | 0.0514 (19) | 0.0403 (18) | 0.060 (2) | 0.0043 (14) | 0.0295 (16) | −0.0006 (15) |
| C5 | 0.068 (2) | 0.062 (2) | 0.089 (3) | −0.0053 (18) | 0.052 (2) | −0.014 (2) |
| C6 | 0.108 (3) | 0.072 (3) | 0.088 (3) | −0.018 (2) | 0.070 (3) | −0.021 (2) |
| C7 | 0.0404 (17) | 0.051 (2) | 0.060 (2) | −0.0002 (14) | 0.0256 (15) | 0.0013 (16) |
| C8 | 0.0389 (16) | 0.0490 (19) | 0.0485 (18) | 0.0029 (14) | 0.0152 (14) | 0.0045 (14) |
| C9 | 0.0457 (18) | 0.053 (2) | 0.0508 (19) | 0.0004 (15) | 0.0113 (16) | 0.0023 (16) |
| C10 | 0.0417 (18) | 0.059 (2) | 0.069 (2) | 0.0016 (16) | 0.0141 (17) | 0.0213 (19) |
| C11 | 0.054 (2) | 0.078 (3) | 0.089 (3) | 0.008 (2) | 0.012 (2) | 0.035 (2) |
| C12 | 0.054 (2) | 0.087 (3) | 0.121 (4) | 0.018 (2) | 0.026 (3) | 0.051 (3) |
| C13 | 0.067 (3) | 0.058 (3) | 0.146 (4) | 0.021 (2) | 0.056 (3) | 0.035 (3) |
| C14 | 0.056 (2) | 0.058 (2) | 0.105 (3) | 0.0092 (18) | 0.043 (2) | 0.015 (2) |
| C15 | 0.0419 (18) | 0.048 (2) | 0.079 (2) | 0.0056 (15) | 0.0291 (18) | 0.0154 (18) |
| C16 | 0.0470 (17) | 0.0441 (17) | 0.0434 (17) | 0.0027 (14) | 0.0191 (14) | 0.0004 (13) |
| C17 | 0.067 (2) | 0.063 (2) | 0.050 (2) | 0.0063 (18) | 0.0021 (17) | −0.0069 (17) |
| C18 | 0.067 (2) | 0.081 (3) | 0.062 (2) | −0.010 (2) | 0.017 (2) | −0.017 (2) |
| C19 | 0.081 (3) | 0.069 (3) | 0.078 (3) | −0.021 (2) | 0.034 (2) | −0.015 (2) |
| F2 | 0.0998 (17) | 0.123 (2) | 0.0704 (14) | 0.0350 (15) | 0.0064 (13) | 0.0357 (14) |
| O2 | 0.0593 (14) | 0.0563 (14) | 0.0670 (15) | −0.0020 (11) | 0.0276 (12) | −0.0159 (11) |
| N2 | 0.0472 (15) | 0.0458 (16) | 0.0392 (14) | 0.0044 (12) | 0.0125 (12) | −0.0029 (11) |
| C20 | 0.068 (2) | 0.066 (2) | 0.047 (2) | 0.0149 (19) | 0.0073 (18) | 0.0145 (17) |
| C21 | 0.048 (2) | 0.081 (3) | 0.071 (2) | 0.0075 (18) | 0.0169 (19) | 0.012 (2) |
| C22 | 0.050 (2) | 0.077 (2) | 0.0510 (19) | 0.0047 (17) | 0.0220 (16) | 0.0131 (17) |
| C23 | 0.0434 (17) | 0.0450 (18) | 0.0416 (16) | 0.0009 (13) | 0.0163 (14) | 0.0029 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24 | 0.059 (2) | 0.078 (2) | 0.057 (2) | 0.0089 (19) | 0.0308 (18) | 0.0174 (18) |
| C25 | 0.087 (3) | 0.082 (3) | 0.054 (2) | 0.020 (2) | 0.034 (2) | 0.0263 (19) |
| C26 | 0.0392 (16) | 0.0477 (19) | 0.0396 (16) | −0.0013 (14) | 0.0169 (14) | 0.0042 (14) |
| C27 | 0.0385 (16) | 0.0423 (18) | 0.0429 (17) | −0.0030 (13) | 0.0135 (13) | 0.0006 (14) |
| C28 | 0.0407 (17) | 0.0497 (19) | 0.0393 (17) | 0.0026 (14) | 0.0128 (14) | −0.0032 (14) |
| C29 | 0.0427 (16) | 0.0439 (18) | 0.0387 (16) | 0.0007 (14) | 0.0148 (14) | −0.0018 (14) |
| C30 | 0.059 (2) | 0.0469 (19) | 0.0448 (18) | 0.0053 (15) | 0.0151 (15) | 0.0016 (15) |
| C31 | 0.066 (2) | 0.050 (2) | 0.054 (2) | 0.0016 (17) | 0.0229 (17) | −0.0078 (16) |
| C32 | 0.067 (2) | 0.059 (2) | 0.0449 (19) | −0.0063 (17) | 0.0213 (17) | −0.0134 (16) |
| C33 | 0.0538 (19) | 0.057 (2) | 0.0369 (17) | 0.0002 (16) | 0.0123 (14) | 0.0000 (15) |
| C34 | 0.0414 (16) | 0.0485 (19) | 0.0402 (16) | −0.0036 (14) | 0.0188 (14) | −0.0002 (14) |
| C35 | 0.0491 (18) | 0.0456 (19) | 0.0523 (19) | −0.0007 (14) | 0.0152 (15) | −0.0012 (15) |
| C36 | 0.056 (2) | 0.0458 (19) | 0.0482 (19) | 0.0075 (15) | 0.0068 (16) | −0.0076 (15) |
| C37 | 0.067 (2) | 0.066 (2) | 0.0423 (18) | −0.0015 (18) | 0.0225 (17) | −0.0071 (16) |
| C38 | 0.052 (2) | 0.062 (2) | 0.0498 (19) | −0.0089 (16) | 0.0122 (16) | −0.0033 (16) |

## Geometric parameters (Å, °)

| | | | |
|---|---|---|---|
| F1—C1 | 1.357 (4) | F2—C20 | 1.356 (4) |
| O1—C16 | 1.426 (3) | O2—C35 | 1.421 (3) |
| O1—H1A | 0.8501 | O2—H2B | 0.8200 |
| N1—C9 | 1.315 (4) | N2—C28 | 1.330 (4) |
| N1—C10 | 1.370 (4) | N2—C29 | 1.373 (3) |
| C1—C2 | 1.361 (5) | C20—C25 | 1.354 (5) |
| C1—C6 | 1.365 (5) | C20—C21 | 1.367 (5) |
| C2—C3 | 1.366 (4) | C21—C22 | 1.381 (4) |
| C2—H2A | 0.9300 | C21—H21A | 0.9300 |
| C3—C4 | 1.391 (4) | C22—C23 | 1.381 (4) |
| C3—H3A | 0.9300 | C22—H22A | 0.9300 |
| C4—C5 | 1.390 (4) | C23—C24 | 1.384 (4) |
| C4—C7 | 1.487 (4) | C23—C26 | 1.490 (4) |
| C5—C6 | 1.370 (5) | C24—C25 | 1.375 (4) |
| C5—H5A | 0.9300 | C24—H24A | 0.9300 |
| C6—H6A | 0.9300 | C25—H25A | 0.9300 |
| C7—C8 | 1.380 (4) | C26—C27 | 1.373 (4) |
| C7—C15 | 1.424 (4) | C26—C34 | 1.429 (4) |
| C8—C9 | 1.425 (4) | C27—C28 | 1.425 (4) |
| C8—C16 | 1.502 (4) | C27—C35 | 1.513 (4) |
| C9—C17 | 1.488 (4) | C28—C36 | 1.479 (4) |
| C10—C11 | 1.407 (4) | C29—C34 | 1.405 (4) |
| C10—C15 | 1.413 (5) | C29—C30 | 1.408 (4) |
| C11—C12 | 1.359 (6) | C30—C31 | 1.360 (4) |
| C11—H11A | 0.9300 | C30—H30A | 0.9300 |
| C12—C13 | 1.399 (6) | C31—C32 | 1.396 (4) |
| C12—H12A | 0.9300 | C31—H31A | 0.9300 |
| C13—C14 | 1.370 (5) | C32—C33 | 1.362 (4) |
| C13—H13A | 0.9300 | C32—H32A | 0.9300 |
| C14—C15 | 1.420 (5) | C33—C34 | 1.416 (4) |

| | | | |
|---|---|---|---|
| C14—H14A | 0.9300 | C33—H33A | 0.9300 |
| C16—H16A | 0.9700 | C35—H35A | 0.9700 |
| C16—H16B | 0.9700 | C35—H35B | 0.9700 |
| C17—C18 | 1.490 (4) | C36—C37 | 1.493 (4) |
| C17—C19 | 1.508 (5) | C36—C38 | 1.498 (4) |
| C17—H17A | 0.9800 | C36—H36A | 0.9800 |
| C18—C19 | 1.469 (5) | C37—C38 | 1.472 (4) |
| C18—H18A | 0.9700 | C37—H37A | 0.9700 |
| C18—H18B | 0.9700 | C37—H37B | 0.9700 |
| C19—H19A | 0.9700 | C38—H38A | 0.9700 |
| C19—H19B | 0.9700 | C38—H38B | 0.9700 |
| | | | |
| C16—O1—H1A | 119.2 | C35—O2—H2B | 109.5 |
| C9—N1—C10 | 117.9 (3) | C28—N2—C29 | 118.9 (2) |
| F1—C1—C2 | 118.4 (4) | C25—C20—F2 | 119.1 (3) |
| F1—C1—C6 | 118.8 (4) | C25—C20—C21 | 122.8 (3) |
| C2—C1—C6 | 122.7 (4) | F2—C20—C21 | 118.1 (3) |
| C1—C2—C3 | 118.4 (3) | C20—C21—C22 | 117.9 (3) |
| C1—C2—H2A | 120.8 | C20—C21—H21A | 121.1 |
| C3—C2—H2A | 120.8 | C22—C21—H21A | 121.1 |
| C2—C3—C4 | 121.5 (3) | C21—C22—C23 | 121.2 (3) |
| C2—C3—H3A | 119.3 | C21—C22—H22A | 119.4 |
| C4—C3—H3A | 119.3 | C23—C22—H22A | 119.4 |
| C5—C4—C3 | 117.7 (3) | C22—C23—C24 | 118.5 (3) |
| C5—C4—C7 | 121.9 (3) | C22—C23—C26 | 120.8 (3) |
| C3—C4—C7 | 120.3 (3) | C24—C23—C26 | 120.7 (3) |
| C6—C5—C4 | 121.3 (3) | C25—C24—C23 | 120.9 (3) |
| C6—C5—H5A | 119.4 | C25—C24—H24A | 119.5 |
| C4—C5—H5A | 119.4 | C23—C24—H24A | 119.5 |
| C1—C6—C5 | 118.3 (3) | C20—C25—C24 | 118.7 (3) |
| C1—C6—H6A | 120.8 | C20—C25—H25A | 120.7 |
| C5—C6—H6A | 120.8 | C24—C25—H25A | 120.7 |
| C8—C7—C15 | 118.4 (3) | C27—C26—C34 | 118.7 (3) |
| C8—C7—C4 | 120.8 (3) | C27—C26—C23 | 122.4 (3) |
| C15—C7—C4 | 120.8 (3) | C34—C26—C23 | 118.9 (3) |
| C7—C8—C9 | 119.2 (3) | C26—C27—C28 | 119.3 (3) |
| C7—C8—C16 | 121.2 (3) | C26—C27—C35 | 120.7 (3) |
| C9—C8—C16 | 119.5 (3) | C28—C27—C35 | 119.9 (3) |
| N1—C9—C8 | 123.6 (3) | N2—C28—C27 | 122.6 (3) |
| N1—C9—C17 | 116.6 (3) | N2—C28—C36 | 117.6 (3) |
| C8—C9—C17 | 119.9 (3) | C27—C28—C36 | 119.8 (3) |
| N1—C10—C11 | 117.9 (4) | N2—C29—C34 | 121.9 (3) |
| N1—C10—C15 | 122.9 (3) | N2—C29—C30 | 119.0 (3) |
| C11—C10—C15 | 119.1 (4) | C34—C29—C30 | 119.1 (3) |
| C12—C11—C10 | 121.0 (4) | C31—C30—C29 | 121.0 (3) |
| C12—C11—H11A | 119.5 | C31—C30—H30A | 119.5 |
| C10—C11—H11A | 119.5 | C29—C30—H30A | 119.5 |
| C11—C12—C13 | 120.1 (4) | C30—C31—C32 | 120.4 (3) |

| | | | |
|---|---|---|---|
| C11—C12—H12A | 119.9 | C30—C31—H31A | 119.8 |
| C13—C12—H12A | 119.9 | C32—C31—H31A | 119.8 |
| C14—C13—C12 | 120.8 (4) | C33—C32—C31 | 119.9 (3) |
| C14—C13—H13A | 119.6 | C33—C32—H32A | 120.0 |
| C12—C13—H13A | 119.6 | C31—C32—H32A | 120.0 |
| C13—C14—C15 | 120.0 (4) | C32—C33—C34 | 121.2 (3) |
| C13—C14—H14A | 120.0 | C32—C33—H33A | 119.4 |
| C15—C14—H14A | 120.0 | C34—C33—H33A | 119.4 |
| C10—C15—C14 | 118.8 (3) | C29—C34—C33 | 118.4 (3) |
| C10—C15—C7 | 118.0 (3) | C29—C34—C26 | 118.6 (3) |
| C14—C15—C7 | 123.2 (3) | C33—C34—C26 | 123.0 (3) |
| O1—C16—C8 | 110.1 (2) | O2—C35—C27 | 113.1 (2) |
| O1—C16—H16A | 109.7 | O2—C35—H35A | 109.0 |
| C8—C16—H16A | 109.7 | C27—C35—H35A | 109.0 |
| O1—C16—H16B | 109.7 | O2—C35—H35B | 109.0 |
| C8—C16—H16B | 109.7 | C27—C35—H35B | 109.0 |
| H16A—C16—H16B | 108.2 | H35A—C35—H35B | 107.8 |
| C9—C17—C18 | 121.6 (3) | C28—C36—C37 | 122.1 (3) |
| C9—C17—C19 | 119.0 (3) | C28—C36—C38 | 120.3 (3) |
| C18—C17—C19 | 58.7 (2) | C37—C36—C38 | 59.0 (2) |
| C9—C17—H17A | 115.3 | C28—C36—H36A | 114.7 |
| C18—C17—H17A | 115.3 | C37—C36—H36A | 114.7 |
| C19—C17—H17A | 115.3 | C38—C36—H36A | 114.7 |
| C19—C18—C17 | 61.3 (2) | C38—C37—C36 | 60.7 (2) |
| C19—C18—H18A | 117.6 | C38—C37—H37A | 117.7 |
| C17—C18—H18A | 117.6 | C36—C37—H37A | 117.7 |
| C19—C18—H18B | 117.6 | C38—C37—H37B | 117.7 |
| C17—C18—H18B | 117.6 | C36—C37—H37B | 117.7 |
| H18A—C18—H18B | 114.7 | H37A—C37—H37B | 114.8 |
| C18—C19—C17 | 60.0 (2) | C37—C38—C36 | 60.4 (2) |
| C18—C19—H19A | 117.8 | C37—C38—H38A | 117.7 |
| C17—C19—H19A | 117.8 | C36—C38—H38A | 117.7 |
| C18—C19—H19B | 117.8 | C37—C38—H38B | 117.7 |
| C17—C19—H19B | 117.8 | C36—C38—H38B | 117.7 |
| H19A—C19—H19B | 114.9 | H38A—C38—H38B | 114.9 |
| | | | |
| F1—C1—C2—C3 | 178.2 (3) | C25—C20—C21—C22 | −1.5 (6) |
| C6—C1—C2—C3 | −2.3 (6) | F2—C20—C21—C22 | 178.6 (3) |
| C1—C2—C3—C4 | 0.7 (5) | C20—C21—C22—C23 | 0.0 (5) |
| C2—C3—C4—C5 | 1.3 (5) | C21—C22—C23—C24 | 1.2 (5) |
| C2—C3—C4—C7 | −176.4 (3) | C21—C22—C23—C26 | −176.9 (3) |
| C3—C4—C5—C6 | −1.9 (5) | C22—C23—C24—C25 | −1.2 (5) |
| C7—C4—C5—C6 | 175.7 (3) | C26—C23—C24—C25 | 176.9 (3) |
| F1—C1—C6—C5 | −178.8 (4) | F2—C20—C25—C24 | −178.5 (3) |
| C2—C1—C6—C5 | 1.7 (6) | C21—C20—C25—C24 | 1.5 (6) |
| C4—C5—C6—C1 | 0.5 (6) | C23—C24—C25—C20 | −0.1 (6) |
| C5—C4—C7—C8 | −107.4 (4) | C22—C23—C26—C27 | −75.3 (4) |
| C3—C4—C7—C8 | 70.2 (4) | C24—C23—C26—C27 | 106.6 (4) |

| C5—C4—C7—C15 | 74.9 (4) | C22—C23—C26—C34 | 103.1 (3) |
| C3—C4—C7—C15 | −107.6 (3) | C24—C23—C26—C34 | −75.0 (4) |
| C15—C7—C8—C9 | 2.3 (4) | C34—C26—C27—C28 | −0.4 (4) |
| C4—C7—C8—C9 | −175.5 (3) | C23—C26—C27—C28 | 178.0 (3) |
| C15—C7—C8—C16 | −175.6 (3) | C34—C26—C27—C35 | −179.1 (3) |
| C4—C7—C8—C16 | 6.6 (4) | C23—C26—C27—C35 | −0.7 (4) |
| C10—N1—C9—C8 | −1.6 (5) | C29—N2—C28—C27 | 0.1 (4) |
| C10—N1—C9—C17 | 178.9 (3) | C29—N2—C28—C36 | −179.3 (3) |
| C7—C8—C9—N1 | −0.2 (5) | C26—C27—C28—N2 | 0.0 (4) |
| C16—C8—C9—N1 | 177.7 (3) | C35—C27—C28—N2 | 178.7 (3) |
| C7—C8—C9—C17 | 179.3 (3) | C26—C27—C28—C36 | 179.4 (3) |
| C16—C8—C9—C17 | −2.7 (4) | C35—C27—C28—C36 | −1.9 (4) |
| C9—N1—C10—C11 | 179.2 (3) | C28—N2—C29—C34 | 0.1 (4) |
| C9—N1—C10—C15 | 1.3 (5) | C28—N2—C29—C30 | −178.3 (3) |
| N1—C10—C11—C12 | 180.0 (3) | N2—C29—C30—C31 | 179.0 (3) |
| C15—C10—C11—C12 | −2.0 (5) | C34—C29—C30—C31 | 0.6 (5) |
| C10—C11—C12—C13 | 1.5 (6) | C29—C30—C31—C32 | −0.7 (5) |
| C11—C12—C13—C14 | −0.7 (6) | C30—C31—C32—C33 | 0.2 (5) |
| C12—C13—C14—C15 | 0.3 (5) | C31—C32—C33—C34 | 0.3 (5) |
| N1—C10—C15—C14 | 179.5 (3) | N2—C29—C34—C33 | −178.4 (3) |
| C11—C10—C15—C14 | 1.6 (5) | C30—C29—C34—C33 | −0.1 (4) |
| N1—C10—C15—C7 | 0.8 (5) | N2—C29—C34—C26 | −0.4 (4) |
| C11—C10—C15—C7 | −177.2 (3) | C30—C29—C34—C26 | 177.9 (3) |
| C13—C14—C15—C10 | −0.8 (5) | C32—C33—C34—C29 | −0.4 (4) |
| C13—C14—C15—C7 | 177.9 (3) | C32—C33—C34—C26 | −178.3 (3) |
| C8—C7—C15—C10 | −2.5 (4) | C27—C26—C34—C29 | 0.6 (4) |
| C4—C7—C15—C10 | 175.3 (3) | C23—C26—C34—C29 | −177.9 (2) |
| C8—C7—C15—C14 | 178.8 (3) | C27—C26—C34—C33 | 178.5 (3) |
| C4—C7—C15—C14 | −3.4 (4) | C23—C26—C34—C33 | 0.0 (4) |
| C7—C8—C16—O1 | −106.7 (3) | C26—C27—C35—O2 | 111.6 (3) |
| C9—C8—C16—O1 | 75.4 (3) | C28—C27—C35—O2 | −67.0 (3) |
| N1—C9—C17—C18 | 25.2 (5) | N2—C28—C36—C37 | −29.2 (4) |
| C8—C9—C17—C18 | −154.4 (3) | C27—C28—C36—C37 | 151.3 (3) |
| N1—C9—C17—C19 | −43.9 (5) | N2—C28—C36—C38 | 41.0 (4) |
| C8—C9—C17—C19 | 136.5 (3) | C27—C28—C36—C38 | −138.4 (3) |
| C9—C17—C18—C19 | −107.0 (4) | C28—C36—C37—C38 | 108.6 (3) |
| C9—C17—C19—C18 | 111.4 (4) | C28—C36—C38—C37 | −111.5 (3) |

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
| --- | --- | --- | --- | --- |
| O1—H1*A*···N2[i] | 0.85 | 2.04 | 2.849 (3) | 159 |
| O2—H2*B*···O1[ii] | 0.82 | 2.10 | 2.909 (3) | 170 |
| C30—H30*A*···O1[i] | 0.93 | 2.57 | 3.307 (3) | 136 |
| C37—H37*B*···O1[i] | 0.97 | 2.59 | 3.372 (4) | 138 |
| C36—H36*A*···O2 | 0.98 | 2.49 | 3.117 (4) | 121 |

| C17—H17*A*···O1 | 0.98 | 2.55 | 3.168 (4) | 121 |
| C12—H12*A*···O2ⁱⁱⁱ | 0.93 | 2.42 | 3.318 (5) | 161 |

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