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# 2-{(*E*)-4-[4-(Trifluoromethyl)phenoxy]-but-2-enyloxy}phenyl *N*-methylcarbamate

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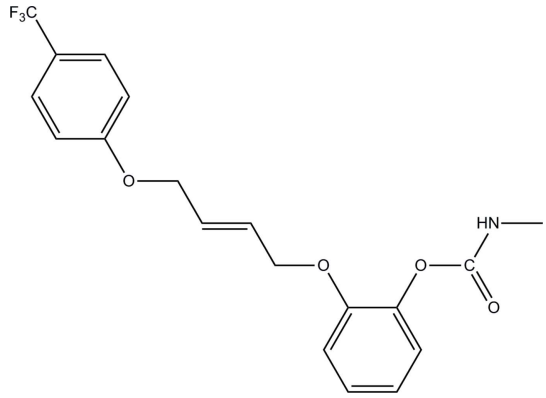
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.044; $wR$ factor = 0.107; data-to-parameter ratio = 11.5.

In the title compound, $C_{19}H_{18}F_3NO_4$, which was designed and synthesized as a dual-site inhibitor of insect AChE (acetylcholinesterase), the dihedral angle between the methylcarbamate group and the benzene ring is 72.47 (6)°. In the crystal, inversion dimers are linked by pairs of N—H···O hydrogen bonds.

## Related literature

For background to multivalent ligand-receptor interactions and their pharmaceutical applications, see: Carlier *et al.* (1999); Hu *et al.* (2002); Kitov *et al.* (2000); Kopytek *et al.* (2000); Kryger *et al.* (1999); Lee & Lee (1995); Luedtke *et al.* (2003); Mammen *et al.* (1998); Pang *et al.* (1996). For agrochemical applications of the cluster effect, see: Ma *et al.* (2010); Zhao *et al.* (2008, 2009). For the structure of AChE from *Torpedo californica* (TcACche), see: Sussman *et al.* (1991); Harel *et al.* (1993).



## Experimental

### Crystal data

$C_{19}H_{18}F_3NO_4$
$M_r$ = 381.34
Monoclinic, $P2_1/c$
$a$ = 12.413 (3) Å
$b$ = 9.3936 (19) Å
$c$ = 16.202 (3) Å
$\beta$ = 111.65 (3)°
$V$ = 1755.9 (6) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 1.05 mm$^{-1}$
$T$ = 173 K
0.47 × 0.30 × 0.25 mm

### Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.639, $T_{max}$ = 0.780
11613 measured reflections
3163 independent reflections
2615 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.107
$S$ = 1.07
3163 reflections
274 parameters
60 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2$^{i}$ | 0.88 | 2.22 | 3.072 (2) | 163 |

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

Data collection: *RAPID-AUTO* (Rigaku 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2102).

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# supporting information

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## 2-{(*E*)-4-[4-(Trifluoromethyl)phenoxy]but-2-enyloxy}phenyl *N*-methylcarbamate

**Hong-Ju Ma, Meng-Han Xu, Jian-Hua Zhang, Jian-Hong Li and Jun Ning**

### S1. Comment

Multivalent ligand-receptor interactions, known as the cluster effect, are defined as specific simultaneous associations of multiple ligands present on a molecular construct that bind to multiple receptors presented on a biological entity (Mammen *et al.*, 1998; Lee *et al.*, 1995). In biological systems, multivalent ligands often possess increased functional affinity for their targets compared with that of monovalent ligands (Kitov *et al.*, 2000; Kopytek *et al.*, 2000; Luedtke *et al.*, 2003). Acetylcholinesterase (AChE; EC 3.1.1.7) is a key enzyme in the nervous system, terminating nerve impulses by catalyzing the hydrolysis of the neurotransmitter acetylcholine. X-ray crystallographic structural analysis of the AChE from *Torpedo californica* (TcAChe) has demonstrated that the active site lies near the bottom of a deep, narrow gorge that reaches half way into the protein and that 14 aromatic residues line a substantial portion of the surface of the gorge (Sussman *et al.*, 1991). This cavity was named the 'active site gorge′ with peripheral sites existing at the gorge mouth and Trp279 being the main site (Harel *et al.*, 1993). On the basis of the structure of AChE, many potential dual-site binding inhibitors of AChE have been synthesized (Pang *et al.*, 1996; Carlier *et al.*, 1999; Hu *et al.*, 2002) and demonstrated in drugs in order to treat or alleviate Alzheimer's disease (Kryger *et al.*, 1999). In the area of pesticide, dual- or multiple-site inhibitors of insect AChE were designed and synthesized in our research group (Zhao *et al.*., 2008; Zhao *et al*., 2009). Recently, we synthesized novel carbamate derivatives as potential dual-binding site acetylcholinesterase inhibitors (Ma *et al.*, 2010). The crystal structure of the title compound (I) is shown in Fig. 1.

### S2. Experimental

2-((*E*)-4-(4-(trifluoromethyl)phenoxy)but-2-enyloxy)phenyl methylcarbamate (0.2 g) was dissolved in 95% ethanol (50 ml) at room temperature. Colorless crystals of compound (I) were obtained through slow evaporation after two weeks.

### S3. Refinement

The trifluoromethyl group showed orientational disorder with two resolved alternative sites which were refined independently leading to a 71:29 occupancy ratio. All non-hydrogen atoms were refined with anisotropic displacement parameters. The carbon-bound H atoms were placed at calculated positions, with C—H = 0.93 - 0.98 Å, and were included in the refinement in the riding model approximation with *U*iso(H) set to 1.2 - 1.5*U*eq(C).

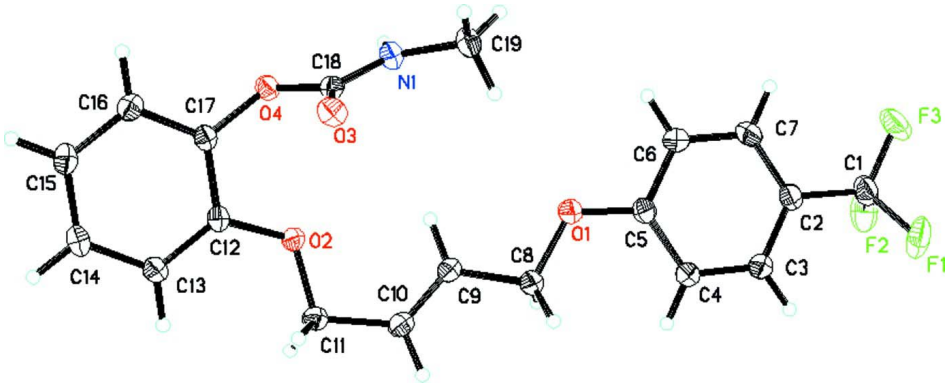


**Figure 1**

The molecular structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

**2-{(*E*)-4-[4-(Trifluoromethyl)phenoxy]but-2-enyloxy}phenyl *N*-methylcarbamate**

*Crystal data*

$C_{19}H_{18}F_3NO_4$
$M_r = 381.34$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.413$ (3) Å
$b = 9.3936$ (19) Å
$c = 16.202$ (3) Å
$\beta = 111.65$ (3)°
$V = 1755.9$ (6) Å$^3$
$Z = 4$
$F(000) = 792$
$D_x = 1.443$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 468 reflections
$\theta = 2.2$–$68.3°$
$\mu = 1.05$ mm$^{-1}$
$T = 173$ K
Block, colorless
0.47 × 0.30 × 0.25 mm

*Data collection*

Rigaku R-AXIS RAPID IP area-detector diffractometer
Radiation source: rotating anode
Graphite monochromator
$\omega$ scans at fixed $\chi = 45°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.639$, $T_{max} = 0.780$
11613 measured reflections
3163 independent reflections
2615 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 68.2°$, $\theta_{min} = 3.8°$
$h = -14 \rightarrow 14$
$k = -11 \rightarrow 10$
$l = -18 \rightarrow 19$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.107$
$S = 1.07$
3163 reflections
274 parameters
60 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
$w = 1/[\sigma^2(F_o^2) + (0.0381P)^2 + 0.8611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å$^{-3}$
$\Delta\rho_{min} = -0.22$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0033 (3)

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| F1 | 0.4769 (4) | −0.2372 (3) | 0.2853 (4) | 0.0698 (14) | 0.710 (12) |
| F2 | 0.4529 (5) | −0.0522 (5) | 0.2121 (3) | 0.0731 (13) | 0.710 (12) |
| F3 | 0.5816 (4) | −0.0554 (8) | 0.3412 (5) | 0.090 (2) | 0.710 (12) |
| F1′ | 0.5251 (13) | −0.2132 (15) | 0.3448 (14) | 0.109 (5) | 0.290 (12) |
| F2′ | 0.4491 (9) | −0.111 (2) | 0.2122 (6) | 0.111 (5) | 0.290 (12) |
| F3′ | 0.5655 (11) | −0.0074 (18) | 0.3219 (13) | 0.092 (5) | 0.290 (12) |
| O1 | 0.13692 (11) | 0.11336 (15) | 0.41856 (9) | 0.0376 (4) | |
| O2 | −0.17712 (11) | 0.32576 (15) | 0.48990 (9) | 0.0348 (3) | |
| O3 | 0.02201 (12) | 0.28785 (14) | 0.67050 (9) | 0.0367 (4) | |
| O4 | −0.03869 (11) | 0.50607 (14) | 0.60863 (9) | 0.0313 (3) | |
| N1 | 0.12414 (13) | 0.41620 (18) | 0.60530 (11) | 0.0336 (4) | |
| H1 | 0.1242 | 0.4945 | 0.5755 | 0.040* | |
| C1 | 0.47480 (19) | −0.0960 (2) | 0.29620 (17) | 0.0477 (6) | |
| C2 | 0.38579 (17) | −0.0443 (2) | 0.32947 (14) | 0.0360 (5) | |
| C3 | 0.27526 (17) | −0.1023 (2) | 0.29649 (13) | 0.0360 (5) | |
| H3 | 0.2584 | −0.1773 | 0.2543 | 0.043* | |
| C4 | 0.18957 (17) | −0.0526 (2) | 0.32412 (13) | 0.0332 (5) | |
| H4 | 0.1141 | −0.0930 | 0.3009 | 0.040* | |
| C5 | 0.21432 (16) | 0.0570 (2) | 0.38617 (13) | 0.0318 (4) | |
| C6 | 0.32588 (18) | 0.1133 (2) | 0.42067 (15) | 0.0422 (5) | |
| H6 | 0.3437 | 0.1868 | 0.4640 | 0.051* | |
| C7 | 0.41034 (18) | 0.0630 (2) | 0.39219 (15) | 0.0439 (5) | |
| H7 | 0.4862 | 0.1022 | 0.4158 | 0.053* | |
| C8 | 0.01688 (16) | 0.0769 (2) | 0.37353 (13) | 0.0354 (5) | |
| H8A | 0.0055 | −0.0264 | 0.3792 | 0.043* | |
| H8B | −0.0081 | 0.1005 | 0.3096 | 0.043* | |
| C9 | −0.05238 (17) | 0.1595 (2) | 0.41472 (13) | 0.0329 (5) | |
| H9 | −0.0182 | 0.2416 | 0.4485 | 0.039* | |
| C10 | −0.15720 (18) | 0.1256 (2) | 0.40707 (14) | 0.0381 (5) | |
| H10 | −0.1877 | 0.0412 | 0.3745 | 0.046* | |
| C11 | −0.23549 (17) | 0.2024 (2) | 0.44281 (13) | 0.0337 (5) | |
| H11A | −0.3074 | 0.2308 | 0.3935 | 0.040* | |
| H11B | −0.2569 | 0.1392 | 0.4832 | 0.040* | |
| C12 | −0.22437 (16) | 0.3914 (2) | 0.54436 (12) | 0.0300 (4) | |
| C13 | −0.33741 (17) | 0.3764 (2) | 0.53971 (13) | 0.0354 (5) | |

| | | | | |
|---|---|---|---|---|
| H13 | −0.3893 | 0.3149 | 0.4967 | 0.042* |
| C14 | −0.37483 (18) | 0.4512 (2) | 0.59798 (14) | 0.0394 (5) |
| H14 | −0.4523 | 0.4402 | 0.5948 | 0.047* |
| C15 | −0.30069 (18) | 0.5415 (2) | 0.66040 (14) | 0.0392 (5) |
| H15 | −0.3271 | 0.5922 | 0.7001 | 0.047* |
| C16 | −0.18725 (17) | 0.5581 (2) | 0.66513 (13) | 0.0347 (5) |
| H16 | −0.1360 | 0.6209 | 0.7076 | 0.042* |
| C17 | −0.14992 (16) | 0.4832 (2) | 0.60820 (12) | 0.0296 (4) |
| C18 | 0.03597 (16) | 0.3915 (2) | 0.63119 (12) | 0.0290 (4) |
| C19 | 0.22029 (18) | 0.3175 (2) | 0.62487 (16) | 0.0446 (6) |
| H19A | 0.2818 | 0.3611 | 0.6091 | 0.067* |
| H19B | 0.1936 | 0.2300 | 0.5904 | 0.067* |
| H19C | 0.2504 | 0.2947 | 0.6884 | 0.067* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.082 (2) | 0.0421 (13) | 0.117 (3) | 0.0125 (13) | 0.073 (2) | 0.0034 (16) |
| F2 | 0.084 (3) | 0.083 (2) | 0.077 (2) | 0.0261 (19) | 0.059 (2) | 0.019 (2) |
| F3 | 0.0276 (13) | 0.136 (5) | 0.100 (3) | −0.001 (2) | 0.0170 (15) | −0.051 (3) |
| F1′ | 0.099 (7) | 0.091 (7) | 0.172 (12) | 0.058 (6) | 0.092 (8) | 0.046 (7) |
| F2′ | 0.038 (4) | 0.192 (13) | 0.093 (7) | −0.003 (6) | 0.011 (4) | −0.102 (8) |
| F3′ | 0.065 (7) | 0.090 (7) | 0.159 (11) | −0.039 (6) | 0.087 (8) | −0.045 (7) |
| O1 | 0.0312 (7) | 0.0435 (8) | 0.0390 (8) | −0.0012 (6) | 0.0141 (6) | −0.0093 (7) |
| O2 | 0.0333 (7) | 0.0358 (8) | 0.0412 (8) | −0.0074 (6) | 0.0207 (6) | −0.0109 (6) |
| O3 | 0.0369 (8) | 0.0314 (8) | 0.0423 (8) | 0.0002 (6) | 0.0151 (6) | 0.0082 (6) |
| O4 | 0.0279 (7) | 0.0274 (7) | 0.0399 (7) | 0.0004 (6) | 0.0139 (6) | 0.0013 (6) |
| N1 | 0.0307 (8) | 0.0351 (9) | 0.0369 (9) | 0.0017 (7) | 0.0148 (7) | 0.0039 (8) |
| C1 | 0.0362 (12) | 0.0442 (13) | 0.0672 (16) | 0.0019 (11) | 0.0243 (11) | 0.0044 (13) |
| C2 | 0.0302 (10) | 0.0354 (11) | 0.0437 (11) | 0.0024 (9) | 0.0151 (9) | 0.0051 (9) |
| C3 | 0.0347 (10) | 0.0354 (11) | 0.0385 (11) | −0.0001 (9) | 0.0141 (9) | −0.0032 (9) |
| C4 | 0.0300 (10) | 0.0346 (11) | 0.0344 (10) | −0.0010 (8) | 0.0111 (8) | −0.0010 (9) |
| C5 | 0.0302 (10) | 0.0330 (10) | 0.0327 (10) | 0.0027 (8) | 0.0121 (8) | 0.0035 (8) |
| C6 | 0.0342 (11) | 0.0405 (12) | 0.0489 (12) | −0.0047 (10) | 0.0118 (9) | −0.0112 (10) |
| C7 | 0.0285 (10) | 0.0434 (12) | 0.0573 (14) | −0.0043 (9) | 0.0130 (10) | −0.0055 (11) |
| C8 | 0.0313 (10) | 0.0384 (11) | 0.0380 (11) | −0.0031 (9) | 0.0145 (9) | −0.0050 (9) |
| C9 | 0.0347 (10) | 0.0314 (10) | 0.0335 (10) | −0.0015 (9) | 0.0137 (8) | −0.0049 (8) |
| C10 | 0.0408 (11) | 0.0331 (11) | 0.0439 (12) | −0.0048 (9) | 0.0200 (9) | −0.0095 (9) |
| C11 | 0.0334 (10) | 0.0322 (10) | 0.0367 (11) | −0.0048 (8) | 0.0142 (8) | −0.0041 (8) |
| C12 | 0.0303 (10) | 0.0313 (10) | 0.0315 (10) | 0.0019 (8) | 0.0147 (8) | 0.0007 (8) |
| C13 | 0.0297 (10) | 0.0400 (12) | 0.0382 (11) | −0.0026 (9) | 0.0145 (9) | −0.0030 (9) |
| C14 | 0.0315 (10) | 0.0457 (13) | 0.0463 (12) | 0.0046 (9) | 0.0205 (9) | 0.0035 (10) |
| C15 | 0.0408 (12) | 0.0441 (12) | 0.0378 (11) | 0.0078 (10) | 0.0206 (10) | 0.0003 (10) |
| C16 | 0.0379 (11) | 0.0333 (11) | 0.0325 (10) | 0.0025 (9) | 0.0125 (9) | −0.0001 (9) |
| C17 | 0.0279 (9) | 0.0291 (10) | 0.0331 (10) | 0.0013 (8) | 0.0129 (8) | 0.0029 (8) |
| C18 | 0.0271 (9) | 0.0294 (10) | 0.0284 (9) | −0.0008 (8) | 0.0077 (8) | −0.0031 (8) |
| C19 | 0.0319 (11) | 0.0475 (13) | 0.0549 (13) | 0.0068 (10) | 0.0168 (10) | 0.0000 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F1—C1 | 1.339 (3) | C6—H6 | 0.9500 |
| F2—C1 | 1.351 (4) | C7—H7 | 0.9500 |
| F3—C1 | 1.312 (5) | C8—C9 | 1.487 (3) |
| F1′—C1 | 1.363 (7) | C8—H8A | 0.9900 |
| F2′—C1 | 1.287 (8) | C8—H8B | 0.9900 |
| F3′—C1 | 1.337 (9) | C9—C10 | 1.300 (3) |
| O1—C5 | 1.361 (2) | C9—H9 | 0.9500 |
| O1—C8 | 1.438 (2) | C10—C11 | 1.488 (3) |
| O2—C12 | 1.373 (2) | C10—H10 | 0.9500 |
| O2—C11 | 1.429 (2) | C11—H11A | 0.9900 |
| O3—C18 | 1.210 (2) | C11—H11B | 0.9900 |
| O4—C18 | 1.379 (2) | C12—C13 | 1.384 (3) |
| O4—C17 | 1.395 (2) | C12—C17 | 1.401 (3) |
| N1—C18 | 1.329 (2) | C13—C14 | 1.387 (3) |
| N1—C19 | 1.451 (3) | C13—H13 | 0.9500 |
| N1—H1 | 0.8800 | C14—C15 | 1.379 (3) |
| C1—C2 | 1.479 (3) | C14—H14 | 0.9500 |
| C2—C7 | 1.383 (3) | C15—C16 | 1.390 (3) |
| C2—C3 | 1.387 (3) | C15—H15 | 0.9500 |
| C3—C4 | 1.379 (3) | C16—C17 | 1.369 (3) |
| C3—H3 | 0.9500 | C16—H16 | 0.9500 |
| C4—C5 | 1.392 (3) | C19—H19A | 0.9800 |
| C4—H4 | 0.9500 | C19—H19B | 0.9800 |
| C5—C6 | 1.393 (3) | C19—H19C | 0.9800 |
| C6—C7 | 1.376 (3) | | |
| | | | |
| C5—O1—C8 | 117.30 (15) | H8A—C8—H8B | 108.4 |
| C12—O2—C11 | 117.06 (15) | C10—C9—C8 | 123.63 (19) |
| C18—O4—C17 | 116.65 (14) | C10—C9—H9 | 118.2 |
| C18—N1—C19 | 121.73 (18) | C8—C9—H9 | 118.2 |
| C18—N1—H1 | 119.1 | C9—C10—C11 | 128.22 (19) |
| C19—N1—H1 | 119.1 | C9—C10—H10 | 115.9 |
| F2′—C1—F3′ | 104.5 (10) | C11—C10—H10 | 115.9 |
| F3—C1—F1 | 107.3 (4) | O2—C11—C10 | 108.98 (16) |
| F3—C1—F2 | 104.9 (4) | O2—C11—H11A | 109.9 |
| F1—C1—F2 | 100.1 (3) | C10—C11—H11A | 109.9 |
| F2′—C1—F1′ | 113.7 (8) | O2—C11—H11B | 109.9 |
| F3′—C1—F1′ | 99.7 (8) | C10—C11—H11B | 109.9 |
| F2′—C1—C2 | 119.7 (6) | H11A—C11—H11B | 108.3 |
| F3—C1—C2 | 116.1 (4) | O2—C12—C13 | 125.72 (17) |
| F3′—C1—C2 | 109.8 (7) | O2—C12—C17 | 115.42 (16) |
| F1—C1—C2 | 115.2 (2) | C13—C12—C17 | 118.84 (18) |
| F2—C1—C2 | 111.6 (3) | C12—C13—C14 | 119.89 (19) |
| F1′—C1—C2 | 107.4 (5) | C12—C13—H13 | 120.1 |
| C7—C2—C3 | 119.2 (2) | C14—C13—H13 | 120.1 |
| C7—C2—C1 | 121.03 (19) | C15—C14—C13 | 120.68 (19) |

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|---|---|---|---|
| C3—C2—C1 | 119.8 (2) | C15—C14—H14 | 119.7 |
| C4—C3—C2 | 120.9 (2) | C13—C14—H14 | 119.7 |
| C4—C3—H3 | 119.5 | C14—C15—C16 | 119.8 (2) |
| C2—C3—H3 | 119.5 | C14—C15—H15 | 120.1 |
| C3—C4—C5 | 119.58 (19) | C16—C15—H15 | 120.1 |
| C3—C4—H4 | 120.2 | C17—C16—C15 | 119.53 (19) |
| C5—C4—H4 | 120.2 | C17—C16—H16 | 120.2 |
| O1—C5—C4 | 124.58 (18) | C15—C16—H16 | 120.2 |
| O1—C5—C6 | 115.86 (18) | C16—C17—O4 | 119.88 (17) |
| C4—C5—C6 | 119.54 (19) | C16—C17—C12 | 121.22 (18) |
| C7—C6—C5 | 120.2 (2) | O4—C17—C12 | 118.71 (17) |
| C7—C6—H6 | 119.9 | O3—C18—N1 | 126.96 (18) |
| C5—C6—H6 | 119.9 | O3—C18—O4 | 123.69 (17) |
| C6—C7—C2 | 120.6 (2) | N1—C18—O4 | 109.33 (16) |
| C6—C7—H7 | 119.7 | N1—C19—H19A | 109.5 |
| C2—C7—H7 | 119.7 | N1—C19—H19B | 109.5 |
| O1—C8—C9 | 108.10 (16) | H19A—C19—H19B | 109.5 |
| O1—C8—H8A | 110.1 | N1—C19—H19C | 109.5 |
| C9—C8—H8A | 110.1 | H19A—C19—H19C | 109.5 |
| O1—C8—H8B | 110.1 | H19B—C19—H19C | 109.5 |
| C9—C8—H8B | 110.1 | | |

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| F2′—C1—C2—C7 | −132.8 (10) | C5—O1—C8—C9 | −175.09 (16) |
| F3—C1—C2—C7 | 12.8 (5) | O1—C8—C9—C10 | −160.9 (2) |
| F3′—C1—C2—C7 | −11.9 (10) | C8—C9—C10—C11 | −177.9 (2) |
| F1—C1—C2—C7 | 139.4 (4) | C12—O2—C11—C10 | −165.39 (16) |
| F2—C1—C2—C7 | −107.3 (3) | C9—C10—C11—O2 | −0.2 (3) |
| F1′—C1—C2—C7 | 95.6 (11) | C11—O2—C12—C13 | −19.5 (3) |
| F2′—C1—C2—C3 | 46.2 (10) | C11—O2—C12—C17 | 161.91 (17) |
| F3—C1—C2—C3 | −168.2 (4) | O2—C12—C13—C14 | −178.79 (18) |
| F3′—C1—C2—C3 | 167.0 (10) | C17—C12—C13—C14 | −0.2 (3) |
| F1—C1—C2—C3 | −41.6 (4) | C12—C13—C14—C15 | 0.4 (3) |
| F2—C1—C2—C3 | 71.7 (3) | C13—C14—C15—C16 | 0.1 (3) |
| F1′—C1—C2—C3 | −85.4 (11) | C14—C15—C16—C17 | −0.7 (3) |
| C7—C2—C3—C4 | 1.2 (3) | C15—C16—C17—O4 | 175.88 (17) |
| C1—C2—C3—C4 | −177.75 (19) | C15—C16—C17—C12 | 0.8 (3) |
| C2—C3—C4—C5 | −0.2 (3) | C18—O4—C17—C16 | 117.69 (19) |
| C8—O1—C5—C4 | −12.6 (3) | C18—O4—C17—C12 | −67.1 (2) |
| C8—O1—C5—C6 | 169.01 (18) | O2—C12—C17—C16 | 178.33 (17) |
| C3—C4—C5—O1 | −179.48 (18) | C13—C12—C17—C16 | −0.4 (3) |
| C3—C4—C5—C6 | −1.1 (3) | O2—C12—C17—O4 | 3.2 (3) |
| O1—C5—C6—C7 | 179.85 (19) | C13—C12—C17—O4 | −175.48 (17) |
| C4—C5—C6—C7 | 1.3 (3) | C19—N1—C18—O3 | −1.9 (3) |
| C5—C6—C7—C2 | −0.3 (3) | C19—N1—C18—O4 | 176.30 (17) |
| C3—C2—C7—C6 | −1.0 (3) | C17—O4—C18—O3 | −18.9 (3) |
| C1—C2—C7—C6 | 178.0 (2) | C17—O4—C18—N1 | 162.82 (15) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2$^{i}$ | 0.88 | 2.22 | 3.072 (2) | 163 |

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.