Ethyl 2-[(E)-{2,4-dimethoxy-6-[2-(4-methoxyphenyl)ethenyl]benzylidene}amino]oxy]acetate

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In the title compound, C_{22}H_{25}NO_{6}, the C≡C double bond linking the benzene rings adopts an E configuration and the dihedral angle between the rings is 47.1 (2)°. The oxime unit contains a C≡N double bond, which also has an E configuration. In the crystal, pairs of C−H⋯N hydrogen bonds generate inversion dimers and weak C−H⋯O interactions link the dimers into chains propagating along the b-axis direction.

Structure description

A recent review has demonstrated that chemically modified resveratrol derivatives have diverse biological activities (Li et al., 2019). Oxime esters are one of the most important pharmacophores in a large number of bioactive compounds (Vessally et al., 2016). As part of our studies in this area, O-methylated resveralol aldehyde (Ge et al., 2013) was treated with hydroxylamine to give the corresponding oxime analogue, which was reacted with ethyl bromoacetate to provide the title resveratrol-oxime ester compound.

The molecular structure of the title compound, C_{22}H_{25}NO_{6}, is shown in Fig. 1. The benzene rings (C1–C6 and C10–C15) are connected by the C8≡C9 double bond, which has an E-configuration [torsion angle of 173.69 (12)° for C3—C8—C9—C10]. The dihedral angle formed by benzene rings is 47.1 (2)°. The C17≡N1 imine double bond in the oxime unit also adopts an E configuration, which is defined by a torsion angle of 178.3 (1)° for C4—C17—N1—O3. There are three methoxy groups attached to carbon atoms C1, C5 and C13 in the benzene rings: those at the meta positions (C1, C5) are essentially co-planar with their attached benzene rings [C6—C1—O1—C7 = −0.2 (2)° and C6—C5—O6—C22 = 3.9 (2)°] whereas the methoxy group at the para position (C13) is slightly twisted from the corresponding ring plane [C12—C13—O2—C16 = 8.9 (2)°]. In the crystal, pairs of C22—H22⋯N1 hydrogen bonds generate inversion dimers (Table 1,
Synthesis and crystallization

A mixture of E-2,4-dimethoxy-6-(4-methoxystyryl)benzaldehyde (298 mg, 1 mmol; Ge *et al.*, 2013) and hydroxylamine hydrochloride (69 mg, 1 mmol) in 15 ml of ethanol–water (1:1) was refluxed for 4 h. After completion of reaction, the mixture was cooled to room temperature to give the corresponding oxime derivative (86%, m.p. = 150–152°C), which was used for the next reaction. To a mixture of the oxime derivative (156 mg, 0.5 mmol) and potassium carbonate (276 mg, 2 mmol) in 10 ml of DMF, 1.2 equivalents of ethyl bromoacetate (100 mg, 0.6 mmol) were added and heated for 5 h at 60°C. After completion of the reaction, the reaction mixture was poured into crushed ice–water to form a precipitate. The resulting solid was separated by filtration and was washed with ethyl acetate. Recrystallization of the solid from ethyl acetate solution gave colourless blocks of the title compound.

Table 1

| Hydrogen-bond geometry (Å, °). |
|--------------------------------|
| D—H···A | D—H | H···A | D···A | D—H···A |
| C22—H22/C···N1i | 0.98 | 2.61 | 3.5633 (19) | 166 |
| C14—H14···O5ii | 0.95 | 2.55 | 3.4834 (16) | 166 |

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

Table 2

| Experimental details. |
|------------------------|
| Crystal data | Chemical formula | C22H25NO6 |
| Mw | 399.43 |
| Crystal system, space group | Monoclinic, P21/n |
| Temperature (K) | 193 |
| a, b, c (Å) | 11.3656 (9), 7.0636 (5), 26.035 (2) |
| V (Å³) | 2057.4 (3) |
| Z | 4 |
| Radiation type | Mo Kα |
| μ (mm⁻¹) | 0.09 |
| Crystal size (mm) | 0.36 × 0.19 × 0.10 |
| Data collection | PHOTON 100 CMOS |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 72604, 5157, 4367 |
| Rint | 0.052 |
| wR2 (F² > 2σ(F²)) | 0.046, 0.133, 1.06 |
| No. of reflections | 5157 |
| No. of parameters | 266 |
| H-atoms treatment | H-atoms parameters constrained |
| Δρmax, Δρmin (e Å⁻³) | 0.32, −0.19 |

Computer programs: APEX2 and SAINT (Bruker, 2012), SHELXS and SHELXTL (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015) and pubICIF (Westrip, 2010).

The next reaction. To a mixture of the oxime derivative (156 mg, 0.5 mmol) and potassium carbonate (276 mg, 2 mmol) in 10 ml of DMF, 1.2 equivalents of ethyl bromoacetate (100 mg, 0.6 mmol) were added and heated for 5 h at 60°C. After completion of the reaction, the reaction mixture was poured into crushed ice–water to form a precipitate. The resulting solid was separated by filtration and was washed with ethyl acetate. Recrystallization of the solid from ethyl acetate solution gave colourless blocks of the title compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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full crystallographic data

*IUCrData* (2021). 6, x210950  [https://doi.org/10.1107/S2414314621009500]

**Ethyl 2-[(E)-{(2,4-dimethoxy-6-[2-(4-methoxyphenyl)ethenyl]benzylidene)amino}oxy]acetate**

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**Crystal data**

| Symbol     | Value                  |
|------------|------------------------|
| C₂₂H₂₅NO₆  |                        |
| Mr         | 399.43                 |
| Monoclinic | P2₁/n Hall symbol: -P 2yn |
| a          | 11.3656 (9) Å          |
| b          | 7.0636 (5) Å           |
| c          | 26.035 (2) Å           |
| β          | 100.148 (3)°           |
| V          | 2057.4 (3) Å³          |
| Z          | 4                      |

**Data collection**

| Instrument                        | 
|-----------------------------------|
| PHOTON 100 CMOS diffractometer    |
| Radiation source: fine-focus sealed tube |
| Graphite monochromator            |
| ϕ and ω scans                     |
| 72604 measured reflections        |
| 5157 independent reflections      |

| Data collection                    |
|-----------------------------------|
| 4367 reflections with I > 2σ(I)   |
| Rint = 0.052                      |
| θmax = 28.4°, θmin = 2.1°         |
| h = -15→15, k = -9→9, l = -34→34  |

**Refinement**

| Refinement on F²                   |
|------------------------------------|
| Least-squares matrix: full        |
| R(F² > 2σ(F²)) = 0.046             |
| wR(F²) = 0.133                     |
| S = 1.06                           |
| 5157 reflections                   |
| 266 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/[σ²(Fo)² + (0.0616P)² + 0.781P] |
| where P = (Fo² + 2Fo²)/3           |
| (Δσ)max = 0.001                   |
| Δρmax = 0.32 e Å⁻³                |
| Δρmin = -0.18 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 F² against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F², conventional R-factors R are based on F, with F set to zero for negative F². The threshold expression of F² > 2sigma(F²) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F² are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

| x   | y    | z    | Uiso*/Ueq |
|-----|------|------|-----------|
| C1  | 0.24155 (11) | 0.2768 (2) | 0.96981 (5) | 0.0339 (3) |
| C2  | 0.27638 (11) | 0.2914 (2) | 0.92163 (5) | 0.0330 (3) |
| H2  | 0.2175 | 0.3046 | 0.8911 | 0.040* |
| C3  | 0.39681 (11) | 0.28708 (17) | 0.91753 (5) | 0.0289 (2) |
| C4  | 0.48435 (11) | 0.26856 (17) | 0.96321 (5) | 0.0277 (2) |
| C5  | 0.44554 (11) | 0.25016 (17) | 1.01146 (5) | 0.0292 (3) |
| C6  | 0.32511 (12) | 0.25393 (19) | 1.01513 (5) | 0.0331 (3) |
| H6  | 0.3005 | 0.2411 | 1.0480 | 0.040* |
| O1  | 0.12111 (9) | 0.28900 (18) | 0.96906 (4) | 0.0448 (3) |
| C7  | 0.08045 (14) | 0.2768 (3) | 1.01766 (7) | 0.0531 (4) |
| H7A | 0.1001 | 0.1517 | 1.0331 | 0.080* |
| H7B | −0.0063 | 0.2954 | 1.1020 | 0.080* |
| C8  | 0.42894 (11) | 0.31089 (18) | 0.86556 (5) | 0.0300 (3) |
| H8  | 0.5016 | 0.3741 | 0.8633 | 0.036* |
| C9  | 0.36217 (12) | 0.24905 (18) | 0.82140 (5) | 0.0318 (3) |
| H9  | 0.2942 | 0.1749 | 0.8247 | 0.038* |
| C10 | 0.38336 (11) | 0.28418 (17) | 0.76843 (5) | 0.0386 (2) |
| C11 | 0.31500 (12) | 0.18938 (19) | 0.72667 (5) | 0.0345 (3) |
| H11 | 0.2584 | 0.0980 | 0.7335 | 0.041* |
| C12 | 0.32681 (12) | 0.2241 (2) | 0.67544 (5) | 0.0349 (3) |
| H12 | 0.2800 | 0.1555 | 0.6478 | 0.042* |
| C13 | 0.40742 (11) | 0.35951 (19) | 0.66487 (5) | 0.0316 (3) |
| C14 | 0.47781 (12) | 0.4548 (2) | 0.70595 (5) | 0.0353 (3) |
| H14 | 0.5341 | 0.5465 | 0.6989 | 0.042* |
| C15 | 0.46637 (11) | 0.41688 (19) | 0.75671 (5) | 0.0326 (3) |
| H15 | 0.5158 | 0.4820 | 0.7843 | 0.039* |
| O2  | 0.42356 (9) | 0.40901 (17) | 0.61580 (4) | 0.0428 (3) |
| C16 | 0.34007 (14) | 0.3337 (2) | 0.57350 (5) | 0.0425 (3) |
| H16A| 0.3487 | 0.1958 | 0.5726 | 0.064* |
| H16B| 0.3554 | 0.3877 | 0.5406 | 0.064* |
| H16C| 0.2587 | 0.3658 | 0.5781 | 0.064* |
| C17 | 0.61356 (11) | 0.27478 (18) | 0.96420 (5) | 0.0303 (3) |
| H17 | 0.6643 | 0.3104 | 0.9957 | 0.036* |
| N1  | 0.66105 (10) | 0.23457 (17) | 0.92473 (5) | 0.0345 (3) |
| O3  | 0.78758 (8) | 0.25945 (16) | 0.93779 (4) | 0.0390 (2) |
| C18 | 0.83580 (12) | 0.2301 (2) | 0.89191 (5) | 0.0375 (3) |
| H18A| 0.8035 | 0.1106 | 0.8752 | 0.045* |
| H18B| 0.9236 | 0.2164 | 0.9014 | 0.045* |
| Atom  | U^11  | U^22  | U^33  | U^12  | U^13  | U^23  |
|-------|-------|-------|-------|-------|-------|-------|
| C1    | 0.0266 (6) | 0.0382 (7) | 0.0379 (7) | -0.0006 (5) | 0.0081 (5) | -0.0013 (5) |
| C2    | 0.0281 (6) | 0.0381 (7) | 0.0321 (6) | -0.0002 (5) | 0.0032 (5) | 0.0024 (5) |
| C3    | 0.0298 (6) | 0.0278 (6) | 0.0294 (6) | -0.0010 (4) | 0.0064 (5) | 0.0012 (4) |
| C4    | 0.0272 (6) | 0.0263 (5) | 0.0301 (6) | -0.0011 (4) | 0.0064 (5) | 0.0013 (4) |
| C5    | 0.0289 (6) | 0.0291 (6) | 0.0292 (6) | -0.0016 (5) | 0.0043 (5) | 0.0006 (4) |
| C6    | 0.0322 (6) | 0.0374 (7) | 0.0311 (6) | -0.0022 (5) | 0.0094 (5) | -0.0001 (5) |
| O1    | 0.0264 (5) | 0.0684 (7) | 0.0408 (6) | 0.0001 (5) | 0.0090 (4) | -0.0012 (5) |
| C7    | 0.0330 (7) | 0.0821 (13) | 0.0477 (9) | -0.0010 (7) | 0.0162 (6) | -0.0021 (8) |
| C8    | 0.0271 (6) | 0.0304 (6) | 0.0326 (6) | 0.0004 (5) | 0.0061 (5) | 0.0048 (5) |
| C9    | 0.0303 (6) | 0.0316 (6) | 0.0341 (6) | -0.0029 (5) | 0.0074 (5) | 0.0039 (5) |
| C10   | 0.0268 (6) | 0.0281 (6) | 0.0309 (6) | 0.0015 (4) | 0.0045 (5) | 0.0018 (5) |
| C11   | 0.0333 (6) | 0.0345 (6) | 0.0358 (7) | -0.0100 (5) | 0.0061 (5) | -0.0003 (5) |
| C12   | 0.0334 (6) | 0.0379 (7) | 0.0321 (6) | -0.0081 (5) | 0.0022 (5) | -0.0044 (5) |
| C13   | 0.0273 (6) | 0.0373 (7) | 0.0304 (6) | -0.0002 (5) | 0.0057 (5) | 0.0016 (5) |
| C14   | 0.0312 (6) | 0.0397 (7) | 0.0350 (6) | -0.0109 (5) | 0.0054 (5) | 0.0017 (5) |
| C15   | 0.0297 (6) | 0.0348 (6) | 0.0322 (6) | -0.0067 (5) | 0.0019 (5) | -0.0017 (5) |
| O2    | 0.0401 (5) | 0.0590 (7) | 0.0291 (5) | -0.0104 (5) | 0.0056 (4) | 0.0025 (4) |
| C16   | 0.0421 (8) | 0.0555 (9) | 0.0295 (6) | -0.0012 (7) | 0.0051 (5) | -0.0033 (6) |
| C17   | 0.0284 (6) | 0.0322 (6) | 0.0300 (6) | -0.0013 (5) | 0.0047 (5) | 0.0033 (5) |
| N1    | 0.0249 (5) | 0.0428 (6) | 0.0359 (6) | -0.0018 (4) | 0.0051 (4) | -0.0024 (5) |
| O3    | 0.0242 (4) | 0.0627 (7) | 0.0298 (5) | -0.0004 (4) | 0.0043 (4) | 0.0036 (4) |
| C18   | 0.0289 (6) | 0.0509 (8) | 0.0338 (7) | 0.0070 (6) | 0.0088 (5) | 0.0046 (6) |
| C19   | 0.0295 (6) | 0.0409 (7) | 0.0321 (6) | 0.0007 (5) | 0.0077 (5) | -0.0026 (5) |
| O4    | 0.0706 (8) | 0.0481 (6) | 0.0457 (6) | 0.0193 (6) | 0.0240 (6) | 0.0018 (5) |
| O5    | 0.0441 (5) | 0.0364 (5) | 0.0340 (5) | 0.0062 (4) | 0.0152 (4) | 0.0023 (4) |
| C20   | 0.0522 (8) | 0.0357 (7) | 0.0373 (7) | 0.0025 (6) | 0.0135 (6) | 0.0047 (6) |
| C21   | 0.0599 (10) | 0.0449 (8) | 0.0402 (7) | -0.0093 (7) | 0.0206 (7) | 0.0001 (6) |
| O6    | 0.0310 (5) | 0.0507 (6) | 0.0272 (4) | -0.0017 (4) | 0.0044 (4) | 0.0043 (4) |
| C22   | 0.0400 (7) | 0.0465 (8) | 0.0268 (6) | -0.0043 (6) | 0.0055 (5) | -0.0001 (5) |
**Geometric parameters (Å, °)**

| Bond/Angle | Length/Distance/Angle |
|------------|-----------------------|
| C1—O1     | 1.3683 (16)           |
| C1—C2     | 1.3842 (18)           |
| C1—C6     | 1.3876 (19)           |
| C2—C3     | 1.3919 (17)           |
| C2—H2     | 0.9500                |
| C3—C4     | 1.4158 (17)           |
| C3—C8     | 1.4719 (17)           |
| C4—C5     | 1.4089 (17)           |
| C4—C17    | 1.4649 (17)           |
| C5—O6     | 1.3628 (15)           |
| C5—C6     | 1.3890 (18)           |
| C6—H6     | 0.9500                |
| O1—C7     | 1.4242 (18)           |
| C7—H7A    | 0.9800                |
| C7—H7B    | 0.9800                |
| C7—H7C    | 0.9800                |
| C8—C9     | 1.3345 (18)           |
| C8—H8     | 0.9500                |
| C9—C10    | 1.4623 (17)           |
| C9—H9     | 0.9500                |
| C10—C11   | 1.3917 (18)           |
| C10—C15   | 1.4012 (17)           |
| C11—C12   | 1.3857 (18)           |
| C11—H11   | 0.9500                |
| C12—C13   | 1.3853 (18)           |
| C12—H12   | 0.9500                |
| C13—O2    | 1.3676 (15)           |
| C13—C14   | 1.3913 (18)           |
| O1—C1—C2 | 115.30 (12)           |
| O1—C1—C6 | 123.55 (12)           |
| C2—C1—C6 | 121.14 (12)           |
| C1—C2—C3 | 120.65 (12)           |
| C1—C2—H2 | 119.7                 |
| C3—C2—H2 | 119.7                 |
| C2—C3—C4 | 119.52 (11)           |
| C2—C3—C8 | 118.33 (11)           |
| C4—C3—C8 | 122.09 (11)           |
| C5—C4—C3 | 118.25 (11)           |
| C5—C4—C17| 117.23 (11)           |
| C3—C4—C17| 124.47 (11)           |
| O6—C5—C6 | 122.35 (11)           |
| O6—C5—C4 | 115.86 (11)           |
| C6—C5—C4 | 121.79 (12)           |
| C1—C6—C5 | 118.61 (12)           |
| C1—C6—H6 | 120.7                 |
| C14—C15  | 1.3768 (18)           |
| C14—H14  | 0.9500                |
| C15—H15  | 0.9500                |
| O2—C16   | 1.4242 (17)           |
| C16—H16A | 0.9800                |
| C16—H16B | 0.9800                |
| C16—H16C | 0.9800                |
| C17—N1   | 1.2742 (17)           |
| C17—H17  | 0.9500                |
| N1—O3    | 1.4291 (14)           |
| O3—C18   | 1.4144 (16)           |
| C18—C19  | 1.515 (2)             |
| C18—H18A | 0.9900                |
| C18—H18B | 0.9900                |
| C19—O4   | 1.1962 (17)           |
| C19—O5   | 1.3362 (15)           |
| O5—C20   | 1.4565 (17)           |
| C20—C21  | 1.498 (2)             |
| C20—H20A | 0.9900                |
| C20—H20B | 0.9900                |
| C21—H21A | 0.9800                |
| C21—H21B | 0.9800                |
| C21—H21C | 0.9800                |
| O6—C22   | 1.4302 (15)           |
| C22—H22A | 0.9800                |
| C22—H22B | 0.9800                |
| C22—H22C | 0.9800                |
| C13—C14  | 119.8                 |
| C14—C15—C10 | 121.36 (12)          |
| C14—C15—H15 | 119.3               |
| C10—C15—H15 | 119.3               |
| C13—O2—C16 | 116.50 (11)          |
| O2—C16—H16A | 109.5              |
| O2—C16—H16B | 109.5              |
| H16A—C16—H16B | 109.5             |
| O2—C16—H16C | 109.5              |
| H16A—C16—H16C | 109.5             |
| N1—C17—C4 | 123.02 (12)          |
| N1—C17—H17 | 118.5               |
| C4—C17—H17 | 118.5               |
| C17—N1—O3 | 109.39 (11)          |
| C18—O3—N1 | 107.72 (10)          |
| C18—C19—O4 | 112.50 (11)         |
| Bond/Angle/Distance | Value 1 | Value 2 | Value 3 |
|--------------------|---------|---------|---------|
| C5—C6—H6          | 120.7   | O3—C18—H18A | 109.1   |
| C1—O1—C7          | 117.64  | C19—C18—H18A | 109.1   |
| O1—C7—H7A         | 109.5   | O3—C18—H18B | 109.1   |
| O1—C7—H7B         | 109.5   | C19—C18—H18B | 109.1   |
| H7A—C7—H7B        | 109.5   | H18A—C18—H18B | 107.8   |
| O1—C7—H7C         | 109.5   | O4—C19—O5    | 124.44  |
| H7A—C7—H7C        | 109.5   | O4—C19—C18   | 125.86  |
| H7B—C7—H7C        | 109.5   | O5—C19—C18   | 109.70  |
| C9—C8—C3          | 123.98  | C19—O5—C20   | 116.35  |
| C9—C8—H8          | 118.0   | O5—C20—C21   | 108.06  |
| C3—C8—H8          | 118.0   | O5—C20—H20A  | 110.1   |
| C8—C9—C10         | 126.42  | C21—C20—H20A | 110.1   |
| C8—C9—H9          | 116.8   | O5—C20—H20B  | 110.1   |
| C10—C9—H9         | 116.8   | C21—C20—H20B | 110.1   |
| C11—C10—C15       | 117.15  | H20A—C20—H20B | 108.4   |
| C11—C10—C9        | 119.55  | C20—C21—H21A | 109.5   |
| C15—C10—C9        | 123.24  | C20—C21—H21B | 109.5   |
| C12—C11—C10       | 122.11  | H21A—C21—H21B | 109.5   |
| C12—C11—H11       | 118.9   | C20—C21—H21C | 109.5   |
| C10—C11—H11       | 118.9   | H21A—C21—H21C | 109.5   |
| C13—C12—C11       | 119.53  | H21B—C21—H21C | 109.5   |
| C13—C12—H12       | 120.2   | C5—O6—C22    | 117.86  |
| C11—C12—H12       | 120.2   | O6—C22—H22A  | 109.5   |
| O2—C13—C12        | 124.35  | O6—C22—H22B  | 109.5   |
| C12—C13—C14       | 116.15  | O6—C22—H22B  | 109.5   |
| C15—C14—C13       | 120.32  | O6—C22—H22C  | 109.5   |
| C15—C14—H14       | 119.8   | O6—C22—H22C  | 109.5   |
| O1—C1—C2—C3       | 177.99  | C9—C10—C11—C12 | 176.62 |
| C6—C1—C2—C3       | −1.2    | C10—C11—C12—C13 | −1.2  |
| C1—C2—C3—C4       | −0.4    | C11—C12—C13—O2 | −177.91 |
| C1—C2—C3—C8       | −177.58 | C11—C12—C13—C14 | 1.9  |
| C2—C3—C4—C5       | 1.62    | O2—C13—C14—C15 | 178.88 |
| C8—C3—C4—C5       | 178.74  | C12—C13—C14—C15 | −0.9 |
| C2—C3—C4—C17      | −175.79 | C13—C14—C15—C10 | −0.8 |
| C8—C3—C4—C17      | 1.32    | C11—C10—C15—C14 | 1.4  |
| C3—C4—C5—O6       | 178.79  | C9—C10—C15—C14 | −175.53 |
| C17—C4—C5—O6      | −3.61   | C12—C13—O2—C16 | 8.9   |
| C3—C4—C5—C6       | −1.41   | C14—C13—O2—C16 | −170.87 |
| C17—C4—C5—C6      | 176.20  | C5—C4—C17—N1   | 158.35 |
| O1—C1—C6—C5       | −177.70 | C3—C4—C17—N1   | −24.2 |
| C2—C1—C6—C5       | 1.4     | C4—C17—N1—O3   | 178.31 |
| O6—C5—C6—C1       | 179.69  | C17—N1—O3—C18  | −174.86 |
| C4—C5—C6—C1       | −0.1    | N1—O3—C18—C19  | 72.08  |
| C2—C1—O1—C7       | −179.36 | O3—C18—C19—O4  | 5.7    |
| C6—C1—O1—C7       | −0.2    | O3—C18—C19—O5  | −174.87 |
| C2—C3—C8—C9       | −33.37  | O4—C19—O5—C20  | 4.5    |
C4—C3—C8—C9 149.49 (13) C18—C19—O5—C20 −174.88 (12)
C3—C8—C9—C10 173.69 (12) C19—O5—C20—C21 176.76 (12)
C8—C9—C10—C11 171.46 (13) C6—C5—O6—C22 3.90 (18)
C8—C9—C10—C15 −11.6 (2) C4—C5—O6—C22 −176.29 (11)
C15—C10—C11—C12 −0.5 (2)

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A   | D—H···A |
|---------|------|-------|---------|---------|
| C22—H22···N1i | 0.98 | 2.61  | 3.5633 (19) | 166     |
| C14—H14···O5ii | 0.95 | 2.55  | 3.4834 (16) | 166     |

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