In the title molecule, C_{27}H_{27}NO, the naphthalene and quinoline groups are both planar and subtend a dihedral angle of 15.47(7)°. They are nearly coplanar with the cis-vinyl bridge and the hexyloxy chain, which adopts an all-trans conformation, resulting in transannular bifurcated intramolecular C—H···N,O contact. The crystal structure features γ-packing of the aromatic moieties, while the parallel packing of alkyl chains resembles that of alkanes.

1. Chemical context

In recent decades, π-conjugated organic molecules with donor–acceptor architectures have received considerable attention regarding their diverse applications in organic optoelectronics and electronics, for example in non-linear optics and as organic semiconductors (Rao et al., 2010; Siram et al., 2011; Wang et al., 2015; Zhang et al., 2015). As for vinyl-bridged donor–acceptor molecules incorporating naphthalene as a donor and quinoline as an acceptor, the poor solubility (which hinders purification and processibility) is due to the good molecular coplanarity (Ishikawa & Hashimoto, 2011). The introduction of long substituents into quinoline or naphthalene cores is an effective method of solving this problem. Hexyloxy-substituted donor–acceptor molecules based on naphthalene and quinoline are a promising class owing to their satisfactory solubility. Moreover, the introduction of alkyl substituents of suitable length can not only increase the capacity for self-assembly, but also improve carrier mobility (Garnier et al., 1993; Halik et al., 2003). The title compound (1) was synthesized by a Wittig reaction and has been shown by single-crystal X-ray diffraction analysis to be a rare example of a stilbene-like donor–π–acceptor (D—π···A) type molecule with a cis configuration, and the first structurally characterized cis-naphthalene-C=C-quinoline derivative. The D—π···A structure is known to favour high-intensity two-photon absorption (Lv, Xu, Cui, et al., 2021; Lv, Xu, Yu, et al., 2021).
2. Structural commentary

Compound (1) crystallizes in the monoclinic centrosymmetric space group $P_{2_1}/n$ with one molecule per asymmetric unit (Fig. 1). The molecule contains four fragments, which are planar within experimental error, viz. the quinoline ($Cg_1$) and naphthalene ($Cg_2$) systems, the $C9—C16\equiv C17—C18$ bridge and the hexyloxy chain, which adopts an all-trans conformation. Planes $Cg_1$ and $Cg_2$ subtend a dihedral angle of 15.46 (5)$^\circ$, and angles of 8.34 (8) and 13.28 (10)$^\circ$, respectively, with the bridge plane. The $Cg_1$ and the hexyloxy planes form an angle of 5.05 (4)$^\circ$. Thus, all non-hydrogen atoms in the molecule are roughly coplanar, with an r.m.s. deviation of 0.23 Å. The intramolecular (transannular) contact $C27—H27\cdots O1$ [$C\cdots O = 3.633 (2)$, $H\cdots O = 2.809 (17)$ Å, $C—H\cdots O = 145.0 (12)^\circ$] corresponds to that of a weakly stabilizing hydrogen bond (Steiner, 1996; Desiraju & Steiner, 1999).

3. Supramolecular features

In the crystal, molecules related by $b$ translation pack face-to-face, forming strongly slanted stacks running along the $b$-axis direction (see Fig. 2). However, $\pi-\pi$ stacking between aromatic moieties (Hunter & Sanders, 1990) is practically absent. Thus, although the quinoline ($Cg_1$) $\pi$-systems are parallel, their overlap is marginal, involving only one carbon atom on either side, with a $C10\cdots C15(x, y + 1, z)$ contact distance of 3.540 (3) Å, while the naphthalene moiety overlaps with the alkyl chain of the next molecule. Molecules belonging to different stacks and related by a screw axis form a typical $\gamma$-motif (Loots & Barbour, 2012), their quinoline and naphthalene moieties contact at an interplanar angle of 68.60 (5)$^\circ$. The packing of the $n$-hexyl chains resembles that of pure alkanes, with a parallel arrangement of the chains, which adopt an all-trans conformation.

4. Database survey

The Cambridge Crystallographic Database (CSD Version 5.42, November 2021; Groom et al., 2016) contains only two structures with a 2-[(2-(naphthalen-2-yl)ethenyl)quinoline moiety, viz. bis[$\mu-2$-[(2-naphthyl)vinyl]quinolin-8-olato]bis(dimethyl sulfoxide)bis(iodo)dicadmium(II) (GAQFIQ; Yuan et al., 2017) and 2-[(2-(6-methoxynaphthalen-2-yl)vinyl]-1-methylquinolin-1-ium iodide (LEWXAP; Tian et al., 2018). Both have a trans-configuration about the vinyl $C\equiv C$ bond, in contrast with the cis-configuration of molecule (1), and adopt interactions (see Database survey), indicating that the $C27—H27\cdots N1$ contact may in fact be a repulsive, ‘collateral damage’ type contact (Gavezzotti, 2010) and the bridge absorbs the resulting strain. On the contrary, the geometry of the longer transannular contact $C27—H27\cdots O1$ [$C\cdots O = 3.633 (2)$, $H\cdots O = 2.809 (17)$ Å, $C—H\cdots O = 145.0 (12)^\circ$] corresponds to that of a weakly stabilizing hydrogen bond (Steiner, 1996; Desiraju & Steiner, 1999).

### Table 1

Hydrogen-bond geometry (Å, $^\circ$).

| $D—H\cdots A$ | $D—H$ | $H\cdots A$ | $D\cdots A$ | $D—H\cdots A$ |
|----------------|--------|-------------|--------------|----------------|
| $C6—H6A\cdots N1$ | 0.97 | 2.68 | 3.600 (2) | 159 |
| $C27—H27\cdots O1$ | 0.955 (16) | 2.809 (17) | 3.633 (2) | 145.0 (12) |
| $C27—H27\cdots N1$ | 0.955 (16) | 2.195 (16) | 3.068 (3) | 151.4 (13) |

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

Figure 1

Molecular structure of compound (1) with atom labelling. Atomic displacement ellipsoids are drawn at the 30% probability level.

Figure 2

Crystal packing of compound (1). Hydrogen atoms are omitted for clarity.
more planar conformation than the latter. In cis-2,5-bis(2-methylbutoxy)- and cis-2,5-dibutoxy-1,4-bis[2-(pyrid-2-yl)vinyl]benzene (SIXQOH and SIXQUN; Liu et al., 2014), the (pyrid-2-yl)vinylbenzene fragments have a cis-configuration about the C=C bond, but in both structures the pyridyl N atom is oriented outward, not intraannually. Thus the pyridyl and benzene rings cannot be coplanar with the ethenyl bridge, due to the steric repulsion between ortho-H atoms, and are inclined to this bridge by 28–47° in a propeller-like fashion. The C–C=C bond angles in the vinyl bridge (129–131°) are narrower than in (I).

5. Synthesis and crystallization

All reactants and solvents were purchased and used without further purification. THF was dried by using Na in the presence of benzophenone. Bromo(naphthalen-2-ylmethyl)triphenylphosphorane (2) was synthesized according to the literature method of our research group (Luo et al., 2018). 1H NMR and 13C NMR spectra were obtained in CDCl3 with tetramethylsilane as internal standard on a Bruker Advance spectrometer. HRMS spectra were obtained on a 650Q-TOF spectrometer. The synthesis procedures for (I)–(4) are shown in Fig. 3.

8-(Hexyloxy)-2-methylquinoline (4): 8-hydroxy-2-methylquinoline (477 mg, 3.0 mmol), 1-bromohexane (495 mg, 3.0 mmol), K2CO3 (207 mg, 1.5 mmol) and DMF (10 ml) were mixed in a three-necked flask, heated to 368 K (100 °C) and stirred at this temperature for 24 h. The reaction solution was extracted with dichloromethane and water. After the solvent had been removed under reduced pressure, the residue was purified by flash chromatography on silica gel using ethyl acetate–petroleum ether (3:50) as the eluent to afford a white solid (495 mg). Yield: 67.8%. 1H NMR (300 MHz, CDCl3, δ) 7.99 (d, J = 8.4 Hz, 1H), 7.40–7.26 (m, 3H), 7.03 (dd, J = 7.2 Hz, 1H), 4.23 (t, J = 7.2 Hz, 2H), 2.78 (s, 3H), 2.08–1.98 (m, 2H), 1.54–1.47 (m, 2H), 1.43–1.33 (m, 4H), 0.98–0.89 (m, 3H). 13C NMR (400 MHz, CDCl3, δ) 157.97, 154.37, 139.97, 135.99, 127.69, 125.64, 122.37, 119.23, 119.01, 69.13, 31.66, 28.82, 25.72, 25.68, 22.60, 14.02.

8-(Hexyloxy)quinoline-2-carbaldehyde (3): Compound (4) (3 g, 12.3 mmol), SeO2 (1.74 g, 15.7 mmol) and 1,4-dioxane (300 ml) were mixed in a three-necked flask, heated to 368 K and stirred at this temperature for 24 h. The reaction solution was extracted with dichloromethane and water. After the solvent had been removed under reduced pressure, the residue was purified by flash chromatography on silica gel using ethyl acetate–petroleum ether (2:25) as the eluent, to obtain a yellow solid (1.63 g). Yield: 51.5%. 1H NMR (300 MHz, CDCl3, δ) 10.29 (d, J = 0.9 Hz, 1H), 8.26 (d, J = 8.4 Hz, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.60 (t, J = 8.1 Hz, 1H), 7.45–7.42 (m, 2H), 7.16–7.13 (m, 1H), 4.29 (t, J = 6.9 Hz, 2H), 2.11–2.01 (m, 2H), 1.62–1.53 (m, 2H), 1.47–1.35 (m, 4H), 0.95–0.90 (m, 3H). 13C NMR (400 MHz, CDCl3, δ) 193.87, 155.68, 151.40, 140.15, 137.20, 131.39, 129.80, 119.33, 117.74, 109.69, 99.44, 31.61, 28.85, 25.69, 22.59, 14.02.

(Z)-8-(Hexyloxy)-2-[2-(naphthalen-2-yl)ethenyl]quinoline (1): bromo(naphthalen-2-ylmethyl)triphenylphosphorane (2) (2250 mg, 4.6 mmol) was dissolved in anhydrous tetrahydrofuran (10 ml) under Ar and the solution was cooled to 273 K. KOtBu (1000 mg, 8.9 mmol) was added and stirred for 15 min. A solution of compound (3) (1290 mg, 5.0 mmol) in dry THF (10 ml) was added dropwise into the reaction mixture. After the addition, the mixture was stirred for 15 min. A few drops of water were added to quench the reaction. The mixture was extracted with CH2Cl2. The organic layer was washed with water three times and dried over anhydrous Na2SO4. The solvent was removed in vacuo and the residue was purified by flash chromatography on silica gel using dichloromethane–petroleum ether (1:10) as the eluent to afford a white solid (1500 mg). Yield: 84.6%. Slow evaporation of compound (1) from dichloromethane/ethanol mixed solutions yielded light-yellow block-shaped crystals of (1). 1H NMR (300 MHz, CDCl3, δ) 8.08 (d, J = 8.0 Hz, 1H), 7.97 (s, 1H), 7.85–7.80 (m, 5H).
7.73 (d, J = 8 Hz, 1H), 7.62–7.58 (m, 1H), 7.49–7.46 (m, 2H), 7.41–7.33 (m, 2H), 7.06 (d, J = 8 Hz, 1H), 4.26 (t, J = 8 Hz, 2H), 2.10–2.07 (m, 2H), 1.60–1.58 (m, 2H), 1.45–1.42 (m, 4H), 0.97–0.93 (m, 3H). 13C NMR (400 MHz, CDCl3, δ) 154.88, 140.44, 136.25, 133.80, 133.65, 133.47, 130.11, 128.56, 128.45, 128.25, 127.92, 127.75, 126.40, 126.38, 126.29, 123.79, 119.47, 119.29, 109.41, 69.30, 31.75, 28.99, 25.81, 22.70, 14.12. HRMS (m/z): 382.2169 [M + H]+ (calculated for C27H27NO: 382.2126).

6. Refinement
Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were refined using a riding model with C—H = 0.93–0.97 Å and Uiso(H) = 1.2–1.5 Ueq(C), except for H27, which was refined in an isotropic approximation.

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Crystal structure of 8-hexyloxy-2-[(Z)-2-(naphthalen-2-yl)ethenyl]quinoline

Xiaozhou Liu, Lu Wang, Ying Feng, Deliang Cui and Zhi Liu

Computing details

Data collection: APEX3 (Bruker, 2017); cell refinement: SAINT (Bruker, 2017); data reduction: SAINT (Bruker, 2017); program(s) used to solve structure: SHELXT2014/4 (Sheldrick, 2015a); program(s) used to refine structure: SHELXL2018/3 (Sheldrick, 2015b); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: PLATON (Spek, 2020).

8-Hexyloxy-2-[(Z)-2-(naphthalen-2-yl)ethenyl]quinoline

Crystal data

C_{27}H_{27}NO

F(000) = 816

D_{x} = 1.190 Mg m^{-3}

Mo Kα radiation, λ = 0.71073 Å

Cell parameters from 2641 reflections

θ = 2.7–19.7°

µ = 0.07 mm^{-1}

T = 293 K

Block, light yellow

0.20 × 0.19 × 0.13 mm

Data collection

Bruker APEXIII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2017)

T_{min} = 0.667, T_{max} = 0.746

Refinement

Refinement on F^{2}

Least-squares matrix: full

R(F^{2} > 2σ(F^{2})) = 0.045

wR(F^{2}) = 0.140

S = 1.00

23828 measured reflections

4844 independent reflections

2314 reflections with I > 2σ(I)

H atoms treated by a mixture of independent and constrained refinement

 Hydrogen site location: inferred from neighbouring sites

w = 1/[σ^{2}(F_{o}^{2}) + (0.0588P)^{2} + 0.0643P]

where P = (F_{o}^{2} + 2F_{c}^{2})/3

Δρ_{max} = 0.12 e Å^{-3}

Δρ_{min} = -0.11 e Å^{-3}
Extinction correction: SHELXL-2018/3  
(Sheldrick, 2015b),  
Fc*=kFc[1+0.001xFc^2λ^3/sin(2θ)]^-1/4  
Extinction coefficient: 0.0047 (10)

**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 > 2sigma(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)**

| Atom | x     | y     | z     | U_iso* | U_eq  |
|------|-------|-------|-------|--------|-------|
| O1   | 0.66156 (7) | 0.62694 (18) | 0.57990 (4) | 0.0757 (3) |
| N1   | 0.75177 (10) | 0.9822 (2) | 0.62699 (6) | 0.0781 (4) |
| C1   | 0.22807 (16) | −0.0537 (4) | 0.58497 (10) | 0.1328 (8) |
| H1A  | 0.237845 | −0.066613 | 0.622896 | 0.199* |
| H1B  | 0.196935 | −0.188067 | 0.570409 | 0.199* |
| H1C  | 0.190330 | 0.078059 | 0.575470 | 0.199* |
| C2   | 0.31962 (13) | −0.0297 (3) | 0.56346 (8) | 0.0949 (6) |
| H2A  | 0.308734 | −0.016894 | 0.525157 | 0.114* |
| H2B  | 0.355594 | −0.167615 | 0.571548 | 0.114* |
| C3   | 0.37715 (11) | 0.1737 (3) | 0.58472 (7) | 0.0776 (5) |
| H3A  | 0.341148 | 0.311844 | 0.576951 | 0.093* |
| H3B  | 0.388916 | 0.160265 | 0.622982 | 0.093* |
| C4   | 0.46867 (11) | 0.1963 (2) | 0.56210 (6) | 0.0700 (4) |
| H4A  | 0.457115 | 0.204372 | 0.523752 | 0.084* |
| H4B  | 0.505672 | 0.060613 | 0.570984 | 0.084* |
| C5   | 0.52431 (10) | 0.4048 (3) | 0.58210 (6) | 0.0672 (4) |
| H5A  | 0.487190 | 0.540674 | 0.573657 | 0.081* |
| H5B  | 0.536989 | 0.395793 | 0.620387 | 0.081* |
| C6   | 0.61429 (10) | 0.4259 (3) | 0.55851 (6) | 0.0700 (4) |
| H6A  | 0.652577 | 0.292010 | 0.567038 | 0.084* |
| H6B  | 0.602656 | 0.437927 | 0.520220 | 0.084* |
| C7   | 0.74858 (12) | 0.6676 (3) | 0.56615 (7) | 0.0764 (5) |
| C8   | 0.79621 (12) | 0.8568 (3) | 0.59206 (7) | 0.0771 (5) |
| C9   | 0.79590 (14) | 1.1602 (3) | 0.65059 (8) | 0.0875 (6) |
| C16  | 0.75188 (17) | 1.3102 (3) | 0.68707 (9) | 0.0982 (7) |
| H16  | 0.785723 | 1.444059 | 0.693853 | 0.118* |
| C17  | 0.67630 (17) | 1.3052 (3) | 0.71303 (8) | 0.0955 (6) |
| H17  | 0.671267 | 1.437542 | 0.732806 | 0.115* |
| C18  | 0.59923 (13) | 1.1490 (3) | 0.71893 (7) | 0.0795 (5) |
| C19  | 0.53998 (16) | 1.2047 (3) | 0.75602 (8) | 0.0898 (6) |
### Atomic displacement parameters (Å²)

|   | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{12}$  | $U^{13}$  | $U^{23}$  |
|---|-----------|-----------|-----------|-----------|-----------|-----------|
| O1 | 0.0716 (7)  | 0.0719 (7)  | 0.0811 (7)  | -0.0082 (6)  | -0.0033 (6)  | -0.0069 (6)  |
| N1 | 0.0824 (10)  | 0.0672 (9)  | 0.0775 (9)  | -0.0120 (8)  | -0.0253 (8)  | -0.0134 (8)  |
| C1 | 0.1192 (17)  | 0.1313 (19)  | 0.153 (2)  | -0.0442 (15)  | 0.0367 (15)  | -0.0115 (16)  |
| C2 | 0.0978 (14)  | 0.0809 (12)  | 0.1056 (15)  | -0.0184 (11)  | 0.0093 (11)  | -0.0081 (11)  |
| C3 | 0.0849 (12)  | 0.0691 (11)  | 0.0775 (11)  | -0.0055 (9)  | 0.0029 (9)  | -0.0039 (9)  |
| C4 | 0.08011 (11)  | 0.0598 (10)  | 0.0680 (10)  | -0.0002 (8)  | -0.0028 (8)  | -0.0060 (8)  |
| C5 | 0.0724 (10)  | 0.0637 (10)  | 0.0628 (9)  | 0.0000 (8)  | -0.0002 (8)  | -0.0066 (8)  |
| C6 | 0.0739 (11)  | 0.0623 (10)  | 0.0699 (10)  | 0.0014 (8)  | -0.0101 (8)  | -0.0044 (8)  |
| C7 | 0.0658 (11)  | 0.0789 (12)  | 0.0820 (12)  | 0.0020 (10)  | -0.0041 (9)  | 0.0127 (10)  |
| C8 | 0.0677 (11)  | 0.0755 (12)  | 0.0823 (12)  | -0.0057 (10)  | -0.0185 (9)  | 0.0214 (10)  |
| C9 | 0.0927 (14)  | 0.0760 (13)  | 0.0842 (13)  | -0.0220 (11)  | -0.0344 (10)  | 0.0202 (11)  |
| C10 | 0.1201 (17)  | 0.0702 (13)  | 0.0935 (15)  | -0.0284 (13)  | -0.0399 (13)  | 0.0032 (12)  |
| C11 | 0.1251 (17)  | 0.0646 (12)  | 0.0876 (14)  | -0.0103 (12)  | -0.0314 (13)  | -0.0030 (10)  |
| C12 | 0.1019 (13)  | 0.0532 (10)  | 0.0750 (12)  | 0.0031 (10)  | -0.0297 (10)  | 0.0013 (9)  |
| C13 | 0.1233 (16)  | 0.0561 (11)  | 0.0825 (13)  | 0.0169 (12)  | -0.0246 (12)  | -0.0110 (10)  |
| C14 | 0.1076 (15)  | 0.0621 (11)  | 0.0804 (12)  | 0.0226 (11)  | -0.0151 (11)  | -0.0041 (10)  |
| C15 | 0.0958 (13)  | 0.0607 (11)  | 0.0734 (11)  | 0.0165 (10)  | -0.0107 (10)  | -0.0039 (9)  |
| C16 | 0.1070 (15)  | 0.0751 (13)  | 0.0999 (15)  | 0.0079 (12)  | 0.0072 (12)  | -0.0066 (11)  |
Geometric parameters (Å, °)

| Bond                              | Distance (Å) |
|-----------------------------------|--------------|
| C1—C2                             | 1.487 (2)    |
| C2—C3                             | 1.517 (2)    |
| C3—C4                             | 1.500 (2)    |
| C4—C5                             | 1.490 (2)    |
| C5—C6                             | 1.518 (2)    |
| C6—C7                             | 1.4374 (17)  |
| O1—C6                             | 1.4374 (17)  |
| O1—C7                             | 1.3582 (19)  |
| N1—C8                             | 1.362 (2)    |
| N1—C9                             | 1.330 (2)    |
| C1—H1A                            | 0.9600       |
| C1—H1B                            | 0.9600       |
| C1—H1C                            | 0.9600       |
| C1—C2                             | 1.487 (3)    |
| C2—H2A                            | 0.9700       |
| C2—H2B                            | 0.9700       |
| C2—C3                             | 1.517 (2)    |
| C3—H3A                            | 0.9700       |
| C3—H3B                            | 0.9700       |
| C3—C4                             | 1.500 (2)    |
| C4—H4A                            | 0.9700       |
| C4—H4B                            | 0.9700       |
| C4—C5                             | 1.518 (2)    |
| C5—H5A                            | 0.9700       |
| C5—H5B                            | 0.9700       |
| C5—C6                             | 1.490 (2)    |
| C6—H6A                            | 0.9700       |
| C6—H6B                            | 0.9700       |
| C7—C8                             | 1.427 (2)    |
| C7—C15                            | 1.360 (2)    |
| C8—C12                            | 1.415 (3)    |
| C9—C16                            | 1.468 (3)    |
| C9—C10                            | 1.419 (3)    |
| C16—H16                           | 0.9300       |
| C16—C17                           | 1.332 (3)    |
| C7—O1                             | 117.42 (13)  |
| C9—N1                             | 118.67 (17)  |
| H1A—C1                            | 109.5        |
| C17—H18                           |              |

Supporting Information
| Bond/Angle | Angle (°) | Bond/Angle | Angle (°) |
|------------|-----------|------------|-----------|
| H1A—C1—H1C | 109.5    | C19—C18—C27 | 117.99 (19) |
| H1B—C1—H1C | 109.5    | C27—C18—C17 | 124.9 (2) |
| C2—C1—H1A  | 109.5    | C18—C19—H19 | 118.5    |
| C2—C1—H1B  | 109.5    | C18—C19—C20 | 123.04 (17) |
| C2—C1—H1C  | 109.5    | C20—C19—H19 | 118.5    |
| C1—C2—H2A  | 108.6    | C19—C20—C25 | 118.06 (19) |
| C1—C2—H2B  | 108.6    | C19—C20—C21 | 123.2 (2) |
| C1—C2—C3   | 114.63 (16) | C21—C20—C25 | 118.7 (2) |
| H2A—C2—H2B | 107.6    | C24—C25—C20 | 118.62 (19) |
| C3—C2—H2A  | 108.6    | C24—C25—C26 | 123.26 (17) |
| C3—C2—H2B  | 108.6    | C26—C25—C20 | 118.10 (19) |
| C2—C3—H3A  | 108.8    | C25—C24—H24 | 119.3    |
| C2—C3—H3B  | 108.8    | C23—C24—C25 | 121.3 (2) |
| H3A—C3—H3B | 107.7    | C23—C24—H24 | 119.3    |
| C4—C3—C2   | 113.78 (14)| C24—C23—H23 | 120.0    |
| C4—C3—H3A  | 108.8    | C24—C23—C22 | 120.0 (2) |
| C4—C3—H3B  | 108.8    | C22—C23—C22 | 120.0    |
| C3—C4—H4A  | 108.9    | C9—C10—H10  | 119.9    |
| C3—C4—H4B  | 108.9    | C11—C10—C9  | 120.3 (2) |
| C3—C4—C5   | 113.47 (13)| C11—C10—H10 | 119.9    |
| H4A—C4—H4B | 107.7    | C10—C11—H11 | 119.6    |
| C5—C4—H4A  | 108.9    | C10—C11—C12 | 120.7 (2) |
| C5—C4—H4B  | 108.9    | C12—C11—H11 | 119.6    |
| C4—C5—H5A  | 109.1    | C11—C12—C8  | 115.9 (2) |
| C4—C5—H5B  | 109.1    | C13—C12—C8  | 120.3 (2) |
| H5A—C5—H5B | 107.8    | C13—C12—C11 | 123.8 (2) |
| C6—C5—C4   | 112.59 (13)| C12—C13—H13 | 119.9    |
| C6—C5—H5A  | 109.1    | C14—C13—C12 | 120.2 (2) |
| C6—C5—H5B  | 109.1    | C14—C13—H13 | 119.9    |
| O1—C6—C5   | 115.49 (17)| C13—C14—H14 | 119.7    |
| O1—C6—H6A  | 110.0    | C13—C14—C15 | 120.6 (2) |
| O1—C6—H6B  | 110.0    | C15—C14—H14 | 119.7    |
| C5—C6—H6A  | 110.0    | C7—C15—C14  | 120.8 (2) |
| C5—C6—H6B  | 110.0    | C7—C15—H15  | 119.6    |
| H6A—C6—H6B | 108.4    | C14—C15—H15 | 119.6    |
| O1—C7—C8   | 115.49 (17)| C20—C21—H21 | 119.7    |
| O1—C7—C15  | 124.23 (17)| C22—C21—C20 | 120.7 (2) |
| C15—C7—C8  | 120.28 (18)| C22—C21—H21 | 119.7    |
| N1—C8—C7   | 118.79 (16)| C23—C22—H22 | 119.7    |
| N1—C8—C12  | 123.38 (19)| C21—C22—C23 | 120.7 (2) |
| C12—C8—C7  | 117.8 (2) | C21—C22—H22 | 119.7    |
| N1—C9—C16  | 122.30 (18)| C25—C26—H26 | 118.5    |
| N1—C9—C10  | 121.1 (2) | C27—C26—C25 | 123.01 (17) |
| C10—C9—C16 | 116.6 (2) | C27—C26—H26 | 118.5    |
| C9—C16—H16 | 111.6    | C18—C27—H27 | 115.8 (10) |
| C17—C16—C9 | 136.87 (19)| C26—C27—C18 | 119.8 (2) |
| C17—C16—H16 | 111.6 | C26—C27—H27 | 124.3 (10) |
| C16—C17—H17 | 111.3 | | |
O1—C7—C8—N1   −1.1 (2)  C17—C18—C27—C26   178.78 (16)
O1—C7—C8—C12   179.39 (14)  C18—C19—C20—C25   −1.6 (2)
O1—C7—C15—C14  −179.77 (16)  C18—C19—C20—C21   176.41 (16)
N1—C8—C12—C11  0.8 (2)  C19—C18—C27—C26   −0.2 (2)
N1—C8—C12—C13  −178.52 (17)  C19—C20—C25—C24   179.35 (15)
N1—C9—C16—C17  13.5 (3)  C19—C20—C25—C26   0.7 (2)
N1—C9—C10—C11  0.0 (3)  C19—C20—C21—C22   −178.30 (18)
C1—C2—C3—C4   −179.36 (17)  C20—C25—C24—C23   −0.9 (3)
C2—C3—C4—C5   177.97 (13)  C20—C25—C26—C27   0.4 (2)
C3—C4—C5—C6   −179.12 (13)  C20—C21—C22—C23   −1.0 (3)
C4—C5—C6—O1   −179.87 (11)  C25—C20—C21—C22   −0.3 (3)
C6—O1—C7—C8   −174.45 (12)  C25—C24—C23—C22   −0.4 (3)
C6—O1—C7—C15  5.9 (2)  C25—C26—C27—C18   −0.7 (3)
C7—O1—C6—C5   175.35 (12)  C24—C25—C26—C27   −178.17 (16)
C7—C8—C12—C11  −179.80 (15)  C24—C23—C22—C21   1.4 (3)
C7—C8—C12—C13  0.9 (3)  C10—C9—C16—C17   −168.3 (2)
C8—C9—C16—C17  177.45 (15)  C10—C9—C12—C8   −1.4 (3)
C8—C9—C10—C11  −0.7 (2)  C10—C11—C12—C13   177.8 (2)
C9—C16—C17—C18  0.6 (3)  C11—C12—C13—C14   −179.8 (2)
C9—C16—C18—C19  −0.5 (3)  C12—C13—C14—C15   0.2 (4)
C9—N1—C8—C7   −179.17 (13)  C13—C14—C15—C7   −0.2 (3)
C9—N1—C8—C12  0.3 (2)  C15—C7—C8—N1   178.53 (15)
C9—C16—C17—C18  0.6 (4)  C15—C7—C8—C12   −0.9 (2)
C9—C10—C11—C12  1.1 (3)  C21—C20—C25—C24   1.2 (2)
C16—C9—C10—C11  −178.2 (2)  C21—C20—C25—C26   −177.45 (15)
C16—C17—C18—C19  172.5 (2)  C26—C25—C24—C23   177.68 (17)
C16—C17—C18—C27  −6.5 (3)  C27—C18—C19—C20   1.4 (2)
C17—C18—C19—C20  −177.69 (15)

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|-----|------|------|---------|
| C6—H6···N1i | 0.97 | 2.68 | 3.600 (2) | 159 |
| C27—H27···O1 | 0.955 (16) | 2.809 (17) | 3.633 (2) | 145.0 (12) |
| C27—H27···N1 | 0.955 (16) | 2.195 (16) | 3.068 (3) | 151.4 (13) |

Symmetry code: (i) x, y−1, z.