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Synthesis, crystal structure and Hirshfeld surface analysis of 4′-cyano-[1,1′-biphenyl]-4-yl 3-(benzyloxy)benzoate

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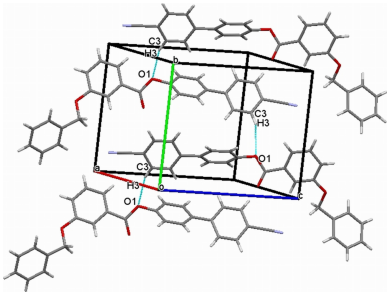
In the title compound, $C_{27}H_{19}O_3N$, the dihedral angle between the aromatic rings of the biphenyl unit is 38.14 (2)° and the C—O—C—C torsion angle in the benzyloxy benzene fragment is 179.1 (2)°. In the crystal, the molecules are linked by weak C—H···O interactions forming $S(9)$ chains propagating along [010]. The most important contributions to the Hirshfeld surface arise from H···H (32.4%) and C···H/H···C (37.0%) contacts.

1. Chemical context

Cyanobiphenyl-substituted derivatives can act as biological inhibitors and potential agents for the treatment of Alzheimer's disease (Godyń *et al.*, 2021) as well as antibacterial and antimalarial drugs (Malani *et al.*, 2013). Benzyloxy derivatives exhibit anti-bacterial, anti-platelet and anti-malarial activities (Kaushik *et al.*, 2018; de Candia *et al.*, 2015; Mohebi *et al.*, 2022) and related pyrimidinylphenylamine derivatives are most active towards the inhibition of HIV-1 (Rai *et al.*, 2013). The cyanobiphenyl and (benzyloxy)benzoate groups exhibit distinct structural geometries and these derivatives play significant roles in the construction of organic liquid crystal materials (Srinivasa *et al.*, 2015), which have been investigated for their display technology applications, such as optoelectronic materials, sensor materials, light-emitting diodes, and photovoltaic solar cells (Goodby *et al.*, 2022; Srinivasa *et al.*, 2024). As part of our studies of this family of materials, we now present the synthesis, structure and Hirshfeld surface analysis of the title compound, $C_{27}H_{19}NO_3$ (I).



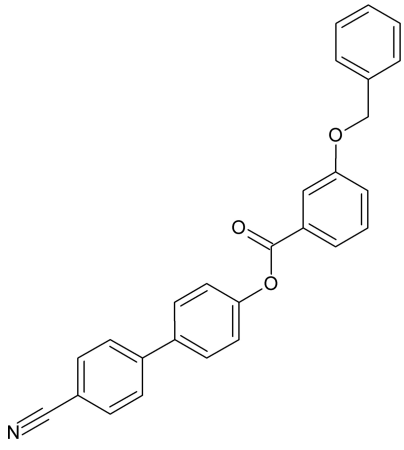


Table 1
Hydrogen-bond geometry (Å, °).

*Cg*4 is the centroid of the C22–C27 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.93	2.52	3.395 (4)	158
CH—H4···*Cg*2^{i}	0.93	2.97	3.805 (3)	151
C9—H9···*Cg*4^{ii}	0.93	2.90	3.579 (3)	131
C12—H12···*Cg*4^{iii}	0.93	2.77	3.485 (13)	135

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

2. Structural commentary

The molecular structure of (I) is shown in Fig. 1. The aromatic rings in the molecule are designated as *A* (C2–C7), *B* (C8–C13), *C* (C15–C20) and *D* (C22–C27) and the dihedral angles between the rings *A*/*B* = 38.14 (2), *A*/*C* = 8.29 (3) and *A*/*D* = 50.66 (2)°, whereas *B*/*C*, *B*/*D* and *C*/*D* are 46.43 (4), 83.95 (2) and 44.01 (2)°, respectively. The torsion angle associated with the phenyl benzoate group (C11—O1—C14—C15) is −177.8 (2)° and that for the benzyloxy group (C22—C21—O3—C17) is 179.1 (2)°. Otherwise, the bond distances and angles may be regarded as normal.

3. Supramolecular features

The crystal structure features a weak C3—H3···O1 interaction (Table 1), which forms an *S*(9) chain propagating along the [010] direction as shown in Fig. 2. Furthermore, the packing is consolidated by three weak C—H···π interactions as shown in Fig. 3. In addition there exists an aromatic π–π stacking interaction between the C2–C7 and C15–C20 rings with a centroid–centroid distance of 3.9282 (19) Å (Fig. 4).

4. Hirshfeld surface analysis

CrystalExplorer17.5 (Turner *et al.*, 2017) was used to perform a Hirshfeld surface analysis to further quantify the various intermolecular interactions. Fig. 5 illustrates the Hirshfeld surface mapped over d_{norm} with red spots corresponding to short contacts. The fingerprint plots (Fig. 6) indicate that the major contributions to the crystal structure are from H···H (36.2%), C···H/H···C (33.8%), O···H/H···O (12.1.6%), N···H/H···N (10.1.8%) and C···C (5.0%) contacts. The characteristic spikes in the O···H/H···O plot indicate the existence of the C—H···O hydrogen bond listed in Table 1.

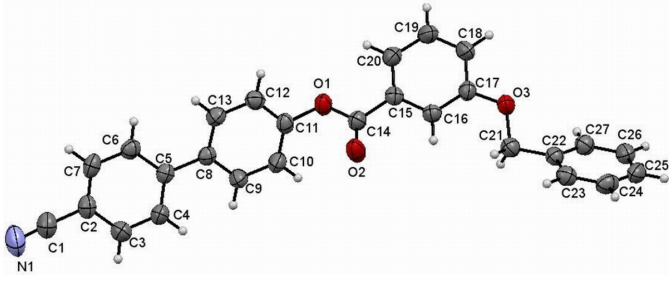


Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level.

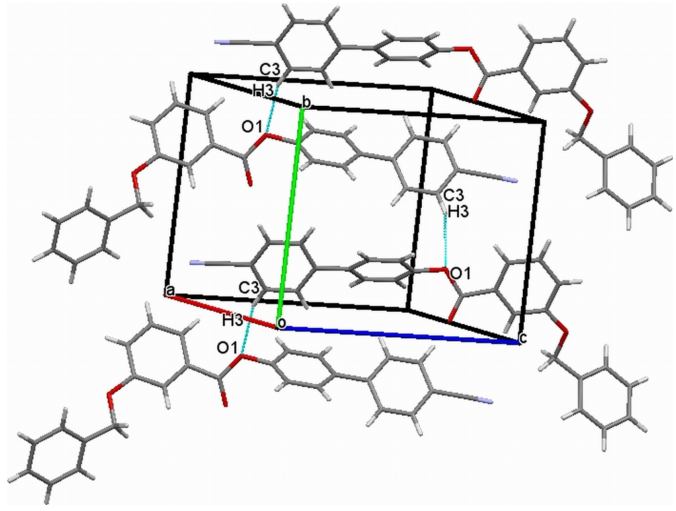


Figure 2
The crystal structure of (I) with a weak C—H ··· O interaction forming an *S*(9) chain running along the [010] direction.

5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.42, update of November 2020; Groom *et al.*, 2016) for molecules containing the 4′-cyano-[1,1′-biphenyl] fragment resulted in two matches with CSD refcodes PIFZEN and PIFZIR (Jakubowski *et al.*, 2023). In these structures, the dihedral angle between the 4-cyanophenoxy ring and the

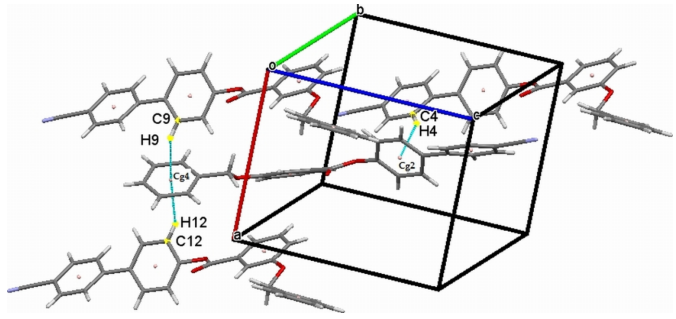


Figure 3
The molecular packing of (I) with C—H···π interactions depicted by dashed lines.

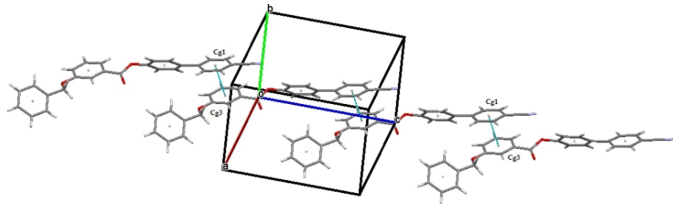


Figure 4
The molecular packing of (I) with π–π interactions depicted by pale green coloured dashed lines.

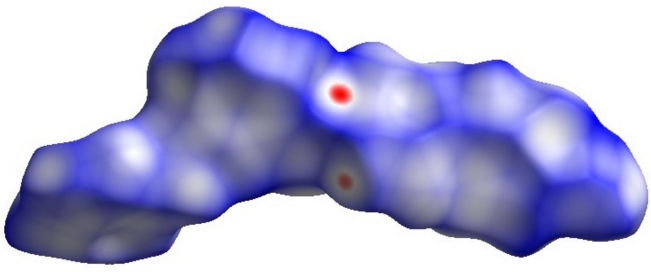


Figure 5
Hirshfeld surface representation for (I) plotted over d_{norm}.

neighbouring ring are 31.71 (2) and 38.95 (3)°, respectively, compared to 38.14 (2)° for (I). For molecules containing the (benzyloxy)benzoate fragment, a search resulted in thirteen matches: in all of these, the torsion angle of the linking C—O—C—C unit indicates a conformation close to *anti*.

6. Synthesis and crystallization

A mixture of 3-(benzyloxy)benzoic acid (1 eq., 0.228 g) and 4′-hydroxy-[1,1′-biphenyl]-4-carbonitrile (1 eq., 0.195 g), dicyclohexylcarbodiimide (1.2 eq.) and a catalytic amount of dimethylaminopyrimidine were stirred in dry dichloromethane at room temperature overnight. After completion of the reaction, the product mass was subjected to column chromatography with silica gel and chloroform as eluent. The crude product was recrystallized from chloroform solution to yield colourless blocks of (I). Melting point = 398 K, analysis (%) calculated for $C_{27}H_{19}NO_3$, C 79.98, H 4.72, N 3.45; found C 78.01; H 4.76, N 3.48. ^{1}H NMR (500 MHz, $CDCl_3$, δ/ppm): 7.82 (*m*, 4H, Ar-H), 7.65 (*m*, 4H, Ar-H), 7.44 (*m*, 4H, Ar-H), 7.23 (*m*, 5H, Ar-H), 5.24 (*s*, 2H, Ar—CH_2—O—).

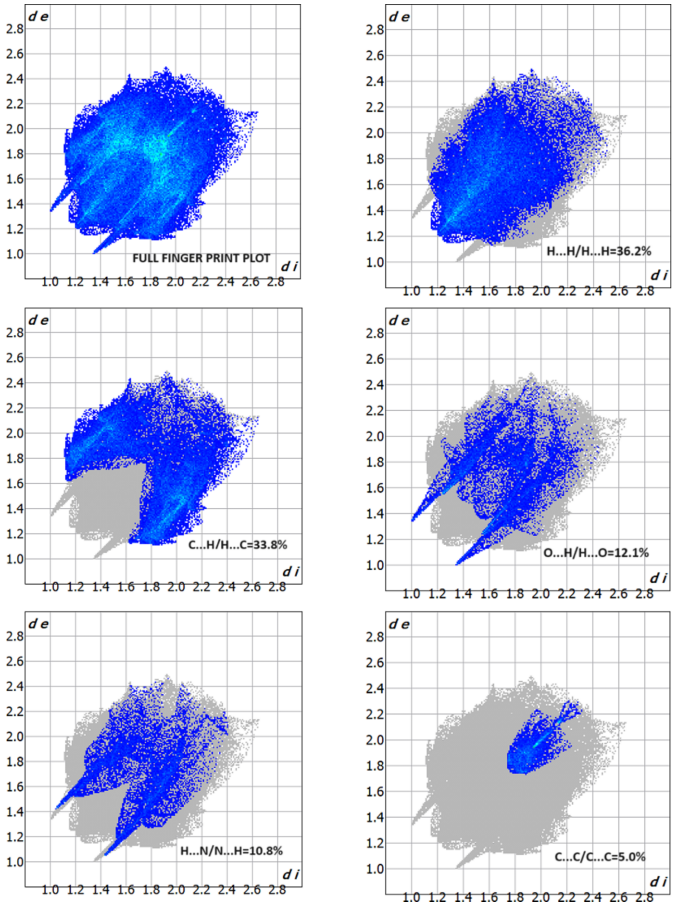


Figure 6
The full two-dimensional fingerprint plots for the title compound, showing all interactions and delineated into H···H, C···H/H···C, O···H/H···O, N···H/H···N and C···C interactions.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{27}H_{19}NO_3$
M_r	405.43
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	270
a, b, c (Å)	9.4289 (10), 9.6739 (9), 11.4872 (11)
β (°)	97.668 (4)
V (Å^3)	1038.43 (18)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.42 × 0.38 × 0.24
Data collection	
Diffractometer	Bruker *SMART* APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.966, 0.981
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27994, 3639, 3308
R_{int}	0.052
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.080, 1.08
No. of reflections	3639
No. of parameters	280
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.11, −0.16
Absolute structure	Flack x determined using 1347 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.0 (5)

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015) and *Mercury* (Macrae *et al.*, 2020).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All the H-atoms were positioned with idealized geometry and refined using a riding model with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Acknowledgements

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supporting information

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M. Harish Kumar, M. Vinduvahini, H. C. Devarajegowda, H. T. Srinivasa and B. S. Palakshamurthy

Computing details

4′-Cyano-[1,1′-biphenyl]-4-yl 3-(benzyloxy)benzoate

Crystal data

$C_{27}H_{19}NO_3$
M_r = 405.43
Monoclinic, $P2_1$
a = 9.4289 (10) Å
b = 9.6739 (9) Å
c = 11.4872 (11) Å
β = 97.668 (4)°
V = 1038.43 (18) Å^3
Z = 2
$F(000)$ = 424
Rod
D_x = 1.297 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3639 reflections
θ = 3.5–25.1°
μ = 0.09 mm^{-1}
T = 270 K
Block, colourless
0.42 × 0.38 × 0.24 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 1.09 pixels mm^{-1}
φ and Ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.966, T_{max} = 0.981
27994 measured reflections
3639 independent reflections
3308 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 25.0°, θ_{min} = 3.6°
h = −11→11
k = −11→11
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.080
S = 1.08
3639 reflections
280 parameters
1 restraint
0.012 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.1198P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack x determined using 1347 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.0 (5)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.7334 (2)	0.77894 (19)	0.21126 (16)	0.0509 (5)
O3	0.8888 (2)	0.5498 (2)	−0.24091 (16)	0.0555 (6)
O2	0.7452 (3)	0.5514 (2)	0.17589 (19)	0.0695 (7)
C11	0.6854 (3)	0.7566 (3)	0.3203 (2)	0.0430 (7)
C13	0.7200 (3)	0.7988 (3)	0.5258 (2)	0.0443 (7)
H13	0.775740	0.834123	0.592030	0.053*
C21	0.8166 (3)	0.4201 (3)	−0.2372 (2)	0.0484 (7)
H21A	0.715024	0.435077	−0.236419	0.058*
H21B	0.853943	0.369863	−0.166652	0.058*
C10	0.5549 (3)	0.6967 (3)	0.3284 (2)	0.0506 (7)
H10	0.498693	0.663636	0.261571	0.061*
C16	0.8197 (3)	0.6095 (3)	−0.0507 (2)	0.0414 (6)
H16	0.783496	0.521562	−0.040255	0.050*
C8	0.5898 (3)	0.7372 (3)	0.5372 (2)	0.0384 (6)
C22	0.8404 (3)	0.3390 (3)	−0.3434 (2)	0.0401 (6)
C12	0.7683 (3)	0.8085 (3)	0.4174 (2)	0.0450 (7)
H12	0.855882	0.849784	0.410635	0.054*
C20	0.8662 (3)	0.8422 (3)	0.0195 (2)	0.0488 (7)
H20	0.860968	0.910130	0.076078	0.059*
C27	0.8103 (3)	0.3941 (3)	−0.4553 (3)	0.0481 (7)
H27	0.775214	0.483768	−0.465142	0.058*
C17	0.8782 (3)	0.6410 (3)	−0.1512 (2)	0.0421 (6)
C9	0.5083 (3)	0.6864 (3)	0.4366 (2)	0.0470 (7)
H9	0.420768	0.644553	0.442524	0.056*
C15	0.8154 (3)	0.7109 (3)	0.0354 (2)	0.0391 (6)
C6	0.5598 (3)	0.8325 (3)	0.7351 (2)	0.0461 (7)
H6	0.611277	0.910110	0.717919	0.055*
C5	0.5377 (3)	0.7261 (3)	0.6536 (2)	0.0393 (6)
C2	0.4316 (3)	0.7098 (3)	0.8675 (2)	0.0493 (7)
C4	0.4646 (3)	0.6095 (3)	0.6828 (2)	0.0496 (7)
H4	0.451143	0.536161	0.630193	0.060*
C19	0.9250 (3)	0.8715 (3)	−0.0818 (3)	0.0550 (8)
H19	0.959121	0.959983	−0.093327	0.066*
C23	0.8922 (3)	0.2051 (3)	−0.3313 (3)	0.0475 (7)
H23	0.911977	0.166328	−0.256862	0.057*
N1	0.3247 (4)	0.6894 (4)	1.0630 (3)	0.0907 (11)
C7	0.5067 (3)	0.8251 (3)	0.8410 (2)	0.0506 (7)
H7	0.521498	0.897631	0.894393	0.061*
C3	0.4113 (3)	0.6006 (3)	0.7889 (3)	0.0552 (8)

H3	0.362120	0.521913	0.807373	0.066*
C14	0.7605 (3)	0.6679 (3)	0.1449 (3)	0.0450 (7)
C18	0.9338 (3)	0.7717 (3)	−0.1657 (2)	0.0515 (8)
H18	0.976819	0.791722	−0.232010	0.062*
C26	0.8322 (3)	0.3164 (3)	−0.5526 (3)	0.0549 (8)
H26	0.811223	0.353879	−0.627419	0.066*
C25	0.8848 (3)	0.1843 (3)	−0.5389 (3)	0.0588 (8)
H25	0.900050	0.132486	−0.604287	0.071*
C1	0.3728 (4)	0.6998 (4)	0.9774 (3)	0.0635 (9)
C24	0.9147 (3)	0.1288 (3)	−0.4283 (3)	0.0561 (8)
H24	0.950410	0.039321	−0.418934	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0725 (14)	0.0391 (10)	0.0449 (11)	0.0014 (10)	0.0219 (10)	−0.0050 (9)
O3	0.0780 (15)	0.0486 (12)	0.0448 (11)	−0.0129 (11)	0.0262 (10)	−0.0078 (9)
O2	0.112 (2)	0.0427 (12)	0.0623 (14)	−0.0043 (13)	0.0450 (13)	−0.0047 (11)
C11	0.0543 (17)	0.0372 (15)	0.0398 (15)	0.0058 (13)	0.0142 (13)	−0.0018 (12)
C13	0.0456 (16)	0.0440 (15)	0.0421 (15)	−0.0021 (13)	0.0016 (12)	−0.0031 (12)
C21	0.0514 (17)	0.0455 (16)	0.0506 (17)	−0.0032 (13)	0.0152 (14)	−0.0025 (14)
C10	0.0530 (17)	0.0555 (18)	0.0437 (16)	−0.0063 (15)	0.0079 (13)	−0.0136 (14)
C16	0.0458 (15)	0.0361 (14)	0.0431 (15)	−0.0021 (12)	0.0085 (12)	0.0004 (12)
C8	0.0385 (14)	0.0334 (14)	0.0435 (15)	0.0041 (11)	0.0066 (11)	−0.0026 (11)
C22	0.0382 (14)	0.0404 (15)	0.0432 (16)	−0.0017 (12)	0.0103 (12)	−0.0023 (12)
C12	0.0445 (15)	0.0408 (15)	0.0508 (17)	−0.0009 (13)	0.0110 (13)	−0.0008 (13)
C20	0.0572 (17)	0.0453 (17)	0.0435 (16)	−0.0077 (14)	0.0050 (13)	−0.0047 (13)
C27	0.0515 (17)	0.0429 (16)	0.0514 (18)	0.0016 (13)	0.0130 (14)	−0.0007 (13)
C17	0.0487 (15)	0.0428 (15)	0.0350 (15)	−0.0007 (13)	0.0060 (12)	−0.0027 (12)
C9	0.0429 (15)	0.0548 (17)	0.0445 (16)	−0.0065 (14)	0.0102 (12)	−0.0083 (14)
C15	0.0385 (14)	0.0403 (15)	0.0386 (14)	0.0012 (12)	0.0048 (11)	−0.0003 (12)
C6	0.0544 (17)	0.0361 (15)	0.0479 (17)	0.0009 (13)	0.0068 (13)	−0.0029 (13)
C5	0.0402 (14)	0.0386 (14)	0.0387 (14)	0.0057 (12)	0.0033 (11)	−0.0012 (12)
C2	0.0559 (18)	0.0544 (18)	0.0377 (15)	0.0068 (15)	0.0067 (13)	−0.0004 (15)
C4	0.0586 (18)	0.0489 (17)	0.0427 (16)	−0.0082 (14)	0.0119 (13)	−0.0097 (13)
C19	0.071 (2)	0.0476 (17)	0.0465 (17)	−0.0191 (16)	0.0078 (15)	−0.0018 (14)
C23	0.0473 (16)	0.0450 (16)	0.0511 (16)	−0.0004 (14)	0.0091 (13)	0.0027 (14)
N1	0.114 (3)	0.112 (3)	0.0516 (18)	0.004 (2)	0.0303 (18)	−0.0054 (19)
C7	0.0602 (18)	0.0490 (17)	0.0418 (16)	0.0078 (15)	0.0039 (14)	−0.0123 (13)
C3	0.063 (2)	0.0538 (17)	0.0510 (17)	−0.0105 (16)	0.0151 (15)	−0.0012 (14)
C14	0.0506 (16)	0.0398 (15)	0.0465 (16)	−0.0002 (13)	0.0131 (13)	−0.0048 (13)
C18	0.0608 (19)	0.0557 (17)	0.0390 (16)	−0.0142 (15)	0.0105 (14)	0.0036 (15)
C26	0.0610 (19)	0.062 (2)	0.0428 (17)	−0.0149 (16)	0.0112 (14)	−0.0030 (15)
C25	0.061 (2)	0.056 (2)	0.063 (2)	−0.0137 (17)	0.0226 (16)	−0.0223 (17)
C1	0.074 (2)	0.070 (2)	0.0475 (19)	0.0047 (19)	0.0114 (16)	−0.0063 (18)
C24	0.0561 (19)	0.0386 (16)	0.076 (2)	−0.0020 (14)	0.0166 (16)	−0.0101 (16)

Geometric parameters (Å, º)

O1—C14	1.361 (3)	C27—H27	0.9300
O1—C11	1.405 (3)	C17—C18	1.387 (4)
O3—C17	1.370 (3)	C9—H9	0.9300
O3—C21	1.431 (3)	C15—C14	1.482 (4)
O2—C14	1.197 (3)	C6—C7	1.378 (4)
C11—C12	1.369 (4)	C6—C5	1.388 (4)
C11—C10	1.374 (4)	C6—H6	0.9300
C13—C12	1.386 (4)	C5—C4	1.386 (4)
C13—C8	1.386 (4)	C2—C7	1.377 (4)
C13—H13	0.9300	C2—C3	1.386 (4)
C21—C22	1.492 (4)	C2—C1	1.448 (4)
C21—H21A	0.9700	C4—C3	1.381 (4)
C21—H21B	0.9700	C4—H4	0.9300
C10—C9	1.376 (4)	C19—C18	1.374 (4)
C10—H10	0.9300	C19—H19	0.9300
C16—C17	1.379 (4)	C23—C24	1.376 (4)
C16—C15	1.398 (4)	C23—H23	0.9300
C16—H16	0.9300	N1—C1	1.141 (4)
C8—C9	1.389 (4)	C7—H7	0.9300
C8—C5	1.488 (3)	C3—H3	0.9300
C22—C27	1.385 (4)	C18—H18	0.9300
C22—C23	1.385 (4)	C26—C25	1.372 (5)
C12—H12	0.9300	C26—H26	0.9300
C20—C15	1.378 (4)	C25—C24	1.373 (4)
C20—C19	1.384 (4)	C25—H25	0.9300
C20—H20	0.9300	C24—H24	0.9300
C27—C26	1.385 (4)		
C14—O1—C11	119.0 (2)	C20—C15—C14	122.5 (2)
C17—O3—C21	117.4 (2)	C16—C15—C14	116.8 (2)
C12—C11—C10	121.2 (2)	C7—C6—C5	121.2 (3)
C12—C11—O1	117.0 (3)	C7—C6—H6	119.4
C10—C11—O1	121.6 (2)	C5—C6—H6	119.4
C12—C13—C8	121.0 (3)	C4—C5—C6	118.3 (2)
C12—C13—H13	119.5	C4—C5—C8	120.7 (2)
C8—C13—H13	119.5	C6—C5—C8	121.0 (2)
O3—C21—C22	108.2 (2)	C7—C2—C3	120.3 (3)
O3—C21—H21A	110.1	C7—C2—C1	120.9 (3)
C22—C21—H21A	110.1	C3—C2—C1	118.8 (3)
O3—C21—H21B	110.1	C3—C4—C5	121.1 (3)
C22—C21—H21B	110.1	C3—C4—H4	119.5
H21A—C21—H21B	108.4	C5—C4—H4	119.5
C11—C10—C9	119.2 (3)	C18—C19—C20	120.9 (3)
C11—C10—H10	120.4	C18—C19—H19	119.5
C9—C10—H10	120.4	C20—C19—H19	119.5
C17—C16—C15	119.4 (2)	C24—C23—C22	120.7 (3)

C17—C16—H16	120.3	C24—C23—H23	119.6
C15—C16—H16	120.3	C22—C23—H23	119.6
C13—C8—C9	118.2 (2)	C2—C7—C6	119.7 (3)
C13—C8—C5	121.2 (2)	C2—C7—H7	120.2
C9—C8—C5	120.6 (2)	C6—C7—H7	120.2
C27—C22—C23	118.6 (3)	C4—C3—C2	119.5 (3)
C27—C22—C21	121.5 (3)	C4—C3—H3	120.3
C23—C22—C21	119.9 (3)	C2—C3—H3	120.3
C11—C12—C13	119.1 (3)	O2—C14—O1	122.5 (3)
C11—C12—H12	120.4	O2—C14—C15	125.9 (3)
C13—C12—H12	120.4	O1—C14—C15	111.5 (2)
C15—C20—C19	119.1 (3)	C19—C18—C17	119.8 (3)
C15—C20—H20	120.5	C19—C18—H18	120.1
C19—C20—H20	120.5	C17—C18—H18	120.1
C22—C27—C26	120.4 (3)	C25—C26—C27	120.3 (3)
C22—C27—H27	119.8	C25—C26—H26	119.9
C26—C27—H27	119.8	C27—C26—H26	119.9
O3—C17—C16	124.4 (2)	C26—C25—C24	119.8 (3)
O3—C17—C18	115.5 (2)	C26—C25—H25	120.1
C16—C17—C18	120.1 (2)	C24—C25—H25	120.1
C10—C9—C8	121.2 (3)	N1—C1—C2	178.4 (4)
C10—C9—H9	119.4	C25—C24—C23	120.3 (3)
C8—C9—H9	119.4	C25—C24—H24	119.9
C20—C15—C16	120.6 (2)	C23—C24—H24	119.9

C14—O1—C11—C12	120.6 (3)	C9—C8—C5—C4	37.8 (4)
C14—O1—C11—C10	−65.3 (4)	C13—C8—C5—C6	38.2 (4)
C17—O3—C21—C22	179.1 (2)	C9—C8—C5—C6	−141.5 (3)
C12—C11—C10—C9	−1.4 (4)	C6—C5—C4—C3	1.8 (4)
O1—C11—C10—C9	−175.3 (3)	C8—C5—C4—C3	−177.6 (3)
C12—C13—C8—C9	−0.5 (4)	C15—C20—C19—C18	−0.3 (5)
C12—C13—C8—C5	179.8 (2)	C27—C22—C23—C24	0.7 (4)
O3—C21—C22—C27	−52.9 (3)	C21—C22—C23—C24	180.0 (3)
O3—C21—C22—C23	127.8 (3)	C3—C2—C7—C6	1.0 (5)
C10—C11—C12—C13	0.8 (4)	C1—C2—C7—C6	−179.1 (3)
O1—C11—C12—C13	174.9 (2)	C5—C6—C7—C2	0.7 (4)
C8—C13—C12—C11	0.2 (4)	C5—C4—C3—C2	−0.2 (4)
C23—C22—C27—C26	−0.2 (4)	C7—C2—C3—C4	−1.2 (5)
C21—C22—C27—C26	−179.5 (3)	C1—C2—C3—C4	178.9 (3)
C21—O3—C17—C16	9.1 (4)	C11—O1—C14—O2	0.0 (4)
C21—O3—C17—C18	−172.0 (3)	C11—O1—C14—C15	−177.8 (2)
C15—C16—C17—O3	179.6 (3)	C20—C15—C14—O2	−162.2 (3)
C15—C16—C17—C18	0.8 (4)	C16—C15—C14—O2	14.9 (4)
C11—C10—C9—C8	1.0 (4)	C20—C15—C14—O1	15.5 (4)
C13—C8—C9—C10	−0.1 (4)	C16—C15—C14—O1	−167.4 (2)
C5—C8—C9—C10	179.6 (3)	C20—C19—C18—C17	2.4 (5)
C19—C20—C15—C16	−1.6 (4)	O3—C17—C18—C19	178.4 (3)
C19—C20—C15—C14	175.4 (3)	C16—C17—C18—C19	−2.7 (4)

C17—C16—C15—C20	1.3 (4)	C22—C27—C26—C25	−0.4 (4)
C17—C16—C15—C14	−175.9 (2)	C27—C26—C25—C24	0.5 (4)
C7—C6—C5—C4	−2.0 (4)	C26—C25—C24—C23	0.0 (4)
C7—C6—C5—C8	177.3 (3)	C22—C23—C24—C25	−0.6 (4)
C13—C8—C5—C4	−142.5 (3)		

Hydrogen-bond geometry (Å, º)

*Cg*4 is the centroid of the C22–C27 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.93	2.52	3.395 (4)	158
CH—H4···*Cg*2^{i}	0.93	2.97	3.805 (3)	151
C9—H9···*Cg*4^{ii}	0.93	2.90	3.579 (3)	131
C12—H12···*Cg*4^{iii}	0.93	2.77	3.485 (13)	135

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