research communications

Crystal structure of N,N′-didecylpyromellitic diimide

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The title compound, $C_{30}H_{44}N_2O_4$ [systematic name: 2,6-didecylpyrrolo[3,4-f]-isoindole-1,3,5,7(2H,6H)-tetraone], consists of a central pyromellitic diimide moiety with terminal decyl groups at the N-atom positions. The centre of the molecule lies on a crystallographic inversion centre so the asymmetric unit contains one half-molecule. The molecule exhibits a rod-shaped conformation, like other similar compounds of this type, the distance between the ends of terminal decyl groups being 32.45 Å. The packing is dominated by a lamellar arrangement of the molecules, which is reinforced by C—H···O hydrogen bonds and C—O···π interactions, forming a classic herringbone structure. The molecular structure is consistent with the theoretical calculations performed by density functional theory (DFT).

1. Chemical context

Previous studies have proposed that pyromellitic diimide derivatives have potential applications in energy storage materials (Song et al., 2010) and photovoltaic devices (Kanosue & Ando, 2016). Additionally, aromatic diimides can act as organic semiconductors (Shao et al., 2014). Recently, our group reported a copper(I) coordination polymer with a pyromellitic diimide ligand, namely N,N′-bis[2-(cyclohexyl-thio)ethyl]pyromellitic diimide, and showed that the ligand has two conformations, syn and anti. In addition, a reversible anti to syn transition was achieved by agitating in mixed organic solvents (Kang et al., 2015). In an extension of our studies of pyromellitic diimide derivatives, we have prepared the title compound by the reaction of pyromellitic dianhydride with decylamine and report its crystal structure herein.
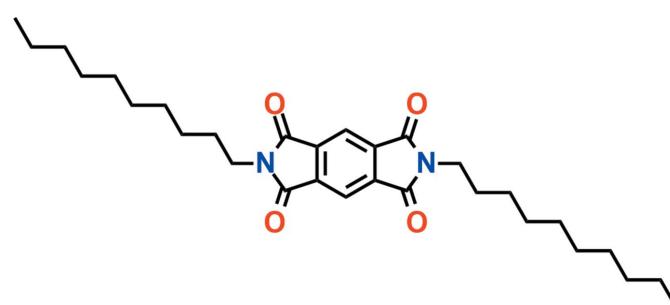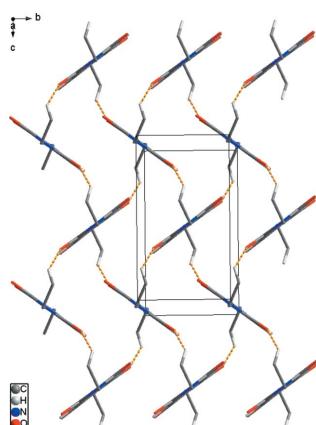

2. Structural commentary

The title compound consists of a central pyromellitic diimide with two terminal decyl groups (Fig. 1). The centre of the
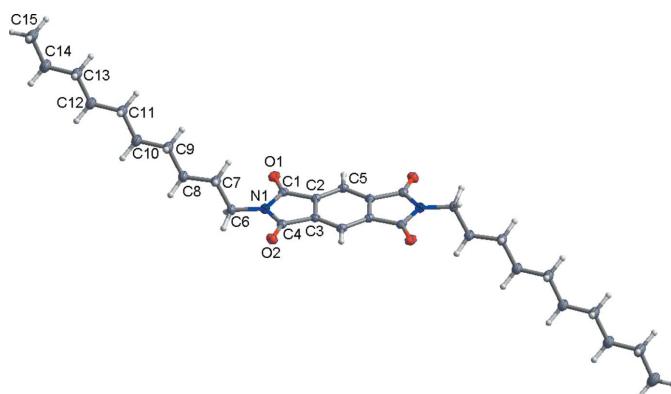
Figure 1
The asymmetric unit of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius. Unlabelled atoms are generated by the symmetry operation $(1 - x, 1 - y, 2 - z)$.

molecule lies on a crystallographic inversion centre and the asymmetric unit of the title compound is composed of one half-molecule. The decyl chains are inclined at an angle of 67.96° to the plane of the pyromellitic diimide ring. The decyl

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

$D-\mathrm{H}\cdots A$	$D-\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D-\mathrm{H}\cdots A$
C7—H7B···O2$^{\mathrm{i}}$	0.99	2.57	3.3929 (14)	141

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

chains point in opposite directions, forming a rod-shaped conformation with a distance of 32.45 Å between the carbon atoms of the terminal decyl groups.

3. Supramolecular features

In the crystal, C7—H7B···O2$^{\mathrm{i}}$ [symmetry code: (i) $x, -y + \frac{3}{2}$, $z - \frac{1}{2}$; Table 1] hydrogen bonds (H···O = 2.57 Å) link adjacent molecules (yellow dashed lines in Fig. 2). In addition,, adjacent molecules are connected by C4—O2$^{\mathrm{ii}}$···Cg1 (Cg1 is the centroid of the N1/C1–C4 ring) interactions [O···π = 3.272 (1) Å; symmetry code: (ii) $x, -y + \frac{3}{2}, z + \frac{1}{2}$], resulting in the formation of a classic herringbone structure (black dashed lines in Fig. 3). One oxygen atom accepts both hydrogen bonds and C—O···π interactions with neighboring molecules, generating a two-dimensional architecture extending parallel to the *bc* plane (Fig. 4).

Figure 2
Intermolecular C—H···O hydrogen bonds (yellow dashed lines) [symmetry code: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$] in the crystal of (I). H atoms and terminal decyl chains not involved in intermolecular interactions have been omitted for clarity.
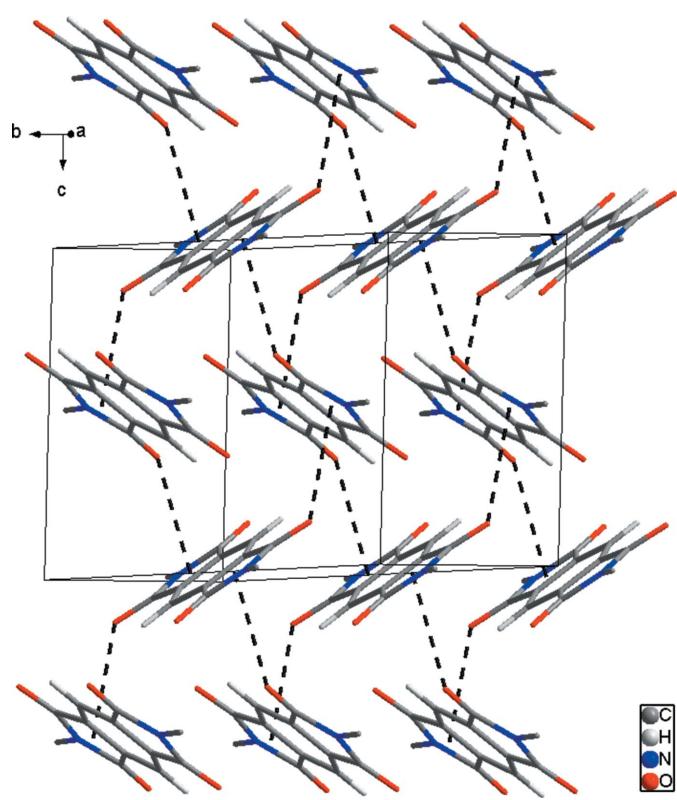
Figure 3
The packing diagram for (I), showing the classic herringbone structure formed by C—O···π interactions (black dashed lines). H atoms and terminal decyl chains not involved in intermolecular interactions have been omitted for clarity.

Table 2
Experimental and calculated bond lengths (Å).

Bond	X-ray	B3LYP (6–311G*)
O1—C1	1.2059 (13)	1.2069
O2—C4	1.2034 (13)	1.2069
N1—C1	1.3924 (14)	1.4019
N1—C4	1.3915 (14)	1.4011
N1—C6	1.4590 (13)	1.4607
C1—C2	1.4933 (14)	1.4972
C2—C3	1.3911 (15)	1.3968
C3—C4	1.4984 (14)	1.4971
C2—C5	1.3869 (14)	1.3896
C6—C7	1.5235 (15)	1.5318
C7—C8	1.5225 (15)	1.5317
C8—C9	1.5238 (16)	1.5323
C9—C10	1.5221 (15)	1.5322
C10—C11	1.5230 (16)	1.5322
C11—C12	1.5223 (16)	1.5323
C12—C13	1.5235 (17)	1.5321
C13—C14	1.5200 (17)	1.5324
C14—C15	1.5236 (19)	1.5303

4. Theoretical calculations

DFT calculations have been performed to support the experimental values on the basis of the diffraction study using the *GAUSSIAN09* software package (Frisch *et al.*, 2009). Full geometry optimizations were performed using B3LYP levels of theory with a 6-311G* basis set. The optimized parameters such as bond lengths and bond angles are in excellent agreement with the experimental crystallographic data (Table 2). In
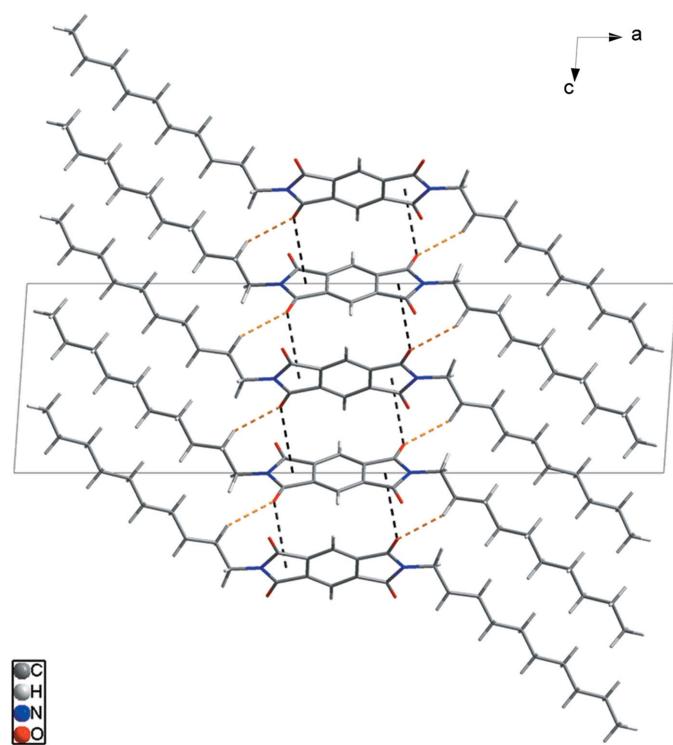
Figure 4
The packing for (I) showing intermolecular hydrogen bonds (yellow dashed lines) and C—O···π interactions (black dashed lines) accepted by the same O atom.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{30}H_{44}N_2O_4$
M_r	496.67
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	30.6365 (16), 5.0149 (3), 8.9393 (5)
β (°)	93.980 (3)
V (Å³)	1370.11 (13)
Z	2
Radiation type	Mo $K\alpha$
μ (mm⁻¹)	0.08
Crystal size (mm)	$0.66 \times 0.65 \times 0.13$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.703, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22193, 3364, 2964
R_{int}	0.026
$(\sin \theta/\lambda)_{max}$ (Å⁻¹)	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.113, 1.09
No. of reflections	3364
No. of parameters	164
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å⁻³)	0.33, −0.20

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2010) and *publCIF* (Westrip, 2010).

particular, the theoretical value (67.07°) for the angle between the decyl chain and the plane of the pyromellitic diimide ring is almost equal that obtained from the experimental crystallographic data (67.96°).

5. Synthesis and crystallization

A mixture of pyromellitic dianhydride (0.55g, 2.5mmol) and decyl amine (0.88 g, 5.3mmol) in toluene (10 ml) and dimethyl sulfoxide (6 ml) was heated at 453 K with stirring for 5 h. Upon cooling to room temperature, an off-white crude solid was filtered and washed with water, methanol and ether. Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a dichloromethane solution of the title compound. ¹H NMR (300 MHz, CDCl₃): d = 8.27 (*s*, 2H, Ar), 3.74 (*t*, 4H, CH₂N), 1.70 (*t*, 4H, CH₂CH₂N), 1.32 (*m*, 28H, CH₂), 0.88 (*t*, 6H, CH₃)

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.95 Å, U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, d(C—H) = 0.99 Å, U_{iso}(H) = 1.2U_{eq}(C) for Csp^3—H, d(C—H) = 0.98 Å, U_{iso} = 1.5U_{eq}(C) for methyl group.

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Crystal structure of *N*,*N*′-didecylpyromellitic diimide

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

2,6-Didecylpyrrolo[3,4-*f*]isoindole-1,3,5,7(2*H*,6*H*)-tetraone

Crystal data

$C_{30}H_{44}N_2O_4$	$F(000) = 540$
$M_r = 496.67$	$D_x = 1.204$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 30.6365$ (16) Å	Cell parameters from 9966 reflections
$b = 5.0149$ (3) Å	$\theta = 3.3–28.1°$
$c = 8.9393$ (5) Å	$\mu = 0.08$ mm^{-1}
$\beta = 93.980$ (3)°	$T = 173$ K
$V = 1370.11$ (13) Å^3	Block, colourless
$Z = 2$	$0.66 \times 0.65 \times 0.13$ mm

Data collection

Bruker APEXII CCD diffractometer	3364 independent reflections
φ and ω scans	2964 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2014)	$R_{int} = 0.026$
	$\theta_{max} = 28.3°$, $\theta_{min} = 1.3°$
$T_{min} = 0.703$, $T_{max} = 0.746$	$h = -40 \rightarrow 40$
22193 measured reflections	$k = -6 \rightarrow 6$
	$l = -11 \rightarrow 10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	
$wR(F^2) = 0.113$	
$S = 1.09$	H-atom parameters constrained
3364 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.4968P]$ where $P = (F_o^2 + 2F_c^2)/3$
164 parameters	
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
	$\Delta\rho_{max} = 0.33$ e Å^{-3}
	$\Delta\rho_{min} = -0.20$ 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.

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

	x	y	z	U_{iso}*/U_{eq}
C3	0.46219 (3)	0.6062 (2)	1.04594 (11)	0.0174 (2)
O1	0.40031 (3)	0.12036 (16)	0.84589 (9)	0.0248 (2)
O2	0.40323 (3)	0.85647 (16)	1.14895 (9)	0.02379 (19)
N1	0.39028 (3)	0.47982 (19)	1.00209 (10)	0.0198 (2)
C2	0.46141 (3)	0.3850 (2)	0.95188 (11)	0.0175 (2)
C4	0.41601 (3)	0.6734 (2)	1.07673 (11)	0.0185 (2)
C5	0.49907 (3)	0.2709 (2)	0.90256 (11)	0.0183 (2)
H5	0.4984	0.1198	0.8383	0.022*
C1	0.41477 (3)	0.3030 (2)	0.92185 (12)	0.0189 (2)
C6	0.34303 (3)	0.4510 (2)	1.00787 (13)	0.0233 (2)
H6A	0.3336	0.5442	1.0977	0.028*
H6B	0.3358	0.2597	1.0174	0.028*
C7	0.31819 (4)	0.5643 (3)	0.86860 (13)	0.0251 (2)
H7A	0.3175	0.7612	0.8764	0.030*
H7B	0.3340	0.5180	0.7793	0.030*
C8	0.27152 (4)	0.4597 (3)	0.84738 (13)	0.0257 (3)
H8A	0.2554	0.5098	0.9355	0.031*
H8B	0.2722	0.2626	0.8417	0.031*
C9	0.24734 (4)	0.5696 (3)	0.70588 (14)	0.0275 (3)
H9A	0.2444	0.7651	0.7165	0.033*
H9B	0.2652	0.5359	0.6197	0.033*
C10	0.20209 (4)	0.4500 (3)	0.67147 (14)	0.0288 (3)
H10A	0.1840	0.4845	0.7570	0.035*
H10B	0.2049	0.2544	0.6607	0.035*
C12	0.13370 (4)	0.4426 (3)	0.49163 (14)	0.0305 (3)
H12A	0.1152	0.4744	0.5765	0.037*
H12B	0.1367	0.2474	0.4797	0.037*
C11	0.17877 (4)	0.5626 (3)	0.52925 (14)	0.0292 (3)
H11A	0.1757	0.7579	0.5408	0.035*
H11B	0.1972	0.5307	0.4442	0.035*
C13	0.11075 (4)	0.5574 (3)	0.34923 (14)	0.0312 (3)
H13A	0.1079	0.7527	0.3611	0.037*
H13B	0.1292	0.5249	0.2644	0.037*
C14	0.06564 (4)	0.4394 (3)	0.31123 (16)	0.0378 (3)
H14A	0.0469	0.4755	0.3948	0.045*
H14B	0.0683	0.2436	0.3012	0.045*
C15	0.04360 (5)	0.5520 (4)	0.16677 (17)	0.0469 (4)
H15A	0.0394	0.7445	0.1778	0.070*
H15B	0.0151	0.4656	0.1460	0.070*

H15C	0.0621	0.5182	0.0836	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C3	0.0191 (5)	0.0168 (5)	0.0161 (5)	0.0019 (4)	0.0005 (4)	0.0016 (4)
O1	0.0268 (4)	0.0240 (4)	0.0230 (4)	−0.0051 (3)	−0.0021 (3)	−0.0033 (3)
O2	0.0258 (4)	0.0219 (4)	0.0241 (4)	0.0038 (3)	0.0050 (3)	−0.0017 (3)
N1	0.0168 (4)	0.0238 (5)	0.0186 (4)	−0.0001 (3)	−0.0004 (3)	0.0000 (4)
C2	0.0200 (5)	0.0165 (5)	0.0157 (5)	−0.0005 (4)	−0.0013 (4)	0.0016 (4)
C4	0.0201 (5)	0.0193 (5)	0.0162 (5)	0.0011 (4)	0.0006 (4)	0.0035 (4)
C5	0.0218 (5)	0.0159 (5)	0.0170 (5)	0.0008 (4)	−0.0002 (4)	−0.0010 (4)
C1	0.0208 (5)	0.0191 (5)	0.0164 (5)	0.0000 (4)	−0.0009 (4)	0.0031 (4)
C6	0.0156 (5)	0.0321 (6)	0.0222 (5)	−0.0020 (4)	0.0008 (4)	0.0023 (4)
C7	0.0184 (5)	0.0313 (6)	0.0252 (6)	−0.0014 (4)	−0.0017 (4)	0.0041 (5)
C8	0.0186 (5)	0.0324 (6)	0.0257 (6)	−0.0017 (4)	−0.0012 (4)	0.0019 (5)
C9	0.0201 (5)	0.0341 (6)	0.0279 (6)	−0.0006 (5)	−0.0026 (4)	0.0019 (5)
C10	0.0215 (6)	0.0345 (7)	0.0296 (6)	−0.0016 (5)	−0.0040 (5)	0.0014 (5)
C12	0.0229 (6)	0.0371 (7)	0.0305 (6)	−0.0020 (5)	−0.0055 (5)	0.0009 (5)
C11	0.0218 (5)	0.0355 (7)	0.0296 (6)	−0.0009 (5)	−0.0043 (5)	0.0017 (5)
C13	0.0241 (6)	0.0388 (7)	0.0298 (6)	−0.0005 (5)	−0.0049 (5)	0.0011 (5)
C14	0.0253 (6)	0.0519 (9)	0.0349 (7)	−0.0032 (6)	−0.0074 (5)	0.0005 (6)
C15	0.0311 (7)	0.0702 (11)	0.0374 (8)	0.0019 (7)	−0.0111 (6)	0.0015 (7)

Geometric parameters (Å, º)

C3—C5^i	1.3873 (14)	C9—C10	1.5221 (15)
C3—C2	1.3911 (15)	C9—H9A	0.9900
C3—C4	1.4984 (14)	C9—H9B	0.9900
O1—C1	1.2059 (13)	C10—C11	1.5230 (16)
O2—C4	1.2034 (13)	C10—H10A	0.9900
N1—C4	1.3915 (14)	C10—H10B	0.9900
N1—C1	1.3924 (14)	C12—C11	1.5223 (16)
N1—C6	1.4590 (13)	C12—C13	1.5235 (17)
C2—C5	1.3869 (14)	C12—H12A	0.9900
C2—C1	1.4933 (14)	C12—H12B	0.9900
C5—C3^i	1.3872 (14)	C11—H11A	0.9900
C5—H5	0.9500	C11—H11B	0.9900
C6—C7	1.5235 (15)	C13—C14	1.5200 (17)
C6—H6A	0.9900	C13—H13A	0.9900
C6—H6B	0.9900	C13—H13B	0.9900
C7—C8	1.5225 (15)	C14—C15	1.5236 (19)
C7—H7A	0.9900	C14—H14A	0.9900
C7—H7B	0.9900	C14—H14B	0.9900
C8—C9	1.5238 (16)	C15—H15A	0.9800
C8—H8A	0.9900	C15—H15B	0.9800
C8—H8B	0.9900	C15—H15C	0.9800

C5ⁱ—C3—C2	122.23 (10)	C10—C9—H9B	108.7
C5ⁱ—C3—C4	129.49 (10)	C8—C9—H9B	108.7
C2—C3—C4	108.27 (9)	H9A—C9—H9B	107.6
C4—N1—C1	112.56 (9)	C9—C10—C11	113.00 (11)
C4—N1—C6	125.64 (9)	C9—C10—H10A	109.0
C1—N1—C6	121.77 (9)	C11—C10—H10A	109.0
C5—C2—C3	122.78 (10)	C9—C10—H10B	109.0
C5—C2—C1	129.49 (10)	C11—C10—H10B	109.0
C3—C2—C1	107.72 (9)	H10A—C10—H10B	107.8
O2—C4—N1	126.50 (10)	C11—C12—C13	113.21 (11)
O2—C4—C3	128.08 (10)	C11—C12—H12A	108.9
N1—C4—C3	105.42 (9)	C13—C12—H12A	108.9
C2—C5—C3ⁱ	114.99 (10)	C11—C12—H12B	108.9
C2—C5—H5	122.5	C13—C12—H12B	108.9
C3ⁱ—C5—H5	122.5	H12A—C12—H12B	107.7
O1—C1—N1	125.71 (10)	C12—C11—C10	113.81 (11)
O1—C1—C2	128.31 (10)	C12—C11—H11A	108.8
N1—C1—C2	105.97 (9)	C10—C11—H11A	108.8
N1—C6—C7	112.01 (9)	C12—C11—H11B	108.8
N1—C6—H6A	109.2	C10—C11—H11B	108.8
C7—C6—H6A	109.2	H11A—C11—H11B	107.7
N1—C6—H6B	109.2	C14—C13—C12	113.54 (11)
C7—C6—H6B	109.2	C14—C13—H13A	108.9
H6A—C6—H6B	107.9	C12—C13—H13A	108.9
C8—C7—C6	112.63 (10)	C14—C13—H13B	108.9
C8—C7—H7A	109.1	C12—C13—H13B	108.9
C6—C7—H7A	109.1	H13A—C13—H13B	107.7
C8—C7—H7B	109.1	C13—C14—C15	112.82 (13)
C6—C7—H7B	109.1	C13—C14—H14A	109.0
H7A—C7—H7B	107.8	C15—C14—H14A	109.0
C7—C8—C9	112.15 (10)	C13—C14—H14B	109.0
C7—C8—H8A	109.2	C15—C14—H14B	109.0
C9—C8—H8A	109.2	H14A—C14—H14B	107.8
C7—C8—H8B	109.2	C14—C15—H15A	109.5
C9—C8—H8B	109.2	C14—C15—H15B	109.5
H8A—C8—H8B	107.9	H15A—C15—H15B	109.5
C10—C9—C8	114.13 (10)	C14—C15—H15C	109.5
C10—C9—H9A	108.7	H15A—C15—H15C	109.5
C8—C9—H9A	108.7	H15B—C15—H15C	109.5
C5ⁱ—C3—C2—C5	0.00 (18)	C4—N1—C1—C2	2.09 (12)
C4—C3—C2—C5	−179.64 (9)	C6—N1—C1—C2	−175.94 (9)
C5ⁱ—C3—C2—C1	178.88 (9)	C5—C2—C1—O1	−1.11 (19)
C4—C3—C2—C1	−0.76 (11)	C3—C2—C1—O1	−179.89 (11)
C1—N1—C4—O2	176.76 (10)	C5—C2—C1—N1	178.05 (10)
C6—N1—C4—O2	−5.30 (17)	C3—C2—C1—N1	−0.73 (11)
C1—N1—C4—C3	−2.53 (11)	C4—N1—C6—C7	101.29 (12)
C6—N1—C4—C3	175.41 (9)	C1—N1—C6—C7	−80.95 (13)

C5ⁱ—C3—C4—O2	3.09 (18)	N1—C6—C7—C8	161.36 (10)
C2—C3—C4—O2	−177.30 (11)	C6—C7—C8—C9	−178.71 (10)
C5ⁱ—C3—C4—N1	−177.63 (10)	C7—C8—C9—C10	174.31 (11)
C2—C3—C4—N1	1.98 (11)	C8—C9—C10—C11	−179.78 (11)
C3—C2—C5—C3ⁱ	0.00 (17)	C13—C12—C11—C10	179.93 (11)
C1—C2—C5—C3ⁱ	−178.62 (10)	C9—C10—C11—C12	179.16 (11)
C4—N1—C1—O1	−178.71 (10)	C11—C12—C13—C14	−179.76 (12)
C6—N1—C1—O1	3.26 (17)	C12—C13—C14—C15	−178.76 (13)

Symmetry code: (i) −x+1, −y+1, −z+2.

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7B···O2ⁱⁱ	0.99	2.57	3.3929 (14)	141

Symmetry code: (ii) x, −y+3/2, z−1/2.