

Crystal structure and Hirshfeld surface analysis of 3-({4-[(4-cyanophenoxy)carbonyl]phenoxy}carbonyl)phenyl 4-(benzyloxy)-3-chlorobenzoate

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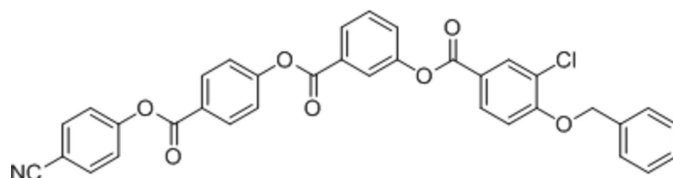
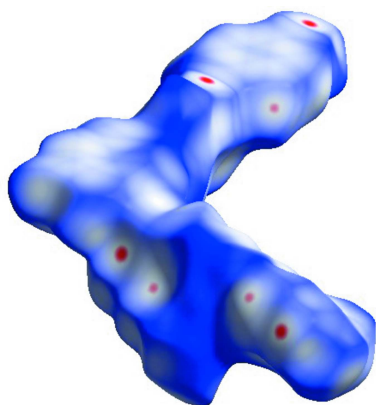
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The title compound, C₃₅H₂₂ClNO₇, is a non-liquid crystal with a bent-shaped molecule. The dihedral angles between adjacent aromatic rings in the molecule (starting from the cyanobenzene ring) are 72.61 (2), 87.69 (4), 64.08 (2) and 88.23 (2)°, indicating that adjacent rings are close to perpendicular to each other. In the crystal, the molecules are linked by weak C—H···N and C—H···π interactions, thereby forming a two-dimensional supramolecular architecture in the *ac* plane. The most important contributions to the crystal packing arise from H···H (59.3%), S···H (27.4%) and O···H (7.5%) interactions, as determined by a Hirshfeld surface analysis.

1. Chemical context

Banana/bent-shaped liquid crystals (LCs) are of great interest in the field of display materials. In particular, the —CN groups at the terminal end (Walba *et al.*, 2000; Reddy & Sadashiva, 2004) of banana-shaped LCs have been linked to their bent or bow (twisted) anisometric phase with C_{2v} symmetry. Furthermore, they exhibit polar order, chirality and spontaneous polarization in the fluid phase. We have reported the crystal structures of LC intermediates and found that benzyloxy group-substituted molecules are prone to be hydrophobic (Kashi *et al.*, 2012; Al-Eryani *et al.*, 2011). Benzyloxy group-substituted molecules also play a significant role in synthesizing bent-shaped LCs and non-LCs (Palakshamurthy *et al.*, 2012). Hence, it is useful to study benzyloxy group-substituted bent-shaped molecules to understand the structural properties and the relationship between LCs and crystal structures.



In a continuation of this work, we investigated the title molecule, which possesses five aromatic rings with three ester groups and a benzyloxy group at one terminal end, presumably making the molecule highly polar. Furthermore, it has a chloro group at one side and a cyano group at the opposite terminal end of the molecule, inducing an unsymmetrical

Table 1

Hydrogen-bond geometry (Å, °).

Cg4 and Cg5 are the centroids of the C23–C28 and C30–C35 rings, respectively.

| <i>D</i> –H··· <i>A</i> | <i>D</i> –H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> –H··· <i>A</i> |
|------------------------------|-------------|---------------|-----------------------|-------------------------|
| C2–H2···O2 | 0.944 (18) | 2.411 (17) | 2.7213 (19) | 98.9 (12) |
| C12–H12···O4 | 0.93 | 2.42 | 2.733 (2) | 100 |
| C24–H24···O6 | 0.93 | 2.40 | 2.721 (2) | 100 |
| C17–H17···N1 ⁱ | 0.93 | 2.62 | 3.504 (3) | 158 |
| C25–H25···Cg5 ⁱⁱ | 0.93 | 2.86 | 3.744 (2) | 158 |
| C31–H31···Cg4 ⁱⁱⁱ | 0.93 | 2.82 | 3.702 (3) | 158 |

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

structure (Hartung *et al.*, 2000). The molecule was subjected to LC characterization studies, but it did not show any LC properties, which may be due to the absence of a flexible alkyl chain. The title compound was synthesized according to the procedure described by Sadashiva *et al.* (2002) and its crystal structure is reported herein.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The dihedral angles between the aromatic rings are as follows: $A/B = 64.08$ (2), $A/C = 29.75$ (2), $A/D = 87.69$ (4), $A/E = 16.07$ (3), $B/C = 88.23$ (2), $B/D = 87.88$ (4), $B/E = 68.87$ (4), $C/D = 82.27$ (3), $E/D = 72.61$ (2) and $C/E = 37.46$ (4)°, where *A*, *B*, *C*, *D* and *E* are the C1–C6, C23–C28, C30–C35, C8–C13 and C15–C20, rings, respectively. The torsion angles associated with the benzyloxy group are -7.2 (3) (C15–O4–C14–O3), -3.1 (3) (C8–O2–C7–O1) and -0.7 (2)° (C3–O6–C22–O5). Three short intramolecular C–H···O contacts (Table 1) may influence the molecular conformation.

3. Supramolecular features

In the crystal, the molecules are linked by weak C–H···N hydrogen bonds and weak C–H···π interactions (Table 1) to generate a two-dimensional supramolecular architecture propagating in the *ac* plane as shown in Fig. 2. Furthermore, the molecules are linked by centrosymmetric aromatic π–π stacking interactions with Cg4···Cg4 and Cg3···Cg3 =

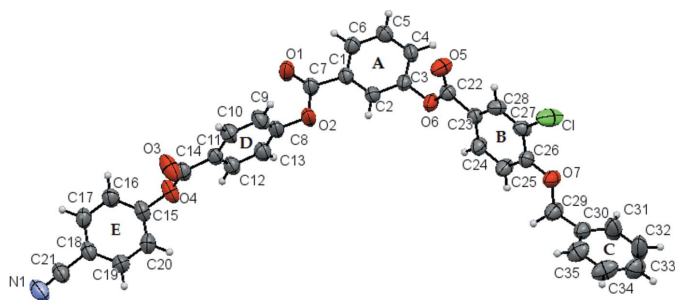


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

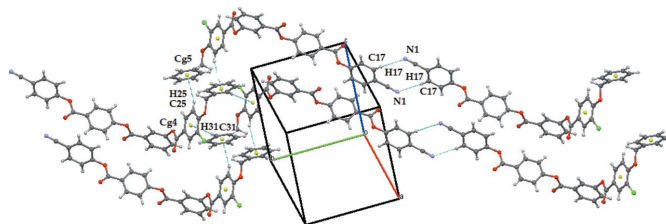


Figure 2

The molecular packing of the title compound. Dashed lines indicate the C–H···π interactions.

3.6387 (10) Å (slippage = 1.086 Å) and 3.7740 (10) Å (slippage = 1.407 Å), respectively, as shown in Fig. 3 (Cg4 is the centroid of the C23–C28 ring and Cg3 is the centroid of the C15–C20 ring).

4. 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-cyanophenoxy)carbonyl fragment resulted in four matches with CSD refcodes EWUSIA (Srinivasa *et al.*, 2015), IBUXOV (Ji *et al.*, 2017), IBUXUB (Yingchun *et al.*, 2016) and OCUTIS (Yingchun *et al.*, 2016). In all these structures there is a 4-cyanophenoxy grouping at the one end of the molecule, similar to the title compound. In IBUXOV, IBUXUB and OCUTIS the same core exists at both ends of the molecule. Sometimes the presence of a –CN group at both terminals of the molecule induces liquid-crystal properties.

In EWUSIA, the dihedral angles between the cyanobenzoate ring and the first neighbouring benzene ring, and between the second neighbour and the first and second benzene rings are 50.47 (2), 10.15 (3) and 50.02 (5)° compared to 72.61 (2), 16.06 (2) and 87.69 (4)° in the title molecule. In IBUXOV, the dihedral angles between the rings (cyanobenzoate ring and the neighbouring benzene ring) are 69.45 (2) and 64.20 (3)°, and 73.60 (3) and 84.16 (3)° between the adjacent cyanobenzoate and benzene rings themselves. In IBUXUB, the dihedral angles between the rings (cyanobenzoate and the neighbouring benzene ring) are 69.68 (2)

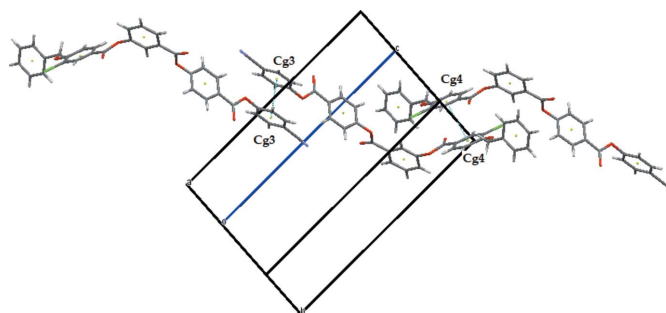


Figure 3

The molecular packing of the title compound. Dashed lines indicate the π–π stacking interactions.

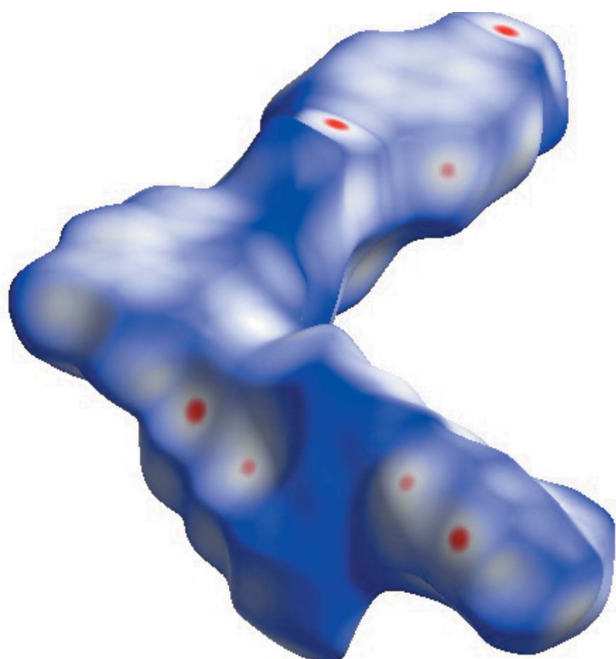


Figure 4
Hirshfeld surface of the title compound mapped with d_{norm} .

and $74.28(4)^\circ$, and $48.87(2)$ and $89.88(4)^\circ$ between the cyanobenzoate and benzene rings. In OCUTIS, the dihedral angles between adjacent cyanobenzoate and benzene rings are $81.21(4)$ and $54.43(2)^\circ$ compared to angles between the cyanobenzoate and benzene rings of $55.02(3)$ and $84.20(3)^\circ$.

5. Hirshfeld surface analysis

CrystalExplorer17.5 (Turner *et al.*, 2017) was used to perform the Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) to further quantify the various intermolecular interactions.

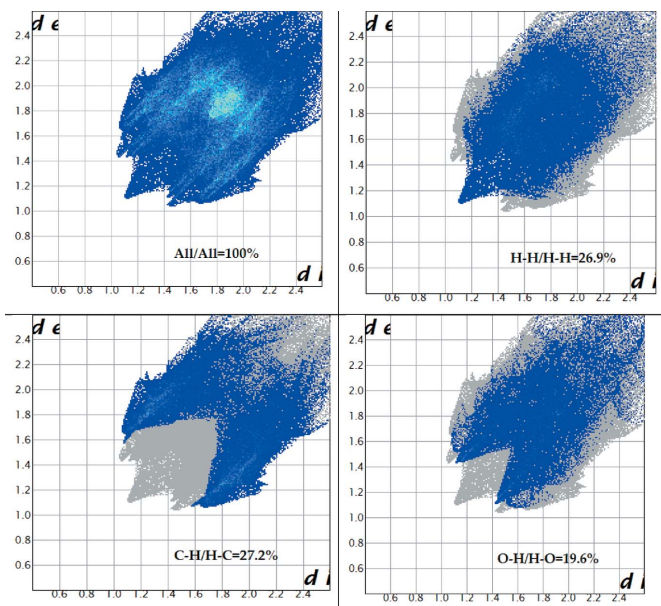


Figure 5
Two-dimensional fingerprint plots for the title compound.

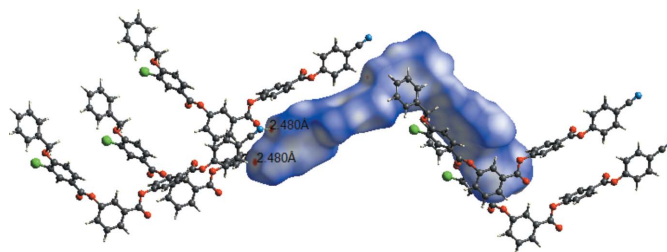


Figure 6
Hirshfeld surface of the title compound mapped over d_{norm} , showing the $\text{C-H}\cdots\text{N}$ interactions.

The Hirshfeld surface mapped over d_{norm} is illustrated in Fig. 4 and the associated two-dimensional fingerprint plots in Fig. 5. The major contributions to the crystal structure are from $\text{H}\cdots\text{H}$ (26.9%), $\text{C}\cdots\text{H}$ (27.2%) and $\text{O}\cdots\text{H}$ (19.6%) contacts. In Figs. 6 and 7, the red spots on the d_{norm} and d_e surfaces represent the $\text{C-H}\cdots\pi$ interactions.

6. Synthesis and crystallization

4-[(4-Cyanophenoxy)carbonyl]phenyl 3-hydroxybenzoate (1 mmol) and 4-(benzyloxy)-3-chlorobenzoic acid (1.2 mmol) were dissolved in dry chloroform (50 ml). After the addition of *N,N*-dicyclohexylcarbodiimide (1.2 mmol) and a catalytic amount of 4-(*N,N*-dimethylamino)pyridine (DMAP), the mixture was stirred at room temperature for about 12 h. The dicyclohexylurea that precipitated was filtered off and the filtrate diluted with chloroform. This solution was washed with 2% aqueous acetic acid solution

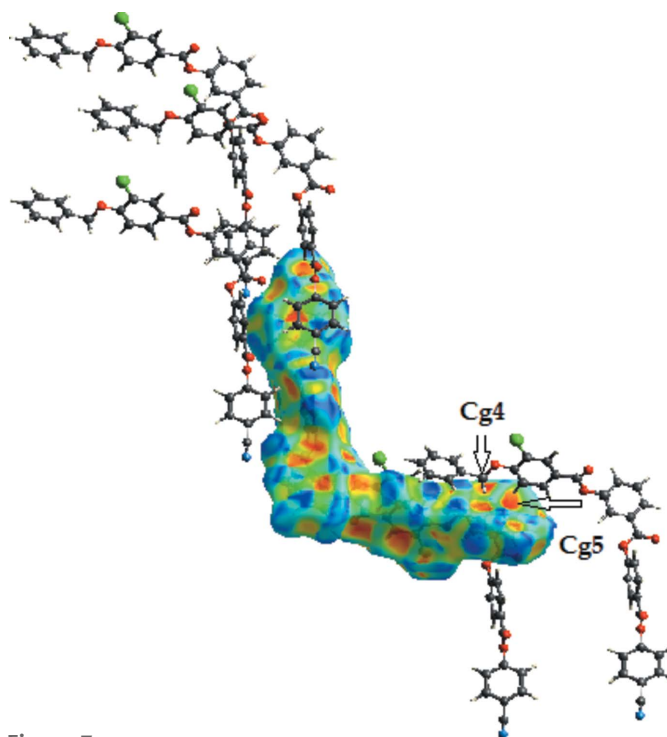


Figure 7
Hirshfeld surface of the title compound mapped over shape-index, showing the $\text{C-H}\cdots\pi$ interactions.

Table 2
Experimental details.

| | |
|---|--|
| Crystal data | |
| Chemical formula | C ₃₅ H ₂₂ ClNO ₇ |
| <i>M_r</i> | 603.98 |
| Crystal system, space group | Triclinic, <i>P</i> $\bar{1}$ |
| Temperature (K) | 296 |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 8.0202 (1), 9.8474 (2), 19.4712 (4) |
| α , β , γ (°) | 95.422 (1), 94.693 (1), 103.857 (1) |
| <i>V</i> (Å ³) | 1477.66 (5) |
| <i>Z</i> | 2 |
| Radiation type | Mo <i>K</i> α |
| μ (mm ⁻¹) | 0.18 |
| Crystal size (mm) | 0.19 × 0.18 × 0.16 |
| Data collection | |
| Diffractometer | Bruker SMART APEXII CCD |
| Absorption correction | Multi-scan (<i>SADABS</i> ; Bruker, 2017) |
| <i>T_{min}</i> , <i>T_{max}</i> | 0.966, 0.971 |
| No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections | 25466, 5207, 4255 |
| <i>R_{int}</i> | 0.024 |
| (<i>sin</i> θ / λ) _{max} (Å ⁻¹) | 0.595 |
| Refinement | |
| <i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i> | 0.038, 0.114, 1.03 |
| No. of reflections | 5207 |
| No. of parameters | 410 |
| No. of restraints | 6 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³) | 0.26, -0.33 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2017), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *Mercury* (Macrae *et al.*, 2020).

(10 ml) and 5% ice-cold sodium hydroxide solution (10 ml) and finally washed with water and dried over anhydrous sodium sulfate. The crude residue obtained was chromatographed on silica gel using chloroform as an eluent. Removal of solvent from the eluate afforded the white target material, which was crystallized from a mixture of chloroform and acetonitrile. Single crystals in the form of colourless prisms suitable for diffraction studies were grown from a solution in ethyl alcohol by slow evaporation.

IR (nujol) λ_{\max} : 3105, 3080, 2237, 1738, 1733, 1614, 1523, 1452, 1253, 1054 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ H: 8.22 (*m*, 3H, Ar-H), 8.19 (*m*, 3H, Ar-H), 8.02 (*m*, 2H, Ar-H), 7.98–7.30 (*m*, 7H, Ar-H), 6.99 (*m*, 5H, Ar-H), 5.22 (*s*, 2H, Ar–O–CH₂–) ppm; ¹³C NMR (125 MHz, CDCl₃) δ : 165.2, 159.8, 154.6, 153.7, 151.2, 136.7, 132.6, 130.2, 129, 128.9, 128.6, 127.6, 127.1, 126.8, 123.9, 122.3, 121.3, 112.4 ppm. Micro elemental analysis calculated for C₃₅H₂₂ClNO₇; C, 69.60; H, 3.67; Cl, 5.87; N, 2.32; found C, 69.68; H, 3.72; Cl, 5.91; N, 2.35%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atoms H2, H4 and H6 were fully refined. Other 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) = 1.2–1.5*U*_{eq}(C).

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Computing details

Data collection: *APEX2* (Bruker, 2017); cell refinement: *SAINTE* (Bruker, 2017); data reduction: *SAINTE* (Bruker, 2017); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *SHELXL* (Sheldrick, 2015b).

3-({4-[(4-Cyanophenoxy)carbonyl]phenoxy}carbonyl)phenyl 4-(benzyloxy)-3-chlorobenzoate

Crystal data

$C_{35}H_{22}ClNO_7$
 $M_r = 603.98$
 Triclinic, $P\bar{1}$
 Hall symbol: -P 1
 $a = 8.0202$ (1) Å
 $b = 9.8474$ (2) Å
 $c = 19.4712$ (4) Å
 $\alpha = 95.422$ (1)°
 $\beta = 94.693$ (1)°
 $\gamma = 103.857$ (1)°
 $V = 1477.66$ (5) Å³
 $Z = 2$

$F(000) = 624$
 Prism
 $D_x = 1.357$ Mg m⁻³
 Melting point: 445 K
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 5212 reflections
 $\theta = 1.0$ – 25.0 °
 $\mu = 0.18$ mm⁻¹
 $T = 296$ K
 Prism, colourless
 $0.19 \times 0.18 \times 0.16$ mm

Data collection

Bruker SMART APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 2.06 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2017)
 $T_{\min} = 0.966$, $T_{\max} = 0.971$

25466 measured reflections
 5207 independent reflections
 4255 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.1$ °
 $h = -9 \rightarrow 9$
 $k = -11 \rightarrow 11$
 $l = -23 \rightarrow 23$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.114$
 $S = 1.03$
 5207 reflections

410 parameters
 6 restraints
 0 constraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 0.2788P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.002$$

$$\Delta\rho_{\max} = 0.26 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$$

Extinction correction: SHELXL2018

(Sheldrick, 2015b),

$$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Extinction coefficient: 0.0158 (18)

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|---------------|--------------|----------------------------------|
| O7 | 0.66155 (14) | 1.37557 (12) | 1.06583 (6) | 0.0604 (3) |
| O6 | 0.23387 (14) | 0.91624 (11) | 0.82866 (6) | 0.0562 (3) |
| O2 | 0.31260 (15) | 0.47851 (13) | 0.70608 (7) | 0.0701 (4) |
| O4 | 0.70509 (18) | 0.04285 (14) | 0.58733 (6) | 0.0691 (4) |
| O5 | 0.07952 (16) | 0.85138 (14) | 0.91636 (6) | 0.0683 (4) |
| O3 | 0.6173 (2) | -0.06006 (17) | 0.67969 (8) | 0.0920 (5) |
| O1 | 0.06206 (16) | 0.37006 (13) | 0.64386 (7) | 0.0734 (4) |
| N1 | 1.2423 (3) | -0.3715 (2) | 0.52599 (11) | 0.0906 (6) |
| C33 | 1.1312 (3) | 1.7706 (3) | 1.18897 (11) | 0.0805 (6) |
| H33 | 1.200300 | 1.842548 | 1.220743 | 0.097* |
| C34 | 1.1522 (3) | 1.6373 (3) | 1.18768 (11) | 0.0812 (6) |
| H34 | 1.235250 | 1.618164 | 1.218912 | 0.097* |
| C35 | 1.0499 (3) | 1.5295 (2) | 1.13982 (10) | 0.0710 (5) |
| H35 | 1.066616 | 1.439064 | 1.138300 | 0.085* |
| C30 | 0.9239 (2) | 1.55720 (18) | 1.09471 (8) | 0.0561 (4) |
| C29 | 0.8184 (2) | 1.44647 (19) | 1.03988 (9) | 0.0652 (5) |
| H29A | 0.790624 | 1.489441 | 0.999036 | 0.078* |
| H29B | 0.883975 | 1.378979 | 1.026758 | 0.078* |
| C26 | 0.5546 (2) | 1.27075 (17) | 1.02142 (8) | 0.0496 (4) |
| C25 | 0.5822 (2) | 1.23457 (18) | 0.95365 (9) | 0.0599 (4) |
| H25 | 0.678848 | 1.285319 | 0.935657 | 0.072* |
| C24 | 0.4681 (2) | 1.12408 (17) | 0.91246 (8) | 0.0550 (4) |
| H24 | 0.488830 | 1.101130 | 0.867042 | 0.066* |
| C23 | 0.32400 (19) | 1.04740 (15) | 0.93774 (8) | 0.0456 (3) |
| C22 | 0.19929 (19) | 0.92835 (16) | 0.89583 (8) | 0.0472 (4) |
| C3 | 0.1246 (2) | 0.80725 (15) | 0.78186 (8) | 0.0476 (4) |
| C2 | 0.1912 (2) | 0.69862 (16) | 0.75737 (8) | 0.0479 (4) |
| C1 | 0.08826 (19) | 0.59329 (16) | 0.70854 (7) | 0.0449 (3) |
| C7 | 0.1464 (2) | 0.46904 (17) | 0.68174 (8) | 0.0517 (4) |
| C8 | 0.3800 (2) | 0.36353 (18) | 0.68774 (9) | 0.0577 (4) |
| C13 | 0.4822 (2) | 0.37070 (19) | 0.63451 (10) | 0.0608 (4) |
| H13 | 0.499046 | 0.447392 | 0.609152 | 0.073* |

| | | | | |
|-----|--------------|---------------|--------------|------------|
| C12 | 0.5600 (2) | 0.26220 (18) | 0.61907 (9) | 0.0572 (4) |
| H12 | 0.630774 | 0.266133 | 0.583388 | 0.069* |
| C11 | 0.53291 (19) | 0.14754 (17) | 0.65663 (8) | 0.0494 (4) |
| C14 | 0.6184 (2) | 0.03171 (19) | 0.64397 (9) | 0.0551 (4) |
| C15 | 0.8124 (2) | -0.04890 (18) | 0.57562 (9) | 0.0566 (4) |
| C20 | 0.9844 (2) | 0.00167 (19) | 0.59635 (10) | 0.0654 (5) |
| H20 | 1.027213 | 0.091840 | 0.619681 | 0.078* |
| C19 | 1.0936 (2) | -0.08343 (19) | 0.58204 (10) | 0.0657 (5) |
| H19 | 1.211388 | -0.050869 | 0.595875 | 0.079* |
| C18 | 1.0288 (2) | -0.21700 (18) | 0.54721 (9) | 0.0564 (4) |
| C21 | 1.1458 (3) | -0.3048 (2) | 0.53442 (10) | 0.0671 (5) |
| C27 | 0.40785 (19) | 1.19401 (19) | 1.04630 (8) | 0.0526 (4) |
| C28 | 0.29494 (19) | 1.08363 (18) | 1.00565 (8) | 0.0530 (4) |
| H28 | 0.198360 | 1.032683 | 1.023589 | 0.064* |
| C9 | 0.3515 (2) | 0.2511 (2) | 0.72563 (10) | 0.0674 (5) |
| H9 | 0.281420 | 0.248249 | 0.761511 | 0.081* |
| C10 | 0.4279 (2) | 0.1426 (2) | 0.70986 (9) | 0.0615 (4) |
| H10 | 0.408968 | 0.065641 | 0.735040 | 0.074* |
| C17 | 0.8540 (2) | -0.26542 (19) | 0.52624 (9) | 0.0621 (5) |
| H17 | 0.810392 | -0.354934 | 0.502276 | 0.074* |
| C16 | 0.7448 (2) | -0.18100 (19) | 0.54090 (9) | 0.0632 (5) |
| H16 | 0.626763 | -0.212940 | 0.527475 | 0.076* |
| C6 | -0.0776 (2) | 0.59977 (17) | 0.68582 (8) | 0.0501 (4) |
| C5 | -0.1410 (2) | 0.71063 (18) | 0.71118 (9) | 0.0558 (4) |
| H5 | -0.252302 | 0.714786 | 0.695759 | 0.067* |
| C4 | -0.0391 (2) | 0.81545 (17) | 0.75948 (9) | 0.0538 (4) |
| C31 | 0.9056 (3) | 1.6916 (2) | 1.09726 (13) | 0.0897 (7) |
| H31 | 0.821394 | 1.711933 | 1.066993 | 0.108* |
| C32 | 1.0097 (3) | 1.7978 (3) | 1.14393 (15) | 0.1065 (9) |
| H32 | 0.996215 | 1.889094 | 1.144422 | 0.128* |
| Cl | 0.37075 (6) | 1.23731 (8) | 1.13083 (2) | 0.0967 (2) |
| H6 | -0.146 (2) | 0.5267 (19) | 0.6546 (9) | 0.057 (5)* |
| H2 | 0.303 (2) | 0.6937 (18) | 0.7740 (9) | 0.061 (5)* |
| H4 | -0.080 (2) | 0.8914 (19) | 0.7778 (9) | 0.057 (5)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| O7 | 0.0531 (6) | 0.0670 (7) | 0.0505 (6) | 0.0008 (5) | 0.0086 (5) | -0.0123 (5) |
| O6 | 0.0596 (7) | 0.0465 (6) | 0.0544 (6) | 0.0017 (5) | 0.0134 (5) | -0.0115 (5) |
| O2 | 0.0542 (7) | 0.0636 (8) | 0.0892 (9) | 0.0284 (6) | -0.0096 (6) | -0.0289 (6) |
| O4 | 0.0899 (9) | 0.0714 (8) | 0.0624 (7) | 0.0493 (7) | 0.0188 (6) | 0.0061 (6) |
| O5 | 0.0600 (7) | 0.0755 (8) | 0.0566 (7) | -0.0063 (6) | 0.0056 (6) | 0.0044 (6) |
| O3 | 0.1290 (13) | 0.0867 (10) | 0.0914 (10) | 0.0694 (10) | 0.0423 (9) | 0.0305 (9) |
| O1 | 0.0672 (8) | 0.0598 (8) | 0.0861 (9) | 0.0257 (6) | -0.0185 (7) | -0.0296 (7) |
| N1 | 0.0917 (13) | 0.0785 (12) | 0.1191 (16) | 0.0446 (10) | 0.0413 (11) | 0.0130 (11) |
| C33 | 0.0729 (13) | 0.0866 (16) | 0.0667 (12) | 0.0043 (11) | -0.0038 (10) | -0.0185 (11) |
| C34 | 0.0696 (12) | 0.0989 (17) | 0.0638 (12) | -0.0017 (11) | -0.0122 (9) | 0.0277 (11) |

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|--------------|--------------|
| C35 | 0.0744 (12) | 0.0626 (11) | 0.0720 (12) | 0.0052 (9) | 0.0026 (10) | 0.0236 (9) |
| C30 | 0.0519 (9) | 0.0587 (10) | 0.0518 (9) | 0.0056 (7) | 0.0090 (7) | -0.0046 (7) |
| C29 | 0.0636 (10) | 0.0634 (11) | 0.0573 (10) | -0.0031 (8) | 0.0135 (8) | -0.0061 (8) |
| C26 | 0.0488 (8) | 0.0514 (9) | 0.0461 (8) | 0.0120 (7) | 0.0033 (6) | -0.0037 (7) |
| C25 | 0.0622 (10) | 0.0569 (10) | 0.0510 (9) | -0.0031 (8) | 0.0164 (8) | -0.0036 (7) |
| C24 | 0.0620 (10) | 0.0524 (9) | 0.0458 (8) | 0.0062 (7) | 0.0139 (7) | -0.0049 (7) |
| C23 | 0.0461 (8) | 0.0443 (8) | 0.0471 (8) | 0.0146 (6) | 0.0034 (6) | 0.0019 (6) |
| C22 | 0.0464 (8) | 0.0473 (8) | 0.0490 (8) | 0.0142 (7) | 0.0053 (7) | 0.0046 (7) |
| C3 | 0.0507 (8) | 0.0411 (8) | 0.0476 (8) | 0.0066 (6) | 0.0103 (7) | -0.0032 (6) |
| C2 | 0.0439 (8) | 0.0497 (9) | 0.0487 (8) | 0.0123 (7) | 0.0051 (7) | -0.0034 (7) |
| C1 | 0.0470 (8) | 0.0447 (8) | 0.0433 (8) | 0.0145 (6) | 0.0046 (6) | -0.0011 (6) |
| C7 | 0.0513 (9) | 0.0517 (9) | 0.0515 (9) | 0.0187 (7) | -0.0001 (7) | -0.0068 (7) |
| C8 | 0.0485 (9) | 0.0568 (10) | 0.0656 (10) | 0.0224 (7) | -0.0064 (8) | -0.0173 (8) |
| C13 | 0.0616 (10) | 0.0555 (10) | 0.0678 (11) | 0.0238 (8) | 0.0021 (8) | 0.0005 (8) |
| C12 | 0.0581 (10) | 0.0600 (10) | 0.0575 (9) | 0.0249 (8) | 0.0076 (8) | -0.0016 (8) |
| C11 | 0.0477 (8) | 0.0524 (9) | 0.0474 (8) | 0.0189 (7) | -0.0041 (6) | -0.0060 (7) |
| C14 | 0.0588 (10) | 0.0564 (10) | 0.0518 (9) | 0.0239 (8) | -0.0010 (7) | -0.0045 (8) |
| C15 | 0.0700 (11) | 0.0565 (10) | 0.0516 (9) | 0.0327 (8) | 0.0109 (8) | 0.0006 (7) |
| C20 | 0.0719 (12) | 0.0497 (10) | 0.0717 (11) | 0.0170 (8) | 0.0076 (9) | -0.0112 (8) |
| C19 | 0.0564 (10) | 0.0588 (11) | 0.0800 (12) | 0.0158 (8) | 0.0080 (9) | -0.0055 (9) |
| C18 | 0.0646 (10) | 0.0527 (10) | 0.0578 (9) | 0.0240 (8) | 0.0177 (8) | 0.0026 (8) |
| C21 | 0.0734 (12) | 0.0601 (11) | 0.0766 (12) | 0.0275 (9) | 0.0263 (10) | 0.0079 (9) |
| C27 | 0.0433 (8) | 0.0724 (11) | 0.0414 (8) | 0.0163 (7) | 0.0051 (6) | -0.0021 (7) |
| C28 | 0.0406 (8) | 0.0688 (10) | 0.0467 (8) | 0.0082 (7) | 0.0061 (6) | 0.0052 (7) |
| C9 | 0.0664 (11) | 0.0776 (13) | 0.0630 (11) | 0.0300 (9) | 0.0144 (9) | -0.0054 (10) |
| C10 | 0.0645 (10) | 0.0645 (11) | 0.0591 (10) | 0.0247 (8) | 0.0076 (8) | 0.0028 (8) |
| C17 | 0.0723 (11) | 0.0507 (10) | 0.0618 (10) | 0.0198 (8) | 0.0057 (8) | -0.0105 (8) |
| C16 | 0.0602 (10) | 0.0657 (11) | 0.0629 (10) | 0.0224 (8) | -0.0004 (8) | -0.0083 (9) |
| C6 | 0.0513 (9) | 0.0478 (9) | 0.0492 (8) | 0.0137 (7) | -0.0005 (7) | -0.0029 (7) |
| C5 | 0.0518 (9) | 0.0562 (10) | 0.0623 (10) | 0.0225 (7) | 0.0017 (7) | 0.0016 (8) |
| C4 | 0.0614 (10) | 0.0446 (9) | 0.0594 (10) | 0.0215 (7) | 0.0121 (8) | -0.0013 (7) |
| C31 | 0.0782 (14) | 0.0788 (14) | 0.1071 (17) | 0.0395 (11) | -0.0310 (12) | -0.0313 (12) |
| C32 | 0.0958 (17) | 0.0809 (15) | 0.133 (2) | 0.0416 (13) | -0.0338 (16) | -0.0495 (15) |
| C1 | 0.0578 (3) | 0.1601 (6) | 0.0491 (3) | -0.0054 (3) | 0.0139 (2) | -0.0263 (3) |

Geometric parameters (Å, °)

| | | | |
|--------|-------------|---------|-----------|
| O7—C26 | 1.3545 (19) | C1—C6 | 1.385 (2) |
| O7—C29 | 1.441 (2) | C1—C7 | 1.476 (2) |
| O6—C22 | 1.3591 (19) | C8—C13 | 1.370 (3) |
| O6—C3 | 1.4086 (17) | C8—C9 | 1.372 (3) |
| O2—C7 | 1.3563 (19) | C13—C12 | 1.382 (2) |
| O2—C8 | 1.396 (2) | C13—H13 | 0.9300 |
| O4—C14 | 1.350 (2) | C12—C11 | 1.386 (2) |
| O4—C15 | 1.4052 (19) | C12—H12 | 0.9300 |
| O5—C22 | 1.1953 (19) | C11—C10 | 1.385 (2) |
| O3—C14 | 1.190 (2) | C11—C14 | 1.477 (2) |
| O1—C7 | 1.1909 (19) | C15—C20 | 1.363 (3) |

| | | | |
|---------------|-------------|-------------|-------------|
| N1—C21 | 1.141 (2) | C15—C16 | 1.371 (2) |
| C33—C32 | 1.349 (3) | C20—C19 | 1.376 (3) |
| C33—C34 | 1.360 (3) | C20—H20 | 0.9300 |
| C33—H33 | 0.9300 | C19—C18 | 1.381 (2) |
| C34—C35 | 1.393 (3) | C19—H19 | 0.9300 |
| C34—H34 | 0.9300 | C18—C17 | 1.382 (3) |
| C35—C30 | 1.378 (3) | C18—C21 | 1.441 (2) |
| C35—H35 | 0.9300 | C27—C28 | 1.370 (2) |
| C30—C31 | 1.363 (3) | C27—C1 | 1.7284 (15) |
| C30—C29 | 1.495 (2) | C28—H28 | 0.9300 |
| C29—H29A | 0.9700 | C9—C10 | 1.376 (3) |
| C29—H29B | 0.9700 | C9—H9 | 0.9300 |
| C26—C25 | 1.384 (2) | C10—H10 | 0.9300 |
| C26—C27 | 1.388 (2) | C17—C16 | 1.372 (2) |
| C25—C24 | 1.379 (2) | C17—H17 | 0.9300 |
| C25—H25 | 0.9300 | C16—H16 | 0.9300 |
| C24—C23 | 1.376 (2) | C6—C5 | 1.378 (2) |
| C24—H24 | 0.9300 | C6—H6 | 0.929 (18) |
| C23—C28 | 1.390 (2) | C5—C4 | 1.380 (2) |
| C23—C22 | 1.471 (2) | C5—H5 | 0.9300 |
| C3—C2 | 1.369 (2) | C4—H4 | 0.940 (18) |
| C3—C4 | 1.373 (2) | C31—C32 | 1.376 (3) |
| C2—C1 | 1.392 (2) | C31—H31 | 0.9300 |
| C2—H2 | 0.944 (18) | C32—H32 | 0.9300 |
| C26—O7—C29 | 115.72 (12) | C8—C13—H13 | 120.5 |
| C22—O6—C3 | 118.29 (12) | C12—C13—H13 | 120.5 |
| C7—O2—C8 | 117.25 (12) | C13—C12—C11 | 120.16 (16) |
| C14—O4—C15 | 117.53 (13) | C13—C12—H12 | 119.9 |
| C32—C33—C34 | 119.68 (19) | C11—C12—H12 | 119.9 |
| C32—C33—H33 | 120.2 | C10—C11—C12 | 119.62 (15) |
| C34—C33—H33 | 120.2 | C10—C11—C14 | 118.11 (16) |
| C33—C34—C35 | 120.33 (19) | C12—C11—C14 | 122.22 (15) |
| C33—C34—H34 | 119.8 | O3—C14—O4 | 122.49 (15) |
| C35—C34—H34 | 119.8 | O3—C14—O4 | 122.49 (15) |
| C30—C35—C34 | 119.8 (2) | O3—C14—C11 | 125.25 (16) |
| C30—C35—H35 | 120.1 | O4—C14—C11 | 112.23 (15) |
| C34—C35—H35 | 120.1 | O4—C14—C11 | 112.23 (15) |
| C31—C30—C35 | 118.56 (17) | C20—C15—C16 | 122.31 (16) |
| C31—C30—C29 | 119.80 (18) | C20—C15—O4 | 117.50 (16) |
| C35—C30—C29 | 121.44 (18) | C16—C15—O4 | 120.08 (16) |
| O7—C29—C30 | 109.61 (13) | C20—C15—O4 | 117.50 (16) |
| O7—C29—H29A | 109.7 | C16—C15—O4 | 120.08 (16) |
| C30—C29—H29A | 109.7 | C15—C20—C19 | 118.63 (16) |
| O7—C29—H29B | 109.7 | C15—C20—H20 | 120.7 |
| C30—C29—H29B | 109.7 | C19—C20—H20 | 120.7 |
| H29A—C29—H29B | 108.2 | C20—C19—C18 | 120.22 (17) |
| O7—C26—C25 | 124.66 (14) | C20—C19—H19 | 119.9 |

| | | | |
|-----------------|--------------|----------------|-------------|
| O7—C26—C27 | 117.23 (13) | C18—C19—H19 | 119.9 |
| C25—C26—C27 | 118.10 (14) | C19—C18—C17 | 120.04 (16) |
| C24—C25—C26 | 120.76 (15) | C19—C18—C21 | 118.90 (17) |
| C24—C25—H25 | 119.6 | C17—C18—C21 | 121.06 (16) |
| C26—C25—H25 | 119.6 | N1—C21—C18 | 177.7 (2) |
| C23—C24—C25 | 120.81 (14) | C28—C27—C26 | 121.24 (14) |
| C23—C24—H24 | 119.6 | C28—C27—C1 | 119.84 (12) |
| C25—C24—H24 | 119.6 | C26—C27—C1 | 118.91 (12) |
| C24—C23—C28 | 118.75 (14) | C27—C28—C23 | 120.32 (14) |
| C24—C23—C22 | 122.69 (14) | C27—C28—H28 | 119.8 |
| C28—C23—C22 | 118.56 (14) | C23—C28—H28 | 119.8 |
| O5—C22—O6 | 122.68 (14) | C8—C9—C10 | 119.15 (17) |
| O5—C22—O6 | 122.68 (14) | C8—C9—H9 | 120.4 |
| O5—C22—C23 | 125.70 (14) | C10—C9—H9 | 120.4 |
| O6—C22—C23 | 111.61 (13) | C9—C10—C11 | 120.26 (18) |
| O6—C22—C23 | 111.61 (13) | C9—C10—H10 | 119.9 |
| C2—C3—C4 | 122.09 (14) | C11—C10—H10 | 119.9 |
| C2—C3—O6 | 117.58 (14) | C16—C17—C18 | 119.79 (16) |
| C4—C3—O6 | 120.24 (14) | C16—C17—H17 | 120.1 |
| C2—C3—O6 | 117.58 (14) | C18—C17—H17 | 120.1 |
| C4—C3—O6 | 120.24 (14) | C15—C16—C17 | 119.01 (17) |
| C3—C2—C1 | 118.53 (15) | C15—C16—H16 | 120.5 |
| C3—C2—H2 | 120.9 (11) | C17—C16—H16 | 120.5 |
| C1—C2—H2 | 120.5 (11) | C5—C6—C1 | 120.23 (15) |
| C6—C1—C2 | 119.99 (14) | C5—C6—H6 | 120.9 (11) |
| C6—C1—C7 | 117.75 (14) | C1—C6—H6 | 118.8 (11) |
| C2—C1—C7 | 122.20 (14) | C6—C5—C4 | 119.93 (15) |
| O1—C7—O2 | 122.12 (14) | C6—C5—H5 | 120.0 |
| O1—C7—O2 | 122.12 (14) | C4—C5—H5 | 120.0 |
| O1—C7—C1 | 126.23 (15) | C3—C4—C5 | 119.21 (15) |
| O2—C7—C1 | 111.65 (13) | C3—C4—H4 | 119.5 (11) |
| O2—C7—C1 | 111.65 (13) | C5—C4—H4 | 121.3 (11) |
| C13—C8—C9 | 121.82 (16) | C30—C31—C32 | 121.0 (2) |
| C13—C8—O2 | 118.33 (17) | C30—C31—H31 | 119.5 |
| C9—C8—O2 | 119.73 (16) | C32—C31—H31 | 119.5 |
| C13—C8—O2 | 118.33 (17) | C33—C32—C31 | 120.6 (2) |
| C9—C8—O2 | 119.73 (16) | C33—C32—H32 | 119.7 |
| C8—C13—C12 | 118.98 (17) | C31—C32—H32 | 119.7 |
| C32—C33—C34—C35 | 0.5 (4) | C15—O4—C14—C11 | 170.88 (14) |
| C33—C34—C35—C30 | -1.6 (3) | C10—C11—C14—O3 | -7.1 (3) |
| C34—C35—C30—C31 | 1.5 (3) | C12—C11—C14—O3 | 170.25 (19) |
| C34—C35—C30—C29 | 176.40 (17) | C10—C11—C14—O4 | 174.84 (15) |
| C26—O7—C29—C30 | -179.10 (15) | C12—C11—C14—O4 | -7.8 (2) |
| C31—C30—C29—O7 | -92.2 (2) | C10—C11—C14—O4 | 174.84 (15) |
| C35—C30—C29—O7 | 93.0 (2) | C12—C11—C14—O4 | -7.8 (2) |
| C29—O7—C26—C25 | -3.6 (3) | C14—O4—C15—C20 | -98.2 (2) |
| C29—O7—C26—C27 | 175.84 (15) | C14—O4—C15—C16 | 85.5 (2) |

| | | | |
|-----------------|--------------|-----------------|--------------|
| O7—C26—C25—C24 | 178.60 (17) | C16—C15—C20—C19 | -0.3 (3) |
| C27—C26—C25—C24 | -0.9 (3) | O4—C15—C20—C19 | -176.45 (16) |
| C26—C25—C24—C23 | 0.1 (3) | O4—C15—C20—C19 | -176.45 (16) |
| C25—C24—C23—C28 | 0.2 (3) | C15—C20—C19—C18 | 0.2 (3) |
| C25—C24—C23—C22 | -179.69 (16) | C20—C19—C18—C17 | 0.4 (3) |
| C3—O6—C22—O5 | -0.7 (2) | C20—C19—C18—C21 | -178.57 (18) |
| C3—O6—C22—C23 | -179.61 (13) | O7—C26—C27—C28 | -178.18 (15) |
| C24—C23—C22—O5 | 173.94 (17) | C25—C26—C27—C28 | 1.3 (3) |
| C28—C23—C22—O5 | -6.0 (3) | O7—C26—C27—C1 | 0.5 (2) |
| C24—C23—C22—O6 | -7.2 (2) | C25—C26—C27—C1 | 179.98 (14) |
| C28—C23—C22—O6 | 172.84 (14) | C26—C27—C28—C23 | -1.0 (3) |
| C24—C23—C22—O6 | -7.2 (2) | C1—C27—C28—C23 | -179.65 (13) |
| C28—C23—C22—O6 | 172.84 (14) | C24—C23—C28—C27 | 0.2 (2) |
| C22—O6—C3—C2 | -110.45 (16) | C22—C23—C28—C27 | -179.86 (15) |
| C22—O6—C3—C4 | 72.9 (2) | C13—C8—C9—C10 | 0.1 (3) |
| C4—C3—C2—C1 | -0.3 (2) | O2—C8—C9—C10 | -175.81 (15) |
| O6—C3—C2—C1 | -176.95 (13) | O2—C8—C9—C10 | -175.81 (15) |
| O6—C3—C2—C1 | -176.95 (13) | C8—C9—C10—C11 | 0.3 (3) |
| C3—C2—C1—C6 | -0.1 (2) | C12—C11—C10—C9 | -0.3 (3) |
| C3—C2—C1—C7 | -177.12 (15) | C14—C11—C10—C9 | 177.15 (16) |
| C8—O2—C7—O1 | -3.1 (3) | C19—C18—C17—C16 | -0.8 (3) |
| C8—O2—C7—C1 | 176.36 (15) | C21—C18—C17—C16 | 178.11 (17) |
| C6—C1—C7—O1 | -2.8 (3) | C20—C15—C16—C17 | -0.2 (3) |
| C2—C1—C7—O1 | 174.35 (17) | O4—C15—C16—C17 | 175.92 (16) |
| C6—C1—C7—O2 | 177.76 (14) | O4—C15—C16—C17 | 175.92 (16) |
| C2—C1—C7—O2 | -5.1 (2) | C18—C17—C16—C15 | 0.7 (3) |
| C6—C1—C7—O2 | 177.76 (14) | C2—C1—C6—C5 | 0.3 (2) |
| C2—C1—C7—O2 | -5.1 (2) | C7—C1—C6—C5 | 177.48 (15) |
| C7—O2—C8—C13 | 99.95 (19) | C1—C6—C5—C4 | -0.1 (3) |
| C7—O2—C8—C9 | -84.0 (2) | C2—C3—C4—C5 | 0.5 (3) |
| C9—C8—C13—C12 | -0.6 (3) | O6—C3—C4—C5 | 177.03 (14) |
| O2—C8—C13—C12 | 175.35 (14) | O6—C3—C4—C5 | 177.03 (14) |
| O2—C8—C13—C12 | 175.35 (14) | C6—C5—C4—C3 | -0.3 (3) |
| C8—C13—C12—C11 | 0.7 (2) | C35—C30—C31—C32 | -0.3 (4) |
| C13—C12—C11—C10 | -0.2 (2) | C29—C30—C31—C32 | -175.3 (2) |
| C13—C12—C11—C14 | -177.55 (15) | C34—C33—C32—C31 | 0.7 (4) |
| C15—O4—C14—O3 | -7.2 (3) | C30—C31—C32—C33 | -0.9 (4) |

Hydrogen-bond geometry (\AA , $^\circ$)

Cg4 and cg5 are the centroids of the C23–C28 and C30–C35 rings, respectively.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|------------|-------------|-------------|---------------|
| C2—H2 \cdots O2 | 0.944 (18) | 2.411 (17) | 2.7213 (19) | 98.9 (12) |
| C12—H12 \cdots O4 | 0.93 | 2.42 | 2.733 (2) | 100 |
| C24—H24 \cdots O6 | 0.93 | 2.40 | 2.721 (2) | 100 |
| C17—H17 \cdots N1 ⁱ | 0.93 | 2.62 | 3.504 (3) | 158 |

| | | | | |
|------------------------------|------|------|-----------|-----|
| C25—H25...Cg5 ⁱⁱ | 0.93 | 2.86 | 3.744 (2) | 158 |
| C31—H31...Cg4 ⁱⁱⁱ | 0.93 | 2.82 | 3.702 (3) | 158 |

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