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Synthesis and structure of 4-[(2,3,4,5,6-pentafluorophenoxy)carbonyl]phenyl 4-(tetradecyloxy)benzoate

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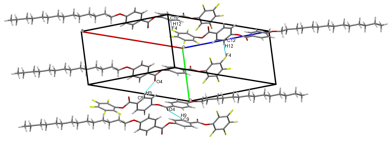
In the title molecule, $C_{34}H_{37}F_5O_5$, the dihedral angles between the central carbonylphenyl and adjacent perfluorophenoxy and (tetradecyloxy)benzoate rings are 74.19 (2) and 67.86 (2)°, respectively and the tetradecyl chain adopts an extended conformation. In the crystal, the molecules are linked by C—H···O and C—H···F hydrogen bonds, forming *C*(7) and *C*(10) chains, respectively, both running infinitely along [010]. The Hirshfeld surface analysis reveals that the major contributions to the two dimensional fingerprint plots are from H···H (49.4%), F···H/H···F (16.7%) and O···H/H···O (9.0%) contacts. An intermolecular interaction energy calculation shows that dispersion energy contributes the most to the consolidation of the structure.

1. Chemical context

Benzophenone derivatives have been reported to inhibit leukotriene release and have been evaluated as inhibitors of HIV reverse transcriptase, where their activity has been attributed to hydrogen-bonding and π–π interactions (Mahendra *et al.*, 2005). In addition to their pharmaceutical importance, aromatic ester systems such as phenyl benzoates have been widely studied in the field of thermotropic liquid crystals. These materials consist of rigid aromatic cores linked to flexible terminal chains, which have played an important role in governing mesophase formation and stability. Structural modifications have significantly influenced phase behaviour; rigid lateral substituents have tended to disrupt molecular packing, whereas flexible alkyl or alkoxy chains have modulated phase transitions depending on chain length (Yao *et al.*, 2021). Furthermore, fluorine substitution has been recognized as an effective strategy for tuning molecular properties, as it can modify dipole moments, enhance thermal and chemical stability, and influence intermolecular interactions.

Recently, liquid-crystalline materials have gained increasing attention due to their interactions with biological systems. Studies have indicated that such materials have influenced biological activity by reducing bacterial viability and affecting biochemical pathways such as peroxisome proliferator-activated receptor gamma (PPARγ) regulation (Li *et al.*, 2024). Finally, alkyl chains have played a significant role in enhancing the biological performance of organic molecules by improving cell membrane permeability. Increased chain length has been associated with improved anticancer, anti-tuberculosis, and



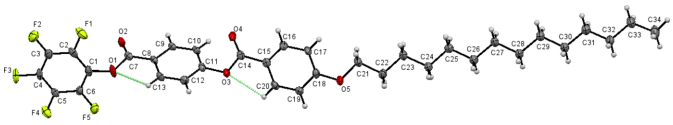
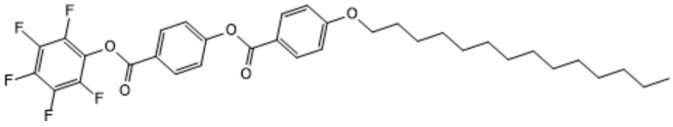


Figure 1
The molecular structure of (**I**) showing 50% probability ellipsoids.

anti-inflammatory activities, owing to better interaction with biological targets (Devarajegowda *et al.*, 2025). As part of our studies in this area, we now describe the synthesis and structure of the title compound, $C_{34}H_{37}F_5O_5$ (**I**).



2. Structural commentary

The molecular structure of (**I**) is presented in Fig. 1. The dihedral angle between the perfluorophenoxy ring (atoms C1–C6) and central carbonylphenyl (C8–C13) and (tetradecyloxy) benzoate (C15–C20) rings are 74.19 (2) and 67.86 (2)°, respectively, indicating that the central aromatic ring is approximately normal to the two adjacent rings. The dihedral angle between the outer rings of 6.93 (3)° indicates that they are approximately parallel to each other. The torsion angle associated with the ester groups between the perfluorophenoxy and carbonylphenyl, and carbonylphenyl and (tetradecyloxy)benzoate rings are −175.8 (3)° for C8—C7—O1—C1 and −172.5 (3)° for C15—C14—O3—C11, whereas the C18—O5—C21—C22 torsion angle across the oxygen atom of the (tetradecyloxy)benzoate ring and the C_{14} alkyl chain is found to be 179.9 (3)°. Otherwise the bond lengths and angles are normal. Two short intramolecular C—H···O contacts (Table 1) may help to consolidate the molecular conformation.

3. Supramolecular features

In the extended structure of (**I**), a C9—H9···O4 hydrogen bond (Table 1) connects molecules into a *C*(7) chain propagating along [010]. The chain is consolidated by a C12—H12···F4 hydrogen bond, which generates a C(10) chain (Fig. 2). Three C—F···π interactions, namely C3—F2···*Cg*3, C5—F4···*Cg*3 and C6—F5···*Cg*2 where *Cg*2 and *Cg*3 are the centroids of central carbonylphenyl and (tetradecyloxy)benzoate rings, respectively, are seen. Weak aromatic π–π stacking interactions, namely *Cg*1···*Cg*3, with a centroid–centroid distance of 4.078 (3) Å (slippage = 2.583 Å) and *Cg*2···*Cg*2 [centroid–centroid separation = 3.792 (3) Å, slippage = 1.726 Å], where *Cg*1 is centroid of the perfluorophenoxy ring (see supplementary figures) may help to consolidate the packing.

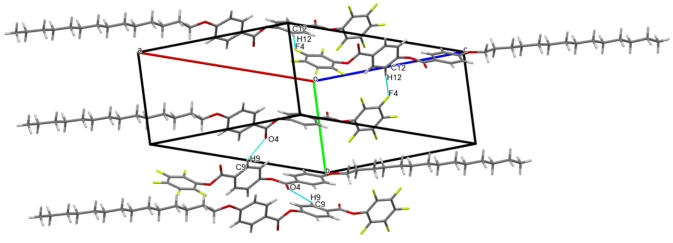


Figure 2
The packing diagram of (**I**) showing C—H···O and C—H···F hydrogen bonds as blue dashed lines.

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, C8–C13 and C15–C20 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···O3	0.93	2.45	2.753 (4)	99
C13—H13···O1	0.93	2.40	2.720 (4)	100
C9—H9···O4^{i}	0.93	2.52	3.177 (4)	128
C12—H12···F4^{ii}	0.93	2.50	3.425 (4)	172
C3—F2···*Cg*3^{iii}	1.33 (1)	3.30 (1)	3.634 (4)	94 (1)
C5—F4···*Cg*3^{iv}	1.34 (1)	3.15 (1)	3.385 (4)	88 (1)
C6—F5···*Cg*2^{v}	1.35 (1)	3.48 (1)	4.077 (4)	107 (1)

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+1, -y+1, -z$; (iv) $-x+1, -y, -z$; (v) $x, -y-\frac{1}{2}, z-\frac{3}{2}$.

4. Database survey

A search of the Cambridge Structural Database (CSD, version 6.01, March 2026; Groom *et al.*, 2016) for structures containing the phenyl benzoate moiety yielded more than 30 hits. Among these, five closely related structures with CSD refcodes HEKLAN (Dey *et al.*, 2017), MEXCOJ (Ambekar *et al.*, 2013), OQALOL (Mandal *et al.*, 2025), CIKTEW (Gowda *et al.*, 2007), and KUTGOW (Moumou *et al.*, 2010) feature substituted aromatic rings or long alkyl chains. In these structures, the dihedral angles between the phenyl ring and the aromatic ring of the benzoate moiety lie between 62 and 76° compared to 67.86 (2)° in (**I**). In all these structures, the ester linkages adopt their expected conformations with C—C—O—C torsion angles close to 180°.

5. Hirshfeld surface analysis

The Hirshfeld surface analysis of (**I**), mapped over d_{norm}, obtained using *CrystalExplorer* (Spackman *et al.*, 2021), is

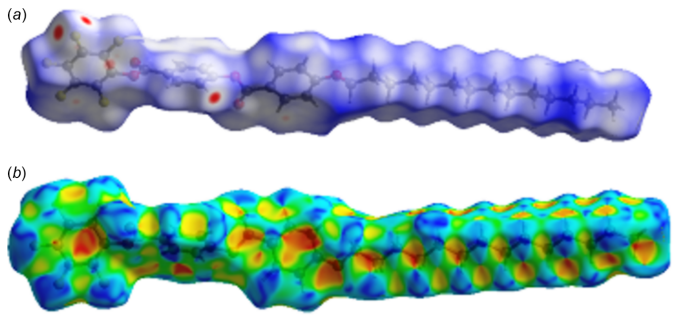


Figure 3
Views of the three-dimensional Hirshfeld surface of (**I**) mapped over (*a*) d_{norm} and (*b*) shape-index.

presented in Fig. 3. The two-dimensional fingerprint plots indicate that the contributions to the crystal packing are from H···H: (49.4%), F···H/H···F: (16.7%), C···H/H···C: (7.3%), C···F/F···C: (7%) F···O/O···F: (2.3%), F···F: (1.9%) contacts as shown in Fig. 4. The interaction energies were computed for (**I**) using the basis set B3LYP\631-G(d,p) for the molecular pairs within a cluster of 3.8 Å radius. The net interaction energies were calculated as E_{ele} = −59.6 kJ mol^{-1}, E_{pol} = −14.1 kJ mol^{-1}, E_{dis} = −464.8 kJ mol^{-1}, E_{rep} = +142.2 kJ mol^{-1} and total interaction energy E_{tot} = -390.4 kJ mol^{-1}. The overall interaction energy is strongly negative, confirming that the crystal packing is energetically favourable and primarily governed by dispersion forces. The topology of energy frameworks for the Coloumbic, dispersion and total energies are shown in Fig. 5.

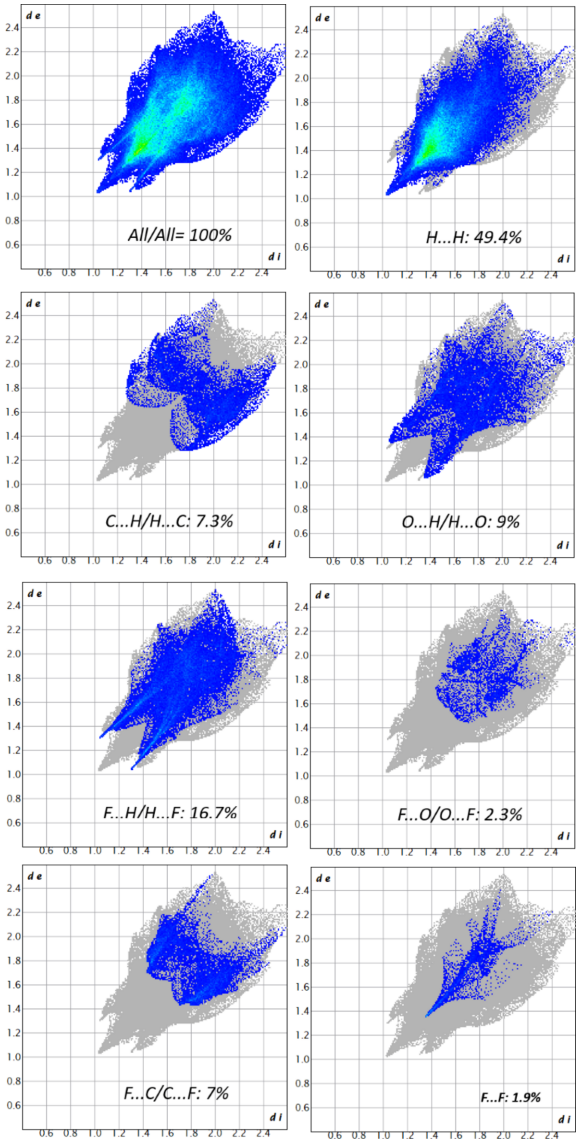


Figure 4
The two-dimensional fingerprint plots for (**I**), showing the contributions of the different contact types to the Hirshfeld surface.

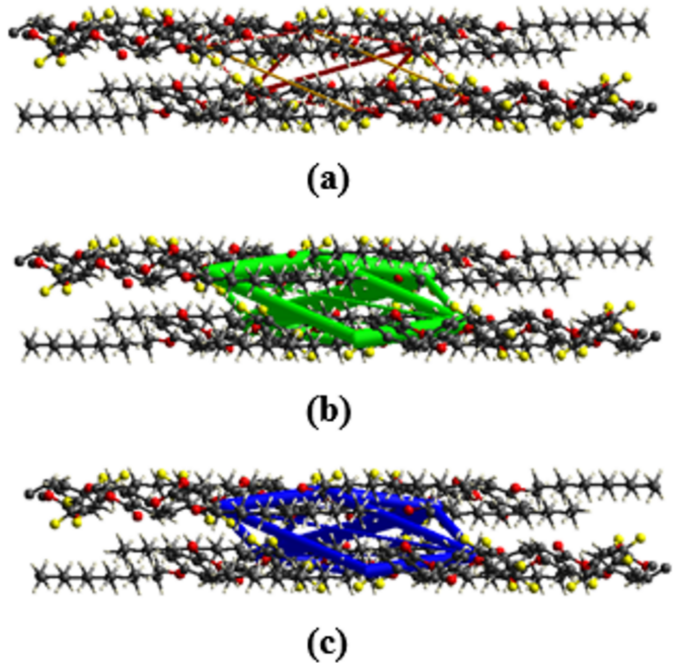


Figure 5
The energy frameworks for the interaction energies of (**I**): (*a*) Coloumbic energy, (*b*) dispersion energy and (*c*) total energy.

6. Synthesis and crystallization

A reaction mixture of 2,3,4,5,6-pentafluorophenol (0.184 g, 1 eq) and 4-{[4-(tetradecyloxy)benzoyl]oxy}benzoic acid (0.454 g, 1 eq) in dichloromethane was stirred at room temperature overnight using the DCC esterification process in the presence of *N*,*N*-dimethylaminopyrimidine as a catalyst. The insoluble byproduct dicyclohexyl urea was removed by filtration. The filtrate was washed with 5% acetic acid solution in water and then with pure water. The filtrate was passed through silica gel, and then left undisturbed for a week to grow crystals of (**I**) for X-ray studies. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.12–8.02 (*m*, 4H, Ar-H), 7.54 (*m*, 2H, Ar-H), 7.10 (*d*, *J* = 8.5Hz, 2H, Ar-H), 4.01 (*t*, *J* = 6.5Hz, 2H, –OCH_2–), 1.74–1.25 (*m*, 24H, –CH_2–alkyl), 0.91 (*t*, *J* = 4.5Hz, 3H, –CH_3) ppm. Elemental analysis (%) calculated: C 65.80; H 6.01; F 15.31; O 12.89; found C 65.85; H 6.05; F 15.28%. Since the title compound has liquid crystal properties, results will be reported in due course.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen-atom positions were calculated geometrically (C—H = 0.93–0.97 Å) and refined using a riding model by applying the constraint U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

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Sheldrick, G. M. (2015*b*). *Acta Cryst.* A**71**, 3–8.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{34}H_{37}F_5O_5$
M_r	620.66
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	423
a, b, c (Å)	27.811 (16), 8.206 (5), 13.975 (8)
β (°)	103.868 (14)
V (Å^3)	3096 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.43 × 0.32 × 0.27
Data collection	
Diffractometer	Bruker *SMART* APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.954, 0.970
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28865, 5466, 4231
R_{int}	0.063
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.078, 0.165, 1.15
No. of reflections	5466
No. of parameters	398
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.29

Computer programs: *APEX2* and *SAINT* (Bruker, 2017), *SHELXT2018/3* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip,2010).

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supporting information

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Synthesis and structure of 4-[(2,3,4,5,6-pentafluorophenoxy)carbonyl]phenyl 4-(tetradecyloxy)benzoate

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Computing details

4-[(2,3,4,5,6-Pentafluorophenoxy)carbonyl]phenyl 4-(tetradecyloxy)benzoate

Crystal data

$C_{34}H_{37}F_5O_5$
M_r = 620.66
Monoclinic, $P2_1/c$
a = 27.811 (16) Å
b = 8.206 (5) Å
c = 13.975 (8) Å
β = 103.868 (14)°
V = 3096 (3) Å^3
Z = 4
$F(000)$ = 1304
prism
D_x = 1.331 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4231 reflections
θ = 2.5–25.0°
μ = 0.11 mm^{-1}
T = 423 K
Prism, colourless
0.43 × 0.32 × 0.27 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 2.09 pixels mm^{-1}
φ and Ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.954, T_{max} = 0.970
28865 measured reflections
5466 independent reflections
4231 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 25.0°, θ_{min} = 2.6°
h = −32→33
k = −9→9
l = −15→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.165
S = 1.15
5466 reflections
398 parameters
0 restraints
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 4.4152P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: SHELXL2019/2 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0020 (6)

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}
O2	0.38024 (8)	0.6170 (3)	0.48615 (16)	0.0262 (5)
F4	0.35716 (8)	0.5541 (2)	0.87454 (14)	0.0381 (5)
F5	0.42775 (7)	0.5653 (2)	0.77188 (14)	0.0353 (5)
O3	0.59440 (7)	0.7225 (3)	0.40331 (16)	0.0251 (5)
O1	0.41978 (8)	0.7700 (3)	0.61509 (17)	0.0345 (6)
O5	0.77655 (8)	0.6657 (3)	0.21290 (16)	0.0300 (6)
C8	0.46276 (11)	0.7110 (3)	0.4931 (2)	0.0183 (7)
C1	0.38045 (12)	0.7534 (4)	0.6592 (2)	0.0266 (8)
C27	0.96003 (12)	0.6387 (5)	−0.2196 (2)	0.0310 (8)
H27A	0.944781	0.736989	−0.251815	0.037*
H27B	0.943268	0.546417	−0.256432	0.037*
C14	0.59713 (12)	0.7989 (4)	0.3177 (2)	0.0230 (7)
C15	0.64528 (11)	0.7663 (4)	0.2936 (2)	0.0219 (7)
C26	0.95197 (12)	0.6331 (5)	−0.1166 (2)	0.0317 (8)
H26A	0.970501	0.721440	−0.078670	0.038*
H26B	0.965523	0.531679	−0.085900	0.038*
F2	0.25856 (8)	0.9160 (3)	0.64890 (16)	0.0486 (6)
C28	1.01423 (12)	0.6359 (5)	−0.2243 (2)	0.0327 (8)
H28A	1.030786	0.729941	−0.189119	0.039*
H28B	1.029729	0.539202	−0.190492	0.039*
F1	0.33047 (9)	0.9358 (3)	0.54875 (15)	0.0470 (6)
C7	0.41639 (12)	0.6913 (4)	0.5266 (2)	0.0208 (7)
C22	0.83173 (12)	0.6435 (4)	0.1067 (2)	0.0296 (8)
H22A	0.837076	0.530673	0.127156	0.036*
H22B	0.856248	0.709328	0.151254	0.036*
O4	0.56406 (8)	0.8788 (3)	0.27024 (17)	0.0318 (6)
C11	0.54874 (11)	0.7260 (4)	0.4293 (2)	0.0208 (7)
C31	1.08395 (12)	0.6394 (5)	−0.4360 (3)	0.0327 (8)
H31A	1.070576	0.537908	−0.466831	0.039*
H31B	1.065120	0.727644	−0.473462	0.039*
C10	0.50888 (11)	0.6382 (4)	0.3745 (2)	0.0211 (7)
H10	0.511179	0.585478	0.316830	0.025*
C24	0.89144 (12)	0.6334 (4)	−0.0056 (2)	0.0287 (8)
H24A	0.901917	0.526046	0.020164	0.034*
H24B	0.912800	0.712690	0.035420	0.034*
C32	1.13746 (12)	0.6541 (5)	−0.4426 (3)	0.0315 (8)
H32A	1.150637	0.757311	−0.414001	0.038*
H32B	1.156626	0.567831	−0.403756	0.038*
C23	0.83867 (12)	0.6616 (4)	0.0023 (2)	0.0290 (8)

H23A	0.817124	0.584640	−0.040248	0.035*
H23B	0.828538	0.770368	−0.021307	0.035*
F3	0.27248 (8)	0.7280 (3)	0.81361 (16)	0.0456 (6)
C20	0.68342 (11)	0.6751 (4)	0.3539 (2)	0.0238 (7)
H20	0.679478	0.633695	0.413501	0.029*
C13	0.50303 (12)	0.7993 (4)	0.5465 (2)	0.0242 (7)
H13	0.500851	0.853027	0.603950	0.029*
C30	1.07635 (12)	0.6437 (5)	−0.3320 (2)	0.0322 (8)
H30A	1.090985	0.742796	−0.299860	0.039*
H30B	1.093700	0.552203	−0.295247	0.039*
C9	0.46602 (11)	0.6307 (4)	0.4067 (2)	0.0193 (7)
H9	0.439060	0.571916	0.370932	0.023*
C19	0.72662 (12)	0.6467 (4)	0.3252 (2)	0.0256 (7)
H19	0.752020	0.588183	0.366316	0.031*
C5	0.35055 (12)	0.6489 (4)	0.7945 (2)	0.0247 (7)
C16	0.65249 (12)	0.8267 (4)	0.2043 (2)	0.0253 (7)
H16	0.627599	0.888183	0.163886	0.030*
C6	0.38649 (11)	0.6553 (4)	0.7414 (2)	0.0227 (7)
C17	0.69537 (12)	0.7975 (4)	0.1749 (2)	0.0260 (8)
H17	0.699454	0.839085	0.115490	0.031*
C25	0.89840 (12)	0.6459 (4)	−0.1102 (2)	0.0292 (8)
H25A	0.879485	0.559996	−0.149846	0.035*
H25B	0.885100	0.749354	−0.138261	0.035*
C18	0.73277 (11)	0.7049 (4)	0.2349 (2)	0.0235 (7)
C12	0.54617 (12)	0.8074 (4)	0.5145 (2)	0.0240 (7)
H12	0.573131	0.866797	0.549667	0.029*
C33	1.14389 (13)	0.6441 (5)	−0.5472 (3)	0.0375 (9)
H33A	1.123245	0.726665	−0.586683	0.045*
H33B	1.132153	0.538652	−0.574443	0.045*
C29	1.02213 (12)	0.6368 (5)	−0.3279 (3)	0.0313 (8)
H29A	1.005045	0.730135	−0.362958	0.038*
H29B	1.007275	0.539454	−0.361860	0.038*
C3	0.30040 (12)	0.8311 (4)	0.6789 (3)	0.0286 (8)
C21	0.78072 (12)	0.6952 (4)	0.1137 (2)	0.0294 (8)
H21A	0.775738	0.809945	0.097782	0.035*
H21B	0.755791	0.633271	0.067471	0.035*
C34	1.19685 (14)	0.6671 (5)	−0.5561 (3)	0.0488 (11)
H34A	1.197913	0.659169	−0.624146	0.073*
H34B	1.208594	0.772407	−0.531093	0.073*
H34C	1.217514	0.584132	−0.518835	0.073*
C4	0.30756 (12)	0.7354 (4)	0.7631 (3)	0.0286 (8)
C2	0.33696 (13)	0.8384 (4)	0.6280 (2)	0.0299 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0286 (12)	0.0312 (13)	0.0225 (12)	−0.0024 (11)	0.0136 (10)	−0.0085 (10)
F4	0.0579 (14)	0.0315 (11)	0.0309 (12)	0.0028 (10)	0.0222 (10)	0.0050 (9)

F5	0.0306 (11)	0.0402 (12)	0.0363 (12)	0.0074 (9)	0.0104 (9)	−0.0101 (10)
O3	0.0229 (12)	0.0322 (13)	0.0238 (12)	0.0042 (10)	0.0126 (9)	0.0100 (10)
O1	0.0363 (14)	0.0457 (15)	0.0301 (14)	−0.0156 (12)	0.0246 (11)	−0.0174 (12)
O5	0.0225 (12)	0.0443 (15)	0.0270 (13)	0.0043 (11)	0.0135 (10)	0.0052 (11)
C8	0.0273 (17)	0.0141 (14)	0.0153 (16)	0.0005 (13)	0.0084 (13)	0.0006 (12)
C1	0.0275 (18)	0.0291 (18)	0.0272 (18)	−0.0072 (15)	0.0144 (14)	−0.0115 (15)
C27	0.0261 (18)	0.044 (2)	0.0242 (19)	−0.0005 (16)	0.0094 (14)	0.0019 (16)
C14	0.0278 (18)	0.0184 (16)	0.0253 (18)	−0.0006 (14)	0.0113 (14)	0.0009 (14)
C15	0.0261 (17)	0.0170 (16)	0.0243 (17)	−0.0011 (13)	0.0092 (14)	−0.0010 (13)
C26	0.0285 (18)	0.042 (2)	0.0262 (19)	0.0014 (16)	0.0100 (15)	0.0040 (17)
F2	0.0381 (12)	0.0579 (15)	0.0480 (14)	0.0220 (11)	0.0069 (10)	−0.0046 (12)
C28	0.0263 (18)	0.048 (2)	0.0249 (19)	0.0040 (17)	0.0089 (14)	0.0027 (17)
F1	0.0722 (16)	0.0470 (13)	0.0250 (12)	0.0064 (12)	0.0180 (11)	0.0074 (10)
C7	0.0307 (18)	0.0146 (15)	0.0179 (17)	0.0019 (14)	0.0075 (14)	−0.0003 (13)
C22	0.0228 (17)	0.037 (2)	0.031 (2)	−0.0023 (15)	0.0109 (14)	−0.0016 (16)
O4	0.0288 (13)	0.0400 (14)	0.0319 (14)	0.0137 (11)	0.0177 (11)	0.0196 (12)
C11	0.0248 (17)	0.0193 (16)	0.0214 (17)	0.0010 (13)	0.0116 (13)	0.0069 (13)
C31	0.0307 (19)	0.039 (2)	0.030 (2)	0.0021 (16)	0.0104 (15)	0.0015 (16)
C10	0.0299 (18)	0.0195 (16)	0.0163 (16)	0.0019 (14)	0.0104 (13)	−0.0012 (13)
C24	0.0261 (18)	0.038 (2)	0.0246 (18)	0.0018 (16)	0.0108 (14)	0.0027 (16)
C32	0.0298 (19)	0.036 (2)	0.032 (2)	0.0052 (16)	0.0140 (15)	0.0034 (16)
C23	0.0267 (18)	0.037 (2)	0.0262 (19)	0.0008 (15)	0.0117 (14)	0.0000 (15)
F3	0.0407 (12)	0.0570 (14)	0.0526 (14)	0.0028 (11)	0.0374 (11)	−0.0035 (12)
C20	0.0280 (18)	0.0277 (18)	0.0178 (17)	−0.0062 (14)	0.0099 (13)	0.0004 (14)
C13	0.0345 (19)	0.0227 (17)	0.0176 (17)	−0.0008 (15)	0.0102 (14)	−0.0067 (14)
C30	0.0280 (19)	0.043 (2)	0.0273 (19)	0.0022 (16)	0.0102 (15)	0.0027 (16)
C9	0.0237 (16)	0.0189 (15)	0.0158 (16)	−0.0002 (13)	0.0062 (13)	0.0009 (13)
C19	0.0236 (17)	0.0317 (18)	0.0213 (18)	0.0013 (15)	0.0049 (13)	0.0029 (15)
C5	0.0344 (19)	0.0229 (16)	0.0191 (17)	0.0003 (15)	0.0112 (14)	−0.0027 (14)
C16	0.0273 (18)	0.0223 (17)	0.0288 (19)	0.0037 (14)	0.0117 (14)	0.0061 (14)
C6	0.0212 (16)	0.0232 (17)	0.0246 (18)	0.0013 (14)	0.0073 (13)	−0.0082 (14)
C17	0.0281 (18)	0.0315 (18)	0.0218 (18)	0.0022 (15)	0.0124 (14)	0.0080 (15)
C25	0.0267 (18)	0.0355 (19)	0.0261 (19)	0.0022 (15)	0.0074 (14)	0.0019 (15)
C18	0.0224 (17)	0.0238 (16)	0.0267 (18)	−0.0066 (14)	0.0107 (14)	−0.0033 (14)
C12	0.0245 (17)	0.0225 (17)	0.0245 (18)	−0.0042 (14)	0.0050 (14)	0.0002 (14)
C33	0.038 (2)	0.046 (2)	0.033 (2)	0.0020 (18)	0.0182 (17)	0.0009 (18)
C29	0.0274 (18)	0.040 (2)	0.0293 (19)	0.0017 (16)	0.0119 (15)	0.0022 (16)
C3	0.0291 (18)	0.0298 (19)	0.0272 (19)	0.0047 (15)	0.0074 (15)	−0.0086 (15)
C21	0.0302 (19)	0.036 (2)	0.0258 (19)	0.0019 (16)	0.0138 (15)	0.0021 (16)
C34	0.047 (2)	0.057 (3)	0.053 (3)	0.004 (2)	0.032 (2)	0.007 (2)
C4	0.0271 (18)	0.0342 (19)	0.031 (2)	−0.0054 (15)	0.0191 (15)	−0.0130 (16)
C2	0.044 (2)	0.0300 (19)	0.0180 (18)	−0.0052 (16)	0.0122 (15)	−0.0046 (15)

Geometric parameters (Å, º)

O2—C7	1.196 (4)	C24—C23	1.516 (4)
F4—C5	1.339 (4)	C24—C25	1.524 (4)
F5—C6	1.345 (4)	C24—H24A	0.9700

O3—C14	1.369 (4)	C24—H24B	0.9700
O3—C11	1.403 (4)	C32—C33	1.517 (5)
O1—C7	1.378 (4)	C32—H32A	0.9700
O1—C1	1.385 (4)	C32—H32B	0.9700
O5—C18	1.363 (4)	C23—H23A	0.9700
O5—C21	1.439 (4)	C23—H23B	0.9700
C8—C13	1.391 (4)	F3—C4	1.335 (4)
C8—C9	1.397 (4)	C20—C19	1.374 (4)
C8—C7	1.482 (4)	C20—H20	0.9300
C1—C2	1.374 (5)	C13—C12	1.379 (4)
C1—C6	1.379 (5)	C13—H13	0.9300
C27—C26	1.510 (4)	C30—C29	1.524 (4)
C27—C28	1.525 (4)	C30—H30A	0.9700
C27—H27A	0.9700	C30—H30B	0.9700
C27—H27B	0.9700	C9—H9	0.9300
C14—O4	1.193 (4)	C19—C18	1.398 (4)
C14—C15	1.481 (4)	C19—H19	0.9300
C15—C16	1.402 (4)	C5—C4	1.369 (5)
C15—C20	1.403 (4)	C5—C6	1.381 (4)
C26—C25	1.517 (4)	C16—C17	1.372 (4)
C26—H26A	0.9700	C16—H16	0.9300
C26—H26B	0.9700	C17—C18	1.394 (5)
F2—C3	1.335 (4)	C17—H17	0.9300
C28—C29	1.515 (5)	C25—H25A	0.9700
C28—H28A	0.9700	C25—H25B	0.9700
C28—H28B	0.9700	C12—H12	0.9300
F1—C2	1.343 (4)	C33—C34	1.520 (5)
C22—C21	1.506 (4)	C33—H33A	0.9700
C22—C23	1.523 (5)	C33—H33B	0.9700
C22—H22A	0.9700	C29—H29A	0.9700
C22—H22B	0.9700	C29—H29B	0.9700
C11—C12	1.381 (4)	C3—C2	1.375 (5)
C11—C10	1.388 (4)	C3—C4	1.389 (5)
C31—C32	1.518 (5)	C21—H21A	0.9700
C31—C30	1.519 (5)	C21—H21B	0.9700
C31—H31A	0.9700	C34—H34A	0.9600
C31—H31B	0.9700	C34—H34B	0.9600
C10—C9	1.373 (4)	C34—H34C	0.9600
C10—H10	0.9300		

C14—O3—C11	117.4 (2)	C22—C23—H23B	108.8
C7—O1—C1	117.5 (3)	H23A—C23—H23B	107.7
C18—O5—C21	117.4 (2)	C19—C20—C15	120.2 (3)
C13—C8—C9	119.9 (3)	C19—C20—H20	119.9
C13—C8—C7	122.5 (3)	C15—C20—H20	119.9
C9—C8—C7	117.6 (3)	C12—C13—C8	120.1 (3)
C2—C1—C6	118.9 (3)	C12—C13—H13	119.9
C2—C1—O1	122.5 (3)	C8—C13—H13	119.9

C6—C1—O1	118.5 (3)	C31—C30—C29	113.6 (3)
C2—C1—O1	122.5 (3)	C31—C30—H30A	108.8
C6—C1—O1	118.5 (3)	C29—C30—H30A	108.8
C26—C27—C28	114.5 (3)	C31—C30—H30B	108.8
C26—C27—H27A	108.6	C29—C30—H30B	108.8
C28—C27—H27A	108.6	H30A—C30—H30B	107.7
C26—C27—H27B	108.6	C10—C9—C8	120.2 (3)
C28—C27—H27B	108.6	C10—C9—H9	119.9
H27A—C27—H27B	107.6	C8—C9—H9	119.9
O4—C14—O3	122.7 (3)	C20—C19—C18	120.7 (3)
O4—C14—O3	122.7 (3)	C20—C19—H19	119.7
O4—C14—C15	126.3 (3)	C18—C19—H19	119.7
O3—C14—C15	111.0 (3)	F4—C5—C4	120.2 (3)
O3—C14—C15	111.0 (3)	F4—C5—C6	119.9 (3)
C16—C15—C20	118.4 (3)	C4—C5—C6	119.8 (3)
C16—C15—C14	117.9 (3)	C17—C16—C15	121.6 (3)
C20—C15—C14	123.7 (3)	C17—C16—H16	119.2
C27—C26—C25	115.2 (3)	C15—C16—H16	119.2
C27—C26—H26A	108.5	F5—C6—C1	120.6 (3)
C25—C26—H26A	108.5	F5—C6—C5	118.8 (3)
C27—C26—H26B	108.5	C1—C6—C5	120.7 (3)
C25—C26—H26B	108.5	C16—C17—C18	119.5 (3)
H26A—C26—H26B	107.5	C16—C17—H17	120.2
C29—C28—C27	114.3 (3)	C18—C17—H17	120.2
C29—C28—H28A	108.7	C26—C25—C24	113.8 (3)
C27—C28—H28A	108.7	C26—C25—H25A	108.8
C29—C28—H28B	108.7	C24—C25—H25A	108.8
C27—C28—H28B	108.7	C26—C25—H25B	108.8
H28A—C28—H28B	107.6	C24—C25—H25B	108.8
O2—C7—O1	122.1 (3)	H25A—C25—H25B	107.7
O2—C7—O1	122.1 (3)	O5—C18—C17	124.8 (3)
O2—C7—C8	127.1 (3)	O5—C18—C19	115.6 (3)
O1—C7—C8	110.8 (3)	C17—C18—C19	119.6 (3)
O1—C7—C8	110.8 (3)	C13—C12—C11	119.0 (3)
C21—C22—C23	111.8 (3)	C13—C12—H12	120.5
C21—C22—H22A	109.2	C11—C12—H12	120.5
C23—C22—H22A	109.2	C32—C33—C34	114.4 (3)
C21—C22—H22B	109.2	C32—C33—H33A	108.7
C23—C22—H22B	109.2	C34—C33—H33A	108.7
H22A—C22—H22B	107.9	C32—C33—H33B	108.7
C12—C11—C10	121.8 (3)	C34—C33—H33B	108.7
C12—C11—O3	118.0 (3)	H33A—C33—H33B	107.6
C10—C11—O3	119.9 (3)	C28—C29—C30	114.1 (3)
C12—C11—O3	118.0 (3)	C28—C29—H29A	108.7
C10—C11—O3	119.9 (3)	C30—C29—H29A	108.7
C32—C31—C30	114.8 (3)	C28—C29—H29B	108.7
C32—C31—H31A	108.6	C30—C29—H29B	108.7
C30—C31—H31A	108.6	H29A—C29—H29B	107.6

C32—C31—H31B	108.6	F2—C3—C2	120.8 (3)
C30—C31—H31B	108.6	F2—C3—C4	119.9 (3)
H31A—C31—H31B	107.5	C2—C3—C4	119.3 (3)
C9—C10—C11	118.9 (3)	O5—C21—C22	108.1 (3)
C9—C10—H10	120.6	O5—C21—H21A	110.1
C11—C10—H10	120.6	C22—C21—H21A	110.1
C23—C24—C25	114.1 (3)	O5—C21—H21B	110.1
C23—C24—H24A	108.7	C22—C21—H21B	110.1
C25—C24—H24A	108.7	H21A—C21—H21B	108.4
C23—C24—H24B	108.7	C33—C34—H34A	109.5
C25—C24—H24B	108.7	C33—C34—H34B	109.5
H24A—C24—H24B	107.6	H34A—C34—H34B	109.5
C33—C32—C31	113.4 (3)	C33—C34—H34C	109.5
C33—C32—H32A	108.9	H34A—C34—H34C	109.5
C31—C32—H32A	108.9	H34B—C34—H34C	109.5
C33—C32—H32B	108.9	F3—C4—C5	120.0 (3)
C31—C32—H32B	108.9	F3—C4—C3	119.9 (3)
H32A—C32—H32B	107.7	C5—C4—C3	120.1 (3)
C24—C23—C22	113.7 (3)	F1—C2—C1	119.9 (3)
C24—C23—H23A	108.8	F1—C2—C3	118.9 (3)
C22—C23—H23A	108.8	C1—C2—C3	121.2 (3)
C24—C23—H23B	108.8		

C7—O1—C1—C2	−77.5 (4)	C2—C1—C6—C5	−3.3 (5)
C7—O1—C1—C6	106.5 (3)	O1—C1—C6—C5	172.8 (3)
C7—O1—C1—O1	0 (100)	O1—C1—C6—C5	172.8 (3)
C11—O3—C14—O4	6.8 (5)	F4—C5—C6—F5	−0.1 (5)
C11—O3—C14—C15	−172.5 (3)	C4—C5—C6—F5	−178.0 (3)
O4—C14—C15—C16	−3.6 (5)	F4—C5—C6—C1	−179.4 (3)
O3—C14—C15—C16	175.6 (3)	C4—C5—C6—C1	2.7 (5)
O3—C14—C15—C16	175.6 (3)	C15—C16—C17—C18	0.3 (5)
O4—C14—C15—C20	178.0 (3)	C27—C26—C25—C24	177.8 (3)
O3—C14—C15—C20	−2.7 (4)	C23—C24—C25—C26	174.7 (3)
O3—C14—C15—C20	−2.7 (4)	C21—O5—C18—C17	−12.3 (5)
C28—C27—C26—C25	176.5 (3)	C21—O5—C18—C19	168.3 (3)
C26—C27—C28—C29	178.4 (3)	C16—C17—C18—O5	178.9 (3)
C1—O1—C7—O2	3.3 (5)	C16—C17—C18—C19	−1.7 (5)
C1—O1—C7—C8	−175.8 (3)	C20—C19—C18—O5	−178.3 (3)
C13—C8—C7—O2	−179.4 (3)	C20—C19—C18—C17	2.3 (5)
C9—C8—C7—O2	−2.3 (5)	C8—C13—C12—C11	−0.4 (5)
C13—C8—C7—O1	−0.4 (4)	C10—C11—C12—C13	0.9 (5)
C9—C8—C7—O1	176.7 (3)	O3—C11—C12—C13	−173.9 (3)
C13—C8—C7—O1	−0.4 (4)	O3—C11—C12—C13	−173.9 (3)
C9—C8—C7—O1	176.7 (3)	C31—C32—C33—C34	177.1 (3)
C14—O3—C11—C12	−115.7 (3)	C27—C28—C29—C30	176.7 (3)
O3—O3—C11—C10	0.00 (11)	C31—C30—C29—C28	178.3 (3)
C14—O3—C11—C10	69.4 (4)	C18—O5—C21—C22	179.9 (3)
C12—C11—C10—C9	−0.9 (5)	C23—C22—C21—O5	176.9 (3)

O3—C11—C10—C9	173.8 (3)	F4—C5—C4—F3	1.4 (5)
O3—C11—C10—C9	173.8 (3)	C6—C5—C4—F3	179.2 (3)
C30—C31—C32—C33	178.2 (3)	F4—C5—C4—C3	−178.8 (3)
C25—C24—C23—C22	178.1 (3)	C6—C5—C4—C3	−0.9 (5)
C21—C22—C23—C24	172.0 (3)	F2—C3—C4—F3	0.2 (5)
C16—C15—C20—C19	0.0 (5)	C2—C3—C4—F3	179.6 (3)
C14—C15—C20—C19	178.4 (3)	F2—C3—C4—C5	−179.6 (3)
C9—C8—C13—C12	−0.1 (5)	C2—C3—C4—C5	−0.3 (5)
C7—C8—C13—C12	176.9 (3)	C6—C1—C2—F1	179.4 (3)
C32—C31—C30—C29	177.3 (3)	O1—C1—C2—F1	3.5 (5)
C11—C10—C9—C8	0.3 (5)	O1—C1—C2—F1	3.5 (5)
C13—C8—C9—C10	0.2 (5)	C6—C1—C2—C3	2.1 (5)
C7—C8—C9—C10	−177.0 (3)	O1—C1—C2—C3	−173.8 (3)
C15—C20—C19—C18	−1.4 (5)	O1—C1—C2—C3	−173.8 (3)
C20—C15—C16—C17	0.6 (5)	F2—C3—C2—F1	1.8 (5)
C14—C15—C16—C17	−177.9 (3)	C4—C3—C2—F1	−177.6 (3)
C2—C1—C6—F5	177.4 (3)	F2—C3—C2—C1	179.0 (3)
O1—C1—C6—F5	−6.5 (4)	C4—C3—C2—C1	−0.4 (5)
O1—C1—C6—F5	−6.5 (4)		

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, C8–C13 and C15–C20 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···O3	0.93	2.45	2.753 (4)	99
C13—H13···O1	0.93	2.40	2.720 (4)	100
C9—H9···O4^{i}	0.93	2.52	3.177 (4)	128
C12—H12···F4^{ii}	0.93	2.50	3.425 (4)	172
C3—F2···*Cg*3^{iii}	1.33 (1)	3.30 (1)	3.634 (4)	94 (1)
C5—F4···*Cg*3^{iv}	1.34 (1)	3.15 (1)	3.385 (4)	88 (1)
C6—F5···*Cg*2^{v}	1.35 (1)	3.48 (1)	4.077 (4)	107 (1)

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