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

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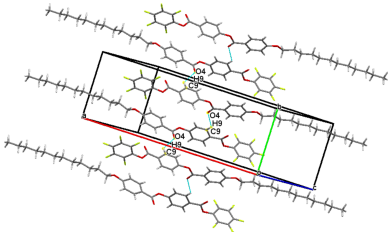
In the title compound, $C_{32}H_{33}F_5O_5$, the dihedral angle between the central carbonylpheyl and peripheral perfluorophenoxy and (dodecyloxy)benzoate rings are 85.24 (2) and 78.98 (2)°, respectively, indicating that the central ring is almost normal to both adjacent rings. The pendant C_{12} alkyl chain adopts an all-*anti* conformation. In the crystal, weak C—H···O hydrogen bonds connect the molecules, forming $S(7)$ chains propagating along the [010] direction. The packing is consolidated by C—F···π interactions and weak π–π stacking. The Hirshfeld surface analysis reveals that the major contributions to the two-dimensional fingerprint plots are from H···H (45%),F···H/H···F (18.5%), O···H/H···O (9.7%), C···H/H···C (9.4%), F···C/C···F (7.3%), and F···F (1.9%) contacts. An energy framework calculation shows that dispersion energy (–383.4 kJ mol^{-1}) makes by far the largest contribution.

1. Chemical context

Phenylbenzoate-based three-ring calamitic liquid crystals incorporating a 4-(dodecyloxy)benzoate terminal unit are well-established mesogens in which the dodecyloxy chain promotes layered organization, while ester linkages preserve the required rod-like geometry (Cakar *et al.*, 2022). The introduction of a perfluorophenoxy group at the opposite terminus is expected to influence both intermolecular interactions and physicochemical properties through fluorination (Ashmawy *et al.*, 2017; Podruczna *et al.*, 2014). Beyond their mesomorphic behaviour, derivatives bearing the 4-(dodecyloxy)benzoate motif have attracted attention due to their biological activities. In closely related systems, structural modification of the terminal substituent and alkyl chain length has been shown to significantly affect biological performance. For instance, bis(dodecyloxy)benzoate–poly(amidoamine) conjugates exhibit pronounced anticancer activity against a range of human cancer cell lines (Castillo-Rodrez *et al.*, 2023), while flutamide-linked 3,5-bis(dodecyloxy)benzoate derivatives demonstrate effective inhibition toward U-251, PC-3, K-562 and HCT-15 cell lines (Medina-Rojas *et al.*, 2020; Lukáč *et al.*, 2024). Similarly, incorporation of long alkyl chains in heterocyclic benzoate derivatives enhances corrosion inhibition efficiency, indicating strong surface adsorption driven by hydrophobic interactions (Kadhim *et al.*, 2023).

More generally, elongation of alkyl chains in organic molecules is known to enhance lipophilicity, thereby improving membrane permeability and facilitating cellular uptake, which is a key factor in drug design. This effect has been demon-



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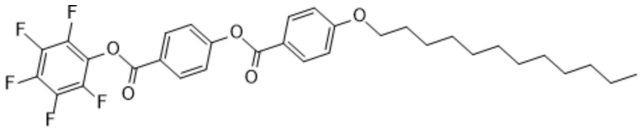
strated in several systems, including alkylated caffeic acid derivatives exhibiting anticancer properties, cinnamic acid analogues showing anti-tuberculosis activity (De *et al.*, 2011), and amide-based compounds with improved anti-inflammatory behaviour upon chain extension (Matta *et al.*, 2020). In this context, the present structural study of the title compound, $C_{32}H_{33}F_5O_5$ (**I**), provides insight into the molecular conformation of the C_{12}-alkyl chain and the intermolecular contacts governing crystal packing, which may contribute to both its mesomorphic characteristics and potential biological interactions (Koshti *et al.*, 2023; Singh *et al.*, 2016).



2. Structural commentary

The molecular structure of (**I**) is shown in Fig. 1. The dihedral angle between the aromatic rings of the perfluorophenoxy (C1–C6) and carbonylphenyl (C8–C13) fragments are 85.24 (2)° and the corresponding dihedral angle for the carbonylphenyl and (dodecyloxy)benzoate (C15–C20) rings is 78.98 (2)°, thus, the central ring is close to normal to both peripheral rings. The torsion angles associated with the C8—C7—O1—C1 and C15—C14—O3—C11 ester linkages are 175.6 (3) and 172.2 (3)°, respectively, indicating the expected *anti*-periplanar conformations. The pendant C_{12} alkyl chain adopts an all-*anti* conformation with the largest torsion angle deviation from ±180° being −173.1 (4)° for C21—C22—C23—C24. Two short intramolecular C—H···O contacts (Table 1) are observed. Otherwise, the bond length and the bond angles may be regarded as normal.

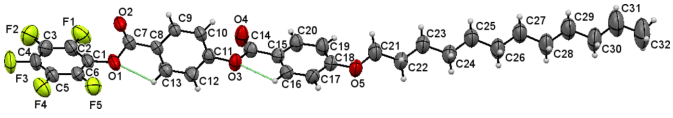


Figure 1
The molecular structure of (**I**) showing 50% probability ellipsoids. Short intramolecular —H···O contacts are shown as green dashed lines.

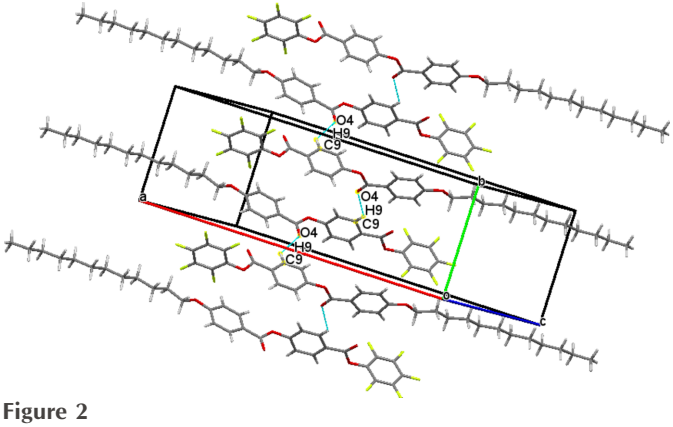


Figure 2
Detail of the packing of (**I**) showing C—H···O hydrogen bonds (blue dashed lines) connecting the molecules into *S*(7) [010] chains.

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O1	0.93	2.39	2.715 (4)	100
C16—H16···O3	0.93	2.42	2.730 (4)	100
C9—H9···O4^{i}	0.93	2.60	3.250 (4)	128
C3—F2···*Cg*3^{ii}	1.34 (1)	3.44 (1)	3.899 (5)	100 (1)
C5—F4···*Cg*3^{iii}	1.33 (1)	3.18 (1)	3.604 (4)	98 (1)
C6—F5···*Cg*2^{iv}	1.33 (1)	3.42 (1)	3.917 (4)	102 (1)

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

3. Supramolecular features

In the crystal, weak C9—H9···O4 hydrogen bonds (Table 1) connect the molecules into infinite *S*(7) chains propagating along the [010] direction as shown in Fig. 2. The packing is consolidated by C—F···π interactions (Fig. 3, Table 1) , *viz.*: C6—F5···*Cg*2, C3—F2···*Cg*3 and C5—F4···*Cg*3, where *Cg*2 and *Cg*3 are the centroids of the C8–C13 and C15–C20 rings, respectively. Very weak aromatic π–π stacking between pairs of *Cg*2 rings related by inversion symmetry with a centroid–centroid distance of 4.079 (2) Å and a slippage of 2.212 Å is also seen (Fig. 4).

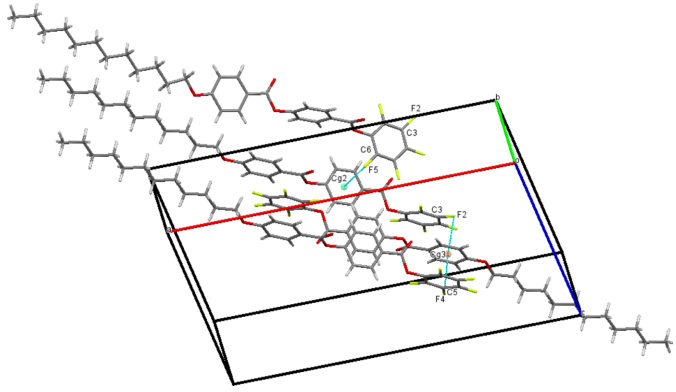


Figure 3
Detail of the packing of (**I**) showing C—F···π interactions as blue dashed lines.

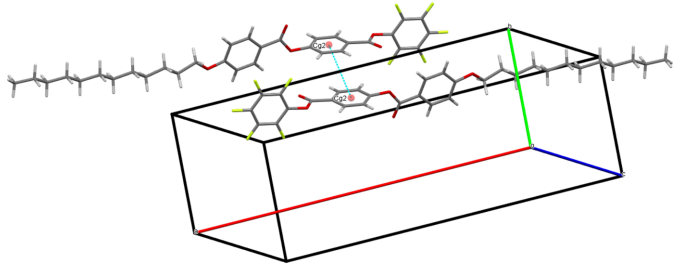


Figure 4
Detail of the packing of (**I**) showing aromatic π–π stacking.

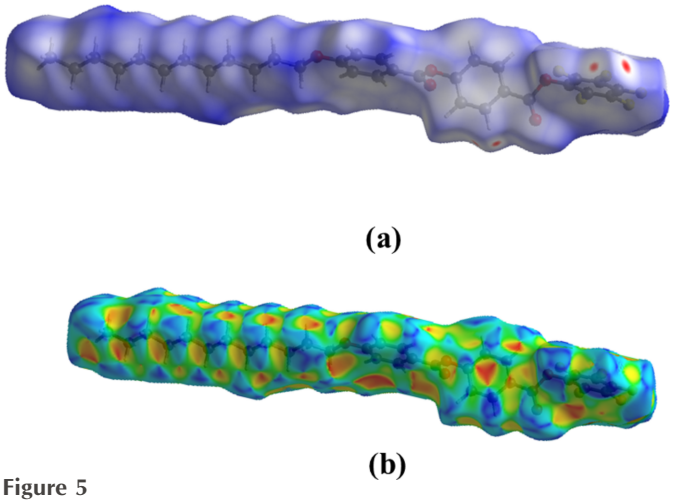


Figure 5
View of the three-dimensional Hirshfeld surface of (**I**) plotted over (*a*) d_{norm} and (*b*) shape-index.

4. Hirshfeld surface analysis

The Hirshfeld surface analysis was performed using *Crystal-Explorer* (Spackman *et al.*, 2021). Fig. 5 illustrates the Hirshfeld surface of (**I**) mapped over d_{norm} and shape-index. The red triangular-shaped region, if viewed normal to the centre of the carbonylphenyl ring indicates the existence of π–π stacking. The two-dimensional fingerprint plots (Fig. 6) indicate that the major contributions to the crystal packing of (**I**) are from H···H: (45%), F···H/H···F: (18.5%), O···H/H···O: (9.7%), C···H/H···C: (9.4%), F···C/C···F: (7.3%),, F···F: (1.9%) contacts. Interaction energies for (**I**) were computed using the basis set B3LYP\\631-G(d,p) for molecular pairs within a cluster of 3.8 Å radius, giving E_{ele} = −37.6 kJ mol^{-1}, E_{pol} = −15.6 kJ mol^{-1}, E_{dis} = −383.4 kJ mol^{-1} and E_{rep} = +128.4 kJ mol^{-1}. The energy framework topologies are shown in Fig. 7.

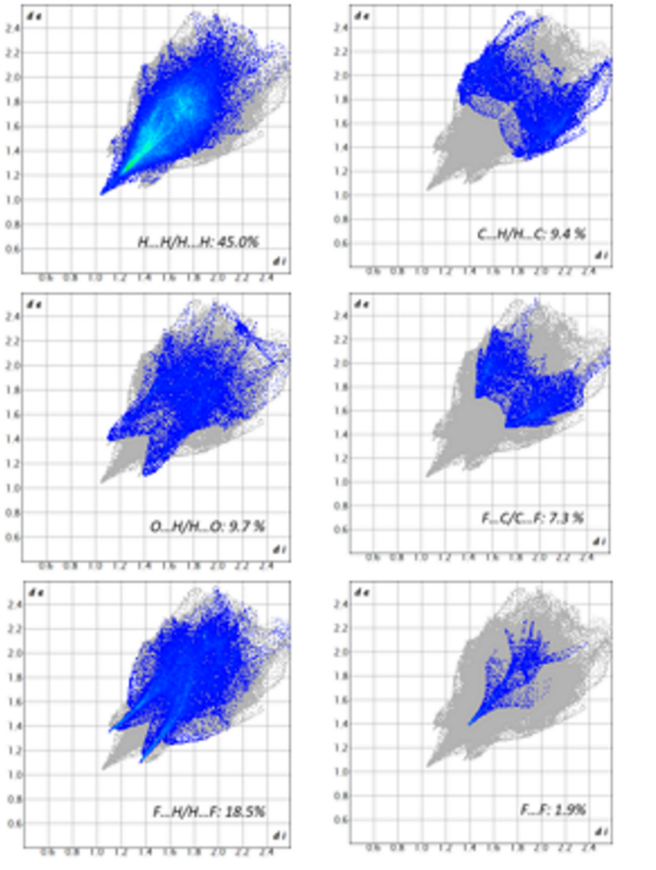


Figure 6
The two-dimensional fingerprint plots for (**I**) for different contact types.

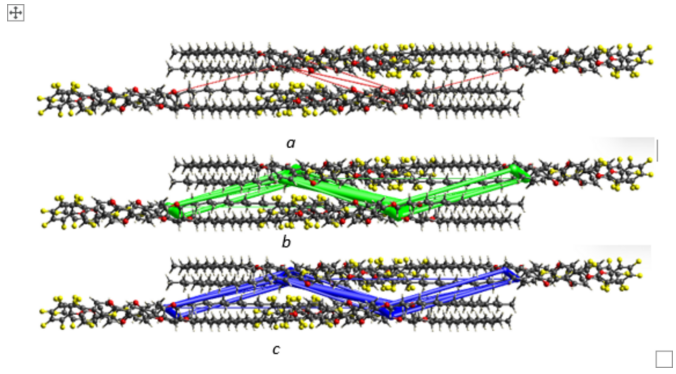


Figure 7
The topology of the energy frameworks for (**I**) representing Coulombic, dispersion and total energy.

5. Database survey

A search of the Cambridge Structural Database (CSD version 6.01, March 2026; Groom *et al.*, 2016) for structures containing the 4-(dodecyloxy) benzoate moiety yielded eleven hits. Among these, five structures with CSD refcodes FOCDIN (Kanji Kubo *et al.*, 2018), PUWDES, SANCAO and PUWREG (Dutronc *et al.*, 2016), and TUVCAP (Cheng *et al.*, 2010) are substituted with long alkyl chains or aromatic rings that are nearly planar, showing only slight deviations. The dihedral angles between these substituent planes and the 4-(dodecyloxy) benzoate moiety are 82.3, 70.1, 47.5, 57.7 and 79.0°, respectively. In the title compound, the dihedral angle between the 4-(dodecyloxy)benzoate ring and the (undecyloxyphenyl)acrylate fragment is 78.98 (2)°, which lies within the range observed for related structures. However, a notable difference is observed in the torsion angle: in the reported structures, the torsion angle between the substituted oxygen atom and the adjacent atom of the almost planar fragment ranges from approximately 1° to 10°, indicating near coplanarity in those segments. In contrast, in the title compound, the torsion angle between the dodecyloxy chain and the phenyl ring is 172.1°, indicating that these groups are nearly coplanar and adopt an anti (extended) conformation, with only a small deviation (∼8°) from the ideal 180°.

6. Synthesis and crystallization

The reaction mixture of 2,3,4,5,6-pentafluorophenol (0.184 g, 1 eq) and 4-{[4-(dodecyloxy)benzoyl]oxy}benzoic acid

(0.426 g, 1 eq) in dichloromethane was stirred at room temperature overnight using a DCC esterification process in the presence of *N*,*N*-dimethylaminopyrimidine as a catalyst. The insoluble byproduct of 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 for a week to grow crystals 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* = 8.5 Hz, 2H, Ar-H), 4.01 (*t*, *J* = 6.5Hz, 2H, –OCH_2–), 1.74–1.25 (*m*, 20H, CH_2-alkyl), 0.91 (*t*, *J* = 4.5Hz, 3H, –CH_3) ppm. Elemental analysis (%) calculated: C, 64.86; H, 5.61; F, 16.03; found C, 64.90; H, 5.65; F, 16.09%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All 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).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{32}H_{33}F_5O_5$
M_r	592.58
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	297
a, *b*, *c* (Å)	25.212 (3), 8.8684 (11), 13.7665 (18)
β (°)	102.518 (4)
V (Å^3)	3004.8 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.32 × 0.27 × 0.21
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.964, 0.976
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	64189, 6157, 3592
R_{int}	0.108
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.087, 0.216, 1.08
No. of reflections	6157
No. of parameters	379
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.20

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

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

Khaleel Ahmed, B. Bommalingaiah, G. N. Venkatareddy, H. T. Srinivasa, H. C. Devarajegowda and B. S. Palakshamurthy

Computing details

4-[(2,3,4,5,6-pentafluorophenoxy)carbonyl]phenyl 4-(dodecyloxy)benzoate

Crystal data

$C_{32}H_{33}F_5O_5$
M_r = 592.58
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 25.212 (3) Å
b = 8.8684 (11) Å
c = 13.7665 (18) Å
β = 102.518 (4)°
V = 3004.8 (7) Å^3
Z = 4
$F(000)$ = 1240
Prism
D_x = 1.310 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3592 reflections
θ = 2–27°
μ = 0.11 mm^{-1}
T = 297 K
Prism, colourless
0.32 × 0.27 × 0.21 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 1.97 pixels mm^{-1}
φ and Ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.964, T_{max} = 0.976
64189 measured reflections
6157 independent reflections
3592 reflections with $I > 2\sigma(I)$
R_{int} = 0.108
θ_{max} = 26.4°, θ_{min} = 2.8°
h = −31→31
k = −11→10
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.087
$wR(F^2)$ = 0.216
S = 1.08
6157 reflections
379 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
$w = 1/[\sigma^2(F_o^2) + (0.0703P)^2 + 1.9288P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 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}
O2	0.62659 (10)	0.8834 (3)	−0.00610 (18)	0.0711 (7)
O3	0.39899 (9)	0.7824 (3)	0.11380 (17)	0.0692 (7)
O1	0.58408 (10)	0.7223 (3)	−0.12246 (18)	0.0797 (8)
O4	0.43103 (11)	0.6248 (3)	0.2388 (2)	0.0893 (9)
O5	0.20585 (10)	0.8468 (3)	0.32820 (19)	0.0843 (8)
C1	0.62584 (15)	0.7373 (4)	−0.1729 (3)	0.0635 (9)
C2	0.67148 (17)	0.6497 (5)	−0.1492 (3)	0.0745 (11)
C3	0.71051 (16)	0.6580 (5)	−0.2045 (3)	0.0820 (12)
C4	0.70352 (17)	0.7543 (5)	−0.2838 (3)	0.0784 (12)
C5	0.65836 (16)	0.8418 (4)	−0.3073 (3)	0.0676 (10)
C6	0.61994 (14)	0.8345 (4)	−0.2515 (3)	0.0628 (9)
C7	0.58815 (15)	0.8070 (4)	−0.0374 (2)	0.0542 (8)
C8	0.53892 (13)	0.7883 (3)	0.0036 (2)	0.0502 (8)
C9	0.53588 (13)	0.8741 (4)	0.0864 (2)	0.0536 (8)
H9	0.564725	0.936244	0.115161	0.064*
C10	0.49039 (14)	0.8676 (4)	0.1260 (2)	0.0573 (9)
H10	0.488360	0.923881	0.182060	0.069*
C11	0.44813 (14)	0.7770 (4)	0.0817 (2)	0.0581 (9)
C12	0.45047 (15)	0.6890 (4)	0.0004 (3)	0.0678 (10)
H12	0.421761	0.625661	−0.027261	0.081*
C13	0.49620 (15)	0.6963 (4)	−0.0393 (3)	0.0649 (9)
H13	0.498183	0.639122	−0.095040	0.078*
C14	0.39587 (14)	0.7057 (4)	0.1983 (3)	0.0598 (9)
C15	0.34493 (13)	0.7394 (4)	0.2292 (2)	0.0576 (8)
C16	0.30507 (14)	0.8343 (4)	0.1765 (3)	0.0622 (9)
H16	0.309606	0.877081	0.117177	0.075*
C17	0.25925 (14)	0.8656 (4)	0.2107 (3)	0.0692 (10)
H17	0.232581	0.927649	0.173849	0.083*
C18	0.25225 (14)	0.8051 (4)	0.3004 (3)	0.0640 (9)
C19	0.29130 (15)	0.7095 (5)	0.3536 (3)	0.0752 (11)
H19	0.286706	0.666733	0.412878	0.090*
C20	0.33676 (15)	0.6785 (4)	0.3181 (3)	0.0713 (10)
H20	0.363031	0.614770	0.354462	0.086*
C21	0.20080 (16)	0.8107 (5)	0.4269 (3)	0.0887 (13)
H21A	0.230112	0.856987	0.474917	0.106*
H21B	0.202828	0.702320	0.436681	0.106*
C22	0.14732 (15)	0.8682 (6)	0.4411 (3)	0.0866 (13)
H22A	0.118463	0.819903	0.393057	0.104*
H22B	0.145254	0.975724	0.427945	0.104*

C23	0.13827 (16)	0.8402 (6)	0.5441 (3)	0.0934 (14)
H23A	0.145117	0.734372	0.559865	0.112*
H23B	0.164865	0.898047	0.590906	0.112*
C24	0.08310 (16)	0.8786 (6)	0.5598 (3)	0.0916 (13)
H24A	0.075818	0.983454	0.541695	0.110*
H24B	0.056675	0.818229	0.514387	0.110*
C25	0.07406 (17)	0.8562 (6)	0.6622 (3)	0.0967 (14)
H25A	0.085332	0.754546	0.683199	0.116*
H25B	0.097722	0.924978	0.706441	0.116*
C26	0.01770 (18)	0.8783 (6)	0.6763 (3)	0.1067 (16)
H26A	0.006387	0.979361	0.653921	0.128*
H26B	−0.005702	0.808603	0.632363	0.128*
C27	0.00738 (18)	0.8593 (6)	0.7763 (3)	0.1045 (16)
H27A	0.029293	0.932870	0.819433	0.125*
H27B	0.020558	0.760344	0.800135	0.125*
C28	−0.04948 (18)	0.8736 (7)	0.7896 (3)	0.1110 (17)
H28A	−0.062671	0.972398	0.765482	0.133*
H28B	−0.071345	0.799824	0.746527	0.133*
C29	−0.06010 (19)	0.8552 (7)	0.8893 (4)	0.1158 (18)
H29A	−0.045840	0.757473	0.913831	0.139*
H29B	−0.038712	0.930481	0.931699	0.139*
C30	−0.1156 (2)	0.8649 (7)	0.9048 (4)	0.1215 (19)
H30A	−0.130530	0.960962	0.878194	0.146*
H30B	−0.136808	0.786771	0.864814	0.146*
C31	−0.1246 (3)	0.8517 (8)	1.0055 (5)	0.152 (3)
H31A	−0.108028	0.757934	1.032921	0.183*
H31B	−0.104544	0.932616	1.044445	0.183*
C32	−0.1787 (3)	0.8546 (9)	1.0231 (5)	0.175 (3)
H32A	−0.177098	0.844603	1.093133	0.263*
H32B	−0.195806	0.948374	0.999799	0.263*
H32C	−0.199313	0.772584	0.988201	0.263*
F5	0.57632 (9)	0.9232 (3)	−0.27505 (17)	0.0880 (7)
F4	0.65212 (11)	0.9356 (3)	−0.38455 (17)	0.0974 (8)
F3	0.74166 (10)	0.7621 (3)	−0.3378 (2)	0.1192 (10)
F1	0.67773 (12)	0.5529 (3)	−0.07250 (18)	0.1108 (9)
F2	0.75492 (11)	0.5723 (4)	−0.1801 (2)	0.1260 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0704 (16)	0.0849 (18)	0.0659 (16)	−0.0158 (14)	0.0323 (13)	−0.0230 (14)
O3	0.0610 (14)	0.0841 (17)	0.0701 (16)	0.0127 (12)	0.0309 (12)	0.0216 (13)
O1	0.0848 (18)	0.101 (2)	0.0663 (16)	−0.0254 (15)	0.0441 (14)	−0.0310 (15)
O4	0.0836 (19)	0.105 (2)	0.092 (2)	0.0353 (17)	0.0459 (16)	0.0468 (17)
O5	0.0609 (15)	0.122 (2)	0.0768 (18)	0.0116 (15)	0.0292 (13)	0.0103 (16)
C1	0.068 (2)	0.075 (2)	0.054 (2)	−0.0108 (19)	0.0287 (18)	−0.0192 (19)
C2	0.087 (3)	0.085 (3)	0.057 (2)	0.004 (2)	0.027 (2)	−0.003 (2)
C3	0.066 (2)	0.097 (3)	0.084 (3)	0.021 (2)	0.017 (2)	−0.013 (2)

C4	0.076 (3)	0.101 (3)	0.072 (3)	−0.005 (2)	0.045 (2)	−0.017 (2)
C5	0.085 (3)	0.072 (2)	0.052 (2)	−0.005 (2)	0.029 (2)	−0.0076 (19)
C6	0.063 (2)	0.070 (2)	0.058 (2)	0.0012 (19)	0.0206 (18)	−0.0172 (19)
C7	0.073 (2)	0.0474 (18)	0.0469 (19)	0.0040 (17)	0.0237 (17)	0.0001 (15)
C8	0.063 (2)	0.0490 (18)	0.0421 (17)	0.0023 (16)	0.0202 (15)	0.0013 (14)
C9	0.061 (2)	0.056 (2)	0.0489 (18)	−0.0051 (15)	0.0213 (15)	−0.0039 (15)
C10	0.067 (2)	0.063 (2)	0.0477 (19)	0.0049 (18)	0.0237 (17)	−0.0023 (16)
C11	0.061 (2)	0.063 (2)	0.055 (2)	0.0074 (18)	0.0221 (17)	0.0130 (17)
C12	0.065 (2)	0.072 (2)	0.071 (2)	−0.0114 (18)	0.0229 (19)	−0.008 (2)
C13	0.075 (2)	0.066 (2)	0.057 (2)	−0.0038 (19)	0.0227 (19)	−0.0104 (18)
C14	0.064 (2)	0.059 (2)	0.060 (2)	0.0009 (18)	0.0204 (18)	0.0140 (18)
C15	0.058 (2)	0.058 (2)	0.060 (2)	0.0003 (16)	0.0205 (17)	0.0056 (17)
C16	0.062 (2)	0.073 (2)	0.053 (2)	−0.0039 (18)	0.0164 (17)	0.0042 (18)
C17	0.054 (2)	0.089 (3)	0.065 (2)	0.0060 (19)	0.0140 (18)	0.009 (2)
C18	0.056 (2)	0.076 (2)	0.064 (2)	−0.0037 (19)	0.0223 (18)	−0.0016 (19)
C19	0.073 (3)	0.090 (3)	0.072 (2)	0.010 (2)	0.035 (2)	0.018 (2)
C20	0.074 (2)	0.077 (3)	0.070 (2)	0.013 (2)	0.031 (2)	0.017 (2)
C21	0.076 (3)	0.115 (4)	0.085 (3)	0.003 (2)	0.039 (2)	0.006 (3)
C22	0.063 (2)	0.120 (4)	0.083 (3)	−0.001 (2)	0.030 (2)	−0.004 (3)
C23	0.070 (3)	0.131 (4)	0.087 (3)	0.004 (3)	0.034 (2)	0.003 (3)
C24	0.072 (3)	0.123 (4)	0.088 (3)	0.009 (3)	0.034 (2)	0.005 (3)
C25	0.077 (3)	0.138 (4)	0.083 (3)	0.007 (3)	0.034 (2)	0.008 (3)
C26	0.083 (3)	0.156 (5)	0.092 (3)	0.021 (3)	0.044 (3)	0.021 (3)
C27	0.082 (3)	0.150 (5)	0.090 (3)	0.017 (3)	0.038 (3)	0.017 (3)
C28	0.090 (3)	0.155 (5)	0.100 (4)	0.030 (3)	0.048 (3)	0.026 (3)
C29	0.096 (3)	0.162 (5)	0.103 (4)	0.025 (3)	0.050 (3)	0.031 (3)
C30	0.096 (3)	0.160 (5)	0.127 (4)	0.029 (3)	0.065 (3)	0.027 (4)
C31	0.143 (5)	0.195 (7)	0.146 (5)	0.024 (5)	0.092 (4)	0.032 (5)
C32	0.164 (6)	0.211 (7)	0.187 (7)	0.032 (6)	0.121 (5)	0.050 (6)
F5	0.0857 (16)	0.0905 (16)	0.0893 (16)	0.0190 (13)	0.0221 (12)	−0.0165 (13)
F4	0.132 (2)	0.0965 (17)	0.0726 (15)	−0.0045 (15)	0.0419 (14)	0.0069 (13)
F3	0.1030 (19)	0.162 (3)	0.119 (2)	−0.0048 (18)	0.0805 (17)	−0.0161 (19)
F1	0.144 (2)	0.119 (2)	0.0723 (16)	0.0181 (17)	0.0282 (15)	0.0150 (15)
F2	0.0914 (19)	0.154 (3)	0.132 (2)	0.0431 (18)	0.0236 (17)	−0.011 (2)

Geometric parameters (Å, º)

O2—C7	1.184 (4)	C19—H19	0.9300
O3—C14	1.365 (4)	C20—H20	0.9300
O3—C11	1.404 (4)	C21—C22	1.494 (5)
O1—C7	1.376 (4)	C21—H21A	0.9700
O1—C1	1.387 (4)	C21—H21B	0.9700
O4—C14	1.182 (4)	C22—C23	1.505 (5)
O5—C18	1.358 (4)	C22—H22A	0.9700
O5—C21	1.428 (4)	C22—H22B	0.9700
C1—C6	1.366 (5)	C23—C24	1.493 (5)
C1—C2	1.368 (5)	C23—H23A	0.9700
C2—F1	1.344 (4)	C23—H23B	0.9700

C2—C3	1.370 (5)	C24—C25	1.490 (5)
C3—F2	1.335 (4)	C24—H24A	0.9700
C3—C4	1.368 (6)	C24—H24B	0.9700
C4—F3	1.338 (4)	C25—C26	1.488 (5)
C4—C5	1.358 (5)	C25—H25A	0.9700
C5—F4	1.333 (4)	C25—H25B	0.9700
C5—C6	1.362 (5)	C26—C27	1.466 (6)
C6—F5	1.334 (4)	C26—H26A	0.9700
C7—C8	1.481 (4)	C26—H26B	0.9700
C8—C13	1.378 (5)	C27—C28	1.489 (5)
C8—C9	1.386 (4)	C27—H27A	0.9700
C9—C10	1.374 (4)	C27—H27B	0.9700
C9—H9	0.9300	C28—C29	1.464 (6)
C10—C11	1.368 (5)	C28—H28A	0.9700
C10—H10	0.9300	C28—H28B	0.9700
C11—C12	1.376 (5)	C29—C30	1.463 (6)
C12—C13	1.380 (5)	C29—H29A	0.9700
C12—H12	0.9300	C29—H29B	0.9700
C13—H13	0.9300	C30—C31	1.458 (7)
C14—C15	1.469 (5)	C30—H30A	0.9700
C15—C16	1.389 (5)	C30—H30B	0.9700
C15—C20	1.393 (4)	C31—C32	1.435 (7)
C16—C17	1.367 (5)	C31—H31A	0.9700
C16—H16	0.9300	C31—H31B	0.9700
C17—C18	1.392 (5)	C32—H32A	0.9600
C17—H17	0.9300	C32—H32B	0.9600
C18—C19	1.382 (5)	C32—H32C	0.9600
C19—C20	1.367 (5)		

C14—O3—C11	118.0 (3)	O5—C21—H21A	110.0
C7—O1—C1	116.6 (3)	C22—C21—H21A	110.0
C18—O5—C21	117.8 (3)	O5—C21—H21B	110.0
C6—C1—C2	119.2 (3)	C22—C21—H21B	110.0
C6—C1—O1	119.5 (3)	H21A—C21—H21B	108.4
C2—C1—O1	121.1 (4)	C21—C22—C23	113.1 (4)
C6—C1—O1	119.5 (3)	C21—C22—H22A	109.0
C2—C1—O1	121.1 (4)	C23—C22—H22A	109.0
F1—C2—C1	119.9 (3)	C21—C22—H22B	109.0
F1—C2—C3	119.6 (4)	C23—C22—H22B	109.0
C1—C2—C3	120.4 (4)	H22A—C22—H22B	107.8
F2—C3—C4	120.8 (4)	C24—C23—C22	115.8 (4)
F2—C3—C2	119.6 (4)	C24—C23—H23A	108.3
C4—C3—C2	119.5 (4)	C22—C23—H23A	108.3
F3—C4—C5	120.4 (4)	C24—C23—H23B	108.3
F3—C4—C3	119.5 (4)	C22—C23—H23B	108.3
C5—C4—C3	120.2 (3)	H23A—C23—H23B	107.4
F4—C5—C4	119.6 (3)	C25—C24—C23	116.4 (4)
F4—C5—C6	120.3 (4)	C25—C24—H24A	108.2

C4—C5—C6	120.1 (4)	C23—C24—H24A	108.2
F5—C6—C5	119.0 (4)	C25—C24—H24B	108.2
F5—C6—C1	120.5 (3)	C23—C24—H24B	108.2
C5—C6—C1	120.6 (4)	H24A—C24—H24B	107.3
O2—C7—O1	121.8 (3)	C26—C25—C24	116.8 (4)
O2—C7—O1	121.8 (3)	C26—C25—H25A	108.1
O2—C7—C8	127.8 (3)	C24—C25—H25A	108.1
O1—C7—C8	110.4 (3)	C26—C25—H25B	108.1
O1—C7—C8	110.4 (3)	C24—C25—H25B	108.1
C13—C8—C9	120.0 (3)	H25A—C25—H25B	107.3
C13—C8—C7	123.0 (3)	C27—C26—C25	118.4 (4)
C9—C8—C7	116.9 (3)	C27—C26—H26A	107.7
C10—C9—C8	120.2 (3)	C25—C26—H26A	107.7
C10—C9—H9	119.9	C27—C26—H26B	107.7
C8—C9—H9	119.9	C25—C26—H26B	107.7
C11—C10—C9	119.0 (3)	H26A—C26—H26B	107.1
C11—C10—H10	120.5	C26—C27—C28	118.5 (4)
C9—C10—H10	120.5	C26—C27—H27A	107.7
C10—C11—C12	122.0 (3)	C28—C27—H27A	107.7
C10—C11—O3	119.7 (3)	C26—C27—H27B	107.7
C12—C11—O3	118.1 (3)	C28—C27—H27B	107.7
C10—C11—O3	119.7 (3)	H27A—C27—H27B	107.1
C12—C11—O3	118.1 (3)	C29—C28—C27	118.8 (4)
C11—C12—C13	118.8 (3)	C29—C28—H28A	107.6
C11—C12—H12	120.6	C27—C28—H28A	107.6
C13—C12—H12	120.6	C29—C28—H28B	107.6
C8—C13—C12	120.0 (3)	C27—C28—H28B	107.6
C8—C13—H13	120.0	H28A—C28—H28B	107.0
C12—C13—H13	120.0	C30—C29—C28	120.3 (4)
O4—C14—O3	121.9 (3)	C30—C29—H29A	107.2
O4—C14—O3	121.9 (3)	C28—C29—H29A	107.2
O4—C14—C15	126.9 (3)	C30—C29—H29B	107.2
O3—C14—C15	111.2 (3)	C28—C29—H29B	107.2
O3—C14—C15	111.2 (3)	H29A—C29—H29B	106.9
C16—C15—C20	117.8 (3)	C31—C30—C29	119.0 (5)
C16—C15—C14	123.4 (3)	C31—C30—H30A	107.6
C20—C15—C14	118.7 (3)	C29—C30—H30A	107.6
C17—C16—C15	120.8 (3)	C31—C30—H30B	107.6
C17—C16—H16	119.6	C29—C30—H30B	107.6
C15—C16—H16	119.6	H30A—C30—H30B	107.0
C16—C17—C18	120.4 (3)	C32—C31—C30	120.6 (6)
C16—C17—H17	119.8	C32—C31—H31A	107.2
C18—C17—H17	119.8	C30—C31—H31A	107.2
O5—C18—C19	125.2 (3)	C32—C31—H31B	107.2
O5—C18—C17	115.3 (3)	C30—C31—H31B	107.2
C19—C18—C17	119.5 (3)	H31A—C31—H31B	106.8
C20—C19—C18	119.4 (3)	C31—C32—H32A	109.5
C20—C19—H19	120.3	C31—C32—H32B	109.5

C18—C19—H19	120.3	H32A—C32—H32B	109.5
C19—C20—C15	122.0 (4)	C31—C32—H32C	109.5
C19—C20—H20	119.0	H32A—C32—H32C	109.5
C15—C20—H20	119.0	H32B—C32—H32C	109.5
O5—C21—C22	108.5 (3)		

C7—O1—C1—C6	−96.2 (4)	C9—C10—C11—O3	−172.5 (3)
C7—O1—C1—C2	87.9 (4)	C9—C10—C11—O3	−172.5 (3)
C6—C1—C2—F1	−179.6 (3)	O3—O3—C11—C10	0.00 (12)
O1—C1—C2—F1	−3.6 (5)	C14—O3—C11—C10	−79.7 (4)
O1—C1—C2—F1	−3.6 (5)	C14—O3—C11—C12	105.6 (4)
C6—C1—C2—C3	−0.8 (6)	C10—C11—C12—C13	−2.1 (5)
O1—C1—C2—C3	175.1 (3)	O3—C11—C12—C13	172.4 (3)
O1—C1—C2—C3	175.1 (3)	O3—C11—C12—C13	172.4 (3)
F1—C2—C3—F2	−1.6 (6)	C9—C8—C13—C12	−0.3 (5)
C1—C2—C3—F2	179.7 (4)	C7—C8—C13—C12	−177.2 (3)
F1—C2—C3—C4	178.6 (4)	C11—C12—C13—C8	1.3 (5)
C1—C2—C3—C4	−0.1 (6)	C11—O3—C14—O4	−7.3 (5)
F2—C3—C4—F3	0.2 (6)	C11—O3—C14—O3	0 (56)
C2—C3—C4—F3	−179.9 (4)	C11—O3—C14—C15	172.2 (3)
F2—C3—C4—C5	−179.4 (4)	O4—C14—C15—C16	−178.9 (4)
C2—C3—C4—C5	0.4 (6)	O3—C14—C15—C16	1.6 (5)
F3—C4—C5—F4	0.1 (6)	O3—C14—C15—C16	1.6 (5)
C3—C4—C5—F4	179.7 (4)	O4—C14—C15—C20	3.8 (6)
F3—C4—C5—C6	−179.3 (3)	O3—C14—C15—C20	−175.6 (3)
C3—C4—C5—C6	0.3 (6)	O3—C14—C15—C20	−175.6 (3)
F4—C5—C6—F5	−0.4 (5)	C20—C15—C16—C17	−0.5 (5)
C4—C5—C6—F5	179.0 (3)	C14—C15—C16—C17	−177.8 (3)
F4—C5—C6—C1	179.3 (3)	C15—C16—C17—C18	1.3 (6)
C4—C5—C6—C1	−1.3 (6)	C21—O5—C18—C19	11.1 (6)
C2—C1—C6—F5	−178.8 (3)	C21—O5—C18—C17	−169.2 (3)
O1—C1—C6—F5	5.2 (5)	C16—C17—C18—O5	178.5 (3)
O1—C1—C6—F5	5.2 (5)	C16—C17—C18—C19	−1.8 (6)
C2—C1—C6—C5	1.6 (5)	O5—C18—C19—C20	−178.9 (4)
O1—C1—C6—C5	−174.4 (3)	C17—C18—C19—C20	1.4 (6)
O1—C1—C6—C5	−174.4 (3)	C18—C19—C20—C15	−0.5 (6)
C1—O1—C7—O2	−3.6 (5)	C16—C15—C20—C19	0.1 (6)
C1—O1—C7—O1	0 (82)	C14—C15—C20—C19	177.5 (4)
C1—O1—C7—C8	175.6 (3)	C18—O5—C21—C22	179.4 (3)
O2—C7—C8—C13	179.8 (3)	O5—C21—C22—C23	−178.3 (4)
O1—C7—C8—C13	0.6 (5)	C21—C22—C23—C24	−173.1 (4)
O1—C7—C8—C13	0.6 (5)	C22—C23—C24—C25	−178.1 (4)
O2—C7—C8—C9	2.8 (5)	C23—C24—C25—C26	−173.6 (5)
O1—C7—C8—C9	−176.4 (3)	C24—C25—C26—C27	−179.2 (5)
O1—C7—C8—C9	−176.4 (3)	C25—C26—C27—C28	−176.9 (5)
C13—C8—C9—C10	0.1 (5)	C26—C27—C28—C29	−179.8 (5)
C7—C8—C9—C10	177.2 (3)	C27—C28—C29—C30	−178.6 (5)
C8—C9—C10—C11	−0.9 (5)	C28—C29—C30—C31	−177.7 (6)

C9—C10—C11—C12	1.9 (5)	C29—C30—C31—C32	−177.4 (6)

Hydrogen-bond geometry (Å, º)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O1	0.93	2.39	2.715 (4)	100
C16—H16···O3	0.93	2.42	2.730 (4)	100
C9—H9···O4^{i}	0.93	2.60	3.250 (4)	128
C3—F2···*Cg*3^{ii}	1.34 (1)	3.44 (1)	3.899 (5)	100 (1)
C5—F4···*Cg*3^{iii}	1.33 (1)	3.18 (1)	3.604 (4)	98 (1)
C6—F5···*Cg*2^{iv}	1.33 (1)	3.42 (1)	3.917 (4)	102 (1)

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