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Fluorenonophane chlorobenzene solvate: molecular and crystal structures

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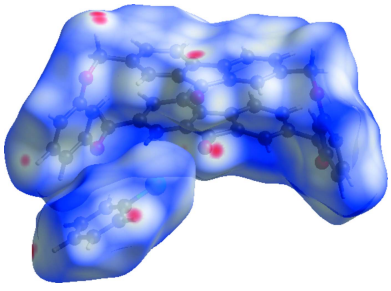
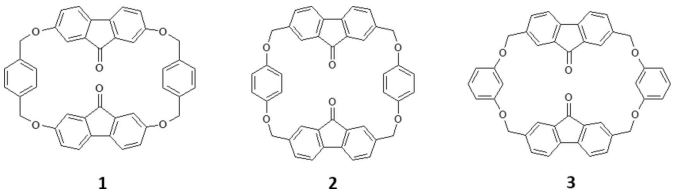
The title compound, $1^9H,7^9H$-3,5,9,11-tetraoxa-1,7(2,7)-difluorena-4,10(1,3)-dibenzenacyclododecaphane-$1^9,7^9$-dione (fluorenonophane), exists as a solvate with chlorobenzene, $C_{42}H_{28}O_6{\cdot}C_6H_5Cl$. The fluorenonophane contains two fluorenone fragments linked by two *m*-substituted benzene fragments. Some decrease in its macrocyclic cavity leads to a stacking interaction between the tricyclic fluorenone fragments. In the crystal, the fluorenonophane and chlorobenzene molecules are linked by weak C—H$\cdots\pi$(ring) interactions and C—H$\cdots$Cl hydrogen bonds. The Cl atom of chlorobenzene does not form a halogen bond. A Hirshfeld surface analysis and two-dimensional fingerprint plots were used to analyse the intermolecular contacts found in the crystal structure.

1. Chemical context

Discovered at the end of the last century, the ability of cyclophanes to form inclusion complexes makes them the central class of synthetic receptors in molecular recognition processes (Diederich, 1991). Particular attention has been paid to the possibility of cationic cyclophanes with box geometries being involved in strong donor–acceptor interactions leading to the formation of 'guest–host' complexes with different guests (Dale *et al.*, 2016; Barnes *et al.*, 2013; Gong *et al.*, 2010). Previously we have obtained fluorenonophane **1** with two fluorenone fragments linked by rigid xylyl groups (Lukyanenko *et al.*, 2003; Simonov *et al.*, 2006). X-ray diffraction analysis of this cyclophane revealed the box geometry with an open intramolecular cavity and the formation of inclusion complexes with DMF and nitrobenzene (Simonov *et al.*, 2006). The other fluorenonophane obtained by our group, **2**, differs from the previous one in the position of the methylene groups, which are located directly at the benzene fragment in **1** or fluorenone in **2**. Fluorenonophane **2** forms inclusion complexes with chloroform and bromoform with a 1:2 stoichiometry. Moreover, C—Cl$\cdots\pi$ and C—Br$\cdots\pi$ halogen bonds (Shishkina *et al.*, 2021) are present in the complexes. In contrast to cationic cyclophanes, there are no charged fragments in fluorenonophanes. Continuing our research in this area, we have obtained fluorenonophane **3** with a different position of attachment of the benzene rings compared to **2** (*m*- and *p*-isomers, respectively) and studied its complexation with chlorobenzene.





2. Structural commentary

Fluorenonophane **3** was crystallized from chlorobenzene and exists in the crystal as a solvate in a 1:1 ratio rather than as an inclusion complex. Fluorenonophane **3** contains two fluorenone fragments linked by two *m*-substituted benzene fragments (Fig. 1). The macrocycle **3** has a boat conformation similar to structure **1** [the torsion angles C41—O6—C1—C2, C37—O5—C36—C33, C20—O3—C22—C23, and C16—O2—C15—C13 are −90.6 (4), 78.4 (4), −80.0 (4) and 91.6 (4)°, respectively]. In structure **3**, the fluorenone fragments are oriented in the same directions (*cis*-orientation) while the orientation of these fragments is *trans* in structures **1** and **2**. *meta*-Substitution of the two benzene fragments results in a smaller macrocycle cavity as compared to fluorenonophanes **1** and **2** with *para*-substituted benzene fragments. As a result, the two fluorenones are slightly bowed inwards [the dihedral angle between C2–C7 and C8-C14 benzene rings is 12.51 (18)° in one fluorenone while the dihedral angle between the C31–C35 and C23–C28 benzene rings is 9.64 (18)° in the other fluorenone). This can be explained by a π-stacking interaction between the C10═O1 carbonyl group and the C25/C26/C31/C30/C29 fluorenone ring [centroid *Cg*2, with O1···*Cg*2 = 3.469 (3) Å, C10···*Cg*2 = 3.492 (4) Å, C10═O1···*Cg*2 = 81.1 (2)°]. In contrast to structures **1** and **2**, the macrocycle in structure **3** does not contain any molecules inside its cavity. Therefore, the structure under study is a chlorobenzene solvate of fluorenonophane.

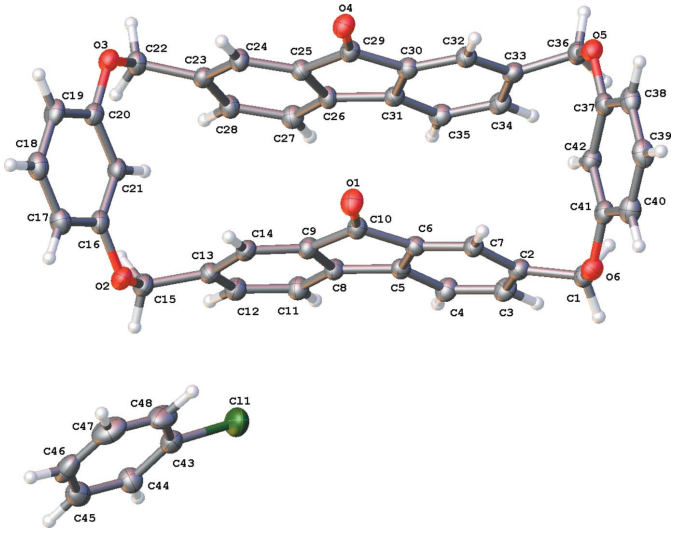


Figure 1
The molecular structure of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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

*Cg*1, *Cg*2 and *Cg*15 are the centroids of the C5/C6/C10/C9/C8, C25/C29/C30/C31/C26 and C43–C48 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···Cl1^{i}	0.95	2.83	3.547 (4)	133
C35—H35···O1^{ii}	0.95	2.58	3.491 (5)	161
C46—H46···O6^{iii}	0.95	2.55	3.418 (5)	152
C1—H1*A*···*Cg*2^{iv}	0.99	2.95	3.610 (4)	125
C22—H22*A*···*Cg*1^{v}	0.99	2.73	3.711 (4)	170
C36—H36*B*···*Cg*15^{vi}	0.99	2.84	3.713 (4)	148

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

3. Supramolecular features

In the crystal, the fluorenonophane and chlorobenzene molecules are linked to each other by weak C46—H46···O6 and C18—H18···Cl1 hydrogen bonds while the fluorenophanes are linked by weak C35—H35···O1 hydrogen bonds (Table 1), forming stepped ribbons. The ribbons are connected by C1—H1*A*···*Cg*2 and C22—H22*A*···*Cg*1 interactions (Table 1) to give the final three-dimensional structure. The halogen atom does not form a halogen bond in the structure of **3**, in contrast to the supramolecular complexes studied earlier (Shishkina *et al.*, 2021). The electrostatic potential for chlorobenzene was calculated using the B3LYP/6–311 G(d,p) method. An area with a positive charge (σ-hole) was not found in the electrostatic potential map around the halogen atom (Fig. 2). The highest electrostatic potential at the chlorine atom is −0.08 eV. This fact can explain the absence of halogen bonds in the structure of **3**.

4. Hirshfeld surface analysis

Crystal Explorer 17.5 (Turner *et al.*, 2017) was used to analyze interactions in the crystal. Molecular Hirshfeld surfaces mapped over $d_{\rm norm}$ with a standard (high) surface resolution

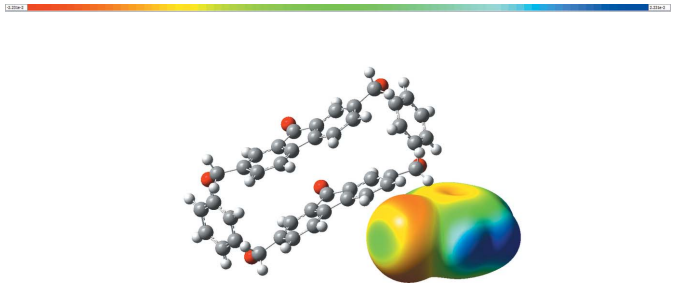


Figure 2
Electrostatic potential map of the chlorobenzene molecule in **3** calculated by the B3LYP/6–311 G(d,p) method.

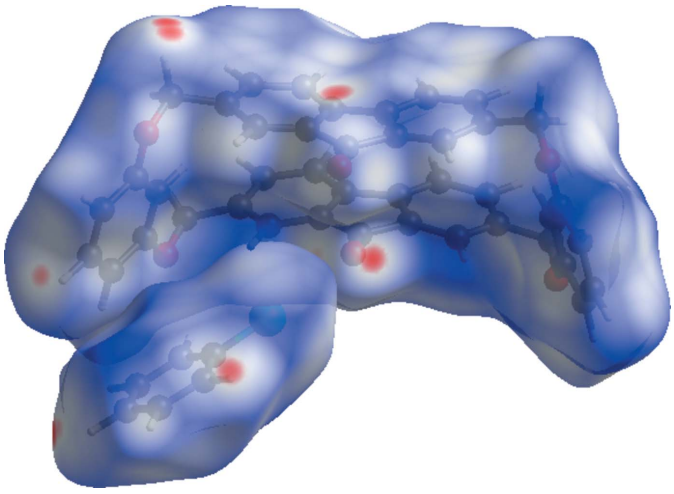


Figure 3
Hirshfeld surface mapped over d_{norm} showing the conformation of the fluorenonophane and chlorobenzene molecules.

and a fixed colour scale of −0.134 (red) to 1.206 (blue) were generated separately (Fig. 3) for the fluorenonophane and chlorobenzene molecules. The areas in red correspond to contacts that are shorter than the sum of the van der Waals radii of the closest atoms. Thus, the red spots at some hydrogen atoms and at the carbonyl oxygen atom as well as in the area of the five-membered ring indicate the existence of short C—H···O and C—H···π(ring) contacts.

To evaluate the contribution of the short contacts of different types to the total Hirshfeld surface, two-dimensional fingerprint plots for the fluorenonophane and chlorobenzene molecules were generated (Fig. 4). The contribution from the C···H/H···C contacts corresponding to the C—H···π(ring) interactions are represented by a pair of sharp spikes (27.7% and 25.9% for fluorenonophane and chlorobenzene, respectively). Analysis of the fingerprint plots also showed a significant contribution from O···H/H···O contacts (19.7%) associated with the C—H···O hydrogen bonds.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.42, update of November 2020; Groom *et al.*, 2016) for cyclophanes containing fluorenone and benzene fragments yielded two hits: two structures with fluorenone fragments linked by rigid xylyl groups (CCDC 263272 and CCDC 263273; Simonov *et al.*, 2006). Recently, two more structures with fluorenonophanes linked by *para*-substituted benzene fragments were published (CCDC 647971 and CCDC 2098245; Shishkina *et al.*, 2021). The structures found are characterized by a larger macrocyclic cavity compared to that in fluorenonophane **3**.

6. Synthesis and crystallization

A solution of 1.75 g (4.78 mmol) of 2,7-bis(bromomethyl)-9*H*-fluoren-9-one (Haenel *et al.*, 1985) in 200 mL of anhydrous DMF was added to a mixture of 0.526 g (4.78 mmol) of resorcinol and 3.96 g (28.7 mmol) of K_2CO_3 in 270 mL of anhydrous DMF with stirring under nitrogen for 10 h at 353–358 K. The reaction mixture was stirred at the same temperature for a further 35 h, cooled and filtered (Fig. 5). The precipitate was washed with DMF and the filtrate was evaporated under reduced pressure. The residue was dissolved

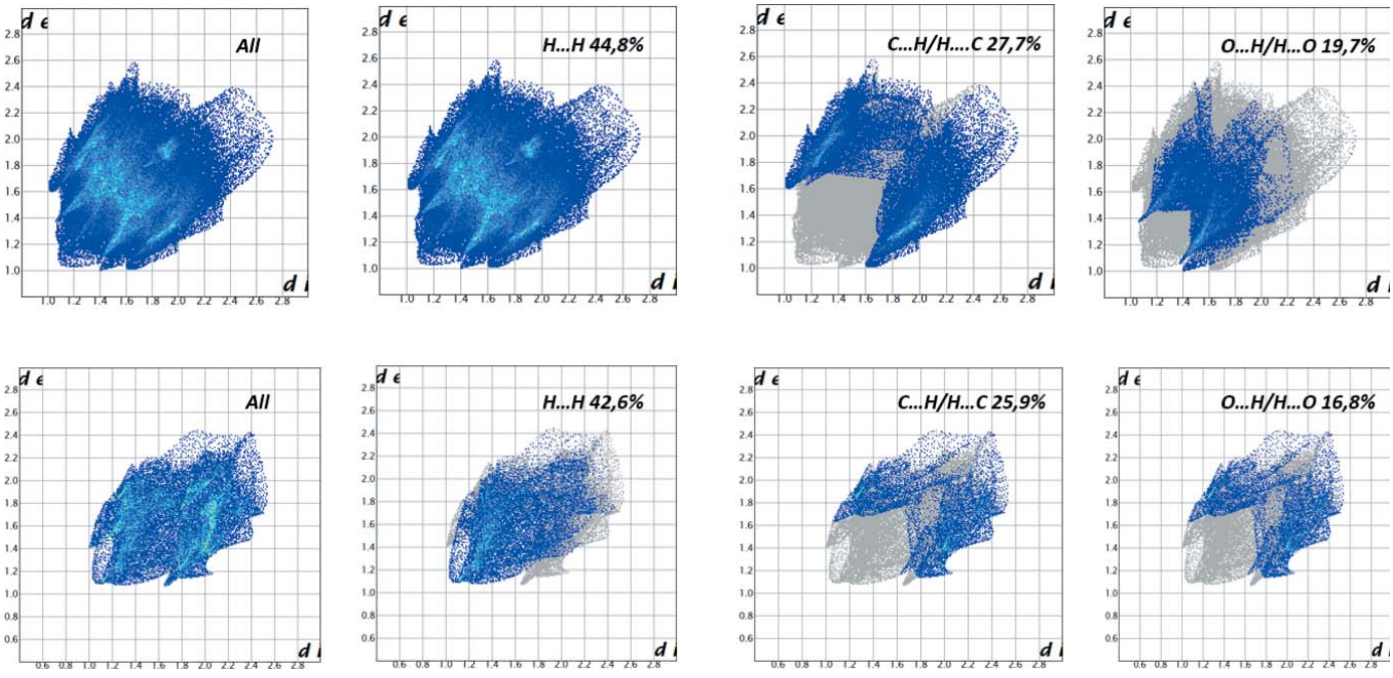


Figure 4
The two-dimensional fingerprint plots for fluorenonophane **3** (top) and chlorobenzene (bottom).

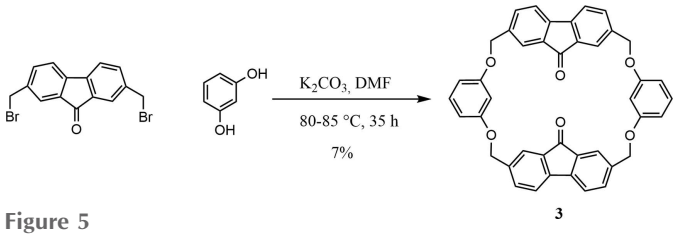


Figure 5
The synthesis of fluorenonophane **3**

in $CHCl_3$ and washed with an aqueous sodium carbonate solution (50 mL), then with water (3 × 50 mL) to a neutral pH. After drying over $MgSO_4$, the $CHCl_3$ was evaporated under reduced pressure. The product was purified by chromatography on silica gel (Acros 0.060 ÷ 1/5), eluent $CHCl_3$–EtOH, 500:1. The yield of cyclophane **3** was 0.11 g (7.2%), m.p. >573 K, dec. ^{1}H NMR (DMSO-d_6), δ, p.p.m.: 5.25 *s* (CH_2, 8H), 6.46–6.56 *m* (H_2, H_4, 6H), 7.04 *t* (H_5, 2H, J = 8.1 Hz), 7.18 *s* (H*a*, 4H), 7.57 *m* (H*b*, HH, 8H). MS: FAB, *m*/*z* 628 [M + H^+]. Analysis calculated for $C_{42}H_{28}O_6$: C, 80.24; H, 4.49. Found: C, 80.44; H, 4.76%. Crystals were obtained by crystallization of fluorenonophane **3** from chlorobenzene.

7. Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. Carbon-bound H atoms were added in calculated positions with C—H bond lengths of 0.95 Å for C—H, 0.92 Å for CH_2 and refined as riding atoms with U_{iso}(H) = 1.2U_{eq}(C).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{42}H_{28}O_6{\cdot}C_6H_5Cl$
M_r	741.19
Crystal system, space group	Triclinic, *P*1
Temperature (K)	100
a, *b*, *c* (Å)	6.2278 (6), 9.6965 (8), 14.9822 (13)
α, β, γ (°)	105.288 (8), 97.126 (7), 96.919 (7)
V (Å^3)	854.83 (13)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.17
Crystal size (mm)	0.6 × 0.4 × 0.2
Data collection	
Diffractometer	Xcalibur, Sapphire3
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018)
T_{min}, T_{max}	0.846, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8226, 7191, 5307
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.808
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.064, 0.171, 1.03
No. of reflections	7191
No. of parameters	496
No. of restraints	3
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.79, −0.42
Absolute structure	Flack *x* determined using 564 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.19 (9)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Funding information

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* (Rigaku OD, 2018); data reduction: *CrysAlis PRO* (Rigaku OD, 2018); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

$1^9H,7^9H$-3,5,9,11-Tetraoxa-1,7(2,7)-difluorena-4,10(1,3)-dibenzenacyclododecaphane-1^9,7^9-dione chlorobenzene monosolvate

Crystal data

$C_{42}H_{28}O_6 \cdot C_6H_5Cl$
$M_r = 741.19$
Triclinic, $P1$
$a = 6.2278$ (6) Å
$b = 9.6965$ (8) Å
$c = 14.9822$ (13) Å
$\alpha = 105.288$ (8)°
$\beta = 97.126$ (7)°
$\gamma = 96.919$ (7)°
$V = 854.83$ (13) Å^3
$Z = 1$
$F(000) = 386$
$D_x = 1.440$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1987 reflections
$\theta = 3.9$–$33.0°$
$\mu = 0.17$ mm^{-1}
$T = 100$ K
Block, colourless
0.6 × 0.4 × 0.2 mm

Data collection

Xcalibur, Sapphire3 diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1827 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2018)
$T_{min} = 0.846$, $T_{max} = 1.000$
8226 measured reflections
7191 independent reflections
5307 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 35.0°$, $\theta_{min} = 3.0°$
$h = -9 \rightarrow 8$
$k = -7 \rightarrow 15$
$l = -24 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.171$
$S = 1.03$
7191 reflections
496 parameters
3 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0825P)^2 + 0.017P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Absolute structure: Flack *x* determined using 564 quotients [(I^+)-(I^-)]/[(I^+)+(I^-)] (Parsons et al.,2013)
Absolute structure parameter: 0.19 (9)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.3386 (4)	0.2409 (3)	0.30318 (19)	0.0294 (6)
O2	0.3907 (5)	0.5919 (3)	0.66155 (19)	0.0298 (6)
O3	0.3627 (5)	0.9250 (3)	0.47327 (18)	0.0265 (5)
O4	0.3771 (4)	0.5007 (3)	0.14591 (18)	0.0265 (5)
O5	0.0097 (4)	−0.0028 (3)	−0.12980 (18)	0.0264 (5)
O6	0.0323 (4)	−0.3103 (3)	0.07559 (18)	0.0259 (5)
C1	−0.1767 (6)	−0.2869 (4)	0.0994 (3)	0.0245 (7)
H1A	−0.238920	−0.369009	0.120950	0.029*
H1B	−0.275117	−0.286764	0.042198	0.029*
C2	−0.1747 (6)	−0.1482 (4)	0.1741 (2)	0.0239 (7)
C3	−0.3613 (6)	−0.1340 (4)	0.2162 (3)	0.0266 (7)
H3	−0.485939	−0.207766	0.193390	0.032*
C4	−0.3703 (6)	−0.0156 (4)	0.2902 (3)	0.0267 (7)
H4	−0.498316	−0.007812	0.318459	0.032*
C5	−0.1889 (6)	0.0909 (4)	0.3217 (2)	0.0222 (6)
C6	−0.0046 (6)	0.0796 (4)	0.2766 (2)	0.0220 (6)
C7	0.0060 (6)	−0.0388 (4)	0.2035 (2)	0.0224 (6)
H7	0.132576	−0.045426	0.174069	0.027*
C8	−0.1381 (6)	0.2194 (4)	0.4039 (2)	0.0225 (6)
C9	0.0774 (6)	0.2848 (4)	0.4097 (2)	0.0244 (7)
C10	0.1658 (6)	0.2076 (4)	0.3267 (2)	0.0231 (7)
C11	−0.2608 (6)	0.2752 (4)	0.4711 (3)	0.0261 (7)
H11	−0.410474	0.235645	0.465987	0.031*
C12	−0.1588 (7)	0.3914 (4)	0.5467 (3)	0.0278 (7)
H12	−0.242323	0.432694	0.592837	0.033*
C13	0.0608 (6)	0.4491 (4)	0.5571 (2)	0.0250 (7)
C14	0.1794 (6)	0.3979 (4)	0.4864 (3)	0.0244 (7)
H14	0.327603	0.439670	0.490436	0.029*
C15	0.1603 (7)	0.5576 (4)	0.6484 (3)	0.0290 (8)
H15A	0.097362	0.647655	0.652418	0.035*
H15B	0.118770	0.519599	0.700067	0.035*
C16	0.4764 (6)	0.7076 (4)	0.6331 (2)	0.0251 (7)
C17	0.6890 (7)	0.7711 (4)	0.6749 (3)	0.0298 (8)
H17	0.766706	0.736390	0.720920	0.036*
C18	0.7850 (7)	0.8861 (5)	0.6479 (3)	0.0316 (8)

H18	0.930083	0.931503	0.676396	0.038*
C19	0.6746 (6)	0.9367 (4)	0.5802 (3)	0.0297 (8)
H19	0.743820	1.015419	0.561995	0.036*
C20	0.4627 (6)	0.8717 (4)	0.5394 (2)	0.0245 (7)
C21	0.3627 (6)	0.7559 (4)	0.5661 (2)	0.0256 (7)
H21	0.217055	0.710835	0.538118	0.031*
C22	0.1320 (6)	0.8832 (4)	0.4482 (3)	0.0260 (7)
H22A	0.071510	0.954612	0.419840	0.031*
H22B	0.068110	0.886179	0.505817	0.031*
C23	0.0619 (6)	0.7348 (4)	0.3806 (2)	0.0231 (7)
C24	0.1890 (6)	0.6774 (4)	0.3150 (2)	0.0242 (7)
H24	0.329679	0.727598	0.314978	0.029*
C25	0.1081 (6)	0.5461 (4)	0.2498 (2)	0.0220 (6)
C26	−0.0988 (6)	0.4699 (4)	0.2487 (2)	0.0222 (6)
C27	−0.2240 (6)	0.5237 (4)	0.3154 (3)	0.0260 (7)
H27	−0.362640	0.471796	0.316539	0.031*
C28	−0.1408 (6)	0.6572 (4)	0.3816 (2)	0.0250 (7)
H28	−0.224639	0.695843	0.428392	0.030*
C29	0.2013 (6)	0.4666 (4)	0.1678 (2)	0.0230 (6)
C30	0.0310 (6)	0.3407 (4)	0.1173 (2)	0.0236 (7)
C31	−0.1468 (6)	0.3419 (4)	0.1661 (2)	0.0222 (6)
C32	0.0253 (6)	0.2392 (4)	0.0333 (2)	0.0232 (6)
H32	0.148081	0.238534	0.001502	0.028*
C33	−0.1620 (6)	0.1380 (4)	−0.0043 (3)	0.0243 (7)
C34	−0.3346 (6)	0.1355 (4)	0.0463 (3)	0.0260 (7)
H34	−0.459675	0.062432	0.021745	0.031*
C35	−0.3285 (6)	0.2373 (4)	0.1318 (3)	0.0258 (7)
H35	−0.447445	0.234509	0.165682	0.031*
C36	−0.1881 (6)	0.0386 (4)	−0.1026 (2)	0.0261 (7)
H36A	−0.292015	−0.049858	−0.107536	0.031*
H36B	−0.253593	0.087410	−0.147047	0.031*
C37	0.0872 (6)	−0.1085 (4)	−0.0968 (2)	0.0243 (7)
C38	0.2524 (6)	−0.1682 (4)	−0.1384 (3)	0.0294 (8)
H38	0.305188	−0.136765	−0.187734	0.035*
C39	0.3404 (6)	−0.2748 (4)	−0.1071 (3)	0.0296 (8)
H39	0.454620	−0.316585	−0.135380	0.036*
C40	0.2643 (6)	−0.3216 (4)	−0.0352 (3)	0.0292 (8)
H40	0.325432	−0.394801	−0.014078	0.035*
C41	0.0986 (6)	−0.2601 (4)	0.0050 (2)	0.0250 (7)
C42	0.0074 (6)	−0.1549 (4)	−0.0254 (3)	0.0246 (7)
H42	−0.108662	−0.114593	0.002177	0.030*
Cl1	0.2053 (2)	0.17453 (13)	0.65929 (9)	0.0542 (4)
C43	0.4128 (7)	0.2615 (4)	0.7525 (3)	0.0306 (8)
C44	0.3680 (7)	0.2937 (5)	0.8418 (3)	0.0320 (8)
H44	0.224785	0.265769	0.853168	0.038*
C45	0.5314 (8)	0.3668 (5)	0.9151 (3)	0.0348 (9)
H45	0.502082	0.389116	0.977568	0.042*
C46	0.7375 (8)	0.4077 (5)	0.8978 (3)	0.0406 (10)

H46	0.850033	0.460205	0.948342	0.049*
C47	0.7812 (9)	0.3732 (6)	0.8083 (4)	0.0484 (12)
H47	0.924417	0.401211	0.796899	0.058*
C48	0.6189 (9)	0.2979 (5)	0.7341 (3)	0.0418 (11)
H48	0.649317	0.271929	0.671735	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0216 (13)	0.0295 (14)	0.0336 (14)	−0.0023 (10)	0.0080 (10)	0.0040 (11)
O2	0.0340 (15)	0.0216 (12)	0.0304 (13)	−0.0017 (10)	0.0013 (11)	0.0058 (10)
O3	0.0278 (14)	0.0216 (12)	0.0279 (13)	0.0000 (10)	0.0036 (10)	0.0051 (9)
O4	0.0219 (13)	0.0244 (13)	0.0315 (13)	0.0004 (10)	0.0054 (10)	0.0058 (10)
O5	0.0267 (14)	0.0236 (12)	0.0270 (12)	−0.0006 (10)	0.0049 (10)	0.0057 (10)
O6	0.0241 (13)	0.0235 (12)	0.0300 (13)	0.0042 (10)	0.0055 (10)	0.0069 (10)
C1	0.0231 (17)	0.0225 (16)	0.0256 (16)	−0.0001 (12)	0.0047 (12)	0.0043 (12)
C2	0.0216 (17)	0.0219 (16)	0.0274 (17)	0.0009 (12)	0.0033 (13)	0.0072 (12)
C3	0.0193 (16)	0.0246 (17)	0.0348 (18)	−0.0007 (13)	0.0064 (13)	0.0077 (14)
C4	0.0204 (16)	0.0256 (17)	0.0326 (18)	−0.0005 (13)	0.0067 (13)	0.0064 (14)
C5	0.0227 (17)	0.0215 (16)	0.0219 (15)	0.0037 (12)	0.0035 (12)	0.0052 (12)
C6	0.0202 (16)	0.0233 (16)	0.0227 (15)	0.0016 (12)	0.0042 (12)	0.0074 (12)
C7	0.0210 (16)	0.0221 (16)	0.0232 (15)	0.0006 (12)	0.0052 (12)	0.0053 (12)
C8	0.0222 (16)	0.0214 (16)	0.0233 (15)	0.0009 (12)	0.0072 (12)	0.0048 (12)
C9	0.0242 (17)	0.0220 (16)	0.0262 (17)	0.0018 (13)	0.0055 (13)	0.0056 (13)
C10	0.0206 (16)	0.0224 (16)	0.0245 (16)	0.0021 (12)	0.0032 (12)	0.0044 (12)
C11	0.0225 (17)	0.0262 (18)	0.0282 (17)	0.0003 (13)	0.0065 (13)	0.0058 (13)
C12	0.0289 (19)	0.0269 (18)	0.0275 (17)	0.0025 (14)	0.0083 (14)	0.0067 (14)
C13	0.0271 (18)	0.0231 (17)	0.0237 (16)	−0.0005 (13)	0.0044 (13)	0.0064 (13)
C14	0.0258 (18)	0.0199 (16)	0.0263 (16)	0.0007 (13)	0.0040 (13)	0.0061 (12)
C15	0.032 (2)	0.0248 (17)	0.0268 (18)	−0.0030 (14)	0.0045 (14)	0.0051 (14)
C16	0.0253 (17)	0.0234 (16)	0.0229 (16)	0.0005 (13)	0.0049 (13)	0.0009 (12)
C17	0.0252 (18)	0.032 (2)	0.0271 (17)	0.0011 (14)	0.0012 (13)	0.0030 (14)
C18	0.0242 (18)	0.035 (2)	0.0291 (18)	−0.0017 (14)	0.0027 (14)	0.0006 (15)
C19	0.0227 (18)	0.0254 (18)	0.0348 (19)	−0.0057 (13)	0.0051 (14)	0.0019 (14)
C20	0.0242 (17)	0.0224 (16)	0.0252 (16)	0.0018 (12)	0.0055 (12)	0.0041 (12)
C21	0.0254 (17)	0.0224 (16)	0.0243 (16)	−0.0028 (13)	0.0027 (12)	0.0022 (12)
C22	0.0239 (17)	0.0257 (17)	0.0255 (16)	0.0027 (13)	0.0027 (13)	0.0031 (13)
C23	0.0229 (17)	0.0220 (16)	0.0240 (16)	0.0032 (13)	0.0021 (12)	0.0067 (12)
C24	0.0222 (17)	0.0242 (16)	0.0235 (16)	−0.0005 (13)	0.0045 (12)	0.0036 (12)
C25	0.0189 (16)	0.0238 (16)	0.0227 (15)	0.0011 (12)	0.0039 (12)	0.0062 (12)
C26	0.0189 (15)	0.0236 (16)	0.0207 (15)	0.0000 (12)	0.0018 (11)	0.0024 (12)
C27	0.0202 (17)	0.0284 (18)	0.0286 (17)	0.0017 (13)	0.0048 (13)	0.0071 (14)
C28	0.0225 (17)	0.0271 (17)	0.0232 (16)	0.0021 (13)	0.0036 (13)	0.0041 (13)
C29	0.0207 (16)	0.0219 (15)	0.0249 (16)	0.0014 (12)	0.0039 (12)	0.0051 (12)
C30	0.0193 (16)	0.0245 (17)	0.0259 (16)	0.0006 (13)	0.0027 (12)	0.0069 (13)
C31	0.0214 (16)	0.0218 (15)	0.0238 (15)	0.0027 (12)	0.0039 (12)	0.0073 (12)
C32	0.0212 (16)	0.0238 (16)	0.0245 (16)	0.0021 (12)	0.0043 (12)	0.0069 (13)
C33	0.0228 (17)	0.0223 (16)	0.0273 (16)	0.0005 (12)	0.0025 (13)	0.0083 (13)

C34	0.0194 (16)	0.0245 (17)	0.0326 (18)	−0.0022 (12)	0.0013 (13)	0.0092 (14)
C35	0.0196 (16)	0.0274 (17)	0.0302 (17)	−0.0004 (13)	0.0043 (13)	0.0095 (13)
C36	0.0274 (18)	0.0229 (16)	0.0246 (16)	0.0010 (13)	0.0028 (13)	0.0031 (12)
C37	0.0223 (17)	0.0241 (16)	0.0221 (16)	−0.0011 (13)	0.0009 (12)	0.0024 (12)
C38	0.0209 (17)	0.0311 (19)	0.0293 (18)	−0.0044 (14)	0.0036 (13)	0.0008 (14)
C39	0.0199 (17)	0.035 (2)	0.0293 (18)	0.0029 (14)	0.0072 (13)	0.0002 (14)
C40	0.0198 (17)	0.0303 (19)	0.0333 (19)	0.0033 (14)	0.0017 (14)	0.0032 (15)
C41	0.0210 (16)	0.0232 (16)	0.0261 (16)	−0.0021 (12)	0.0025 (12)	0.0024 (13)
C42	0.0220 (17)	0.0218 (16)	0.0278 (16)	0.0012 (12)	0.0051 (12)	0.0036 (12)
Cl1	0.0703 (9)	0.0375 (6)	0.0415 (6)	−0.0101 (5)	−0.0137 (5)	0.0074 (5)
C43	0.035 (2)	0.0242 (18)	0.0315 (19)	0.0030 (15)	0.0041 (15)	0.0075 (14)
C44	0.028 (2)	0.036 (2)	0.0318 (19)	0.0023 (15)	0.0064 (15)	0.0088 (15)
C45	0.040 (2)	0.034 (2)	0.033 (2)	0.0101 (17)	0.0089 (17)	0.0093 (16)
C46	0.037 (2)	0.0231 (19)	0.056 (3)	0.0001 (16)	−0.005 (2)	0.0093 (18)
C47	0.036 (3)	0.042 (3)	0.074 (4)	−0.001 (2)	0.014 (2)	0.028 (3)
C48	0.053 (3)	0.038 (2)	0.042 (2)	0.004 (2)	0.024 (2)	0.0173 (19)

Geometric parameters (Å, º)

O1—C10	1.207 (4)	C22—H22B	0.9900
O2—C15	1.410 (5)	C22—C23	1.502 (5)
O2—C16	1.374 (5)	C23—C24	1.383 (5)
O3—C20	1.353 (5)	C23—C28	1.393 (5)
O3—C22	1.420 (5)	C24—H24	0.9500
O4—C29	1.214 (4)	C24—C25	1.377 (5)
O5—C36	1.415 (5)	C25—C26	1.402 (5)
O5—C37	1.362 (4)	C25—C29	1.492 (5)
O6—C1	1.420 (4)	C26—C27	1.377 (5)
O6—C41	1.363 (4)	C26—C31	1.473 (5)
C1—H1A	0.9900	C27—H27	0.9500
C1—H1B	0.9900	C27—C28	1.401 (5)
C1—C2	1.504 (5)	C28—H28	0.9500
C2—C3	1.393 (5)	C29—C30	1.479 (5)
C2—C7	1.389 (5)	C30—C31	1.400 (5)
C3—H3	0.9500	C30—C32	1.371 (5)
C3—C4	1.382 (5)	C31—C35	1.370 (5)
C4—H4	0.9500	C32—H32	0.9500
C4—C5	1.376 (5)	C32—C33	1.382 (5)
C5—C6	1.404 (5)	C33—C34	1.392 (5)
C5—C8	1.472 (5)	C33—C36	1.509 (5)
C6—C7	1.377 (5)	C34—H34	0.9500
C6—C10	1.491 (5)	C34—C35	1.389 (5)
C7—H7	0.9500	C35—H35	0.9500
C8—C9	1.396 (5)	C36—H36A	0.9900
C8—C11	1.376 (5)	C36—H36B	0.9900
C9—C10	1.479 (5)	C37—C38	1.377 (5)
C9—C14	1.383 (5)	C37—C42	1.388 (5)
C11—H11	0.9500	C38—H38	0.9500

C11—C12	1.390 (5)	C38—C39	1.384 (6)
C12—H12	0.9500	C39—H39	0.9500
C12—C13	1.387 (5)	C39—C40	1.387 (6)
C13—C14	1.386 (5)	C40—H40	0.9500
C13—C15	1.495 (5)	C40—C41	1.377 (5)
C14—H14	0.9500	C41—C42	1.375 (5)
C15—H15A	0.9900	C42—H42	0.9500
C15—H15B	0.9900	Cl1—C43	1.732 (4)
C16—C17	1.385 (5)	C43—C44	1.362 (5)
C16—C21	1.372 (5)	C43—C48	1.371 (6)
C17—H17	0.9500	C44—H44	0.9500
C17—C18	1.378 (6)	C44—C45	1.372 (6)
C18—H18	0.9500	C45—H45	0.9500
C18—C19	1.383 (6)	C45—C46	1.373 (7)
C19—H19	0.9500	C46—H46	0.9500
C19—C20	1.382 (5)	C46—C47	1.364 (7)
C20—C21	1.392 (5)	C47—H47	0.9500
C21—H21	0.9500	C47—C48	1.381 (7)
C22—H22A	0.9900	C48—H48	0.9500

C16—O2—C15	117.1 (3)	C24—C23—C28	119.8 (3)
C20—O3—C22	116.5 (3)	C28—C23—C22	118.7 (3)
C37—O5—C36	116.8 (3)	C23—C24—H24	120.6
C41—O6—C1	118.1 (3)	C25—C24—C23	118.8 (3)
O6—C1—H1A	108.6	C25—C24—H24	120.6
O6—C1—H1B	108.6	C24—C25—C26	121.5 (3)
O6—C1—C2	114.5 (3)	C24—C25—C29	129.7 (3)
H1A—C1—H1B	107.6	C26—C25—C29	108.5 (3)
C2—C1—H1A	108.6	C25—C26—C31	108.6 (3)
C2—C1—H1B	108.6	C27—C26—C25	120.2 (3)
C3—C2—C1	117.3 (3)	C27—C26—C31	131.1 (3)
C7—C2—C1	122.5 (3)	C26—C27—H27	121.0
C7—C2—C3	120.2 (3)	C26—C27—C28	118.0 (3)
C2—C3—H3	119.1	C28—C27—H27	121.0
C4—C3—C2	121.9 (3)	C23—C28—C27	121.6 (3)
C4—C3—H3	119.1	C23—C28—H28	119.2
C3—C4—H4	120.9	C27—C28—H28	119.2
C5—C4—C3	118.3 (3)	O4—C29—C25	127.1 (3)
C5—C4—H4	120.9	O4—C29—C30	127.5 (3)
C4—C5—C6	119.9 (3)	C30—C29—C25	105.3 (3)
C4—C5—C8	131.2 (3)	C31—C30—C29	109.1 (3)
C6—C5—C8	108.7 (3)	C32—C30—C29	129.5 (3)
C5—C6—C10	107.9 (3)	C32—C30—C31	121.3 (3)
C7—C6—C5	122.1 (3)	C30—C31—C26	108.4 (3)
C7—C6—C10	129.9 (3)	C35—C31—C26	131.4 (3)
C2—C7—H7	121.2	C35—C31—C30	120.1 (3)
C6—C7—C2	117.7 (3)	C30—C32—H32	120.5
C6—C7—H7	121.2	C30—C32—C33	119.0 (3)

C9—C8—C5	108.5 (3)	C33—C32—H32	120.5
C11—C8—C5	131.3 (3)	C32—C33—C34	119.5 (3)
C11—C8—C9	120.1 (3)	C32—C33—C36	120.7 (3)
C8—C9—C10	108.7 (3)	C34—C33—C36	119.7 (3)
C14—C9—C8	121.4 (3)	C33—C34—H34	119.2
C14—C9—C10	129.8 (3)	C35—C34—C33	121.6 (3)
O1—C10—C6	126.6 (3)	C35—C34—H34	119.2
O1—C10—C9	127.7 (3)	C31—C35—C34	118.4 (3)
C9—C10—C6	105.7 (3)	C31—C35—H35	120.8
C8—C11—H11	121.1	C34—C35—H35	120.8
C8—C11—C12	117.9 (3)	O5—C36—C33	114.3 (3)
C12—C11—H11	121.1	O5—C36—H36A	108.7
C11—C12—H12	118.9	O5—C36—H36B	108.7
C13—C12—C11	122.3 (4)	C33—C36—H36A	108.7
C13—C12—H12	118.9	C33—C36—H36B	108.7
C12—C13—C15	117.1 (3)	H36A—C36—H36B	107.6
C14—C13—C12	119.3 (3)	O5—C37—C38	116.1 (3)
C14—C13—C15	123.4 (3)	O5—C37—C42	123.0 (3)
C9—C14—C13	118.6 (3)	C38—C37—C42	120.9 (4)
C9—C14—H14	120.7	C37—C38—H38	120.5
C13—C14—H14	120.7	C37—C38—C39	118.9 (3)
O2—C15—C13	114.4 (3)	C39—C38—H38	120.5
O2—C15—H15A	108.7	C38—C39—H39	119.5
O2—C15—H15B	108.7	C38—C39—C40	121.0 (4)
C13—C15—H15A	108.7	C40—C39—H39	119.5
C13—C15—H15B	108.7	C39—C40—H40	120.6
H15A—C15—H15B	107.6	C41—C40—C39	118.8 (4)
O2—C16—C17	115.7 (3)	C41—C40—H40	120.6
C21—C16—O2	122.8 (3)	O6—C41—C40	115.9 (3)
C21—C16—C17	121.5 (3)	O6—C41—C42	122.9 (3)
C16—C17—H17	120.9	C42—C41—C40	121.2 (3)
C18—C17—C16	118.3 (4)	C37—C42—H42	120.5
C18—C17—H17	120.9	C41—C42—C37	119.1 (3)
C17—C18—H18	119.3	C41—C42—H42	120.5
C17—C18—C19	121.5 (4)	C44—C43—Cl1	119.8 (3)
C19—C18—H18	119.3	C44—C43—C48	121.6 (4)
C18—C19—H19	120.3	C48—C43—Cl1	118.6 (3)
C20—C19—C18	119.3 (3)	C43—C44—H44	120.3
C20—C19—H19	120.3	C43—C44—C45	119.5 (4)
O3—C20—C19	116.9 (3)	C45—C44—H44	120.3
O3—C20—C21	123.1 (3)	C44—C45—H45	120.1
C19—C20—C21	120.0 (4)	C44—C45—C46	119.8 (4)
C16—C21—C20	119.4 (3)	C46—C45—H45	120.1
C16—C21—H21	120.3	C45—C46—H46	119.9
C20—C21—H21	120.3	C47—C46—C45	120.2 (4)
O3—C22—H22A	108.7	C47—C46—H46	119.9
O3—C22—H22B	108.7	C46—C47—H47	119.7
O3—C22—C23	114.1 (3)	C46—C47—C48	120.6 (4)

H22A—C22—H22B	107.6	C48—C47—H47	119.7
C23—C22—H22A	108.7	C43—C48—C47	118.3 (4)
C23—C22—H22B	108.7	C43—C48—H48	120.8
C24—C23—C22	121.4 (3)	C47—C48—H48	120.8
O2—C16—C17—C18	178.9 (3)	C19—C20—C21—C16	0.1 (5)
O2—C16—C21—C20	−178.5 (3)	C20—O3—C22—C23	−80.0 (4)
O3—C20—C21—C16	179.4 (3)	C21—C16—C17—C18	0.5 (6)
O3—C22—C23—C24	−30.7 (5)	C22—O3—C20—C19	−165.2 (3)
O3—C22—C23—C28	152.4 (3)	C22—O3—C20—C21	15.4 (5)
O4—C29—C30—C31	−179.6 (4)	C22—C23—C24—C25	−174.6 (3)
O4—C29—C30—C32	−3.9 (7)	C22—C23—C28—C27	174.6 (3)
O5—C37—C38—C39	179.1 (3)	C23—C24—C25—C26	−0.1 (5)
O5—C37—C42—C41	−178.6 (3)	C23—C24—C25—C29	174.4 (3)
O6—C1—C2—C3	−165.4 (3)	C24—C23—C28—C27	−2.3 (5)
O6—C1—C2—C7	12.6 (5)	C24—C25—C26—C27	−1.9 (5)
O6—C41—C42—C37	179.0 (3)	C24—C25—C26—C31	174.7 (3)
C1—O6—C41—C40	−160.6 (3)	C24—C25—C29—O4	4.5 (6)
C1—O6—C41—C42	19.3 (5)	C24—C25—C29—C30	−173.6 (4)
C1—C2—C3—C4	175.2 (4)	C25—C26—C27—C28	1.8 (5)
C1—C2—C7—C6	−175.9 (3)	C25—C26—C31—C30	0.0 (4)
C2—C3—C4—C5	0.5 (6)	C25—C26—C31—C35	−177.1 (4)
C3—C2—C7—C6	2.1 (5)	C25—C29—C30—C31	−1.5 (4)
C3—C4—C5—C6	2.3 (5)	C25—C29—C30—C32	174.2 (4)
C3—C4—C5—C8	−172.2 (4)	C26—C25—C29—O4	179.6 (4)
C4—C5—C6—C7	−3.1 (5)	C26—C25—C29—C30	1.5 (4)
C4—C5—C6—C10	−179.0 (3)	C26—C27—C28—C23	0.3 (6)
C4—C5—C8—C9	174.1 (4)	C26—C31—C35—C34	174.0 (4)
C4—C5—C8—C11	−3.6 (7)	C27—C26—C31—C30	176.1 (4)
C5—C6—C7—C2	0.8 (5)	C27—C26—C31—C35	−1.0 (7)
C5—C6—C10—O1	−173.4 (4)	C28—C23—C24—C25	2.2 (5)
C5—C6—C10—C9	6.1 (4)	C29—C25—C26—C27	−177.5 (3)
C5—C8—C9—C10	4.8 (4)	C29—C25—C26—C31	−0.9 (4)
C5—C8—C9—C14	−172.1 (3)	C29—C30—C31—C26	1.0 (4)
C5—C8—C11—C12	173.4 (4)	C29—C30—C31—C35	178.4 (3)
C6—C5—C8—C9	−0.9 (4)	C29—C30—C32—C33	−174.1 (4)
C6—C5—C8—C11	−178.6 (4)	C30—C31—C35—C34	−2.8 (5)
C7—C2—C3—C4	−2.9 (5)	C30—C32—C33—C34	−4.0 (5)
C7—C6—C10—O1	11.1 (6)	C30—C32—C33—C36	171.1 (3)
C7—C6—C10—C9	−169.4 (4)	C31—C26—C27—C28	−173.9 (4)
C8—C5—C6—C7	172.6 (3)	C31—C30—C32—C33	1.2 (5)
C8—C5—C6—C10	−3.3 (4)	C32—C30—C31—C26	−175.2 (3)
C8—C9—C10—O1	172.7 (4)	C32—C30—C31—C35	2.3 (5)
C8—C9—C10—C6	−6.7 (4)	C32—C33—C34—C35	3.5 (5)
C8—C9—C14—C13	−2.0 (5)	C32—C33—C36—O5	33.9 (5)
C8—C11—C12—C13	−1.6 (6)	C33—C34—C35—C31	0.0 (6)
C9—C8—C11—C12	−4.0 (5)	C34—C33—C36—O5	−151.0 (3)
C10—C6—C7—C2	175.7 (3)	C36—O5—C37—C38	167.2 (3)

C10—C9—C14—C13	−178.2 (4)	C36—O5—C37—C42	−13.0 (5)
C11—C8—C9—C10	−177.2 (3)	C36—C33—C34—C35	−171.7 (3)
C11—C8—C9—C14	5.9 (6)	C37—O5—C36—C33	78.4 (4)
C11—C12—C13—C14	5.5 (6)	C37—C38—C39—C40	0.1 (6)
C11—C12—C13—C15	−170.5 (4)	C38—C37—C42—C41	1.3 (5)
C12—C13—C14—C9	−3.6 (5)	C38—C39—C40—C41	0.0 (6)
C12—C13—C15—O2	168.8 (3)	C39—C40—C41—O6	−179.6 (3)
C14—C9—C10—O1	−10.7 (7)	C39—C40—C41—C42	0.5 (5)
C14—C9—C10—C6	169.9 (4)	C40—C41—C42—C37	−1.2 (5)
C14—C13—C15—O2	−7.0 (5)	C41—O6—C1—C2	−90.6 (4)
C15—O2—C16—C17	158.0 (3)	C42—C37—C38—C39	−0.7 (5)
C15—O2—C16—C21	−23.6 (5)	Cl1—C43—C44—C45	−177.9 (3)
C15—C13—C14—C9	172.1 (3)	Cl1—C43—C48—C47	177.0 (4)
C16—O2—C15—C13	91.6 (4)	C43—C44—C45—C46	0.5 (6)
C16—C17—C18—C19	−0.7 (6)	C44—C43—C48—C47	−2.2 (7)
C17—C16—C21—C20	−0.2 (6)	C44—C45—C46—C47	−1.4 (7)
C17—C18—C19—C20	0.7 (6)	C45—C46—C47—C48	0.5 (7)
C18—C19—C20—O3	−179.7 (3)	C46—C47—C48—C43	1.3 (7)
C18—C19—C20—C21	−0.3 (6)	C48—C43—C44—C45	1.3 (7)

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2 and *Cg*15 are the centroids of the C5/C6/C10/C9/C8, C25/C29/C30/C31/C26 and C43–C48 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···Cl1^{i}	0.95	2.83	3.547 (4)	133
C35—H35···O1^{ii}	0.95	2.58	3.491 (5)	161
C46—H46···O6^{iii}	0.95	2.55	3.418 (5)	152
C1—H1*A*···*Cg*2^{iv}	0.99	2.95	3.610 (4)	125
C22—H22*A*···*Cg*1^{v}	0.99	2.73	3.711 (4)	170
C36—H36*B*···*Cg*15^{vi}	0.99	2.84	3.713 (4)	148

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