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[3,4-Bis(2,3-dichlorophenyl)cyclobutane-1,2-diyl]-bis(furan-2-ylmethanone) monohydrate

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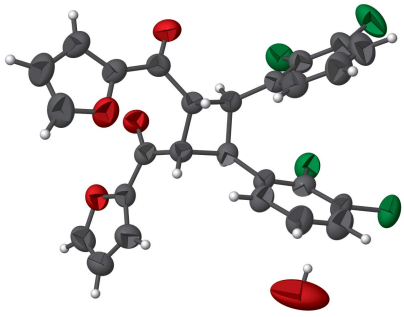
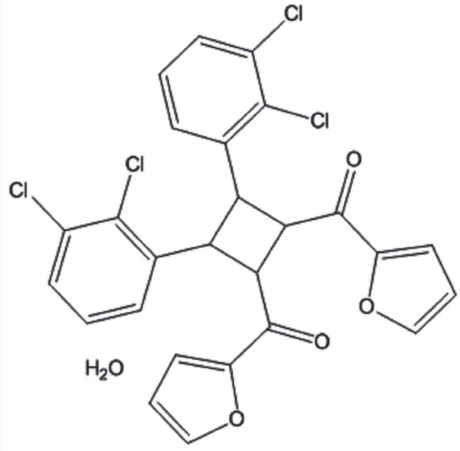
In the title hydrate, $C_{26}H_{16}Cl_4O_4\cdot H_2O$, the cyclobutane ring carries two 2,3-dichlorophenyl and two furan-2-ylmethanone substituents. It subtends dihedral angles of 86.6 (3) and 37.3 (3)° with the furan rings and 77.0 (5) and 77.0 (3)° with the dichlorophenyl rings. In the crystal, molecules are linked *via* weak C—H···O hydrogen bonds, forming chains propagating along the *a*-axis direction. Additional C—H···O and C—H···Cl hydrogen bonds generate a three-dimensional network of molecules stacked along the *b* axis.

3D view



Chemical scheme



Structure description

Recently, a new route to polysubstituted cyclobutanes *via* a $K_2S_2O_8$-promoted intramolecular [2 + 2]-cycloaddition (Zhu *et al.*, 2016) and an efficient intermolecular [2 + 2]-cycloaddition (Raghavendra *et al.*, 2017) were reported. We herein report the synthesis and crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. The dihedral angles between the central cyclobutane ring and the two furan rings (O1/C1–C4 and O3/C14–C17) bridged by the carbonyl group are 86.6 (3) and 37.3 (3)°, respectively, whereas the two dichlorophenyl rings subtend angles of 77.0 (5) and 77.0 (3)°, respectively, with the cyclobutane ring. The furan rings are inclined at 68.6 (3)° to one another while the angle between the two dichlorophenyl rings is 40.8 (2)°. The carbonyl substituents at C5 and C18 on the (O1/C1–C4 and O3/C14–C17) furan rings lie close to the ring planes, as

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O4^{i}	0.93	2.54	3.424 (7)	159
C9—H9···O2^{ii}	0.93	2.48	3.184 (6)	133
C19—H19···O2^{ii}	0.98	2.41	3.267 (5)	146

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

indicated by the torsion angles O1—C4—C5—O2 = 2.6 (6)° and O3—C17—C18—O4 = −179.0 (4)°.

In the crystal, molecules are linked *via* weak C—H···O hydrogen bonds (Table 1), forming chains propagating along the *a*-axis direction (Fig. 2). Additional C—H···O and C—H···Cl hydrogen bonds generate a three-dimensional network of molecules stacked along the *b* axis (Fig. 3).

Synthesis and crystallization

A mixture of 2,3-dichlorobenzaldehyde (5 mmol), 2-acetylfuran (5 mmol) and sodium hydroxide (5 mmol) in 95%

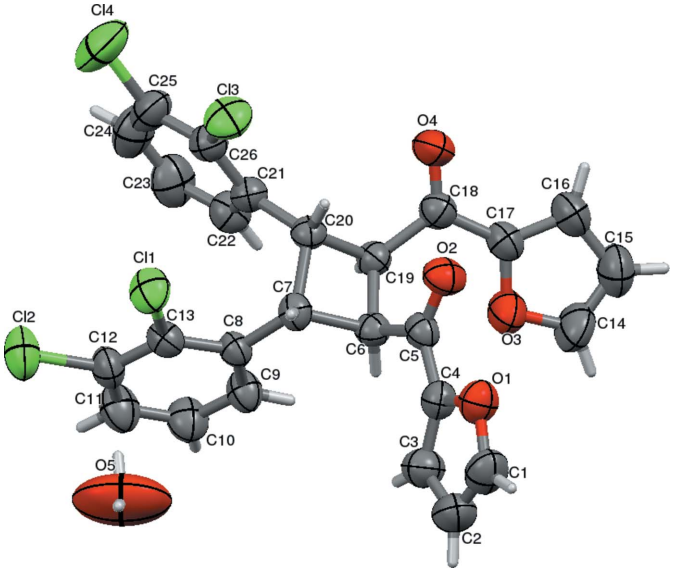


Figure 1
The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

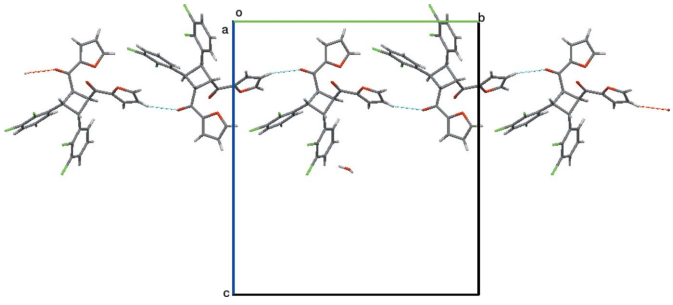


Figure 2
C—H···O hydrogen bonds forming chains propagating along the *b*-axis direction. Hydrogen bonds are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{16}Cl_4O_4{\cdot}H_2O$
M_r	552.20
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, *b*, *c* (Å)	10.9673 (12), 20.211 (2), 22.491 (2)
V (Å^3)	4985.4 (9)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.63
Crystal size (mm)	0.28 × 0.26 × 0.24
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.357, 0.403
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25946, 4144, 2605
R_{int}	0.110
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.587
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.184, 1.03
No. of reflections	4144
No. of parameters	320
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.31

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

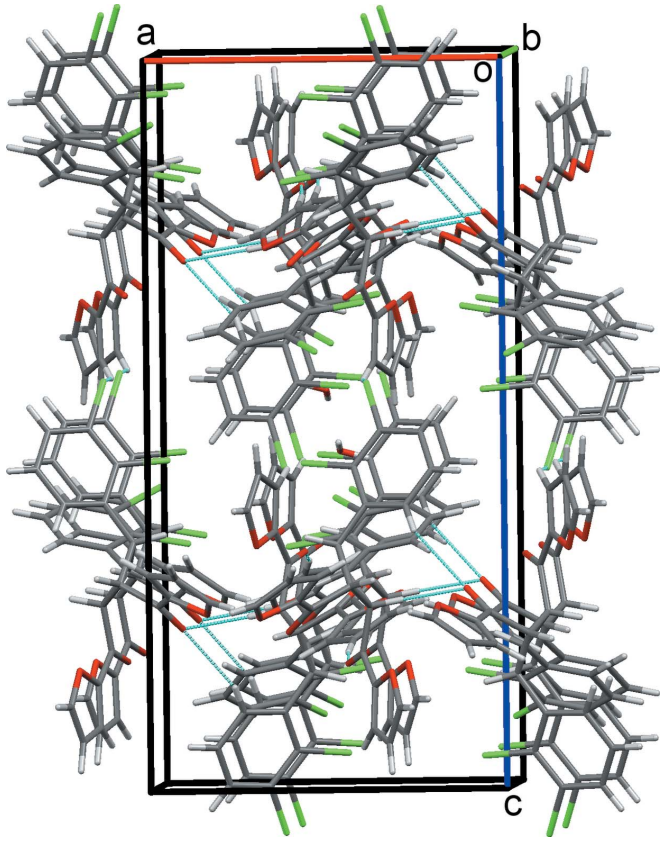


Figure 3
C—H···O and C—H···Cl hydrogen bonds generating a three-dimensional network of molecules stacked along the *b* axis. Hydrogen bonds are shown as dashed lines.

ethanol (25 ml) was refluxed on a water bath for 2 h. The progress of the reaction was monitored by TLC. After the completion of the reaction, the mixture was poured into ice-cold water and kept in a refrigerator overnight. The solid formed was filtered, and washed with cold hydrochloric acid (5%). Yellow rectangular crystals were obtained from 60% aqueous methanol solution by slow evaporation (yield 82%, m.p. 391–393 K).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170318 [https://doi.org/10.1107/S2414314617003182]

[3,4-Bis(2,3-dichlorophenyl)cyclobutane-1,2-diyl]bis(furan-2-ylmethanone) monohydrate

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(3,4-bis(2,3-dichlorophenyl)cyclobutane-1,2-diyl)bis(furan-2-ylmethanone) hydrate

Crystal data

$C_{26}H_{16}Cl_4O_4·H_2O$
M_r = 552.20
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 10.9673 (12) Å
b = 20.211 (2) Å
c = 22.491 (2) Å
V = 4985.4 (9) Å^3
Z = 8
F(000) = 2256
D_x = 1.471 Mg m^{-3}
Cu *Kα* radiation, λ = 1.54178 Å
Cell parameters from 2605 reflections
θ = 4.8–64.8°
μ = 4.63 mm^{-1}
T = 296 K
Rectangle, yellow
0.28 × 0.26 × 0.24 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.357, T_{max} = 0.403
25946 measured reflections
4144 independent reflections
2605 reflections with $I > 2\sigma(I)$
R_{int} = 0.110
θ_{max} = 64.7°, θ_{min} = 4.8°
h = −12→10
k = −23→23
l = −26→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.184
S = 1.03
4144 reflections
320 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0851P)^2 + 1.6075P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $FC^*=KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-1/4}$
Extinction coefficient: 0.0025 (2)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.45306 (10)	0.30473 (6)	0.45130 (6)	0.0683 (4)
Cl2	0.63057 (13)	0.30057 (8)	0.55980 (6)	0.0851 (5)
Cl3	0.40331 (10)	0.18694 (6)	0.33566 (7)	0.0753 (5)
Cl4	0.53084 (17)	0.07000 (7)	0.40060 (9)	0.1110 (7)
O1	0.3358 (3)	0.52823 (15)	0.24221 (15)	0.0638 (11)
O2	0.4107 (3)	0.40209 (15)	0.22127 (15)	0.0623 (11)
O3	0.6993 (3)	0.43530 (18)	0.16593 (15)	0.0747 (12)
O4	0.5712 (3)	0.27567 (16)	0.17591 (15)	0.0740 (12)
C1	0.3265 (5)	0.5923 (3)	0.2602 (3)	0.076 (2)
C2	0.4214 (5)	0.6099 (3)	0.2929 (3)	0.078 (2)
C3	0.4973 (4)	0.5542 (2)	0.2967 (2)	0.0680 (19)
C4	0.4428 (4)	0.5049 (2)	0.2654 (2)	0.0507 (14)
C5	0.4746 (3)	0.4370 (2)	0.25304 (19)	0.0487 (12)
C6	0.5854 (3)	0.40991 (19)	0.28332 (19)	0.0473 (14)
C7	0.5482 (3)	0.3692 (2)	0.33959 (18)	0.0456 (11)
C8	0.6285 (3)	0.3744 (2)	0.39355 (18)	0.0467 (12)
C9	0.7404 (4)	0.4062 (2)	0.3933 (2)	0.0557 (16)
C10	0.8164 (4)	0.4050 (3)	0.4419 (2)	0.0687 (17)
C11	0.7832 (4)	0.3727 (3)	0.4929 (2)	0.0730 (19)
C12	0.6713 (4)	0.3412 (2)	0.49532 (19)	0.0593 (17)
C13	0.5936 (4)	0.3428 (2)	0.44642 (19)	0.0503 (14)
C14	0.7232 (5)	0.4715 (3)	0.1170 (3)	0.085 (2)
C15	0.6914 (5)	0.4393 (3)	0.0684 (3)	0.083 (2)
C16	0.6448 (5)	0.3776 (3)	0.0870 (2)	0.0723 (19)
C17	0.6498 (4)	0.3768 (2)	0.1469 (2)	0.0567 (16)
C18	0.6140 (4)	0.3287 (2)	0.1908 (2)	0.0540 (14)
C19	0.6361 (3)	0.34523 (19)	0.25510 (18)	0.0463 (12)
C20	0.5666 (3)	0.30417 (19)	0.30123 (18)	0.0448 (11)
C21	0.6263 (3)	0.2453 (2)	0.33068 (19)	0.0497 (14)
C22	0.7508 (4)	0.2449 (2)	0.3429 (2)	0.0617 (16)
C23	0.8034 (5)	0.1936 (3)	0.3734 (3)	0.082 (2)
C24	0.7369 (6)	0.1410 (3)	0.3914 (3)	0.086 (2)
C25	0.6137 (5)	0.1381 (2)	0.3792 (2)	0.072 (2)
C26	0.5583 (4)	0.1908 (2)	0.3490 (2)	0.0553 (14)
O5	0.4797 (7)	0.4741 (4)	0.5418 (5)	0.210 (5)

H1	0.26180	0.62010	0.25080	0.0910*
H2	0.43510	0.65110	0.31000	0.0930*
H3	0.57120	0.55150	0.31690	0.0820*
H6	0.64820	0.44330	0.29110	0.0570*
H7	0.46220	0.37600	0.34970	0.0550*
H9	0.76480	0.42890	0.35930	0.0670*
H10	0.89130	0.42650	0.44020	0.0820*
H11	0.83520	0.37190	0.52560	0.0870*
H14	0.75750	0.51350	0.11740	0.1020*
H15	0.69840	0.45430	0.02950	0.1000*
H16	0.61600	0.34390	0.06260	0.0870*
H19	0.72370	0.34220	0.26330	0.0560*
H20	0.48800	0.29060	0.28450	0.0540*
H22	0.79900	0.28000	0.33010	0.0740*
H23	0.88630	0.19500	0.38190	0.0980*
H24	0.77430	0.10660	0.41200	0.1030*
H5A	0.40680	0.48360	0.55150	0.3150*
H5B	0.48290	0.43430	0.52980	0.3150*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0594 (6)	0.0815 (8)	0.0641 (8)	−0.0145 (5)	0.0089 (5)	0.0080 (6)
Cl2	0.0958 (9)	0.1063 (11)	0.0533 (8)	−0.0027 (8)	−0.0004 (6)	0.0212 (7)
Cl3	0.0603 (7)	0.0729 (8)	0.0927 (10)	−0.0198 (6)	0.0031 (6)	0.0031 (7)
Cl4	0.1362 (13)	0.0602 (8)	0.1365 (16)	0.0082 (8)	0.0522 (11)	0.0300 (9)
O1	0.0601 (18)	0.0644 (19)	0.067 (2)	0.0081 (14)	−0.0037 (15)	0.0059 (16)
O2	0.0562 (16)	0.0627 (19)	0.068 (2)	−0.0027 (14)	−0.0140 (16)	−0.0085 (16)
O3	0.086 (2)	0.078 (2)	0.060 (2)	−0.0212 (18)	−0.0029 (17)	0.0087 (18)
O4	0.103 (2)	0.060 (2)	0.059 (2)	−0.0121 (18)	0.0065 (18)	−0.0118 (17)
C1	0.089 (4)	0.062 (3)	0.076 (4)	0.022 (3)	0.011 (3)	0.005 (3)
C2	0.103 (4)	0.057 (3)	0.074 (4)	0.004 (3)	0.002 (3)	−0.004 (3)
C3	0.073 (3)	0.061 (3)	0.070 (4)	0.000 (2)	−0.005 (3)	−0.006 (2)
C4	0.051 (2)	0.053 (2)	0.048 (3)	0.0021 (19)	0.0017 (19)	0.005 (2)
C5	0.048 (2)	0.056 (2)	0.042 (2)	−0.0055 (19)	0.0027 (19)	−0.0005 (19)
C6	0.047 (2)	0.046 (2)	0.049 (3)	−0.0056 (17)	0.0006 (19)	−0.0021 (19)
C7	0.0397 (19)	0.054 (2)	0.043 (2)	−0.0005 (17)	0.0027 (17)	0.0014 (19)
C8	0.050 (2)	0.053 (2)	0.037 (2)	−0.0011 (18)	0.0017 (18)	−0.0020 (18)
C9	0.048 (2)	0.072 (3)	0.047 (3)	−0.006 (2)	0.003 (2)	0.003 (2)
C10	0.058 (3)	0.082 (3)	0.066 (3)	−0.011 (2)	−0.007 (2)	0.004 (3)
C11	0.061 (3)	0.097 (4)	0.061 (3)	−0.007 (3)	−0.012 (2)	0.003 (3)
C12	0.069 (3)	0.070 (3)	0.039 (3)	0.003 (2)	0.001 (2)	0.003 (2)
C13	0.049 (2)	0.055 (2)	0.047 (3)	−0.0016 (19)	−0.0003 (19)	−0.006 (2)
C14	0.096 (4)	0.083 (4)	0.077 (4)	−0.022 (3)	0.007 (3)	0.025 (3)
C15	0.095 (4)	0.100 (4)	0.055 (4)	0.006 (3)	0.009 (3)	0.015 (3)
C16	0.086 (3)	0.081 (4)	0.050 (3)	0.000 (3)	0.004 (3)	−0.006 (3)
C17	0.058 (2)	0.065 (3)	0.047 (3)	0.000 (2)	0.002 (2)	−0.004 (2)
C18	0.058 (2)	0.051 (2)	0.053 (3)	0.002 (2)	0.005 (2)	−0.002 (2)

C19	0.046 (2)	0.047 (2)	0.046 (2)	−0.0033 (17)	0.0017 (18)	−0.0003 (18)
C20	0.0413 (19)	0.046 (2)	0.047 (2)	−0.0066 (16)	−0.0023 (17)	−0.0007 (18)
C21	0.052 (2)	0.046 (2)	0.051 (3)	−0.0011 (18)	−0.0004 (19)	−0.0009 (19)
C22	0.052 (2)	0.067 (3)	0.066 (3)	0.002 (2)	−0.002 (2)	−0.001 (2)
C23	0.066 (3)	0.098 (4)	0.081 (4)	0.024 (3)	−0.010 (3)	0.008 (3)
C24	0.090 (4)	0.079 (4)	0.089 (4)	0.032 (3)	0.012 (3)	0.023 (3)
C25	0.091 (4)	0.050 (3)	0.074 (4)	0.009 (2)	0.022 (3)	0.009 (2)
C26	0.056 (2)	0.053 (2)	0.057 (3)	−0.0014 (19)	0.005 (2)	−0.002 (2)
O5	0.172 (6)	0.142 (6)	0.316 (12)	0.016 (5)	0.032 (7)	−0.107 (7)

Geometric parameters (Å, º)

Cl1—C13	1.726 (4)	C15—C16	1.411 (8)
Cl2—C12	1.725 (4)	C16—C17	1.348 (6)
Cl3—C26	1.728 (5)	C17—C18	1.440 (6)
Cl4—C25	1.718 (5)	C18—C19	1.504 (6)
O1—C1	1.361 (7)	C19—C20	1.532 (5)
O1—C4	1.368 (5)	C20—C21	1.511 (5)
O2—C5	1.225 (5)	C21—C26	1.393 (6)
O3—C14	1.347 (7)	C21—C22	1.393 (6)
O3—C17	1.370 (5)	C22—C23	1.371 (7)
O4—C18	1.217 (5)	C23—C24	1.351 (9)
O5—H5B	0.8500	C24—C25	1.380 (9)
O5—H5A	0.8500	C25—C26	1.402 (6)
C1—C2	1.323 (8)	C1—H1	0.9300
C2—C3	1.403 (7)	C2—H2	0.9300
C3—C4	1.359 (6)	C3—H3	0.9300
C4—C5	1.443 (6)	C6—H6	0.9800
C5—C6	1.497 (5)	C7—H7	0.9800
C6—C7	1.564 (6)	C9—H9	0.9300
C6—C19	1.556 (5)	C10—H10	0.9300
C7—C20	1.585 (6)	C11—H11	0.9300
C7—C8	1.503 (5)	C14—H14	0.9300
C8—C9	1.385 (6)	C15—H15	0.9300
C8—C13	1.403 (6)	C16—H16	0.9300
C9—C10	1.375 (6)	C19—H19	0.9800
C10—C11	1.369 (7)	C20—H20	0.9800
C11—C12	1.384 (6)	C22—H22	0.9300
C12—C13	1.392 (6)	C23—H23	0.9300
C14—C15	1.319 (9)	C24—H24	0.9300
C1—O1—C4	106.2 (4)	C22—C21—C26	117.5 (4)
C14—O3—C17	106.9 (4)	C21—C22—C23	121.1 (4)
H5A—O5—H5B	110.00	C22—C23—C24	121.2 (5)
O1—C1—C2	111.2 (5)	C23—C24—C25	120.2 (6)
C1—C2—C3	106.6 (5)	Cl4—C25—C24	119.8 (4)
C2—C3—C4	107.2 (4)	C24—C25—C26	119.2 (4)
O1—C4—C3	108.8 (4)	Cl4—C25—C26	121.0 (4)

O1—C4—C5	117.5 (4)	Cl3—C26—C21	120.7 (3)
C3—C4—C5	133.7 (4)	C21—C26—C25	120.8 (4)
O2—C5—C6	121.3 (4)	Cl3—C26—C25	118.4 (3)
C4—C5—C6	117.2 (3)	O1—C1—H1	124.00
O2—C5—C4	121.5 (4)	C2—C1—H1	124.00
C5—C6—C19	114.3 (3)	C3—C2—H2	127.00
C7—C6—C19	88.9 (3)	C1—C2—H2	127.00
C5—C6—C7	110.4 (3)	C2—C3—H3	126.00
C6—C7—C20	87.9 (3)	C4—C3—H3	126.00
C8—C7—C20	115.0 (3)	C7—C6—H6	114.00
C6—C7—C8	117.6 (3)	C19—C6—H6	114.00
C7—C8—C9	123.2 (4)	C5—C6—H6	114.00
C7—C8—C13	119.5 (3)	C6—C7—H7	111.00
C9—C8—C13	117.2 (4)	C8—C7—H7	112.00
C8—C9—C10	121.7 (4)	C20—C7—H7	111.00
C9—C10—C11	120.9 (4)	C8—C9—H9	119.00
C10—C11—C12	119.2 (4)	C10—C9—H9	119.00
Cl2—C12—C13	121.1 (3)	C11—C10—H10	119.00
C11—C12—C13	120.1 (4)	C9—C10—H10	120.00
Cl2—C12—C11	118.8 (3)	C10—C11—H11	120.00
Cl1—C13—C12	119.1 (3)	C12—C11—H11	120.00
C8—C13—C12	120.9 (4)	C15—C14—H14	124.00
Cl1—C13—C8	120.0 (3)	O3—C14—H14	125.00
O3—C14—C15	111.0 (5)	C14—C15—H15	127.00
C14—C15—C16	106.6 (6)	C16—C15—H15	127.00
C15—C16—C17	107.0 (5)	C17—C16—H16	126.00
O3—C17—C18	118.5 (4)	C15—C16—H16	127.00
C16—C17—C18	133.0 (4)	C6—C19—H19	109.00
O3—C17—C16	108.5 (4)	C18—C19—H19	109.00
O4—C18—C17	120.7 (4)	C20—C19—H19	109.00
C17—C18—C19	117.7 (4)	C7—C20—H20	109.00
O4—C18—C19	121.5 (4)	C19—C20—H20	109.00
C6—C19—C18	121.4 (3)	C21—C20—H20	109.00
C18—C19—C20	116.8 (3)	C23—C22—H22	120.00
C6—C19—C20	90.1 (3)	C21—C22—H22	119.00
C7—C20—C19	89.0 (3)	C22—C23—H23	119.00
C7—C20—C21	118.0 (3)	C24—C23—H23	119.00
C19—C20—C21	120.5 (3)	C23—C24—H24	120.00
C20—C21—C22	121.1 (3)	C25—C24—H24	120.00
C20—C21—C26	121.4 (3)		

C4—O1—C1—C2	0.2 (6)	C9—C10—C11—C12	−0.3 (8)
C1—O1—C4—C3	−0.2 (5)	C10—C11—C12—Cl2	179.9 (4)
C1—O1—C4—C5	179.7 (4)	C10—C11—C12—C13	−0.3 (7)
C17—O3—C14—C15	0.2 (6)	Cl2—C12—C13—Cl1	1.3 (5)
C14—O3—C17—C16	0.5 (5)	Cl2—C12—C13—C8	−178.3 (3)
C14—O3—C17—C18	−179.2 (4)	C11—C12—C13—Cl1	−178.5 (4)
O1—C1—C2—C3	−0.1 (7)	C11—C12—C13—C8	1.9 (7)

C1—C2—C3—C4	0.0 (6)	O3—C14—C15—C16	−0.7 (6)
C2—C3—C4—O1	0.1 (5)	C14—C15—C16—C17	0.9 (6)
C2—C3—C4—C5	−179.7 (5)	C15—C16—C17—O3	−0.8 (6)
O1—C4—C5—O2	2.6 (6)	C15—C16—C17—C18	178.8 (5)
O1—C4—C5—C6	−174.2 (4)	O3—C17—C18—O4	−179.0 (4)
C3—C4—C5—O2	−177.6 (5)	O3—C17—C18—C19	−1.4 (6)
C3—C4—C5—C6	5.6 (7)	C16—C17—C18—O4	1.5 (8)
O2—C5—C6—C7	−78.4 (5)	C16—C17—C18—C19	179.0 (5)
O2—C5—C6—C19	20.1 (5)	O4—C18—C19—C6	−127.4 (4)
C4—C5—C6—C7	98.4 (4)	O4—C18—C19—C20	−19.4 (6)
C4—C5—C6—C19	−163.2 (3)	C17—C18—C19—C6	55.1 (5)
C5—C6—C7—C8	−142.2 (3)	C17—C18—C19—C20	163.1 (4)
C5—C6—C7—C20	100.6 (3)	C6—C19—C20—C7	−15.4 (3)
C19—C6—C7—C8	102.2 (3)	C6—C19—C20—C21	−137.7 (4)
C19—C6—C7—C20	−15.1 (2)	C18—C19—C20—C7	−141.1 (3)
C5—C6—C19—C18	25.5 (5)	C18—C19—C20—C21	96.5 (4)
C5—C6—C19—C20	−96.4 (3)	C7—C20—C21—C22	−73.1 (5)
C7—C6—C19—C18	137.5 (3)	C7—C20—C21—C26	104.0 (4)
C7—C6—C19—C20	15.6 (3)	C19—C20—C21—C22	33.8 (6)
C6—C7—C8—C9	−8.5 (6)	C19—C20—C21—C26	−149.1 (4)
C6—C7—C8—C13	175.1 (3)	C20—C21—C22—C23	175.3 (5)
C20—C7—C8—C9	92.9 (5)	C26—C21—C22—C23	−1.9 (7)
C20—C7—C8—C13	−83.5 (4)	C20—C21—C26—Cl3	2.9 (6)
C6—C7—C20—C19	15.3 (2)	C20—C21—C26—C25	−176.5 (4)
C6—C7—C20—C21	139.8 (3)	C22—C21—C26—Cl3	−179.9 (3)
C8—C7—C20—C19	−104.4 (3)	C22—C21—C26—C25	0.7 (6)
C8—C7—C20—C21	20.1 (4)	C21—C22—C23—C24	1.6 (9)
C7—C8—C9—C10	−174.1 (4)	C22—C23—C24—C25	0.0 (10)
C13—C8—C9—C10	2.3 (6)	C23—C24—C25—Cl4	178.3 (5)
C7—C8—C13—Cl1	−5.9 (5)	C23—C24—C25—C26	−1.2 (9)
C7—C8—C13—C12	173.7 (4)	Cl4—C25—C26—Cl3	1.9 (5)
C9—C8—C13—Cl1	177.6 (3)	Cl4—C25—C26—C21	−178.7 (3)
C9—C8—C13—C12	−2.9 (6)	C24—C25—C26—Cl3	−178.6 (4)
C8—C9—C10—C11	−0.8 (8)	C24—C25—C26—C21	0.8 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O4^{i}	0.93	2.54	3.424 (7)	159
C9—H9···O2^{ii}	0.93	2.48	3.184 (6)	133
C19—H19···O2^{ii}	0.98	2.41	3.267 (5)	146

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