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(1*E*,4*E*)-1,5-Bis(2,6-dichlorophenyl)penta-1,4-dien-3-one

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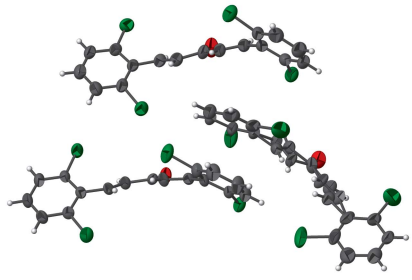
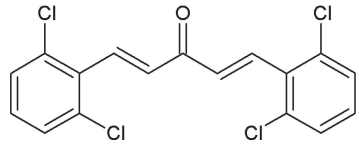
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{17}H_{10}Cl_4O$, consists of one independent molecule and two molecules each located on twofold symmetry axes through the central C═O bond such that they each contribute half a molecule each to the asymmetric unit. The dihedral angles between the rings in the three molecules are 73.1 (3), 65.3 (3) and 75.4 (3)°. In the crystal, molecules are linked through C—H···O hydrogen bonds, generating undulated molecular sheets lying parallel to (110).

3D view



Chemical scheme



Structure description

In the asymmetric unit of the title compound (Fig. 1), one independent molecule and two molecules each located on twofold symmetry axes through the central C═O bond such that they each contribute half a molecule each to the asymmetric unit. The atoms C33 and C34 of the *B* molecule (C27–C35/Cl1/Cl2/O) are disordered over two sets of sites with occupancy factors of 0.471 (14) and 0.529 (14). No abnormalities are observed in the bond lengths and angles of the asymmetric unit molecules and are typical of such compounds (Huang *et al.*, 2011).

In the crystal, the molecules are linked primarily *via* C—H···O hydrogen bonds, forming molecular chains (Table 1 and Fig. 2) with C—H···Cl hydrogen bonds also contributing to the cohesion of the crystal.

Synthesis and crystallization

The title compound was synthesized by following the published procedure (Lee *et al.*, 2009). A mixture of 2,6 dicholorobenzaldehyde (4.8 g, 0.027 mol) and acetone (1 ml) in

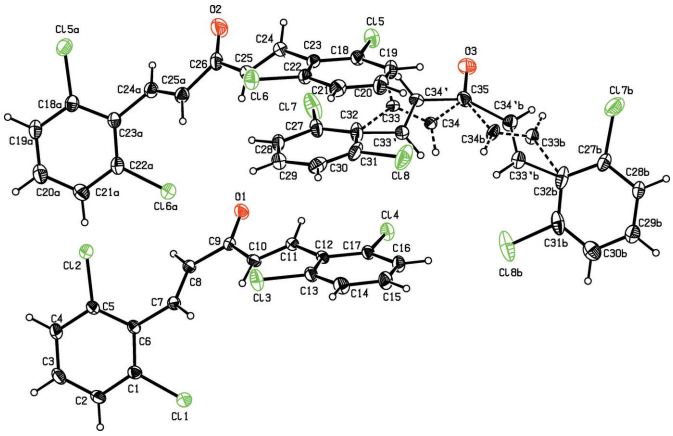


Figure 1
An *ORTEP* plot of the title compound with three molecules in the asymmetric unit, with displacement ellipsoids drawn at 20% probability level. Both disorder components are shown. [Symmetry codes: (a) $-x$, $1-y$, z; (b) $-x+\frac{1}{2}$, $-y+\frac{3}{2}$, z.]

the presence of 10% NaOH along with 50 ml methanol was prepared and the solution was stirred for about 15 h. Ice cubes were added to enhance the precipitation. The resultant precipitate was collected and washed with distilled water to drain excess NaOH from the product. Single crystals of diffraction quality were grown from chloroform solution by slow evaporation (m.p. 371 K).

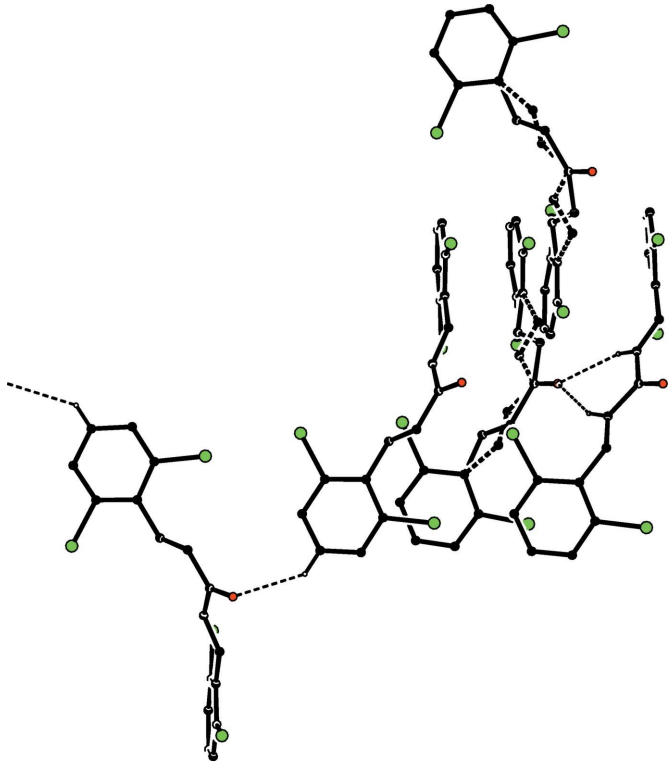


Figure 2
Crystal packing of the title compound. The dashed lines indicate hydrogen bonding. Hydrogen atoms not involved in hydrogen bonding are omitted for clarity.

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···Cl4^{i}	0.93	2.86	3.750 (6)	162
C25—H25···O3^{ii}	0.93	2.57	3.444 (8)	156
C30—H30···Cl7^{i}	0.93	2.90	3.784 (8)	159

Symmetry codes: (i) $-x+\frac{1}{4}, y-\frac{1}{4}, z-\frac{1}{4}$; (ii) $x-\frac{1}{4}, -y+\frac{5}{4}, z-\frac{1}{4}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{10}Cl_4O$
M_r	372.05
Crystal system, space group	Orthorhombic, *Fdd*2
Temperature (K)	296
a, b, c (Å)	28.1477 (8), 17.3385 (7), 26.1837 (10)
V (Å^3)	12778.7 (8)
Z	32
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.74
Crystal size (mm)	0.20 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.863, 0.895
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37791, 5641, 4336
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.085, 1.03
No. of reflections	5633
No. of parameters	418
No. of restraints	64
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.47
Absolute structure	Flack x determined using 1755 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter	−0.01 (2)

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *ORTEP-3 for Windows* (Farrugia, 2012).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atoms C33 and C34 are disordered over two sets of sites [occupancy ratio 0.471 (14):0.529 (14)].

Acknowledgements

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References

Bruker (2004). *APEX2*, *SAINT*, *XPREP* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Huang, J.-D., Tang, Q.-Q., Chen, X.-Y., Ye, Y. & Wang, Y. (2011). *Acta Cryst.* E**67**, o758.
Lee, K., Ab Aziz, F. H., Syahida, A., Abas, F., Shaari, K., Israf, D. A. & Lajis, N. H. (2009). *Eur. J. Med. Chem.* **44**, 3195–3200.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2018). **3**, x171822 [https://doi.org/10.1107/S2414314617018223]

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(1*E*,4*E*)-1,5-Bis(2,6-dichlorophenyl)penta-1,4-dien-3-one

Crystal data

$C_{17}H_{10}Cl_4O$
M_r = 372.05
Orthorhombic, *Fdd*2
a = 28.1477 (8) Å
b = 17.3385 (7) Å
c = 26.1837 (10) Å
V = 12778.7 (8) Å^3
Z = 32
F(000) = 6016
D_x = 1.547 Mg m^{-3}
Melting point: 371 K
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 6475 reflections
θ = 2.7–21.9°
μ = 0.74 mm^{-1}
T = 296 K
Block, yellow
0.20 × 0.20 × 0.15 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.863, T_{max} = 0.895
37791 measured reflections
5641 independent reflections
4336 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 25.0°, θ_{min} = 2.1°
h = −32→33
k = −20→20
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.085
S = 1.03
5633 reflections
418 parameters
64 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2 + 21.0031P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack *x* determined using 1755 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter: −0.01 (2)

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.

Refinement. H atoms were positioned geometrically and treated as riding on their parent atoms and refined with, C—H distance of 0.93 Å.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	−0.11267 (18)	1.0169 (3)	0.15237 (19)	0.0423 (13)	
C2	−0.15359 (19)	1.0469 (3)	0.1311 (2)	0.0496 (14)	
H2	−0.1518	1.0793	0.1029	0.060*	
C3	−0.1968 (2)	1.0285 (3)	0.1519 (2)	0.0572 (16)	
H3	−0.2245	1.0489	0.1380	0.069*	
C4	−0.19913 (18)	0.9798 (3)	0.1935 (2)	0.0525 (15)	
H4	−0.2284	0.9661	0.2071	0.063*	
C5	−0.15811 (18)	0.9516 (3)	0.2146 (2)	0.0446 (13)	
C6	−0.11302 (17)	0.9690 (3)	0.19511 (19)	0.0389 (12)	
C7	−0.06800 (17)	0.9365 (3)	0.2143 (2)	0.0404 (12)	
H7	−0.0469	0.9185	0.1896	0.049*	
C8	−0.05401 (16)	0.9301 (3)	0.2622 (2)	0.0407 (12)	
H8	−0.0745	0.9484	0.2873	0.049*	
C9	−0.00870 (15)	0.8964 (3)	0.2793 (2)	0.0394 (12)	
C10	0.02339 (18)	0.8609 (3)	0.2416 (2)	0.0453 (13)	
H10	0.0133	0.8548	0.2080	0.054*	
C11	0.06613 (17)	0.8379 (3)	0.2548 (2)	0.0403 (12)	
H11	0.0734	0.8433	0.2893	0.048*	
C12	0.10397 (16)	0.8048 (3)	0.22319 (19)	0.0398 (12)	
C13	0.09792 (18)	0.7573 (3)	0.1799 (2)	0.0478 (14)	
C14	0.1352 (2)	0.7286 (4)	0.1525 (2)	0.0584 (16)	
H14	0.1297	0.6973	0.1243	0.070*	
C15	0.18132 (19)	0.7462 (4)	0.1668 (2)	0.0590 (17)	
H15	0.2068	0.7271	0.1480	0.071*	
C16	0.18946 (18)	0.7915 (3)	0.2083 (2)	0.0510 (14)	
H16	0.2204	0.8033	0.2179	0.061*	
C17	0.15191 (17)	0.8196 (3)	0.23576 (19)	0.0403 (12)	
C18	0.16222 (18)	0.4241 (3)	0.3399 (2)	0.0491 (14)	
C19	0.2023 (2)	0.4001 (3)	0.3140 (3)	0.0608 (17)	
H19	0.2322	0.4166	0.3244	0.073*	
C20	0.1977 (2)	0.3517 (4)	0.2729 (3)	0.0699 (19)	
H20	0.2246	0.3357	0.2551	0.084*	
C21	0.1535 (2)	0.3268 (4)	0.2580 (2)	0.0608 (17)	
H21	0.1503	0.2934	0.2304	0.073*	
C22	0.11380 (17)	0.3517 (3)	0.2843 (2)	0.0513 (15)	
C23	0.11649 (17)	0.4019 (3)	0.3262 (2)	0.0431 (13)	
C24	0.07580 (18)	0.4322 (3)	0.3552 (2)	0.0490 (14)	
H24	0.0772	0.4289	0.3907	0.059*	
C25	0.03839 (19)	0.4629 (3)	0.3354 (2)	0.0507 (14)	
H25	0.0351	0.4620	0.3000	0.061*	
C26	0.0000	0.5000	0.3665 (4)	0.057 (2)	
C27	0.09628 (19)	0.6931 (3)	0.3546 (2)	0.0588 (16)	
C28	0.05807 (18)	0.6714 (3)	0.3254 (2)	0.0537 (15)	
H28	0.0275	0.6858	0.3350	0.064*	
C29	0.0650 (2)	0.6288 (4)	0.2826 (3)	0.0643 (17)	

H29	0.0391	0.6139	0.2629	0.077*	
C30	0.1100 (2)	0.6077 (4)	0.2681 (3)	0.0722 (19)	
H30	0.1146	0.5779	0.2390	0.087*	
C31	0.1477 (2)	0.6308 (4)	0.2967 (3)	0.074 (2)	
C32	0.14291 (19)	0.6749 (4)	0.3408 (3)	0.071 (2)	
C33	0.1775 (4)	0.6990 (8)	0.3877 (6)	0.045 (4)	0.471 (14)
H33	0.1691	0.6870	0.4211	0.054*	0.471 (14)
C34	0.2169 (4)	0.7348 (8)	0.3785 (6)	0.052 (4)	0.471 (14)
H34	0.2235	0.7510	0.3454	0.063*	0.471 (14)
C33′	0.1895 (4)	0.7043 (6)	0.3532 (5)	0.050 (3)	0.529 (14)
H33′	0.2107	0.7175	0.3274	0.060*	0.529 (14)
C34′	0.2015 (5)	0.7121 (9)	0.4010 (5)	0.054 (4)	0.529 (14)
H34′	0.1808	0.6947	0.4261	0.064*	0.529 (14)
C35	0.2500	0.7500	0.4180 (3)	0.056 (2)	
O1	0.00129 (11)	0.8985 (2)	0.32475 (14)	0.0559 (10)	
O2	0.0000	0.5000	0.4127 (3)	0.081 (2)	
O3	0.2500	0.7500	0.4629 (2)	0.0734 (18)	
Cl1	−0.05851 (5)	1.04252 (9)	0.12522 (6)	0.0594 (4)	
Cl2	−0.16449 (5)	0.88981 (11)	0.26605 (7)	0.0744 (5)	
Cl3	0.04160 (5)	0.72921 (11)	0.16049 (7)	0.0731 (5)	
Cl4	0.16511 (5)	0.87707 (9)	0.28818 (6)	0.0567 (4)	
Cl5	0.16975 (6)	0.48515 (9)	0.39223 (6)	0.0666 (5)	
Cl6	0.05927 (5)	0.31438 (10)	0.26448 (6)	0.0669 (4)	
Cl7	0.08458 (7)	0.74969 (13)	0.40754 (9)	0.1053 (8)	
Cl8	0.20421 (6)	0.60238 (12)	0.27670 (11)	0.1188 (10)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.045 (3)	0.048 (3)	0.034 (3)	0.001 (3)	−0.002 (2)	−0.001 (3)
C2	0.052 (3)	0.052 (3)	0.045 (4)	0.007 (3)	−0.007 (3)	0.010 (3)
C3	0.046 (3)	0.061 (4)	0.065 (4)	0.007 (3)	−0.019 (3)	0.007 (3)
C4	0.035 (3)	0.059 (4)	0.064 (4)	0.005 (3)	−0.005 (3)	0.006 (3)
C5	0.039 (3)	0.045 (3)	0.050 (3)	0.003 (2)	−0.007 (2)	0.009 (3)
C6	0.038 (3)	0.038 (3)	0.040 (3)	0.005 (2)	−0.003 (2)	−0.002 (2)
C7	0.036 (3)	0.042 (3)	0.043 (3)	0.008 (2)	0.003 (2)	0.003 (3)
C8	0.036 (3)	0.051 (3)	0.035 (3)	0.007 (2)	0.004 (2)	0.002 (3)
C9	0.032 (3)	0.047 (3)	0.039 (3)	−0.004 (2)	0.002 (2)	0.004 (3)
C10	0.041 (3)	0.061 (4)	0.034 (3)	0.012 (3)	0.001 (2)	0.008 (3)
C11	0.037 (3)	0.043 (3)	0.040 (3)	0.002 (2)	0.000 (2)	0.005 (2)
C12	0.035 (3)	0.045 (3)	0.039 (3)	0.007 (2)	−0.004 (2)	0.005 (3)
C13	0.037 (3)	0.058 (4)	0.048 (4)	0.005 (3)	−0.005 (2)	0.001 (3)
C14	0.056 (4)	0.075 (4)	0.044 (4)	0.007 (3)	−0.002 (3)	−0.013 (3)
C15	0.038 (3)	0.078 (4)	0.061 (4)	0.015 (3)	0.007 (3)	−0.010 (4)
C16	0.034 (3)	0.062 (4)	0.057 (4)	0.004 (3)	0.000 (3)	−0.003 (3)
C17	0.033 (3)	0.042 (3)	0.046 (3)	0.005 (2)	−0.002 (2)	0.001 (3)
C18	0.043 (3)	0.047 (3)	0.058 (4)	0.000 (3)	−0.003 (3)	0.007 (3)
C19	0.036 (3)	0.055 (4)	0.091 (5)	0.000 (3)	0.001 (3)	0.003 (4)

C20	0.048 (4)	0.066 (4)	0.096 (6)	0.003 (3)	0.011 (4)	0.000 (4)
C21	0.060 (4)	0.057 (4)	0.066 (4)	0.007 (3)	0.010 (3)	−0.003 (3)
C22	0.038 (3)	0.054 (3)	0.062 (4)	0.003 (3)	0.001 (3)	0.010 (3)
C23	0.039 (3)	0.042 (3)	0.049 (3)	0.000 (2)	0.002 (2)	0.008 (3)
C24	0.043 (3)	0.055 (4)	0.048 (4)	−0.001 (3)	−0.002 (3)	0.006 (3)
C25	0.045 (3)	0.059 (4)	0.049 (4)	−0.001 (3)	−0.005 (3)	0.004 (3)
C26	0.034 (4)	0.063 (6)	0.074 (7)	0.001 (4)	0.000	0.000
C27	0.041 (3)	0.052 (4)	0.083 (5)	−0.005 (3)	−0.016 (3)	−0.002 (3)
C28	0.034 (3)	0.056 (4)	0.070 (4)	−0.005 (3)	−0.004 (3)	0.003 (3)
C29	0.051 (4)	0.074 (5)	0.067 (5)	−0.005 (3)	−0.006 (3)	0.007 (4)
C30	0.076 (5)	0.064 (4)	0.077 (5)	−0.002 (4)	0.019 (4)	0.013 (4)
C31	0.042 (4)	0.057 (4)	0.123 (7)	−0.001 (3)	0.024 (4)	0.028 (4)
C32	0.037 (3)	0.047 (4)	0.129 (6)	−0.007 (3)	−0.016 (4)	0.014 (4)
C33	0.042 (7)	0.060 (7)	0.034 (8)	−0.008 (6)	−0.003 (6)	0.015 (7)
C34	0.042 (7)	0.080 (9)	0.034 (8)	−0.022 (6)	−0.012 (6)	0.014 (7)
C33′	0.043 (7)	0.049 (6)	0.058 (8)	−0.003 (5)	−0.004 (6)	0.013 (6)
C34′	0.050 (9)	0.071 (8)	0.040 (8)	−0.008 (7)	−0.007 (7)	0.013 (6)
C35	0.042 (5)	0.083 (6)	0.042 (5)	0.012 (4)	0.000	0.000
O1	0.044 (2)	0.087 (3)	0.038 (2)	0.0066 (19)	−0.0018 (17)	−0.001 (2)
O2	0.060 (4)	0.118 (6)	0.066 (5)	0.016 (4)	0.000	0.000
O3	0.074 (4)	0.106 (5)	0.040 (4)	−0.001 (3)	0.000	0.000
Cl1	0.0509 (8)	0.0797 (11)	0.0476 (9)	−0.0002 (7)	0.0032 (7)	0.0106 (8)
Cl2	0.0428 (8)	0.0948 (13)	0.0857 (12)	−0.0048 (8)	−0.0023 (8)	0.0453 (11)
Cl3	0.0445 (9)	0.0937 (12)	0.0811 (12)	0.0003 (8)	−0.0166 (8)	−0.0252 (10)
Cl4	0.0433 (8)	0.0685 (10)	0.0581 (9)	−0.0003 (7)	−0.0047 (7)	−0.0120 (8)
Cl5	0.0561 (9)	0.0670 (10)	0.0768 (12)	−0.0040 (7)	−0.0114 (8)	−0.0088 (9)
Cl6	0.0511 (8)	0.0788 (11)	0.0707 (11)	−0.0064 (8)	−0.0010 (8)	−0.0184 (9)
Cl7	0.0755 (14)	0.1122 (16)	0.1282 (18)	0.0179 (11)	−0.0433 (12)	−0.0494 (14)
Cl8	0.0568 (10)	0.0889 (15)	0.211 (3)	0.0153 (10)	0.0501 (14)	0.0386 (17)

Geometric parameters (Å, º)

C1—C2	1.381 (7)	C20—C21	1.374 (8)
C1—C6	1.394 (7)	C20—H20	0.9300
C1—Cl1	1.740 (5)	C21—C22	1.383 (7)
C2—C3	1.370 (8)	C21—H21	0.9300
C2—H2	0.9300	C22—C23	1.402 (8)
C3—C4	1.380 (8)	C22—Cl6	1.745 (5)
C3—H3	0.9300	C23—C24	1.472 (7)
C4—C5	1.370 (7)	C24—C25	1.290 (7)
C4—H4	0.9300	C24—H24	0.9300
C5—C6	1.401 (7)	C25—C26	1.498 (8)
C5—Cl2	1.731 (5)	C25—H25	0.9300
C6—C7	1.474 (7)	C26—O2	1.211 (10)
C7—C8	1.320 (7)	C26—C25^{i}	1.498 (8)
C7—H7	0.9300	C27—C28	1.371 (7)
C8—C9	1.473 (7)	C27—C32	1.397 (8)
C8—H8	0.9300	C27—Cl7	1.731 (7)

C9—O1	1.224 (6)	C28—C29	1.357 (8)
C9—C10	1.473 (7)	C28—H28	0.9300
C10—C11	1.314 (7)	C29—C30	1.371 (8)
C10—H10	0.9300	C29—H29	0.9300
C11—C12	1.466 (7)	C30—C31	1.360 (9)
C11—H11	0.9300	C30—H30	0.9300
C12—C13	1.411 (7)	C31—C32	1.393 (10)
C12—C17	1.413 (7)	C31—Cl8	1.744 (6)
C13—C14	1.367 (7)	C32—C33′	1.444 (11)
C13—Cl3	1.735 (5)	C32—C33	1.622 (15)
C14—C15	1.385 (8)	C33—C34	1.293 (16)
C14—H14	0.9300	C33—H33	0.9300
C15—C16	1.360 (8)	C34—C35	1.418 (12)
C15—H15	0.9300	C34—C34^{ii}	1.94 (2)
C16—C17	1.368 (7)	C34—H34	0.9300
C16—H16	0.9300	C33′—C34′	1.303 (16)
C17—Cl4	1.736 (5)	C33′—H33′	0.9300
C18—C19	1.380 (8)	C34′—C35	1.578 (13)
C18—C23	1.391 (7)	C34′—H34′	0.9300
C18—Cl5	1.744 (6)	C35—O3	1.177 (9)
C19—C20	1.371 (9)	C35—C34^{ii}	1.418 (12)
C19—H19	0.9300	C35—C34′^{ii}	1.578 (13)

C2—C1—C6	122.8 (5)	C20—C21—C22	119.5 (6)
C2—C1—Cl1	118.0 (4)	C20—C21—H21	120.3
C6—C1—Cl1	119.1 (4)	C22—C21—H21	120.3
C3—C2—C1	119.6 (5)	C21—C22—C23	122.8 (5)
C3—C2—H2	120.2	C21—C22—Cl6	116.5 (5)
C1—C2—H2	120.2	C23—C22—Cl6	120.7 (4)
C2—C3—C4	119.8 (5)	C18—C23—C22	115.1 (5)
C2—C3—H3	120.1	C18—C23—C24	119.2 (5)
C4—C3—H3	120.1	C22—C23—C24	125.7 (5)
C5—C4—C3	119.8 (5)	C25—C24—C23	125.1 (5)
C5—C4—H4	120.1	C25—C24—H24	117.5
C3—C4—H4	120.1	C23—C24—H24	117.5
C4—C5—C6	122.7 (5)	C24—C25—C26	123.1 (6)
C4—C5—Cl2	116.6 (4)	C24—C25—H25	118.4
C6—C5—Cl2	120.7 (4)	C26—C25—H25	118.4
C1—C6—C5	115.3 (4)	O2—C26—C25	122.9 (4)
C1—C6—C7	119.6 (5)	O2—C26—C25^{i}	122.9 (4)
C5—C6—C7	125.0 (5)	C25—C26—C25^{i}	114.1 (8)
C8—C7—C6	127.8 (5)	C28—C27—C32	122.1 (6)
C8—C7—H7	116.1	C28—C27—Cl7	116.9 (5)
C6—C7—H7	116.1	C32—C27—Cl7	120.9 (5)
C7—C8—C9	125.5 (5)	C29—C28—C27	119.7 (5)
C7—C8—H8	117.2	C29—C28—H28	120.1
C9—C8—H8	117.2	C27—C28—H28	120.1
O1—C9—C8	118.9 (4)	C28—C29—C30	120.5 (6)

O1—C9—C10	121.6 (4)	C28—C29—H29	119.8
C8—C9—C10	119.5 (5)	C30—C29—H29	119.8
C11—C10—C9	120.7 (5)	C31—C30—C29	119.3 (7)
C11—C10—H10	119.6	C31—C30—H30	120.3
C9—C10—H10	119.6	C29—C30—H30	120.3
C10—C11—C12	129.4 (5)	C30—C31—C32	122.8 (6)
C10—C11—H11	115.3	C30—C31—Cl8	117.6 (7)
C12—C11—H11	115.3	C32—C31—Cl8	119.5 (6)
C13—C12—C17	114.1 (4)	C31—C32—C27	115.4 (6)
C13—C12—C11	126.4 (5)	C31—C32—C33′	107.0 (8)
C17—C12—C11	119.4 (5)	C27—C32—C33′	135.7 (8)
C14—C13—C12	122.8 (5)	C31—C32—C33	135.3 (7)
C14—C13—Cl3	116.5 (4)	C27—C32—C33	108.1 (8)
C12—C13—Cl3	120.7 (4)	C34—C33—C32	119.8 (12)
C13—C14—C15	119.8 (5)	C34—C33—H33	120.1
C13—C14—H14	120.1	C32—C33—H33	120.1
C15—C14—H14	120.1	C33—C34—C35	121.1 (13)
C16—C15—C14	120.1 (5)	C33—C34—C34^{ii}	162.7 (14)
C16—C15—H15	119.9	C35—C34—C34^{ii}	46.9 (6)
C14—C15—H15	119.9	C33—C34—H34	119.4
C15—C16—C17	119.7 (5)	C35—C34—H34	119.4
C15—C16—H16	120.1	C34^{ii}—C34—H34	74.0
C17—C16—H16	120.1	C34′—C33′—C32	119.3 (13)
C16—C17—C12	123.4 (5)	C34′—C33′—H33′	120.3
C16—C17—Cl4	117.0 (4)	C32—C33′—H33′	120.3
C12—C17—Cl4	119.5 (4)	C33′—C34′—C35	122.6 (13)
C19—C18—C23	123.0 (5)	C33′—C34′—H34′	118.7
C19—C18—Cl5	118.1 (4)	C35—C34′—H34′	118.7
C23—C18—Cl5	118.9 (4)	O3—C35—C34^{ii}	136.9 (6)
C20—C19—C18	119.7 (5)	O3—C35—C34	136.9 (6)
C20—C19—H19	120.2	C34^{ii}—C35—C34	86.3 (12)
C18—C19—H19	120.2	O3—C35—C34′	106.4 (6)
C19—C20—C21	120.0 (6)	O3—C35—C34′^{ii}	106.4 (6)
C19—C20—H20	120.0	C34′—C35—C34′^{ii}	147.3 (12)
C21—C20—H20	120.0		

C6—C1—C2—C3	−1.0 (8)	C19—C18—C23—C22	1.2 (8)
Cl1—C1—C2—C3	−179.3 (4)	Cl5—C18—C23—C22	−178.9 (4)
C1—C2—C3—C4	−0.6 (9)	C19—C18—C23—C24	−178.3 (5)
C2—C3—C4—C5	1.7 (9)	Cl5—C18—C23—C24	1.6 (7)
C3—C4—C5—C6	−1.3 (9)	C21—C22—C23—C18	−0.9 (8)
C3—C4—C5—Cl2	−179.1 (4)	Cl6—C22—C23—C18	176.5 (4)
C2—C1—C6—C5	1.4 (8)	C21—C22—C23—C24	178.5 (5)
Cl1—C1—C6—C5	179.7 (4)	Cl6—C22—C23—C24	−4.1 (8)
C2—C1—C6—C7	177.4 (5)	C18—C23—C24—C25	130.7 (6)
Cl1—C1—C6—C7	−4.3 (7)	C22—C23—C24—C25	−48.8 (9)
C4—C5—C6—C1	−0.3 (8)	C23—C24—C25—C26	−173.8 (4)
Cl2—C5—C6—C1	177.5 (4)	C24—C25—C26—O2	−4.3 (6)

C4—C5—C6—C7	−176.0 (5)	C24—C25—C26—C25^{i}	175.7 (6)
Cl2—C5—C6—C7	1.7 (8)	C32—C27—C28—C29	2.1 (9)
C1—C6—C7—C8	137.8 (6)	Cl7—C27—C28—C29	178.1 (5)
C5—C6—C7—C8	−46.6 (9)	C27—C28—C29—C30	−0.4 (10)
C6—C7—C8—C9	179.3 (5)	C28—C29—C30—C31	−0.9 (10)
C7—C8—C9—O1	175.2 (5)	C29—C30—C31—C32	0.5 (10)
C7—C8—C9—C10	−4.9 (8)	C29—C30—C31—Cl8	179.9 (5)
O1—C9—C10—C11	−7.4 (8)	C30—C31—C32—C27	1.2 (10)
C8—C9—C10—C11	172.7 (5)	Cl8—C31—C32—C27	−178.3 (5)
C9—C10—C11—C12	−177.0 (5)	C30—C31—C32—C33′	−165.8 (7)
C10—C11—C12—C13	−32.9 (9)	Cl8—C31—C32—C33′	14.8 (8)
C10—C11—C12—C17	147.6 (6)	C30—C31—C32—C33	167.2 (9)
C17—C12—C13—C14	−0.3 (8)	Cl8—C31—C32—C33	−12.2 (12)
C11—C12—C13—C14	−179.9 (5)	C28—C27—C32—C31	−2.5 (9)
C17—C12—C13—Cl3	177.0 (4)	Cl7—C27—C32—C31	−178.3 (5)
C11—C12—C13—Cl3	−2.5 (7)	C28—C27—C32—C33′	159.5 (9)
C12—C13—C14—C15	−0.3 (9)	Cl7—C27—C32—C33′	−16.3 (13)
Cl3—C13—C14—C15	−177.7 (5)	C28—C27—C32—C33	−172.2 (7)
C13—C14—C15—C16	0.5 (9)	Cl7—C27—C32—C33	12.0 (8)
C14—C15—C16—C17	−0.1 (9)	C31—C32—C33—C34	57.6 (17)
C15—C16—C17—C12	−0.6 (9)	C27—C32—C33—C34	−135.7 (13)
C15—C16—C17—Cl4	−179.9 (5)	C32—C33—C34—C35	−173.8 (9)
C13—C12—C17—C16	0.8 (7)	C32—C33—C34—C34^{ii}	−132 (4)
C11—C12—C17—C16	−179.7 (5)	C31—C32—C33′—C34′	−145.2 (11)
C13—C12—C17—Cl4	−179.9 (4)	C27—C32—C33′—C34′	51.7 (16)
C11—C12—C17—Cl4	−0.3 (7)	C32—C33′—C34′—C35	−174.9 (9)
C23—C18—C19—C20	−0.5 (9)	C33—C34—C35—O3	−15.6 (19)
Cl5—C18—C19—C20	179.6 (5)	C34^{ii}—C34—C35—O3	179.999 (1)
C18—C19—C20—C21	−0.6 (10)	C33—C34—C35—C34^{ii}	164.4 (19)
C19—C20—C21—C22	0.9 (10)	C33′—C34′—C35—O3	178.7 (11)
C20—C21—C22—C23	−0.1 (9)	C33′—C34′—C35—C34′^{ii}	−1.3 (11)
C20—C21—C22—Cl6	−177.6 (5)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···Cl3	0.93	2.63	3.160 (6)	117
C14—H14···Cl4^{iii}	0.93	2.86	3.750 (6)	162
C25—H25···O3^{iv}	0.93	2.57	3.444 (8)	156
C30—H30···Cl7^{iii}	0.93	2.90	3.784 (8)	159
C34′—H34′···Cl7	0.93	2.91	3.361 (14)	111

Symmetry codes: (iii) −*x*+1/4, *y*−1/4, *z*−1/4; (iv) *x*−1/4, −*y*+5/4, *z*−1/4.