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(*E*)-*N*′-[4-(2,4-Dichlorobenzyloxy)-3-methoxybenzylidene]-2-methoxybenzohydrazide sesquihydrate

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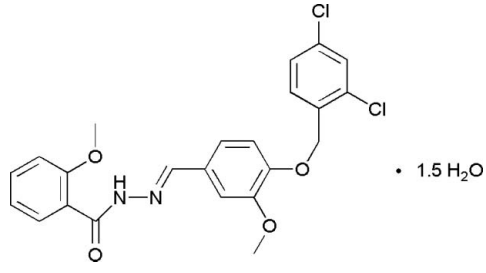
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.049; wR factor = 0.130; data-to-parameter ratio = 13.6.

In the title compound, $C_{23}H_{20}Cl_2N_2O_4\cdot1.5H_2O$, the vanillin group makes dihedral angles of 0.52 (14) and 81.22 (7)° with the benzohydrazide residue and the dichlorobenzene ring, respectively. An intramolecular N—H···O hydrogen bond helps to stabilize the molecular conformation, while intermolecular O—H···O and bifurcated O—H···(N,O) hydrogen bonds link the molecules, forming an infinite network. One of the water molecule sites is half-occupied.

Related literature

For general background, Santos *et al.* (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{23}H_{20}Cl_2N_2O_4\cdot1.5H_2O$
M_r = 486.34
Triclinic, $P\overline{1}$
a = 7.7689 (16) Å
b = 8.3390 (17) Å
c = 18.345 (4) Å
α = 80.93 (3)°
β = 77.85 (3)°
γ = 86.50 (3)°
V = 1146.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.902, T_{max} = 0.943
5880 measured reflections
4015 independent reflections
2630 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.130
S = 1.02
4015 reflections
295 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···O17^{i}	0.85	2.02	2.852 (3)	164
O2—H2A···O1^{ii}	0.85	2.10	2.918 (6)	161
O2—H2B···O1^{iii}	0.85	1.89	2.711 (6)	162
O1—H1A···O17	0.85	2.19	2.987 (3)	155
O1—H1A···N27	0.85	2.54	3.180 (3)	133
N17—H17···O12	0.86	1.93	2.625 (3)	137

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $-x+1, -y+1, -z+1$; (iii) $x-1, y, z+1$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2588).

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supplementary materials

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(*E*)-*N*'-[4-(2,4-Dichlorobenzyloxy)-3-methoxybenzylidene]-2-methoxybenzohydrazide sesquihydrate

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Comment

One of the aims of investigating the structural chemistry of Schiff bases is to develop protein and enzyme mimics (Santos *et al.*, 2001). As part of an investigation of the coordination properties of Schiff bases functioning as ligands, we report the synthesis and structure of the title compound, (I).

In (I) (Fig. 1), the vanillin group (C21—C27/O21/O22) is nearly planar, with an r.m.s. deviation for fitted atoms of 0.0229 Å. This plane makes dihedral angles of 0.52 (14)° and 81.22 (7)° with the benzohydrazide residue (C11—C16) and the dichlorobenzene ring (C31—C36), respectively. The dihedral angle between the benzohydrazide residue and the dichlorobenzene ring is 81.74 (9)°. Otherwise, all bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

An intramolecular hydrogen bond links the NH group to O12, thereby influencing the molecular conformation (Table 1). A bifurcated O—H···(N,*O*) and an O—H···O hydrogen bond link the water molecules to the main molecule, resulting in dimeric associations of two main molecules and two water molecules. Then, further O—H···O hydrogen bonds link the molecules into an infinite network (Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 4-(2,4-dichlorobenzyloxy)-3-methoxybenzaldehyde (3.11 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 2-methoxybenzohydrazide (1.66 g, 10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, giving a white precipitate. The product was isolated, recrystallized from ethanol and then dried in a vacuum to give the pure compound in 81% yield. Colourless blocks of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution. Presumably the water of crystallization in (I) was absorbed from the atmosphere.

Refinement

Due to a close O2···O2 contact, the O2 water molecule has a site occupancy of 0.5.

The H atoms of the water molecule and imine group were located in difference maps and then treated as riding atoms. All other H atoms were included in calculated positions and refined using a riding model approximation: 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2—H; 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene C—H; 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl C—H; 0.85 Å and U_{iso}(H) = 1.2U_{eq}(O) for water O—H; 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N) for imino N—H.

Figures

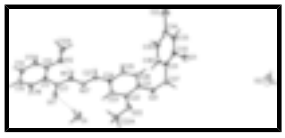

Fig. 1. The structure of (I) with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

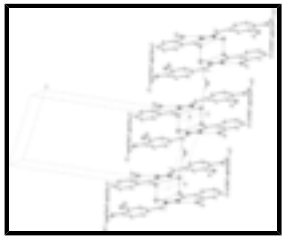

Fig. 2. Packing diagram for (I), with H bonds drawn as dashed lines. For the sake of clarity, H atoms bonded to C atoms have been omitted.

(*E*)—*N*'-[4-(2,4-Dichlorobenzyloxy)-3-methoxybenzylidene]-2-methoxybenzohydrazide sesquihydrate

Crystal data

$C_{23}H_{20}Cl_2N_2O_4 \cdot 1.5H_2O$	$Z = 2$
$M_r = 486.34$	$F_{000} = 506$
Triclinic, $P\overline{1}$	$D_x = 1.408$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.7689$ (16) Å	Cell parameters from 1784 reflections
$b = 8.3390$ (17) Å	$\theta = 2.3$–25.6º
$c = 18.345$ (4) Å	$\mu = 0.33$ mm^{-1}
$\alpha = 80.93$ (3)º	$T = 294$ (2) K
$\beta = 77.85$ (3)º	Block, colorless
$\gamma = 86.50$ (3)º	0.24 × 0.20 × 0.18 mm
$V = 1146.9$ (4) Å^3	

Data collection

Bruker SMART APEX CCD diffractometer	4015 independent reflections
Radiation source: fine-focus sealed tube	2630 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 294(2)$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.2$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -4 \rightarrow 9$
$T_{min} = 0.902$, $T_{max} = 0.943$	$k = -9 \rightarrow 9$
5880 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.5064P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
4015 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
295 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness 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 threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	−0.13680 (11)	0.79097 (10)	0.38426 (5)	0.0694 (3)	
Cl2	−0.39945 (15)	0.19415 (15)	0.47328 (6)	0.1037 (4)	
N27	0.5507 (3)	0.2392 (3)	0.01833 (11)	0.0398 (5)	
N17	0.5335 (3)	0.1920 (3)	−0.04870 (11)	0.0408 (5)	
H17	0.4404	0.2209	−0.0663	0.049*	
O21	0.3807 (2)	0.5372 (2)	0.32719 (10)	0.0482 (5)	
O22	0.6607 (2)	0.3832 (3)	0.27045 (10)	0.0555 (5)	
O17	0.7940 (3)	0.0557 (3)	−0.06310 (11)	0.0590 (6)	
O12	0.3475 (2)	0.1888 (2)	−0.15247 (11)	0.0555 (5)	
C24	0.4146 (3)	0.3881 (3)	0.11807 (13)	0.0367 (6)	
C22	0.5358 (3)	0.4077 (3)	0.22718 (14)	0.0385 (6)	
C11	0.6317 (3)	0.0618 (3)	−0.16009 (14)	0.0368 (6)	
C26	0.2499 (3)	0.5272 (3)	0.21774 (14)	0.0401 (6)	
H26	0.1491	0.5849	0.2375	0.048*	
C25	0.2655 (3)	0.4755 (3)	0.14804 (14)	0.0408 (6)	
H25	0.1755	0.4996	0.1213	0.049*	
C17	0.6597 (3)	0.1018 (3)	−0.08664 (14)	0.0391 (6)	
C21	0.3828 (3)	0.4934 (3)	0.25773 (14)	0.0385 (6)	
C12	0.4826 (3)	0.1046 (3)	−0.19211 (15)	0.0406 (6)	
C23	0.5507 (3)	0.3560 (3)	0.15837 (14)	0.0384 (6)	
H23	0.6519	0.2992	0.1384	0.046*	

C27	0.4222 (3)	0.3281 (3)	0.04695 (14)	0.0398 (6)	
H27	0.3304	0.3555	0.0215	0.048*	
C13	0.4770 (4)	0.0628 (3)	−0.26198 (16)	0.0495 (7)	
H13	0.3790	0.0927	−0.2832	0.059*	
C31	0.0713 (4)	0.5174 (3)	0.39109 (14)	0.0424 (7)	
C16	0.7684 (3)	−0.0254 (3)	−0.20037 (15)	0.0434 (7)	
H16	0.8676	−0.0564	−0.1801	0.052*	
C14	0.6156 (4)	−0.0228 (4)	−0.30015 (16)	0.0532 (8)	
H14	0.6103	−0.0505	−0.3468	0.064*	
C37	0.2280 (4)	0.6251 (3)	0.36038 (15)	0.0472 (7)	
H37A	0.1978	0.7116	0.3228	0.057*	
H37B	0.2547	0.6746	0.4010	0.057*	
C15	0.7606 (4)	−0.0670 (3)	−0.26974 (16)	0.0517 (8)	
H15	0.8537	−0.1248	−0.2955	0.062*	
C32	−0.1006 (4)	0.5803 (4)	0.40135 (14)	0.0469 (7)	
C36	0.0922 (4)	0.3508 (4)	0.40978 (15)	0.0525 (8)	
H36	0.2054	0.3046	0.4045	0.063*	
C33	−0.2460 (4)	0.4836 (4)	0.42571 (16)	0.0584 (8)	
H33	−0.3596	0.5288	0.4305	0.070*	
C34	−0.2185 (5)	0.3197 (5)	0.44249 (16)	0.0617 (9)	
C22A	0.8218 (4)	0.3038 (4)	0.24026 (19)	0.0682 (10)	
H22A	0.7993	0.1941	0.2360	0.102*	
H22B	0.9031	0.3032	0.2731	0.102*	
H22C	0.8713	0.3607	0.1913	0.102*	
C35	−0.0504 (5)	0.2514 (4)	0.43596 (16)	0.0621 (9)	
H35	−0.0336	0.1400	0.4490	0.074*	
C12A	0.1899 (4)	0.2271 (4)	−0.1805 (2)	0.0722 (10)	
H12A	0.2160	0.2976	−0.2278	0.108*	
H12B	0.1063	0.2805	−0.1450	0.108*	
H12C	0.1411	0.1289	−0.1874	0.108*	
O1	0.9358 (4)	0.1894 (3)	0.05343 (18)	0.1153 (11)	
H1A	0.8732	0.1775	0.0217	0.138*	
H1B	1.0302	0.1305	0.0513	0.138*	
O2	0.0665 (6)	0.4574 (6)	0.9588 (3)	0.0901 (15)*	0.50
H2A	0.0498	0.5567	0.9654	0.108*	0.50
H2B	0.0095	0.3882	0.9929	0.108*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0655 (6)	0.0677 (6)	0.0727 (6)	0.0170 (4)	−0.0173 (4)	−0.0068 (4)
Cl2	0.0972 (8)	0.1244 (9)	0.0865 (7)	−0.0596 (7)	0.0000 (6)	−0.0102 (6)
N27	0.0412 (13)	0.0448 (13)	0.0342 (12)	−0.0012 (11)	−0.0058 (10)	−0.0108 (10)
N17	0.0413 (13)	0.0489 (14)	0.0343 (12)	0.0053 (11)	−0.0102 (10)	−0.0115 (10)
O21	0.0424 (11)	0.0659 (13)	0.0403 (11)	0.0044 (9)	−0.0078 (8)	−0.0230 (9)
O22	0.0390 (11)	0.0858 (15)	0.0483 (12)	0.0109 (10)	−0.0158 (9)	−0.0257 (11)
O17	0.0498 (12)	0.0776 (15)	0.0594 (13)	0.0183 (11)	−0.0236 (10)	−0.0311 (11)
O12	0.0440 (11)	0.0722 (14)	0.0567 (12)	0.0161 (10)	−0.0185 (10)	−0.0247 (11)

C24	0.0393 (15)	0.0366 (15)	0.0322 (14)	−0.0030 (12)	−0.0023 (11)	−0.0051 (11)
C22	0.0322 (14)	0.0448 (16)	0.0392 (15)	−0.0009 (12)	−0.0068 (12)	−0.0091 (12)
C11	0.0410 (15)	0.0322 (14)	0.0366 (14)	−0.0021 (12)	−0.0054 (12)	−0.0063 (11)
C26	0.0379 (15)	0.0429 (16)	0.0376 (15)	0.0040 (12)	−0.0024 (12)	−0.0095 (12)
C25	0.0403 (15)	0.0446 (16)	0.0369 (15)	0.0012 (13)	−0.0099 (12)	−0.0027 (12)
C17	0.0385 (15)	0.0382 (15)	0.0412 (15)	−0.0006 (12)	−0.0079 (12)	−0.0085 (12)
C21	0.0387 (15)	0.0427 (16)	0.0332 (14)	−0.0055 (12)	−0.0026 (12)	−0.0076 (12)
C12	0.0415 (16)	0.0376 (15)	0.0425 (16)	0.0025 (12)	−0.0072 (13)	−0.0088 (12)
C23	0.0331 (14)	0.0434 (16)	0.0376 (15)	0.0013 (12)	−0.0020 (11)	−0.0100 (12)
C27	0.0399 (15)	0.0443 (16)	0.0354 (15)	−0.0017 (13)	−0.0083 (12)	−0.0050 (12)
C13	0.0552 (18)	0.0507 (18)	0.0472 (17)	0.0017 (14)	−0.0199 (14)	−0.0100 (14)
C31	0.0510 (17)	0.0505 (18)	0.0267 (13)	0.0007 (14)	−0.0039 (12)	−0.0145 (12)
C16	0.0406 (16)	0.0410 (16)	0.0470 (17)	0.0021 (13)	−0.0049 (13)	−0.0080 (13)
C14	0.069 (2)	0.0534 (19)	0.0392 (16)	−0.0015 (16)	−0.0099 (15)	−0.0146 (14)
C37	0.0477 (17)	0.0549 (18)	0.0417 (16)	0.0031 (14)	−0.0049 (13)	−0.0228 (14)
C15	0.0593 (19)	0.0484 (18)	0.0462 (17)	0.0067 (15)	−0.0029 (15)	−0.0173 (14)
C32	0.0510 (18)	0.0581 (19)	0.0327 (15)	0.0012 (15)	−0.0084 (13)	−0.0111 (13)
C36	0.0581 (19)	0.057 (2)	0.0415 (16)	0.0014 (16)	−0.0054 (14)	−0.0129 (14)
C33	0.0478 (18)	0.085 (3)	0.0421 (17)	−0.0043 (18)	−0.0072 (14)	−0.0106 (17)
C34	0.070 (2)	0.076 (2)	0.0386 (17)	−0.0263 (19)	−0.0016 (15)	−0.0110 (16)
C22A	0.0397 (17)	0.103 (3)	0.070 (2)	0.0175 (17)	−0.0213 (16)	−0.032 (2)
C35	0.088 (3)	0.054 (2)	0.0407 (17)	−0.0094 (19)	−0.0046 (17)	−0.0075 (15)
C12A	0.052 (2)	0.092 (3)	0.083 (2)	0.0193 (18)	−0.0267 (18)	−0.034 (2)
O1	0.105 (2)	0.102 (2)	0.177 (3)	0.0502 (17)	−0.088 (2)	−0.080 (2)

Geometric parameters (Å, °)

Cl1—C32	1.751 (3)	C13—H13	0.9300
Cl2—C34	1.747 (3)	C31—C36	1.386 (4)
N27—C27	1.279 (3)	C31—C32	1.391 (4)
N27—N17	1.383 (3)	C31—C37	1.513 (4)
N17—C17	1.341 (3)	C16—C15	1.385 (4)
N17—H17	0.8600	C16—H16	0.9300
O21—C21	1.377 (3)	C14—C15	1.365 (4)
O21—C37	1.431 (3)	C14—H14	0.9300
O22—C22	1.365 (3)	C37—H37A	0.9700
O22—C22A	1.426 (3)	C37—H37B	0.9700
O17—C17	1.229 (3)	C15—H15	0.9300
O12—C12	1.369 (3)	C32—C33	1.383 (4)
O12—C12A	1.425 (3)	C36—C35	1.382 (4)
C24—C25	1.389 (3)	C36—H36	0.9300
C24—C23	1.403 (3)	C33—C34	1.367 (5)
C24—C27	1.458 (3)	C33—H33	0.9300
C22—C23	1.377 (3)	C34—C35	1.381 (5)
C22—C21	1.407 (3)	C22A—H22A	0.9600
C11—C16	1.396 (3)	C22A—H22B	0.9600
C11—C12	1.409 (4)	C22A—H22C	0.9600
C11—C17	1.499 (4)	C35—H35	0.9300
C26—C21	1.379 (4)	C12A—H12A	0.9600

C26—C25	1.392 (4)	C12A—H12B	0.9600
C26—H26	0.9300	C12A—H12C	0.9600
C25—H25	0.9300	O1—H1A	0.8532
C12—C13	1.390 (4)	O1—H1B	0.8547
C23—H23	0.9300	O2—H2A	0.8539
C27—H27	0.9300	O2—H2B	0.8485
C13—C14	1.380 (4)		
C27—N27—N17	114.0 (2)	C15—C16—H16	119.1
C17—N17—N27	121.1 (2)	C11—C16—H16	119.1
C17—N17—H17	119.5	C15—C14—C13	120.3 (3)
N27—N17—H17	119.5	C15—C14—H14	119.9
C21—O21—C37	117.1 (2)	C13—C14—H14	119.9
C22—O22—C22A	117.1 (2)	O21—C37—C31	112.3 (2)
C12—O12—C12A	119.8 (2)	O21—C37—H37A	109.1
C25—C24—C23	118.9 (2)	C31—C37—H37A	109.1
C25—C24—C27	118.9 (2)	O21—C37—H37B	109.1
C23—C24—C27	122.1 (2)	C31—C37—H37B	109.1
O22—C22—C23	125.1 (2)	H37A—C37—H37B	107.9
O22—C22—C21	115.0 (2)	C14—C15—C16	119.8 (3)
C23—C22—C21	119.9 (2)	C14—C15—H15	120.1
C16—C11—C12	117.5 (2)	C16—C15—H15	120.1
C16—C11—C17	116.1 (2)	C33—C32—C31	122.8 (3)
C12—C11—C17	126.4 (2)	C33—C32—Cl1	118.0 (2)
C21—C26—C25	120.4 (2)	C31—C32—Cl1	119.2 (2)
C21—C26—H26	119.8	C35—C36—C31	121.8 (3)
C25—C26—H26	119.8	C35—C36—H36	119.1
C24—C25—C26	120.5 (2)	C31—C36—H36	119.1
C24—C25—H25	119.8	C34—C33—C32	118.2 (3)
C26—C25—H25	119.8	C34—C33—H33	120.9
O17—C17—N17	121.8 (2)	C32—C33—H33	120.9
O17—C17—C11	121.2 (2)	C33—C34—C35	121.4 (3)
N17—C17—C11	117.1 (2)	C33—C34—Cl2	119.3 (3)
O21—C21—C26	125.3 (2)	C35—C34—Cl2	119.3 (3)
O21—C21—C22	115.1 (2)	O22—C22A—H22A	109.5
C26—C21—C22	119.5 (2)	O22—C22A—H22B	109.5
O12—C12—C13	122.3 (2)	H22A—C22A—H22B	109.5
O12—C12—C11	117.6 (2)	O22—C22A—H22C	109.5
C13—C12—C11	120.0 (2)	H22A—C22A—H22C	109.5
C22—C23—C24	120.7 (2)	H22B—C22A—H22C	109.5
C22—C23—H23	119.7	C34—C35—C36	119.1 (3)
C24—C23—H23	119.7	C34—C35—H35	120.5
N27—C27—C24	122.2 (2)	C36—C35—H35	120.5
N27—C27—H27	118.9	O12—C12A—H12A	109.5
C24—C27—H27	118.9	O12—C12A—H12B	109.5
C14—C13—C12	120.6 (3)	H12A—C12A—H12B	109.5
C14—C13—H13	119.7	O12—C12A—H12C	109.5
C12—C13—H13	119.7	H12A—C12A—H12C	109.5
C36—C31—C32	116.7 (3)	H12B—C12A—H12C	109.5
C36—C31—C37	121.6 (3)	H1A—O1—H1B	115.6

C32—C31—C37	121.8 (3)	H2A—O2—H2B	116.3
C15—C16—C11	121.8 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1B···O17^{i}	0.85	2.02	2.852 (3)	164
O2—H2A···O1^{ii}	0.85	2.10	2.918 (6)	161
O2—H2B···O1^{iii}	0.85	1.89	2.711 (6)	162
O1—H1A···O17	0.85	2.19	2.987 (3)	155
O1—H1A···N27	0.85	2.54	3.180 (3)	133
N17—H17···O12	0.86	1.93	2.625 (3)	137

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

Fig. 1

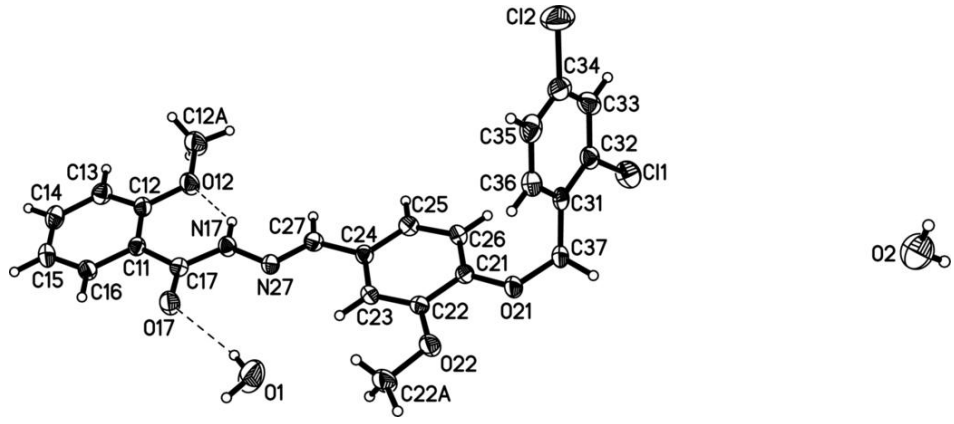
Cl2
C34
C33
C12A
C35
C32
C13
C12
O12
C36
Cl1
C14
C31
C25
N17
C27
C24
C26
C37
C11
C21
C15
C16
C17
N27
C23
C22
O21
O17
O22
O1
C22A
O2

Fig. 2