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2,4-Dichloro-6-[(2-hydroxy-5-methylanilino)-methylidene]cyclohexa-2,4-dienone

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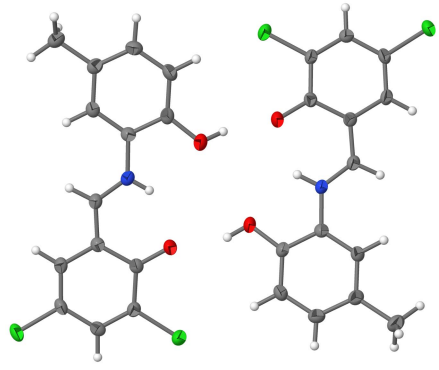
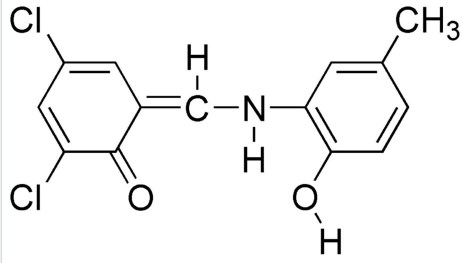
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{14}H_{11}Cl_2NO_2$, has been prepared by the condensation of 3,5-dichlorosalicylaldehyde and 2-amino-4-methylphenol. The asymmetric unit consists of two independent molecules, both of which are almost planar; the dihedral angle between the two benzene rings is 10.61 (8)° for one molecule and 2.46 (8)° for the other. There is an intramolecular N—H···O hydrogen bond that generates $S(6)$ ring motifs in each molecule. In the crystal, the two independent molecules are linked by O—H···O and C—H···Cl hydrogen bonds, forming a pseudo-inversion dimer. A π–π interaction, with a centroid–centroid distance of 3.6065 (12) Å, is also observed.

3D view



Chemical scheme



Structure description

Halogen atoms in Schiff base ligands (Dong *et al.*, 2015; Pal *et al.*, 2018) and their metal complexes are interesting because of their possible bioactivities (Dong *et al.*, 2015; Rani & Bheeter, 2016). In view of the biological activities of these compounds, which are related to structural aspects, and as part of our studies on 2,4-dibromo-6-[(2-hydroxy-5-methylanilino)methylidene]cyclohexa-2,4-dienone, we report herein the synthesis and crystal structure of 2,4-dichloro-6-[(2-hydroxy-5-methylanilino)methylidene]cyclohexa-2,4-dienone.

The C2—O1 and C16—O3 bond lengths reveal double-bond character, while the C7—N1 and C15—N2 bonds show single-bond character (Khalaji *et al.*, 2015; Pal *et al.*, 2018). There is an intramolecular N—H···O hydrogen bond (Table 1) that generates $S(6)$ ring

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O3	0.84 (3)	1.87 (3)	2.693 (2)	168 (3)
O4—H4···O1	0.83 (3)	1.89 (3)	2.685 (2)	160 (3)
N1—H1···O1	0.80 (2)	1.96 (2)	2.617 (2)	139 (2)
N2—H3···O3	0.87 (2)	1.90 (2)	2.603 (2)	137 (2)
C10—H10···Cl3	0.95	2.88	3.660 (2)	140
C24—H24···Cl1	0.95	2.72	3.661 (2)	172

motifs in each molecule. In the crystal, the two independent molecules are linked through two O—H···O hydrogen bonds, creating a pseudo-inversion dimer, with an $R_2^2(18)$ ring motif, in which C—H···Cl interactions further link the molecules (Fig. 1 and Table 1). A π–π stacking interaction, with a centroid–centroid distance of 3.6065 (12) Å, is also observed between the C16–C21 and C22–C27 rings.

Synthesis and crystallization

An ethanol solution of 3,5-dichlorosalicylaldehyde (100 mg, 0.52 mmol) was added dropwise to an ethanol solution of 2-amino-4-methylphenol (77 mg, 0.62 mmol) with continuous stirring at 333 K. A bright-orange coloured precipitate of the title compound formed immediately. The resulting mixture was stirred for a further 1 h at room temperature for completion of the reaction. On cooling, an orange solid product was isolated by filtration, washed with hot ethanol and dried in a vacuum (yield 125 mg, 77%). Orange needle-like single crystals were obtained from an *N*,*N*-dimethylformamide–acetonitrile (1:7 *v*/*v*) solution by slow evaporation of the solvent at room temperature over a period of 15 d (m.p. 457 K).

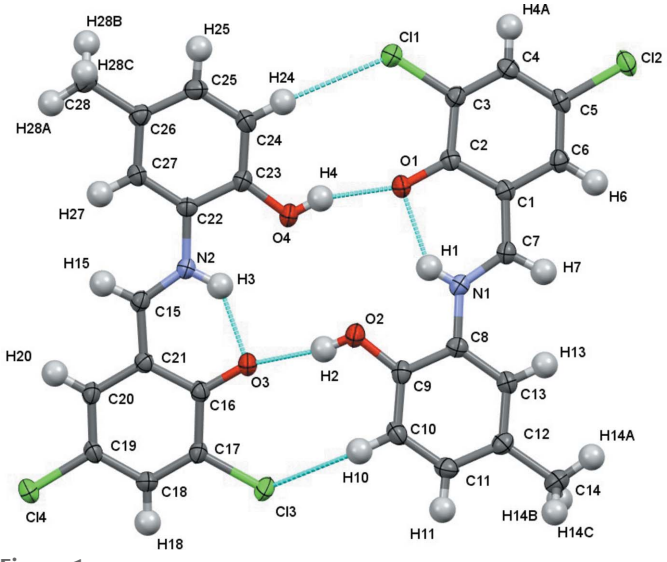


Figure 1
The asymmetric unit of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. Intermolecular C—H···Cl and O—H···O and intramolecular N—H···O hydrogen bonds are indicated by dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{11}Cl_2NO_2$
M_r	296.15
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	173
a, b, c (Å)	16.6119 (5), 6.83947 (16), 22.5749 (6)
β (°)	98.255 (7)
V (Å^3)	2538.30 (12)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.51
Crystal size (mm)	0.37 × 0.15 × 0.07
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.697, 0.965
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	24092, 5794, 4366
R_{int}	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.100, 1.03
No. of reflections	5794
No. of parameters	361
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.39

Computer programs: *RAPID-AUTO* (Rigaku, 2001), *SIR92* (Altomare *et al.*, 1993), *SHELXL97* (Sheldrick, 2008) and *CrystalStructure* (Rigaku, 2018).

Refinement

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

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full crystallographic data

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Crystal data

$C_{14}H_{11}Cl_2NO_2$
M_r = 296.15
Monoclinic, $P2_1/n$
a = 16.6119 (5) Å
b = 6.83947 (16) Å
c = 22.5749 (6) Å
β = 98.255 (7)°
V = 2538.30 (12) Å^3
Z = 8
$F(000)$ = 1216.00
D_x = 1.550 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 16379 reflections
θ = 1.8–27.5°
μ = 0.51 mm^{-1}
T = 173 K
Needle, orange
0.37 × 0.14 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.697, T_{max} = 0.965
24092 measured reflections
5794 independent reflections
4366 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.049
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −21→21
k = −8→8
l = −27→29

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.100
S = 1.02
5794 reflections
361 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 1.2427P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 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.

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.25495 (3)	0.09343 (10)	−0.08874 (3)	0.03921 (16)
Cl2	0.51221 (3)	0.11130 (8)	−0.20767 (2)	0.03353 (14)
Cl3	0.50788 (3)	0.19328 (9)	0.35698 (3)	0.03368 (14)
Cl4	0.26343 (4)	0.11237 (10)	0.48780 (2)	0.04106 (16)
O1	0.37601 (9)	0.2150 (2)	0.01624 (6)	0.0307 (4)
O2	0.45249 (9)	0.3530 (2)	0.16615 (7)	0.0319 (4)
O3	0.37348 (9)	0.2238 (2)	0.25471 (6)	0.0312 (4)
O4	0.28678 (9)	0.1500 (3)	0.10445 (7)	0.0335 (4)
N1	0.52248 (11)	0.3018 (3)	0.06875 (8)	0.0238 (4)
N2	0.22374 (11)	0.1714 (3)	0.20494 (8)	0.0240 (4)
C1	0.49095 (12)	0.2179 (3)	−0.03532 (9)	0.0224 (4)
C2	0.40586 (12)	0.1912 (3)	−0.03220 (9)	0.0230 (4)
C3	0.35810 (12)	0.1351 (3)	−0.08807 (9)	0.0252 (4)
C4	0.39050 (13)	0.1133 (3)	−0.14003 (9)	0.0264 (4)
H4A	0.356340	0.078181	−0.175870	0.032*
C5	0.47392 (13)	0.1425 (3)	−0.14064 (9)	0.0253 (4)
C6	0.52355 (13)	0.1907 (3)	−0.08924 (9)	0.0258 (4)
H6	0.580302	0.206062	−0.089665	0.031*
C7	0.54515 (12)	0.2706 (3)	0.01641 (9)	0.0246 (4)
H7	0.601196	0.284176	0.012926	0.029*
C8	0.57277 (12)	0.3531 (3)	0.12254 (9)	0.0226 (4)
C9	0.53468 (12)	0.3730 (3)	0.17345 (9)	0.0253 (4)
C10	0.58203 (13)	0.4161 (3)	0.22768 (9)	0.0297 (5)
H10	0.557122	0.429067	0.262812	0.036*
C11	0.66529 (13)	0.4401 (3)	0.23091 (10)	0.0299 (5)
H11	0.696733	0.468769	0.268450	0.036*
C12	0.70405 (12)	0.4233 (3)	0.18025 (10)	0.0269 (5)
C13	0.65650 (12)	0.3793 (3)	0.12615 (9)	0.0252 (4)
H13	0.681486	0.366869	0.091027	0.030*
C14	0.79483 (13)	0.4497 (4)	0.18360 (11)	0.0359 (5)
H14A	0.808814	0.463165	0.143078	0.043*
H14B	0.822829	0.335619	0.203108	0.043*
H14C	0.811765	0.567534	0.206801	0.043*
C15	0.20603 (12)	0.1554 (3)	0.25913 (9)	0.0236 (4)
H15	0.150757	0.136914	0.264204	0.028*
C16	0.34976 (12)	0.1928 (3)	0.30534 (9)	0.0234 (4)

C17	0.40453 (12)	0.1814 (3)	0.36060 (9)	0.0243 (4)
C18	0.37823 (12)	0.1580 (3)	0.41483 (9)	0.0256 (5)
H18	0.416378	0.153527	0.450438	0.031*
C19	0.29454 (13)	0.1406 (3)	0.41776 (9)	0.0266 (5)
C20	0.23901 (12)	0.1389 (3)	0.36714 (9)	0.0251 (4)
H20	0.182907	0.120713	0.369653	0.030*
C21	0.26538 (12)	0.1643 (3)	0.31084 (9)	0.0225 (4)
C22	0.16925 (12)	0.1673 (3)	0.15075 (9)	0.0231 (4)
C23	0.20467 (12)	0.1583 (3)	0.09815 (9)	0.0260 (5)
C24	0.15371 (14)	0.1588 (3)	0.04366 (10)	0.0304 (5)
H24	0.176341	0.152636	0.007370	0.037*
C25	0.07038 (13)	0.1681 (3)	0.04194 (10)	0.0300 (5)
H25	0.036697	0.168583	0.004192	0.036*
C26	0.03407 (12)	0.1770 (3)	0.09397 (10)	0.0270 (5)
C27	0.08532 (12)	0.1767 (3)	0.14838 (9)	0.0257 (4)
H27	0.062516	0.183028	0.184586	0.031*
C28	−0.05674 (13)	0.1887 (4)	0.09160 (11)	0.0360 (5)
H28A	−0.071234	0.159467	0.131228	0.043*
H28B	−0.082835	0.093679	0.062499	0.043*
H28C	−0.075315	0.320734	0.079520	0.043*
H1	0.4750 (14)	0.283 (3)	0.0701 (10)	0.025 (6)*
H2	0.4343 (18)	0.314 (4)	0.1968 (14)	0.060 (9)*
H3	0.2752 (15)	0.184 (4)	0.2018 (10)	0.033 (7)*
H4	0.3040 (18)	0.164 (4)	0.0721 (14)	0.060 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0229 (3)	0.0649 (4)	0.0302 (3)	−0.0034 (3)	0.0053 (2)	−0.0073 (3)
Cl2	0.0391 (3)	0.0394 (3)	0.0252 (3)	−0.0016 (3)	0.0151 (2)	−0.0022 (2)
Cl3	0.0186 (2)	0.0485 (3)	0.0346 (3)	0.0009 (2)	0.0061 (2)	0.0030 (3)
Cl4	0.0320 (3)	0.0703 (4)	0.0227 (3)	−0.0026 (3)	0.0102 (2)	−0.0022 (3)
O1	0.0237 (8)	0.0454 (9)	0.0240 (8)	0.0020 (7)	0.0074 (6)	−0.0025 (7)
O2	0.0231 (8)	0.0434 (10)	0.0303 (9)	−0.0021 (7)	0.0079 (7)	0.0034 (7)
O3	0.0226 (8)	0.0473 (10)	0.0252 (8)	−0.0007 (7)	0.0084 (6)	0.0008 (7)
O4	0.0200 (8)	0.0538 (11)	0.0279 (8)	−0.0023 (7)	0.0081 (6)	−0.0002 (8)
N1	0.0197 (9)	0.0249 (9)	0.0270 (9)	−0.0011 (7)	0.0038 (7)	0.0006 (7)
N2	0.0186 (9)	0.0301 (10)	0.0239 (9)	−0.0012 (7)	0.0051 (7)	−0.0019 (7)
C1	0.0249 (10)	0.0199 (10)	0.0230 (10)	0.0000 (8)	0.0048 (8)	0.0017 (8)
C2	0.0237 (10)	0.0221 (10)	0.0236 (10)	0.0027 (8)	0.0044 (8)	0.0021 (8)
C3	0.0207 (10)	0.0282 (11)	0.0269 (11)	0.0010 (8)	0.0045 (8)	0.0005 (9)
C4	0.0304 (11)	0.0266 (11)	0.0220 (10)	0.0012 (9)	0.0029 (8)	0.0026 (9)
C5	0.0323 (11)	0.0244 (11)	0.0212 (10)	0.0008 (9)	0.0110 (9)	0.0020 (8)
C6	0.0258 (11)	0.0262 (11)	0.0268 (11)	−0.0030 (9)	0.0082 (9)	0.0022 (9)
C7	0.0229 (10)	0.0254 (11)	0.0264 (11)	−0.0013 (8)	0.0066 (8)	0.0008 (9)
C8	0.0253 (10)	0.0191 (10)	0.0232 (10)	−0.0001 (8)	0.0026 (8)	−0.0007 (8)
C9	0.0245 (10)	0.0247 (11)	0.0278 (11)	0.0015 (9)	0.0077 (8)	0.0038 (9)
C10	0.0335 (12)	0.0347 (12)	0.0224 (10)	0.0022 (10)	0.0089 (9)	0.0007 (9)

C11	0.0313 (12)	0.0337 (13)	0.0236 (11)	0.0004 (9)	−0.0005 (9)	−0.0003 (9)
C12	0.0232 (10)	0.0258 (11)	0.0311 (11)	0.0017 (9)	0.0018 (9)	0.0017 (9)
C13	0.0262 (11)	0.0260 (11)	0.0243 (10)	0.0007 (9)	0.0069 (8)	0.0000 (9)
C14	0.0253 (11)	0.0458 (14)	0.0358 (13)	−0.0036 (10)	0.0009 (10)	−0.0039 (11)
C15	0.0202 (10)	0.0241 (11)	0.0270 (11)	−0.0005 (8)	0.0056 (8)	−0.0020 (8)
C16	0.0233 (10)	0.0242 (10)	0.0235 (10)	0.0009 (8)	0.0064 (8)	−0.0021 (8)
C17	0.0188 (10)	0.0280 (11)	0.0269 (11)	0.0004 (8)	0.0061 (8)	−0.0012 (9)
C18	0.0236 (10)	0.0298 (12)	0.0228 (10)	−0.0011 (9)	0.0017 (8)	−0.0023 (9)
C19	0.0279 (11)	0.0319 (12)	0.0218 (10)	−0.0010 (9)	0.0100 (8)	−0.0027 (9)
C20	0.0192 (10)	0.0294 (11)	0.0280 (11)	0.0011 (8)	0.0079 (8)	−0.0018 (9)
C21	0.0217 (10)	0.0223 (10)	0.0238 (10)	0.0006 (8)	0.0048 (8)	−0.0035 (8)
C22	0.0233 (10)	0.0235 (10)	0.0225 (10)	−0.0018 (8)	0.0030 (8)	−0.0025 (8)
C23	0.0201 (10)	0.0312 (12)	0.0272 (11)	−0.0021 (9)	0.0056 (8)	−0.0012 (9)
C24	0.0311 (12)	0.0385 (13)	0.0231 (11)	−0.0034 (10)	0.0087 (9)	−0.0027 (9)
C25	0.0280 (11)	0.0346 (12)	0.0262 (11)	−0.0004 (9)	−0.0009 (9)	−0.0031 (9)
C26	0.0227 (10)	0.0282 (11)	0.0297 (11)	0.0011 (9)	0.0030 (9)	−0.0056 (9)
C27	0.0240 (10)	0.0299 (11)	0.0240 (10)	0.0006 (9)	0.0068 (8)	−0.0035 (9)
C28	0.0223 (11)	0.0455 (14)	0.0394 (13)	0.0029 (10)	0.0020 (9)	−0.0063 (11)

Geometric parameters (Å, º)

Cl1—C3	1.735 (2)	C11—C12	1.395 (3)
Cl2—C5	1.737 (2)	C11—H11	0.9500
Cl3—C17	1.732 (2)	C12—C13	1.389 (3)
Cl4—C19	1.743 (2)	C12—C14	1.510 (3)
O1—C2	1.274 (2)	C13—H13	0.9500
O2—C9	1.358 (2)	C14—H14A	0.9800
O2—H2	0.84 (3)	C14—H14B	0.9800
O3—C16	1.279 (2)	C14—H14C	0.9800
O4—C23	1.352 (2)	C15—C21	1.417 (3)
O4—H4	0.83 (3)	C15—H15	0.9500
N1—C7	1.308 (3)	C16—C17	1.437 (3)
N1—C8	1.416 (3)	C16—C21	1.438 (3)
N1—H1	0.80 (2)	C17—C18	1.367 (3)
N2—C15	1.303 (3)	C18—C19	1.406 (3)
N2—C22	1.414 (3)	C18—H18	0.9500
N2—H3	0.87 (2)	C19—C20	1.362 (3)
C1—C6	1.414 (3)	C20—C21	1.413 (3)
C1—C7	1.415 (3)	C20—H20	0.9500
C1—C2	1.437 (3)	C22—C27	1.389 (3)
C2—C3	1.442 (3)	C22—C23	1.400 (3)
C3—C4	1.367 (3)	C23—C24	1.390 (3)
C4—C5	1.402 (3)	C24—C25	1.381 (3)
C4—H4A	0.9500	C24—H24	0.9500
C5—C6	1.364 (3)	C25—C26	1.396 (3)
C6—H6	0.9500	C25—H25	0.9500
C7—H7	0.9500	C26—C27	1.390 (3)
C8—C13	1.393 (3)	C26—C28	1.504 (3)

C8—C9	1.396 (3)	C27—H27	0.9500
C9—C10	1.388 (3)	C28—H28A	0.9800
C10—C11	1.384 (3)	C28—H28B	0.9800
C10—H10	0.9500	C28—H28C	0.9800

C9—O2—H2	114 (2)	H14A—C14—H14B	109.5
C23—O4—H4	112 (2)	C12—C14—H14C	109.5
C7—N1—C8	127.17 (18)	H14A—C14—H14C	109.5
C7—N1—H1	114.9 (16)	H14B—C14—H14C	109.5
C8—N1—H1	117.8 (16)	N2—C15—C21	123.07 (19)
C15—N2—C22	127.43 (18)	N2—C15—H15	118.5
C15—N2—H3	116.1 (16)	C21—C15—H15	118.5
C22—N2—H3	116.4 (16)	O3—C16—C17	123.15 (18)
C6—C1—C7	117.84 (18)	O3—C16—C21	121.93 (18)
C6—C1—C2	121.77 (18)	C17—C16—C21	114.91 (18)
C7—C1—C2	120.38 (18)	C18—C17—C16	122.67 (18)
O1—C2—C1	122.18 (18)	C18—C17—Cl3	119.61 (16)
O1—C2—C3	123.47 (18)	C16—C17—Cl3	117.70 (15)
C1—C2—C3	114.35 (18)	C17—C18—C19	119.83 (19)
C4—C3—C2	122.99 (19)	C17—C18—H18	120.1
C4—C3—Cl1	118.98 (16)	C19—C18—H18	120.1
C2—C3—Cl1	118.03 (15)	C20—C19—C18	121.09 (19)
C3—C4—C5	120.29 (19)	C20—C19—Cl4	120.45 (16)
C3—C4—H4A	119.9	C18—C19—Cl4	118.42 (16)
C5—C4—H4A	119.9	C19—C20—C21	119.58 (19)
C6—C5—C4	120.24 (19)	C19—C20—H20	120.2
C6—C5—Cl2	121.25 (17)	C21—C20—H20	120.2
C4—C5—Cl2	118.50 (16)	C20—C21—C15	117.83 (18)
C5—C6—C1	120.32 (19)	C20—C21—C16	121.75 (18)
C5—C6—H6	119.8	C15—C21—C16	120.40 (18)
C1—C6—H6	119.8	C27—C22—C23	120.73 (19)
N1—C7—C1	123.73 (19)	C27—C22—N2	123.16 (18)
N1—C7—H7	118.1	C23—C22—N2	116.09 (18)
C1—C7—H7	118.1	O4—C23—C24	124.8 (2)
C13—C8—C9	120.40 (19)	O4—C23—C22	116.94 (19)
C13—C8—N1	122.91 (19)	C24—C23—C22	118.29 (19)
C9—C8—N1	116.68 (18)	C25—C24—C23	120.4 (2)
O2—C9—C10	124.10 (19)	C25—C24—H24	119.8
O2—C9—C8	117.18 (19)	C23—C24—H24	119.8
C10—C9—C8	118.70 (19)	C24—C25—C26	122.1 (2)
C11—C10—C9	120.5 (2)	C24—C25—H25	119.0
C11—C10—H10	119.8	C26—C25—H25	119.0
C9—C10—H10	119.8	C27—C26—C25	117.34 (19)
C10—C11—C12	121.5 (2)	C27—C26—C28	121.0 (2)
C10—C11—H11	119.3	C25—C26—C28	121.6 (2)
C12—C11—H11	119.3	C22—C27—C26	121.20 (19)
C13—C12—C11	117.86 (19)	C22—C27—H27	119.4
C13—C12—C14	120.5 (2)	C26—C27—H27	119.4

C11—C12—C14	121.61 (19)	C26—C28—H28A	109.5
C12—C13—C8	121.09 (19)	C26—C28—H28B	109.5
C12—C13—H13	119.5	H28A—C28—H28B	109.5
C8—C13—H13	119.5	C26—C28—H28C	109.5
C12—C14—H14A	109.5	H28A—C28—H28C	109.5
C12—C14—H14B	109.5	H28B—C28—H28C	109.5
C6—C1—C2—O1	179.81 (19)	C22—N2—C15—C21	−179.03 (19)
C7—C1—C2—O1	0.6 (3)	O3—C16—C17—C18	176.6 (2)
C6—C1—C2—C3	0.1 (3)	C21—C16—C17—C18	−4.1 (3)
C7—C1—C2—C3	−179.18 (19)	O3—C16—C17—Cl3	−4.7 (3)
O1—C2—C3—C4	178.8 (2)	C21—C16—C17—Cl3	174.60 (15)
C1—C2—C3—C4	−1.4 (3)	C16—C17—C18—C19	1.1 (3)
O1—C2—C3—Cl1	−1.3 (3)	Cl3—C17—C18—C19	−177.52 (16)
C1—C2—C3—Cl1	178.49 (15)	C17—C18—C19—C20	2.6 (3)
C2—C3—C4—C5	1.1 (3)	C17—C18—C19—Cl4	−179.65 (17)
Cl1—C3—C4—C5	−178.84 (16)	C18—C19—C20—C21	−3.0 (3)
C3—C4—C5—C6	0.8 (3)	Cl4—C19—C20—C21	179.27 (16)
C3—C4—C5—Cl2	179.56 (16)	C19—C20—C21—C15	178.05 (19)
C4—C5—C6—C1	−2.1 (3)	C19—C20—C21—C16	−0.2 (3)
Cl2—C5—C6—C1	179.16 (16)	N2—C15—C21—C20	−178.05 (19)
C7—C1—C6—C5	−179.09 (19)	N2—C15—C21—C16	0.2 (3)
C2—C1—C6—C5	1.7 (3)	O3—C16—C21—C20	−177.08 (19)
C8—N1—C7—C1	179.40 (19)	C17—C16—C21—C20	3.6 (3)
C6—C1—C7—N1	179.33 (19)	O3—C16—C21—C15	4.7 (3)
C2—C1—C7—N1	−1.4 (3)	C17—C16—C21—C15	−174.60 (19)
C7—N1—C8—C13	0.6 (3)	C15—N2—C22—C27	10.8 (3)
C7—N1—C8—C9	−178.1 (2)	C15—N2—C22—C23	−170.8 (2)
C13—C8—C9—O2	177.48 (18)	C27—C22—C23—O4	179.84 (19)
N1—C8—C9—O2	−3.8 (3)	N2—C22—C23—O4	1.4 (3)
C13—C8—C9—C10	−1.1 (3)	C27—C22—C23—C24	−0.1 (3)
N1—C8—C9—C10	177.64 (19)	N2—C22—C23—C24	−178.47 (19)
O2—C9—C10—C11	−177.9 (2)	O4—C23—C24—C25	−179.8 (2)
C8—C9—C10—C11	0.5 (3)	C22—C23—C24—C25	0.1 (3)
C9—C10—C11—C12	0.4 (3)	C23—C24—C25—C26	−0.1 (3)
C10—C11—C12—C13	−0.7 (3)	C24—C25—C26—C27	0.2 (3)
C10—C11—C12—C14	179.9 (2)	C24—C25—C26—C28	179.5 (2)
C11—C12—C13—C8	0.1 (3)	C23—C22—C27—C26	0.1 (3)
C14—C12—C13—C8	179.5 (2)	N2—C22—C27—C26	178.4 (2)
C9—C8—C13—C12	0.8 (3)	C25—C26—C27—C22	−0.2 (3)
N1—C8—C13—C12	−177.85 (19)	C28—C26—C27—C22	−179.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3	0.84 (3)	1.87 (3)	2.693 (2)	168 (3)
O4—H4···O1	0.83 (3)	1.89 (3)	2.685 (2)	160 (3)
N1—H1···O1	0.80 (2)	1.96 (2)	2.617 (2)	139 (2)

N2—H3···O3	0.87 (2)	1.90 (2)	2.603 (2)	137 (2)
C10—H10···Cl3	0.95	2.88	3.660 (2)	140
C24—H24···Cl1	0.95	2.72	3.661 (2)	172