Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structures of salen-type ligands 2-[(1*E*)-({1-(3-chlorophenyl)-2-[(*E*)-(2-hydroxybenzylidene)amino]propyl}imino)methyl]phenol and 2-[(1*E*)-({1-(4-chlorophenyl)-2-[(*E*)-(2-hydroxybenzylidene)amino]propyl}imino)methyl]phenol

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Received 8 October 2017
Accepted 12 November 2017

Edited by O. Blacque, University of Zürich, Switzerland

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Keywords: crystal structure; salen ligand; schiff base; O—H···N intramolecular hydrogen bonds; C—H···O and C—H···π intermolecular interactions.

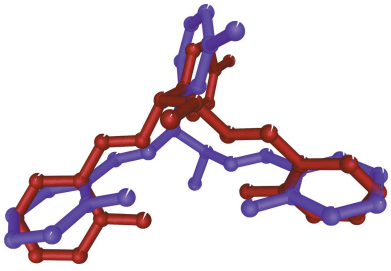
CCDC references: 1412946; 1412945

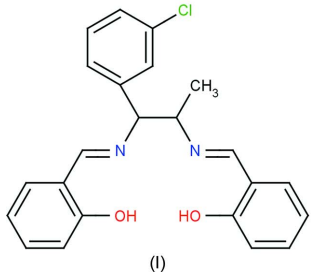
Supporting information: this article has supporting information at journals.iucr.org/e

The title compounds, $C_{23}H_{21}ClN_2O_2$, differ from each other only by the position of the Cl atom on the corresponding benzene ring: *meta* relative to the central sp^3 C atom for (I) and *para* for (II). In (I), the hydroxyphenyl rings are almost parallel, the dihedral angle between the mean planes being 9.2 (2)°, but in (II), the relative position of the ring is different, characterized by a dihedral angle of 48.5 (1)°. Compound (I) features intramolecular O—H···N and intermolecular C—H···O hydrogen bonds, while in (II), intramolecular O—H···N, C—H···N hydrogen bonds and weak intermolecular C—H···π interactions are observed. Compound (I) was refined as an inversion twin.

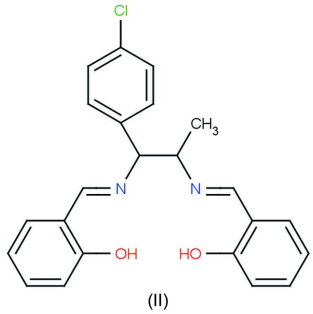
1. Chemical context

Salen-type Schiff bases possessing an unsymmetrical vicinal diamine backbone are promising candidates in synthetic and material science research. Salen ligands and their complexes are widely studied for their extensive applications in various fields, for their luminescent property (Chakraborty *et al.*, 2015; Chen *et al.*, 2013), photophysical properties (Cheng *et al.*, 2013), NLO activity (Nayar & Ravikumar, 2014; Zeyrek, 2013) *etc*. Recent reports on a single-crystal study (Habibi *et al.*, 2007), spectroscopic and DFT calculations (de Toledo *et al.*, 2015) and the utility in asymmetric syntheses (Yang *et al.*, 2011) of this type of ligand address the novelty of these compounds and speak of the impact of their efficacy. In view of the importance of the title compounds, we have undertaken a single-crystal X-ray diffraction study and the results are presented here.





(I)



(II)

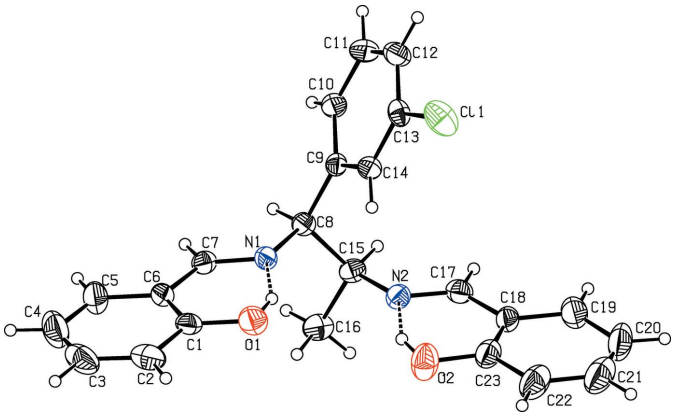


Figure 1
A view of the molecular structure of compound (I), showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines represent intramolecular O—H···N hydrogen bonds (Table 1).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82 (1)	1.88 (3)	2.596 (3)	146 (4)
O2—H2···N2	0.82 (1)	1.88 (3)	2.588 (3)	143 (4)
C16—H16*C*···O1^{i}	0.96	2.52	3.448 (4)	161

Symmetry code: (i) $x, y+1, z$.

Table 2
Hydrogen-bond geometry (Å, °) for (II).

Cg is the centroid of the C18–C23 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.83 (1)	1.83 (2)	2.589 (2)	150 (3)
O2—H2···N2	0.82 (1)	1.81 (2)	2.557 (3)	150 (3)
C14—H14···N1	0.93	2.52	2.845 (3)	101
C5—H5···*Cg*^{i}	0.93	2.76	3.449 (3)	132

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

2. Structural commentary

The molecular structure of the title compounds, (I) and (II), are illustrated in Figs. 1 and 2, respectively. Fig. 3 shows a superposition of the two compounds except for Cl1 using *Qmol* (Gans & Shalloway, 2001); the r.m.s. deviation is 2.3 Å. Compound (I) has two chiral centers with the absolute configuration determined as C8(*S*), C15(*S*). The chlorophenyl group is almost planar with atom Cl1 deviating by 0.013 (1) Å from the ring in (I) whereas in (II) the chlorine atom deviates by 0.079 (1) Å. In (I), hydroxy atoms O1 and O2 deviate by 0.051 (3) and 0.012 (3) Å, respectively, from the phenyl ring to which they are attached. In (II), hydroxy atoms O1 and O2 deviate by 0.006 (2) and 0.002 (2) Å, respectively, from the ring. The dihedral angle between these two rings is 9.2 (2)° in (I) and 48.5 (1)° in (II).

In compounds (I) and (II), the molecular structure maybe influenced by two intramolecular O—H···N hydrogen bonds (Tables 1 and 2). These two hydrogen bonds form $R_1^1(6)$ ring motifs; see Figs. 1 and 2. C—H···N intramolecular hydrogen bonds are also observed in compound (II).

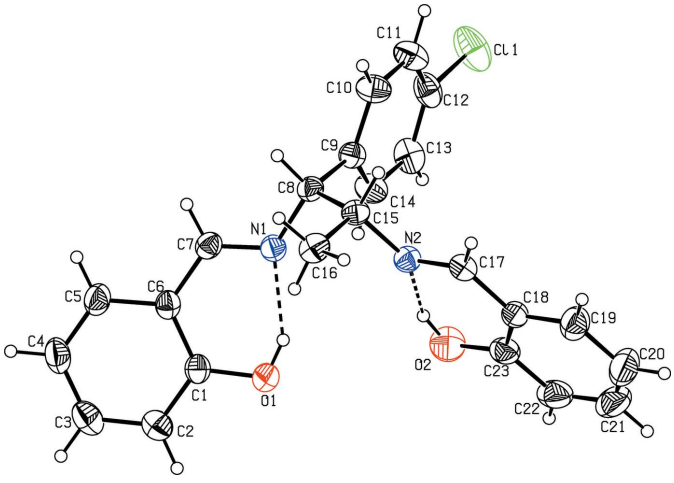


Figure 2
A view of the molecular structure of compound (II), showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines represent intramolecular O—H···N hydrogen bonds (Table 2).

3. Supramolecular features

In the crystal of (I), C—H···O interactions link the molecules to form *C*(9) chains propagating along [010]; see Fig. 4 and Table 1. In compound (II), the molecules are connected only by C—H···π interactions, which form *C*(11) chains propagating along the *ab* plane of the unit cell; see Fig. 5.

4. Synthesis and crystallization

The synthesis of the salen ligand 2-[(1*E*)-({1-(3-chlorophenyl)-2-[(*E*)-(2-hydroxybenzylidene)amino]propyl}imino)methyl]-phenol was achieved by the condensation of salicylaldehyde

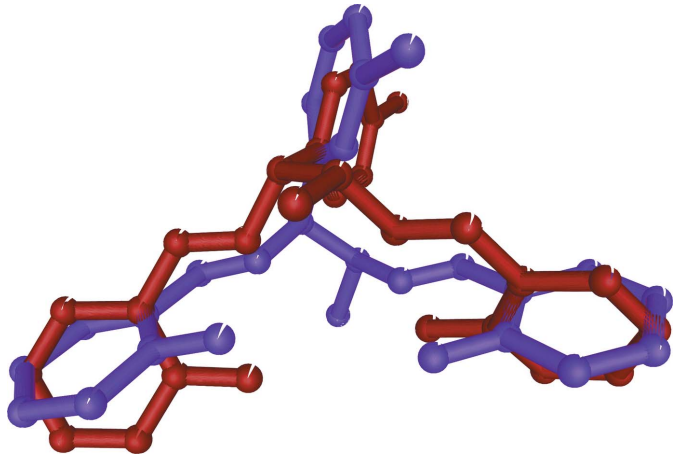


Figure 3
Superposition (excluding atom Cl1) of compound (I) (blue) and compound (II) (red).

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{23}H_{21}ClN_2O_2$	$C_{23}H_{21}ClN_2O_2$
M_r	392.87	392.87
Crystal system, space group	Monoclinic, $P2_1$	Monoclinic, $P2_1/c$
Temperature (K)	296	296
a, b, c (Å)	12.8126 (7), 7.0224 (3), 12.8169 (6)	6.7923 (2), 20.8261 (8), 14.1744 (6)
β (°)	117.207 (3)	92.435 (2)
V (Å^3)	1025.61 (9)	2003.26 (13)
Z	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.21	0.21
Crystal size (mm)	0.35 × 0.30 × 0.25	0.35 × 0.30 × 0.25
Data collection		
Diffractometer	Bruker Kappa APEXII CCD	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.921, 0.959	0.927, 0.959
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15137, 4892, 2738	42044, 4182, 2599
R_{int}	0.039	0.044
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.679	0.629
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.087, 0.98	0.047, 0.140, 1.08
No. of reflections	4892	4182
No. of parameters	263	262
No. of restraints	3	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.21	0.30, −0.29
Absolute structure	Refined as an inversion twin	–
Absolute structure parameter	0.27 (8)	–

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

(0.02 mol) and 1-(3-chlorophenyl)propane-1,2-diamine (0.01 mol) in ethanol (25 ml, 99%). The completion of the reaction was monitored by TLC. The obtained yellow solid was purified by recrystallization from ethanol. Single crystals suitable for X-ray analysis were obtained by slow evaporation from ethanol. The above procedure was repeated with 1-(4-chlorophenyl)propane-1,2-diamine (0.01 mol) instead of 1-(3-chlorophenyl)propane-1,2-diamine to synthesise 2-[(1*E*)-({1-(4-chlorophenyl)-2-[(*E*)-(2-hydroxybenzylidene)amino]propyl}imino)methyl]phenol.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. In both compounds, hydroxy H atoms H1 and H2 were located from difference-Fourier maps. All other H atoms were placed in idealized positions and allowed to ride on their parent atoms: C—H = 0.93–0.97 Å, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms. Pairs of O—H bond distances were restrained to 0.82 (1) Å. Compound (I) was refined as an inversion twin.

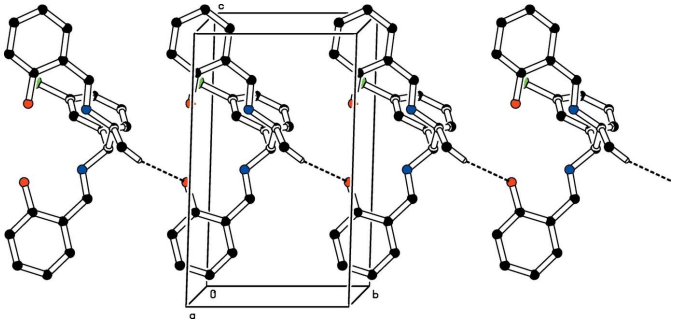


Figure 4
The crystal packing of the title compound (I) viewed along the *a* axis. The C—H···O hydrogen bonds are shown as dashed lines (see Table 1). For clarity, H atoms not involved in these interactions have been omitted.

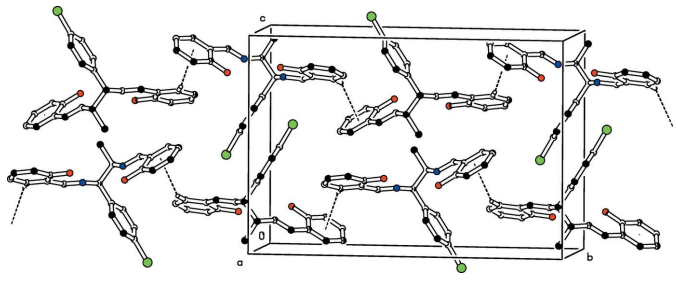


Figure 5
The crystal packing of the title compound (II) viewed along the *a* axis. The C—H···π interactions are shown as dashed lines. For clarity, H atoms not involved in these interactions have been omitted.

Acknowledgements

The authors thank the SAIF, IIT-Madras, for support during the single-crystal data collection and gratefully acknowledge the UGC for financial support under the MRP scheme.

References

Bruker (2004). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chakraborty, S., Bhattacharjee, C. R., Mondal, P., Prasad, S. K. & Rao, D. S. S. (2015). *Dalton Trans.* **44**, 7477–7488.
Chen, C.-H., Liao, D.-J., Wan, C.-F. & Wu, A.-T. (2013). *Analyst*, **138**, 2527–2530.
Cheng, J., Wei, K., Ma, X., Zhou, X. & Xiang, H. (2013). *J. Phys. Chem.* **117**, 16552–16563.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Gans, J. D. & Shalloway, D. (2001). *J. Mol. Graph. Model.* **19**, 557–559.
Habibi, M. H., Sardashti, M. K., Barati, K., Harrington, R. W. & Clegg, W. (2007). *Z. Naturforsch. Teil B*, **62**, 621–624.
Nayar, C. R. & Ravikumar, R. (2014). *J. Coord. Chem.* **67**, 1–16.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Toledo, T. A. de, Pizani, P. S., da Silva, L. E., Teixeira, A. M. & Freire, P. T. (2015). *J. Mol. Struct.* **1097**, 106–111.
Yang, X., Liu, X., Shen, K., Fu, Y., Zhang, M., Zhu, C. & Cheng, Y. (2011). *Org. Biomol. Chem.* **9**, 6011–6021.
Zeyrek, T. C. (2013). *J. Korean Chem. Soc.* **57**, 461–471.

supporting information

Acta Cryst. (2017). E**73**, 1878-1881 [https://doi.org/10.1107/S2056989017016292]

Crystal structures of salen-type ligands 2-[(1*E*)-({1-(3-chlorophenyl)-2-[(*E*)-(2-hydroxybenzylidene)amino]propyl}imino)methyl]phenol and 2-[(1*E*)-({1-(4-chlorophenyl)-2-[(*E*)-(2-hydroxybenzylidene)amino]propyl}imino)methyl]phenol

A. Gayathri, K. Rajeswari, T. Vidhyasagar and S. Selvanayagam

Computing details

For both structures, data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

2-[(1*E*)-({1-(3-Chlorophenyl)-2-[(*E*)-(2-hydroxybenzylidene)amino]propyl}imino)methyl]phenol (I)

Crystal data

$C_{23}H_{21}ClN_2O_2$
M_r = 392.87
Monoclinic, $P2_1$
a = 12.8126 (7) Å
b = 7.0224 (3) Å
c = 12.8169 (6) Å
β = 117.207 (3)°
V = 1025.61 (9) Å^3
Z = 2
$F(000)$ = 412
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4564 reflections
θ = 3.1–28.7°
μ = 0.21 mm^{-1}
T = 296 K
Block, yellow
0.35 × 0.30 × 0.25 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} = 0.921, T_{max} = 0.959
15137 measured reflections
4892 independent reflections
2738 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.9°, θ_{min} = 3.1°
h = −17→17
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.087
S = 0.98
4892 reflections
263 parameters
3 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.27 (8)

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. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.12595 (9)	−0.08259 (13)	0.75791 (8)	0.0764 (3)
O1	0.2698 (2)	−0.1099 (3)	0.4005 (2)	0.0608 (6)
H1	0.267 (4)	−0.021 (4)	0.440 (3)	0.093 (15)*
O2	0.5035 (2)	−0.0707 (4)	0.7066 (2)	0.0756 (7)
H2	0.460 (3)	0.018 (4)	0.671 (3)	0.094 (15)*
N1	0.2403 (2)	0.2414 (3)	0.4445 (2)	0.0392 (6)
N2	0.4325 (2)	0.2792 (3)	0.6800 (2)	0.0447 (6)
C1	0.2232 (3)	−0.0598 (5)	0.2872 (3)	0.0484 (8)
C2	0.2161 (3)	−0.1952 (6)	0.2053 (4)	0.0696 (11)
H2A	0.2458	−0.3170	0.2295	0.084*
C3	0.1651 (4)	−0.1487 (7)	0.0886 (4)	0.0826 (13)
H3	0.1599	−0.2402	0.0340	0.099*
C4	0.1219 (4)	0.0292 (8)	0.0510 (4)	0.0901 (14)
H4	0.0859	0.0578	−0.0286	0.108*
C5	0.1319 (3)	0.1664 (6)	0.1320 (3)	0.0696 (10)
H5	0.1040	0.2887	0.1065	0.083*
C6	0.1828 (3)	0.1248 (4)	0.2505 (3)	0.0457 (8)
C7	0.1946 (2)	0.2720 (4)	0.3347 (3)	0.0425 (7)
H7	0.1676	0.3939	0.3071	0.051*
C8	0.2472 (2)	0.3981 (4)	0.5223 (2)	0.0400 (7)
H8	0.2130	0.5111	0.4737	0.048*
C9	0.1745 (2)	0.3515 (4)	0.5843 (2)	0.0376 (7)
C10	0.1000 (3)	0.4861 (4)	0.5917 (3)	0.0472 (8)
H10	0.0941	0.6051	0.5576	0.057*
C11	0.0340 (3)	0.4461 (5)	0.6495 (3)	0.0586 (9)
H11	−0.0158	0.5386	0.6537	0.070*
C12	0.0411 (3)	0.2721 (5)	0.7004 (3)	0.0539 (8)
H12	−0.0032	0.2453	0.7393	0.065*
C13	0.1150 (3)	0.1387 (4)	0.6927 (2)	0.0444 (8)
C14	0.1816 (2)	0.1744 (4)	0.6362 (2)	0.0413 (7)
H14	0.2312	0.0809	0.6325	0.050*
C15	0.3754 (2)	0.4435 (4)	0.6076 (3)	0.0437 (7)
H15	0.3765	0.5478	0.6589	0.052*
C16	0.4443 (3)	0.5057 (4)	0.5432 (3)	0.0568 (9)

H16A	0.4503	0.4010	0.4981	0.085*
H16B	0.5215	0.5454	0.5991	0.085*
H16C	0.4045	0.6098	0.4918	0.085*
C17	0.4838 (3)	0.2952 (4)	0.7907 (3)	0.0495 (8)
H17	0.4803	0.4115	0.8237	0.059*
C18	0.5477 (3)	0.1402 (5)	0.8680 (3)	0.0492 (8)
C19	0.6041 (3)	0.1668 (6)	0.9894 (3)	0.0740 (11)
H19	0.5978	0.2828	1.0211	0.089*
C20	0.6697 (4)	0.0201 (8)	1.0629 (4)	0.0911 (14)
H20	0.7092	0.0385	1.1437	0.109*
C21	0.6755 (4)	−0.1514 (8)	1.0155 (5)	0.0927 (14)
H21	0.7182	−0.2500	1.0652	0.111*
C22	0.6206 (3)	−0.1822 (6)	0.8973 (4)	0.0805 (12)
H22	0.6265	−0.2998	0.8671	0.097*
C23	0.5557 (3)	−0.0364 (5)	0.8225 (3)	0.0567 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1129 (8)	0.0564 (5)	0.0816 (7)	−0.0087 (6)	0.0632 (6)	0.0050 (5)
O1	0.0708 (16)	0.0535 (15)	0.0610 (17)	0.0124 (12)	0.0325 (14)	0.0025 (13)
O2	0.096 (2)	0.0583 (16)	0.0555 (17)	0.0182 (16)	0.0201 (15)	0.0044 (15)
N1	0.0428 (15)	0.0390 (14)	0.0373 (16)	0.0061 (11)	0.0197 (13)	0.0049 (11)
N2	0.0425 (15)	0.0451 (15)	0.0438 (18)	0.0026 (12)	0.0173 (14)	0.0009 (13)
C1	0.0370 (18)	0.064 (2)	0.050 (2)	−0.0029 (17)	0.0250 (17)	−0.0075 (19)
C2	0.062 (2)	0.074 (2)	0.086 (3)	−0.009 (2)	0.046 (2)	−0.021 (2)
C3	0.078 (3)	0.109 (4)	0.075 (3)	−0.029 (3)	0.048 (3)	−0.045 (3)
C4	0.092 (3)	0.130 (4)	0.047 (3)	−0.020 (3)	0.030 (3)	−0.019 (3)
C5	0.071 (3)	0.091 (3)	0.044 (2)	−0.001 (2)	0.023 (2)	0.004 (2)
C6	0.0387 (19)	0.063 (2)	0.038 (2)	−0.0010 (16)	0.0197 (16)	0.0002 (17)
C7	0.0394 (18)	0.0428 (17)	0.047 (2)	0.0040 (15)	0.0214 (16)	0.0106 (16)
C8	0.0457 (18)	0.0336 (15)	0.0426 (17)	0.0089 (14)	0.0220 (15)	0.0074 (15)
C9	0.0373 (17)	0.0402 (17)	0.0320 (16)	0.0044 (13)	0.0129 (15)	−0.0016 (13)
C10	0.049 (2)	0.0468 (19)	0.047 (2)	0.0117 (14)	0.0228 (17)	0.0036 (14)
C11	0.053 (2)	0.065 (2)	0.064 (2)	0.0155 (17)	0.0332 (18)	−0.0042 (19)
C12	0.051 (2)	0.067 (2)	0.053 (2)	−0.0044 (19)	0.0318 (18)	−0.0093 (18)
C13	0.051 (2)	0.0461 (17)	0.0346 (18)	−0.0079 (16)	0.0185 (16)	−0.0057 (15)
C14	0.0426 (19)	0.0418 (17)	0.0412 (18)	0.0036 (14)	0.0206 (16)	−0.0035 (14)
C15	0.0427 (19)	0.0355 (17)	0.0521 (19)	0.0031 (15)	0.0211 (16)	−0.0009 (15)
C16	0.055 (2)	0.0485 (18)	0.072 (3)	0.0040 (16)	0.034 (2)	0.0124 (17)
C17	0.0440 (19)	0.056 (2)	0.052 (2)	−0.0053 (16)	0.0257 (18)	−0.0095 (18)
C18	0.0395 (19)	0.068 (2)	0.038 (2)	−0.0039 (17)	0.0165 (17)	0.0065 (18)
C19	0.062 (3)	0.108 (3)	0.050 (2)	−0.015 (2)	0.025 (2)	−0.002 (2)
C20	0.068 (3)	0.142 (4)	0.046 (3)	−0.010 (3)	0.011 (2)	0.027 (3)
C21	0.064 (3)	0.115 (4)	0.079 (4)	0.002 (3)	0.016 (3)	0.040 (3)
C22	0.067 (3)	0.082 (3)	0.077 (3)	0.010 (2)	0.020 (2)	0.031 (2)
C23	0.047 (2)	0.066 (3)	0.051 (2)	−0.0002 (17)	0.0165 (18)	0.0131 (19)

Geometric parameters (Å, º)

Cl1—C13	1.740 (3)	C10—C11	1.384 (4)
O1—C1	1.341 (3)	C10—H10	0.9300
O1—H1	0.820 (13)	C11—C12	1.369 (4)
O2—C23	1.343 (4)	C11—H11	0.9300
O2—H2	0.823 (13)	C12—C13	1.368 (4)
N1—C7	1.271 (3)	C12—H12	0.9300
N1—C8	1.461 (3)	C13—C14	1.371 (4)
N2—C17	1.266 (4)	C14—H14	0.9300
N2—C15	1.452 (4)	C15—C16	1.522 (4)
C1—C2	1.388 (4)	C15—H15	0.9800
C1—C6	1.395 (4)	C16—H16A	0.9600
C2—C3	1.370 (6)	C16—H16B	0.9600
C2—H2A	0.9300	C16—H16C	0.9600
C3—C4	1.362 (6)	C17—C18	1.448 (4)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.379 (5)	C18—C23	1.394 (4)
C4—H4	0.9300	C18—C19	1.396 (4)
C5—C6	1.383 (4)	C19—C20	1.389 (6)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.452 (4)	C20—C21	1.367 (6)
C7—H7	0.9300	C20—H20	0.9300
C8—C9	1.510 (4)	C21—C22	1.364 (6)
C8—C15	1.534 (4)	C21—H21	0.9300
C8—H8	0.9800	C22—C23	1.389 (4)
C9—C10	1.377 (4)	C22—H22	0.9300
C9—C14	1.394 (4)		
C1—O1—H1	111 (3)	C13—C12—H12	120.9
C23—O2—H2	110 (3)	C11—C12—H12	120.9
C7—N1—C8	118.8 (2)	C12—C13—C14	122.1 (3)
C17—N2—C15	119.8 (2)	C12—C13—Cl1	118.9 (2)
O1—C1—C2	118.8 (3)	C14—C13—Cl1	119.0 (2)
O1—C1—C6	121.5 (3)	C13—C14—C9	119.7 (3)
C2—C1—C6	119.7 (3)	C13—C14—H14	120.2
C3—C2—C1	119.7 (4)	C9—C14—H14	120.2
C3—C2—H2A	120.1	N2—C15—C16	109.1 (2)
C1—C2—H2A	120.1	N2—C15—C8	110.7 (2)
C4—C3—C2	121.3 (4)	C16—C15—C8	111.8 (2)
C4—C3—H3	119.4	N2—C15—H15	108.4
C2—C3—H3	119.4	C16—C15—H15	108.4
C3—C4—C5	119.5 (4)	C8—C15—H15	108.4
C3—C4—H4	120.3	C15—C16—H16A	109.5
C5—C4—H4	120.3	C15—C16—H16B	109.5
C4—C5—C6	120.9 (4)	H16A—C16—H16B	109.5
C4—C5—H5	119.5	C15—C16—H16C	109.5
C6—C5—H5	119.5	H16A—C16—H16C	109.5

C5—C6—C1	118.9 (3)	H16B—C16—H16C	109.5
C5—C6—C7	120.2 (3)	N2—C17—C18	122.8 (3)
C1—C6—C7	121.0 (3)	N2—C17—H17	118.6
N1—C7—C6	122.8 (3)	C18—C17—H17	118.6
N1—C7—H7	118.6	C23—C18—C19	119.0 (3)
C6—C7—H7	118.6	C23—C18—C17	120.6 (3)
N1—C8—C9	109.7 (2)	C19—C18—C17	120.3 (3)
N1—C8—C15	110.7 (2)	C20—C19—C18	120.1 (4)
C9—C8—C15	112.8 (2)	C20—C19—H19	120.0
N1—C8—H8	107.8	C18—C19—H19	120.0
C9—C8—H8	107.8	C21—C20—C19	119.4 (4)
C15—C8—H8	107.8	C21—C20—H20	120.3
C10—C9—C14	118.4 (3)	C19—C20—H20	120.3
C10—C9—C8	120.1 (2)	C22—C21—C20	121.9 (4)
C14—C9—C8	121.6 (2)	C22—C21—H21	119.1
C9—C10—C11	120.7 (3)	C20—C21—H21	119.1
C9—C10—H10	119.7	C21—C22—C23	119.4 (4)
C11—C10—H10	119.7	C21—C22—H22	120.3
C12—C11—C10	120.9 (3)	C23—C22—H22	120.3
C12—C11—H11	119.6	O2—C23—C22	118.0 (3)
C10—C11—H11	119.6	O2—C23—C18	121.8 (3)
C13—C12—C11	118.3 (3)	C22—C23—C18	120.1 (4)

O1—C1—C2—C3	177.8 (3)	C11—C12—C13—Cl1	179.5 (2)
C6—C1—C2—C3	−2.6 (5)	C12—C13—C14—C9	−0.1 (4)
C1—C2—C3—C4	0.6 (6)	Cl1—C13—C14—C9	−179.5 (2)
C2—C3—C4—C5	1.5 (7)	C10—C9—C14—C13	0.0 (4)
C3—C4—C5—C6	−1.5 (6)	C8—C9—C14—C13	179.3 (3)
C4—C5—C6—C1	−0.6 (5)	C17—N2—C15—C16	110.4 (3)
C4—C5—C6—C7	178.8 (3)	C17—N2—C15—C8	−126.2 (3)
O1—C1—C6—C5	−177.8 (3)	N1—C8—C15—N2	−60.4 (3)
C2—C1—C6—C5	2.6 (4)	C9—C8—C15—N2	62.9 (3)
O1—C1—C6—C7	2.8 (4)	N1—C8—C15—C16	61.3 (3)
C2—C1—C6—C7	−176.8 (3)	C9—C8—C15—C16	−175.3 (2)
C8—N1—C7—C6	−179.3 (2)	C15—N2—C17—C18	−176.7 (2)
C5—C6—C7—N1	179.7 (3)	N2—C17—C18—C23	0.3 (5)
C1—C6—C7—N1	−0.9 (4)	N2—C17—C18—C19	179.0 (3)
C7—N1—C8—C9	117.0 (3)	C23—C18—C19—C20	1.7 (5)
C7—N1—C8—C15	−117.9 (3)	C17—C18—C19—C20	−177.1 (3)
N1—C8—C9—C10	−134.2 (3)	C18—C19—C20—C21	−1.8 (6)
C15—C8—C9—C10	101.9 (3)	C19—C20—C21—C22	1.3 (7)
N1—C8—C9—C14	46.5 (3)	C20—C21—C22—C23	−0.7 (6)
C15—C8—C9—C14	−77.4 (3)	C21—C22—C23—O2	179.4 (3)
C14—C9—C10—C11	0.0 (5)	C21—C22—C23—C18	0.5 (5)
C8—C9—C10—C11	−179.2 (3)	C19—C18—C23—O2	−179.9 (3)
C9—C10—C11—C12	0.0 (5)	C17—C18—C23—O2	−1.1 (5)
C10—C11—C12—C13	−0.1 (5)	C19—C18—C23—C22	−1.0 (5)
C11—C12—C13—C14	0.2 (5)	C17—C18—C23—C22	177.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82 (1)	1.88 (3)	2.596 (3)	146 (4)
O2—H2···N2	0.82 (1)	1.88 (3)	2.588 (3)	143 (4)
C16—H16*C*···O1^{i}	0.96	2.52	3.448 (4)	161

Symmetry code: (i) *x*, *y*+1, *z*.

2-[(1*E*)-({1-(4-Chlorophenyl)-2-[(*E*)-(2-hydroxybenzylidene)amino]propyl}imino)methyl]phenol (II)

Crystal data

$C_{23}H_{21}ClN_2O_2$
M_r = 392.87
Monoclinic, $P2_1/c$
a = 6.7923 (2) Å
b = 20.8261 (8) Å
c = 14.1744 (6) Å
β = 92.435 (2)°
V = 2003.26 (13) Å^3
Z = 4
$F(000)$ = 824
D_x = 1.303 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9979 reflections
θ = 2.4–23.5°
μ = 0.21 mm^{-1}
T = 296 K
Block, brown
0.35 × 0.30 × 0.25 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} = 0.927, T_{max} = 0.959
42044 measured reflections
4182 independent reflections
2599 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 26.6°, θ_{min} = 2.4°
h = −8→8
k = −26→26
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.140
S = 1.08
4182 reflections
262 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 0.8955P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.78279 (15)	0.12547 (4)	0.58629 (6)	0.1006 (3)
O1	0.2304 (3)	−0.08496 (8)	0.15527 (14)	0.0637 (5)

H1	0.334 (3)	−0.0660 (13)	0.171 (2)	0.087 (10)*
O2	0.2661 (3)	0.08746 (11)	0.18436 (16)	0.0770 (6)
H2	0.370 (3)	0.0672 (14)	0.182 (2)	0.098 (12)*
N1	0.5917 (2)	−0.06874 (9)	0.21615 (13)	0.0467 (5)
N2	0.6144 (2)	0.05789 (9)	0.13809 (13)	0.0462 (4)
C1	0.2600 (3)	−0.14842 (11)	0.16815 (16)	0.0482 (5)
C2	0.1094 (4)	−0.19034 (13)	0.14300 (19)	0.0622 (7)
H2A	−0.0098	−0.1747	0.1178	0.075*
C3	0.1357 (5)	−0.25512 (14)	0.1552 (2)	0.0707 (8)
H3	0.0332	−0.2831	0.1391	0.085*
C4	0.3108 (5)	−0.27897 (13)	0.1909 (2)	0.0700 (8)
H4	0.3275	−0.3230	0.1986	0.084*
C5	0.4615 (4)	−0.23786 (12)	0.21510 (18)	0.0614 (7)
H5	0.5805	−0.2543	0.2393	0.074*
C6	0.4400 (3)	−0.17188 (10)	0.20426 (15)	0.0464 (5)
C7	0.6050 (3)	−0.12931 (11)	0.22487 (15)	0.0478 (5)
H7	0.7252	−0.1470	0.2452	0.057*
C8	0.7683 (3)	−0.02938 (10)	0.22775 (15)	0.0452 (5)
H8	0.8834	−0.0578	0.2314	0.054*
C9	0.7673 (3)	0.01045 (11)	0.31730 (15)	0.0463 (5)
C10	0.9417 (4)	0.03504 (14)	0.35463 (18)	0.0633 (7)
H10	1.0577	0.0274	0.3239	0.076*
C11	0.9481 (4)	0.07086 (14)	0.4368 (2)	0.0696 (7)
H11	1.0674	0.0866	0.4617	0.084*
C12	0.7775 (4)	0.08287 (12)	0.48094 (18)	0.0632 (7)
C13	0.6031 (4)	0.06095 (13)	0.44453 (19)	0.0651 (7)
H13	0.4870	0.0704	0.4742	0.078*
C14	0.5981 (4)	0.02444 (13)	0.36300 (18)	0.0595 (6)
H14	0.4779	0.0090	0.3386	0.071*
C15	0.7810 (3)	0.01313 (11)	0.13977 (15)	0.0454 (5)
H15	0.9041	0.0377	0.1442	0.054*
C16	0.7758 (4)	−0.02621 (12)	0.04999 (17)	0.0566 (6)
H16A	0.8808	−0.0571	0.0531	0.085*
H16B	0.7916	0.0016	−0.0031	0.085*
H16C	0.6517	−0.0481	0.0430	0.085*
C17	0.6244 (3)	0.11048 (11)	0.09408 (15)	0.0459 (5)
H17	0.7395	0.1207	0.0642	0.055*
C18	0.4608 (3)	0.15533 (11)	0.08902 (16)	0.0481 (5)
C19	0.4742 (4)	0.21199 (13)	0.03970 (19)	0.0697 (7)
H19	0.5890	0.2213	0.0090	0.084*
C20	0.3212 (6)	0.25477 (16)	0.0351 (3)	0.0959 (11)
H20	0.3309	0.2927	0.0011	0.115*
C21	0.1538 (6)	0.2408 (2)	0.0815 (3)	0.1000 (13)
H21	0.0501	0.2700	0.0789	0.120*
C22	0.1349 (4)	0.18543 (17)	0.1312 (2)	0.0796 (9)
H22	0.0197	0.1771	0.1622	0.096*
C23	0.2875 (3)	0.14176 (13)	0.13520 (18)	0.0582 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1458 (8)	0.0881 (6)	0.0693 (5)	−0.0325 (5)	0.0213 (5)	−0.0277 (4)
O1	0.0522 (10)	0.0485 (11)	0.0897 (14)	0.0042 (9)	−0.0063 (9)	0.0005 (9)
O2	0.0553 (12)	0.0837 (15)	0.0935 (15)	−0.0041 (11)	0.0232 (10)	0.0027 (12)
N1	0.0449 (10)	0.0437 (11)	0.0516 (11)	−0.0004 (8)	0.0032 (8)	−0.0005 (9)
N2	0.0425 (10)	0.0489 (11)	0.0473 (11)	−0.0010 (8)	0.0039 (8)	0.0023 (9)
C1	0.0546 (13)	0.0437 (13)	0.0466 (13)	0.0012 (11)	0.0074 (10)	−0.0004 (10)
C2	0.0591 (15)	0.0630 (17)	0.0646 (16)	−0.0075 (13)	0.0039 (12)	−0.0038 (13)
C3	0.085 (2)	0.0631 (18)	0.0637 (17)	−0.0232 (15)	0.0040 (15)	−0.0013 (14)
C4	0.103 (2)	0.0419 (14)	0.0641 (17)	−0.0084 (15)	−0.0036 (15)	0.0040 (12)
C5	0.0808 (18)	0.0473 (15)	0.0553 (15)	0.0065 (13)	−0.0069 (13)	0.0069 (12)
C6	0.0596 (14)	0.0414 (13)	0.0384 (12)	0.0007 (10)	0.0032 (10)	0.0018 (9)
C7	0.0522 (13)	0.0484 (14)	0.0424 (12)	0.0061 (11)	−0.0011 (10)	0.0022 (10)
C8	0.0376 (11)	0.0473 (13)	0.0507 (13)	0.0025 (9)	0.0020 (9)	0.0011 (10)
C9	0.0475 (12)	0.0484 (13)	0.0430 (12)	−0.0037 (10)	0.0009 (10)	0.0056 (10)
C10	0.0507 (14)	0.0825 (19)	0.0568 (16)	−0.0062 (13)	0.0037 (11)	−0.0040 (14)
C11	0.0683 (17)	0.079 (2)	0.0609 (17)	−0.0178 (15)	−0.0056 (13)	−0.0072 (15)
C12	0.090 (2)	0.0511 (15)	0.0490 (15)	−0.0159 (14)	0.0090 (14)	0.0003 (12)
C13	0.0709 (17)	0.0623 (17)	0.0638 (17)	−0.0060 (13)	0.0219 (14)	−0.0050 (13)
C14	0.0521 (14)	0.0703 (17)	0.0568 (15)	−0.0080 (12)	0.0093 (11)	−0.0071 (13)
C15	0.0375 (11)	0.0535 (13)	0.0454 (13)	−0.0009 (10)	0.0049 (9)	0.0014 (10)
C16	0.0570 (14)	0.0645 (16)	0.0486 (14)	0.0080 (12)	0.0064 (11)	−0.0025 (12)
C17	0.0461 (12)	0.0503 (14)	0.0415 (12)	−0.0061 (10)	0.0048 (9)	−0.0024 (10)
C18	0.0539 (13)	0.0473 (13)	0.0427 (13)	0.0021 (11)	−0.0044 (10)	−0.0062 (10)
C19	0.088 (2)	0.0596 (17)	0.0606 (17)	0.0096 (15)	−0.0041 (14)	0.0024 (14)
C20	0.125 (3)	0.064 (2)	0.096 (3)	0.025 (2)	−0.025 (2)	0.0008 (18)
C21	0.092 (3)	0.092 (3)	0.112 (3)	0.046 (2)	−0.037 (2)	−0.037 (2)
C22	0.0538 (16)	0.090 (2)	0.094 (2)	0.0128 (16)	−0.0105 (14)	−0.035 (2)
C23	0.0504 (14)	0.0625 (16)	0.0610 (16)	0.0018 (12)	−0.0041 (11)	−0.0171 (13)

Geometric parameters (Å, º)

Cl1—C12	1.736 (3)	C10—C11	1.383 (4)
O1—C1	1.348 (3)	C10—H10	0.9300
O1—H1	0.833 (10)	C11—C12	1.363 (4)
O2—C23	1.339 (3)	C11—H11	0.9300
O2—H2	0.822 (10)	C12—C13	1.351 (4)
N1—C7	1.270 (3)	C13—C14	1.383 (4)
N1—C8	1.456 (3)	C13—H13	0.9300
N2—C17	1.264 (3)	C14—H14	0.9300
N2—C15	1.465 (3)	C15—C16	1.513 (3)
C1—C2	1.380 (3)	C15—H15	0.9800
C1—C6	1.394 (3)	C16—H16A	0.9600
C2—C3	1.371 (4)	C16—H16B	0.9600
C2—H2A	0.9300	C16—H16C	0.9600
C3—C4	1.366 (4)	C17—C18	1.451 (3)

C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.367 (4)	C18—C19	1.376 (3)
C4—H4	0.9300	C18—C23	1.400 (3)
C5—C6	1.389 (3)	C19—C20	1.368 (4)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.449 (3)	C20—C21	1.368 (5)
C7—H7	0.9300	C20—H20	0.9300
C8—C9	1.516 (3)	C21—C22	1.361 (5)
C8—C15	1.535 (3)	C21—H21	0.9300
C8—H8	0.9800	C22—C23	1.378 (4)
C9—C14	1.374 (3)	C22—H22	0.9300
C9—C10	1.375 (3)		

C1—O1—H1	108 (2)	C13—C12—Cl1	119.1 (2)
C23—O2—H2	108 (2)	C11—C12—Cl1	120.1 (2)
C7—N1—C8	119.55 (18)	C12—C13—C14	119.7 (2)
C17—N2—C15	120.13 (18)	C12—C13—H13	120.2
O1—C1—C2	118.7 (2)	C14—C13—H13	120.2
O1—C1—C6	121.1 (2)	C9—C14—C13	121.3 (2)
C2—C1—C6	120.1 (2)	C9—C14—H14	119.4
C3—C2—C1	119.9 (3)	C13—C14—H14	119.4
C3—C2—H2A	120.1	N2—C15—C16	109.91 (18)
C1—C2—H2A	120.1	N2—C15—C8	108.07 (17)
C4—C3—C2	120.8 (3)	C16—C15—C8	111.79 (19)
C4—C3—H3	119.6	N2—C15—H15	109.0
C2—C3—H3	119.6	C16—C15—H15	109.0
C3—C4—C5	119.7 (3)	C8—C15—H15	109.0
C3—C4—H4	120.1	C15—C16—H16A	109.5
C5—C4—H4	120.1	C15—C16—H16B	109.5
C4—C5—C6	121.2 (2)	H16A—C16—H16B	109.5
C4—C5—H5	119.4	C15—C16—H16C	109.5
C6—C5—H5	119.4	H16A—C16—H16C	109.5
C5—C6—C1	118.3 (2)	H16B—C16—H16C	109.5
C5—C6—C7	120.4 (2)	N2—C17—C18	121.7 (2)
C1—C6—C7	121.2 (2)	N2—C17—H17	119.2
N1—C7—C6	122.5 (2)	C18—C17—H17	119.2
N1—C7—H7	118.8	C19—C18—C23	119.0 (2)
C6—C7—H7	118.8	C19—C18—C17	120.6 (2)
N1—C8—C9	111.71 (17)	C23—C18—C17	120.3 (2)
N1—C8—C15	107.90 (17)	C20—C19—C18	121.1 (3)
C9—C8—C15	111.53 (18)	C20—C19—H19	119.5
N1—C8—H8	108.5	C18—C19—H19	119.5
C9—C8—H8	108.5	C21—C20—C19	118.9 (3)
C15—C8—H8	108.5	C21—C20—H20	120.5
C14—C9—C10	117.6 (2)	C19—C20—H20	120.5
C14—C9—C8	122.9 (2)	C22—C21—C20	121.8 (3)
C10—C9—C8	119.5 (2)	C22—C21—H21	119.1
C9—C10—C11	121.4 (2)	C20—C21—H21	119.1

C9—C10—H10	119.3	C21—C22—C23	119.6 (3)
C11—C10—H10	119.3	C21—C22—H22	120.2
C12—C11—C10	119.3 (2)	C23—C22—H22	120.2
C12—C11—H11	120.4	O2—C23—C22	118.7 (3)
C10—C11—H11	120.4	O2—C23—C18	121.7 (2)
C13—C12—C11	120.8 (2)	C22—C23—C18	119.6 (3)
O1—C1—C2—C3	179.9 (2)	C11—C12—C13—C14	1.8 (4)
C6—C1—C2—C3	1.2 (4)	Cl1—C12—C13—C14	−177.0 (2)
C1—C2—C3—C4	−1.0 (4)	C10—C9—C14—C13	−1.1 (4)
C2—C3—C4—C5	0.3 (4)	C8—C9—C14—C13	−180.0 (2)
C3—C4—C5—C6	0.1 (4)	C12—C13—C14—C9	−0.7 (4)
C4—C5—C6—C1	0.2 (4)	C17—N2—C15—C16	−81.7 (2)
C4—C5—C6—C7	−176.2 (2)	C17—N2—C15—C8	156.0 (2)
O1—C1—C6—C5	−179.5 (2)	N1—C8—C15—N2	65.8 (2)
C2—C1—C6—C5	−0.8 (3)	C9—C8—C15—N2	−57.2 (2)
O1—C1—C6—C7	−3.1 (3)	N1—C8—C15—C16	−55.3 (2)
C2—C1—C6—C7	175.6 (2)	C9—C8—C15—C16	−178.30 (17)
C8—N1—C7—C6	−173.12 (19)	C15—N2—C17—C18	178.55 (19)
C5—C6—C7—N1	−179.8 (2)	N2—C17—C18—C19	−179.2 (2)
C1—C6—C7—N1	3.9 (3)	N2—C17—C18—C23	1.5 (3)
C7—N1—C8—C9	−110.4 (2)	C23—C18—C19—C20	−0.2 (4)
C7—N1—C8—C15	126.6 (2)	C17—C18—C19—C20	−179.5 (3)
N1—C8—C9—C14	−20.7 (3)	C18—C19—C20—C21	0.7 (5)
C15—C8—C9—C14	100.2 (2)	C19—C20—C21—C22	−0.6 (5)
N1—C8—C9—C10	160.5 (2)	C20—C21—C22—C23	−0.2 (5)
C15—C8—C9—C10	−78.6 (3)	C21—C22—C23—O2	−179.9 (3)
C14—C9—C10—C11	2.0 (4)	C21—C22—C23—C18	0.7 (4)
C8—C9—C10—C11	−179.1 (2)	C19—C18—C23—O2	−179.9 (2)
C9—C10—C11—C12	−1.0 (4)	C17—C18—C23—O2	−0.6 (3)
C10—C11—C12—C13	−0.9 (4)	C19—C18—C23—C22	−0.6 (4)
C10—C11—C12—Cl1	177.9 (2)	C17—C18—C23—C22	178.8 (2)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C18–C23 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.83 (1)	1.83 (2)	2.589 (2)	150 (3)
O2—H2···N2	0.82 (1)	1.81 (2)	2.557 (3)	150 (3)
C14—H14···N1	0.93	2.52	2.845 (3)	101
C5—H5···*Cg*^{i}	0.93	2.76	3.449 (3)	132

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