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(2*E*)-2-[(4-Ethoxyphenyl)imino]-1,2-diphenylethanone

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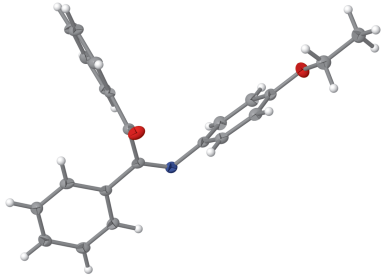
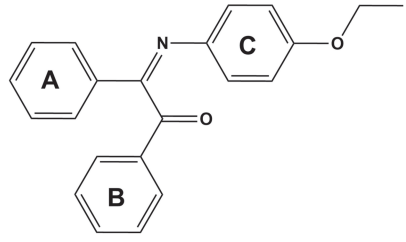
The title compound, $C_{22}H_{19}NO_2$, is an imino-ketone Schiff base. The configuration about the azomethine bond is *E*. The aromatic rings of the 1,2-diphenylethanone moiety are inclined to each other by 80.43 (7)°. The 4-ethoxyphenyl ring is inclined to the phenylethanone ring by 81.91 (7)° and to the phenyl ring to which it is *trans* by 68.56 (7)°. In the crystal, four symmetry-related molecules are linked by C—H···O hydrogen bonds to form square-like units with an $R_4^3(36)$ ring motif, which are linked through bifurcated C—H···O hydrogen bonds to form sheets parallel to the $(10\bar{1})$ plane.

3D view



Chemical scheme



Structure description

As part of our ongoing studies of Schiff bases (Ziani *et al.*, 2023; Bouchama *et al.*, 2007), we describe herein the synthesis and crystal structure of the title imino-ketone compound, (**I**). The molecular structure of (**I**) is illustrated in Fig. 1. The configuration about the azomethine bond, C1═N1, is *E*, with a bond length of 1.278 (2) Å. This value is essentially identical to that observed for the 4-methoxyphenyl analogue (**II**), *viz.* 1.277 (2) Å (Wang *et al.*, 2021). In the 1,2-diphenylethan-1-one unit, the aromatic rings *A* (C2–C7) and *B* (C9–C14) are inclined to each other by 80.43 (7)°. The 4-ethoxyphenyl ring *C* (C15–C20) is inclined to rings *A* and *B* by 68.56 (7) and 81.91 (7)°, respectively. In the 4-methoxyphenyl analogue (**II**), these dihedral angles are similar; *A*/*B* is 79.85 (6)°,

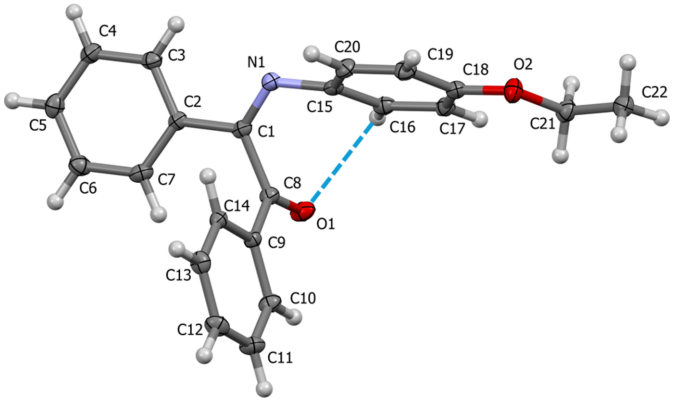


Figure 1
A view of the molecular structure of (**I**) with displacement ellipsoids drawn at the 50% probability level. The intramolecular C—H···O hydrogen bond (Table 1) is shown as a dashed blue line.

A/*C* is 70.06 (6)° and *B*/*C* is 77.26 (6)°. The 4-ethoxyphenyl moiety is almost co-planar with the ethoxy unit (O2/C21/C22), being inclined to aromatic ring *C* by only 1.33 (15)°. There is a short intramolecular C16—H16···O1 contact in the molecule (Fig. 1 and Table 1).

In the crystal, four symmetry-related molecules are linked by C—H···O hydrogen bonds, forming a square-like unit with an $R_4^3(36)$ ring motif (Table 1 and Fig. 2). These units are linked by bifurcated C—H···O hydrogen bonds, forming sheets lying parallel to the $(10\bar{1})$ plane (Fig. 3).

Synthesis and crystallization

Equimolar amounts of benzil (0.210 g, 0.01 mmol) and 4-ethoxyaniline (0.137 g, 0.01 mmol) were mixed in absolute ethanol (30 ml) and refluxed under stirring for 3 h. After cooling to room temperature, the solvent was allowed to

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O1	0.95	2.56	3.068 (2)	114
C12—H12···O1^{i}	0.95	2.41	3.279 (2)	151
C22—H22*A*···O1^{ii}	0.98	2.55	3.462 (2)	155

Symmetry codes: (i) $x, y-1, z$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{19}NO_2$
M_r	329.38
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, *b*, *c* (Å)	13.0674 (4), 8.0633 (2), 16.4309 (5)
β (°)	101.412 (3)
V (Å^3)	1697.04 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.32 × 0.17 × 0.05
Data collection	
Diffractometer	Xcalibur, Eos, Nova
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.568, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22651, 4240, 3037
R_{int}	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.691
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.117, 1.04
No. of reflections	4240
No. of parameters	227
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.26

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2025/1* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020), *OLEX2* (Dolomanov *et al.*, 2009), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

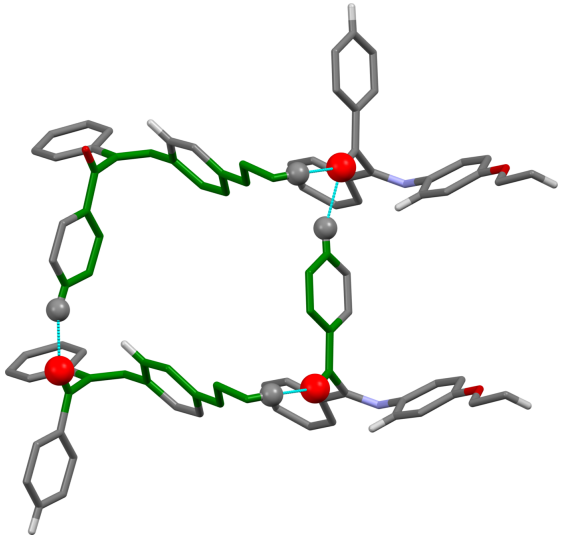


Figure 2
A view of four symmetry-related molecules of (**I**) that are linked by C—H···O hydrogen bonds (Table 1) to form a square-like unit with an $R_4^3(36)$ ring motif. (The acceptor O atoms are red, the donor H atoms are grey and the ring atoms are green.)

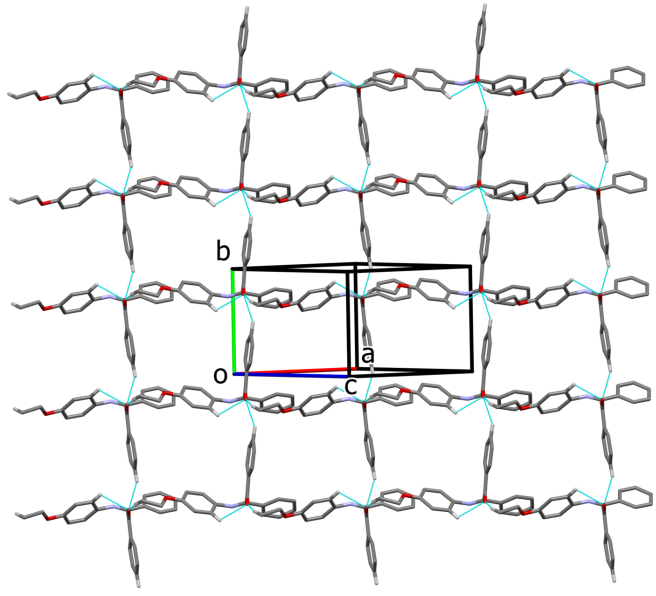


Figure 3
A view of the sheet-like hydrogen-bonded arrangement of symmetry-related molecules in the crystal of (**I**), lying parallel to the $(10\bar{1})$ plane.

evaporate slowly, yielding yellow needle-like crystals (yield 0.249 g, 76%, m.p. 529.5 K).

Refinement

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

References

Bouchama, A., Bendaâs, A., Bouacida, S., Yahiaoui, M., Benard-Rocherulle, P. & Djedouani, A. (2007). *Acta Cryst.* E**63**, o1990–o1992.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.

Rigaku OD (2022). *CrysAlis PRO*. Rigaku Oxford Diffraction Ltd, Yarnton, England.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* C**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* A**71**, 3–8.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

Wang, J., Lin, X., Shao, P.-L., Song, J., Wen, J. & Zhang, X. (2021). *ACS Catal.* **11**, 12729–12735.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

Ziani, N., Ouarda, B., Kadri, S., Jeanneau, E., Warad, I. & Djedouani, A. (2023). *IUCrData* **8**, x230065.

full crystallographic data

IUCrData (2026). **11**, x260740 [https://doi.org/10.1107/S2414314626007406]

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Crystal data

$C_{22}H_{19}NO_2$
M_r = 329.38
Monoclinic, $P2_1/n$
a = 13.0674 (4) Å
b = 8.0633 (2) Å
c = 16.4309 (5) Å
β = 101.412 (3)°
V = 1697.04 (9) Å^3
Z = 4
$F(000)$ = 696
D_x = 1.289 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7263 reflections
θ = 4.0–28.9°
μ = 0.08 mm^{-1}
T = 100 K
Plate, yellow
0.32 × 0.17 × 0.05 mm

Data collection

Xcalibur, Eos, Nova diffractometer
Detector resolution: 15.9897 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.568, T_{max} = 1.000
22651 measured reflections
4240 independent reflections
3037 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 29.4°, θ_{min} = 3.4°
h = −17→17
k = −11→10
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.117
S = 1.04
4240 reflections
227 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.5117P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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. The hydrogen atoms were fixed geometrically (C—H = 0.95–0.99 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 1.5U_{eq}(*C*-methyl) and 1.2U_{eq}(C) for other H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.37863 (9)	0.72732 (14)	0.72318 (7)	0.0230 (3)
O2	−0.00143 (8)	0.65400 (14)	0.42270 (7)	0.0233 (3)
N1	0.42408 (10)	0.75710 (16)	0.54025 (8)	0.0177 (3)
C1	0.47276 (12)	0.72080 (18)	0.61342 (9)	0.0159 (3)
C2	0.58625 (11)	0.75382 (18)	0.63777 (9)	0.0150 (3)
C3	0.63793 (12)	0.84505 (19)	0.58563 (9)	0.0187 (3)
H3	0.599688	0.888983	0.535014	0.022*
C4	0.74416 (12)	0.8714 (2)	0.60744 (10)	0.0210 (3)
H4	0.778474	0.934724	0.572067	0.025*
C5	0.80129 (12)	0.8062 (2)	0.68071 (10)	0.0220 (4)
H5	0.874683	0.822321	0.694735	0.026*
C6	0.75096 (12)	0.7176 (2)	0.73313 (10)	0.0221 (4)
H6	0.789725	0.673329	0.783465	0.026*
C7	0.64419 (12)	0.6935 (2)	0.71241 (10)	0.0208 (4)
H7	0.609858	0.634988	0.749469	0.025*
C8	0.42051 (11)	0.64005 (19)	0.67898 (9)	0.0164 (3)
C9	0.42599 (11)	0.45736 (18)	0.68773 (9)	0.0150 (3)
C10	0.39198 (12)	0.3842 (2)	0.75483 (9)	0.0195 (3)
H10	0.362780	0.450853	0.792138	0.023*
C11	0.40093 (13)	0.2151 (2)	0.76670 (10)	0.0232 (4)
H11	0.377345	0.165044	0.812001	0.028*
C12	0.44422 (12)	0.1181 (2)	0.71271 (10)	0.0229 (4)
H12	0.451685	0.002030	0.721944	0.027*
C13	0.47678 (12)	0.1891 (2)	0.64523 (10)	0.0199 (3)
H13	0.505542	0.121833	0.607927	0.024*
C14	0.46712 (11)	0.35854 (19)	0.63259 (9)	0.0166 (3)
H14	0.488628	0.407542	0.586138	0.020*
C15	0.31464 (12)	0.73071 (19)	0.51553 (9)	0.0175 (3)
C16	0.24190 (12)	0.80883 (19)	0.55370 (9)	0.0189 (3)
H16	0.265110	0.877720	0.600625	0.023*
C17	0.13555 (12)	0.78732 (19)	0.52400 (10)	0.0195 (3)
H17	0.086599	0.841725	0.550558	0.023*
C18	0.10068 (12)	0.6867 (2)	0.45574 (9)	0.0188 (3)
C19	0.17346 (12)	0.6111 (2)	0.41623 (10)	0.0212 (4)
H19	0.150243	0.543058	0.368988	0.025*
C20	0.27838 (12)	0.6342 (2)	0.44505 (9)	0.0213 (4)
H20	0.327052	0.583954	0.416726	0.026*
C21	−0.07850 (12)	0.7274 (2)	0.46183 (11)	0.0232 (4)
H21A	−0.071613	0.849674	0.462343	0.028*
H21B	−0.069898	0.688132	0.519880	0.028*
C22	−0.18352 (12)	0.6770 (2)	0.41299 (10)	0.0250 (4)
H22A	−0.189758	0.711703	0.355052	0.038*

H22B	−0.238460	0.730179	0.436621	0.038*
H22C	−0.190857	0.556242	0.415420	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0319 (7)	0.0175 (6)	0.0236 (6)	0.0029 (5)	0.0153 (5)	−0.0003 (5)
O2	0.0178 (6)	0.0292 (7)	0.0237 (6)	0.0011 (5)	0.0058 (5)	−0.0046 (5)
N1	0.0174 (7)	0.0182 (7)	0.0183 (6)	0.0001 (5)	0.0057 (5)	0.0024 (5)
C1	0.0205 (8)	0.0118 (7)	0.0174 (7)	0.0008 (6)	0.0086 (6)	−0.0011 (6)
C2	0.0179 (8)	0.0110 (7)	0.0177 (7)	0.0005 (6)	0.0072 (6)	−0.0023 (6)
C3	0.0223 (8)	0.0173 (8)	0.0178 (7)	0.0014 (6)	0.0073 (6)	0.0013 (6)
C4	0.0226 (8)	0.0185 (8)	0.0244 (8)	−0.0015 (7)	0.0109 (7)	0.0000 (7)
C5	0.0188 (8)	0.0201 (8)	0.0273 (9)	−0.0017 (7)	0.0052 (7)	−0.0045 (7)
C6	0.0229 (9)	0.0219 (9)	0.0201 (8)	−0.0017 (7)	0.0011 (7)	0.0012 (7)
C7	0.0258 (9)	0.0189 (8)	0.0191 (8)	−0.0042 (7)	0.0079 (7)	0.0007 (6)
C8	0.0173 (8)	0.0167 (8)	0.0158 (7)	−0.0006 (6)	0.0049 (6)	0.0003 (6)
C9	0.0138 (7)	0.0142 (7)	0.0169 (7)	−0.0012 (6)	0.0029 (6)	0.0008 (6)
C10	0.0235 (8)	0.0184 (8)	0.0183 (8)	−0.0014 (7)	0.0081 (6)	−0.0015 (6)
C11	0.0289 (9)	0.0210 (9)	0.0210 (8)	−0.0048 (7)	0.0078 (7)	0.0033 (7)
C12	0.0283 (9)	0.0135 (8)	0.0261 (8)	−0.0011 (7)	0.0037 (7)	0.0008 (7)
C13	0.0207 (8)	0.0172 (8)	0.0215 (8)	0.0017 (6)	0.0034 (6)	−0.0043 (7)
C14	0.0156 (7)	0.0185 (8)	0.0162 (7)	−0.0013 (6)	0.0046 (6)	−0.0002 (6)
C15	0.0180 (8)	0.0180 (8)	0.0178 (7)	−0.0004 (6)	0.0066 (6)	0.0054 (6)
C16	0.0233 (8)	0.0156 (8)	0.0185 (8)	−0.0015 (6)	0.0060 (6)	0.0007 (6)
C17	0.0211 (8)	0.0179 (8)	0.0217 (8)	0.0029 (6)	0.0097 (6)	0.0022 (7)
C18	0.0183 (8)	0.0199 (8)	0.0189 (8)	0.0000 (6)	0.0056 (6)	0.0042 (6)
C19	0.0233 (8)	0.0241 (9)	0.0169 (7)	−0.0003 (7)	0.0058 (6)	−0.0018 (7)
C20	0.0215 (8)	0.0259 (9)	0.0187 (8)	0.0029 (7)	0.0094 (6)	0.0010 (7)
C21	0.0213 (8)	0.0228 (9)	0.0277 (9)	0.0025 (7)	0.0103 (7)	−0.0003 (7)
C22	0.0216 (9)	0.0285 (9)	0.0262 (9)	0.0027 (7)	0.0078 (7)	0.0021 (7)

Geometric parameters (Å, º)

O1—C8	1.2162 (18)	C11—H11	0.9500
O2—C18	1.3630 (19)	C11—C12	1.385 (2)
O2—C21	1.4263 (18)	C12—H12	0.9500
N1—C1	1.2779 (19)	C12—C13	1.387 (2)
N1—C15	1.423 (2)	C13—H13	0.9500
C1—C2	1.482 (2)	C13—C14	1.384 (2)
C1—C8	1.530 (2)	C14—H14	0.9500
C2—C3	1.400 (2)	C15—C16	1.389 (2)
C2—C7	1.395 (2)	C15—C20	1.398 (2)
C3—H3	0.9500	C16—H16	0.9500
C3—C4	1.380 (2)	C16—C17	1.390 (2)
C4—H4	0.9500	C17—H17	0.9500
C4—C5	1.388 (2)	C17—C18	1.386 (2)
C5—H5	0.9500	C18—C19	1.394 (2)

C5—C6	1.381 (2)	C19—H19	0.9500
C6—H6	0.9500	C19—C20	1.372 (2)
C6—C7	1.383 (2)	C20—H20	0.9500
C7—H7	0.9500	C21—H21A	0.9900
C8—C9	1.481 (2)	C21—H21B	0.9900
C9—C10	1.398 (2)	C21—C22	1.502 (2)
C9—C14	1.392 (2)	C22—H22A	0.9800
C10—H10	0.9500	C22—H22B	0.9800
C10—C11	1.380 (2)	C22—H22C	0.9800

C18—O2—C21	117.58 (12)	C13—C12—H12	119.7
C1—N1—C15	121.28 (13)	C12—C13—H13	120.2
N1—C1—C2	119.89 (13)	C14—C13—C12	119.62 (14)
N1—C1—C8	123.46 (13)	C14—C13—H13	120.2
C2—C1—C8	116.64 (13)	C9—C14—H14	119.9
C3—C2—C1	120.48 (13)	C13—C14—C9	120.19 (14)
C7—C2—C1	120.99 (13)	C13—C14—H14	119.9
C7—C2—C3	118.53 (14)	C16—C15—N1	122.83 (14)
C2—C3—H3	119.9	C16—C15—C20	118.45 (14)
C4—C3—C2	120.29 (14)	C20—C15—N1	118.45 (14)
C4—C3—H3	119.9	C15—C16—H16	119.6
C3—C4—H4	119.8	C15—C16—C17	120.73 (15)
C3—C4—C5	120.49 (15)	C17—C16—H16	119.6
C5—C4—H4	119.8	C16—C17—H17	119.9
C4—C5—H5	120.1	C18—C17—C16	120.20 (14)
C6—C5—C4	119.73 (15)	C18—C17—H17	119.9
C6—C5—H5	120.1	O2—C18—C17	125.09 (14)
C5—C6—H6	120.0	O2—C18—C19	115.73 (14)
C5—C6—C7	120.06 (15)	C17—C18—C19	119.18 (14)
C7—C6—H6	120.0	C18—C19—H19	119.8
C2—C7—H7	119.6	C20—C19—C18	120.49 (15)
C6—C7—C2	120.85 (15)	C20—C19—H19	119.8
C6—C7—H7	119.6	C15—C20—H20	119.6
O1—C8—C1	119.36 (14)	C19—C20—C15	120.89 (15)
O1—C8—C9	122.45 (13)	C19—C20—H20	119.6
C9—C8—C1	118.16 (12)	O2—C21—H21A	110.2
C10—C9—C8	118.64 (13)	O2—C21—H21B	110.2
C14—C9—C8	121.59 (13)	O2—C21—C22	107.39 (13)
C14—C9—C10	119.73 (14)	H21A—C21—H21B	108.5
C9—C10—H10	120.1	C22—C21—H21A	110.2
C11—C10—C9	119.81 (14)	C22—C21—H21B	110.2
C11—C10—H10	120.1	C21—C22—H22A	109.5
C10—C11—H11	119.9	C21—C22—H22B	109.5
C10—C11—C12	120.12 (15)	C21—C22—H22C	109.5
C12—C11—H11	119.9	H22A—C22—H22B	109.5
C11—C12—H12	119.7	H22A—C22—H22C	109.5
C11—C12—C13	120.51 (15)	H22B—C22—H22C	109.5

O1—C8—C9—C10	−7.1 (2)	C8—C1—C2—C3	−172.28 (13)
O1—C8—C9—C14	175.02 (14)	C8—C1—C2—C7	8.5 (2)
O2—C18—C19—C20	−179.23 (14)	C8—C9—C10—C11	−176.86 (14)
N1—C1—C2—C3	8.9 (2)	C8—C9—C14—C13	176.21 (14)
N1—C1—C2—C7	−170.37 (14)	C9—C10—C11—C12	0.5 (2)
N1—C1—C8—O1	−86.83 (19)	C10—C9—C14—C13	−1.6 (2)
N1—C1—C8—C9	95.03 (18)	C10—C11—C12—C13	−1.5 (2)
N1—C15—C16—C17	175.87 (14)	C11—C12—C13—C14	0.9 (2)
N1—C15—C20—C19	−176.97 (14)	C12—C13—C14—C9	0.7 (2)
C1—N1—C15—C16	61.3 (2)	C14—C9—C10—C11	1.0 (2)
C1—N1—C15—C20	−124.78 (16)	C15—N1—C1—C2	−178.45 (13)
C1—C2—C3—C4	−178.13 (14)	C15—N1—C1—C8	2.8 (2)
C1—C2—C7—C6	176.87 (14)	C15—C16—C17—C18	0.2 (2)
C1—C8—C9—C10	170.95 (13)	C16—C15—C20—C19	−2.8 (2)
C1—C8—C9—C14	−6.9 (2)	C16—C17—C18—O2	178.41 (14)
C2—C1—C8—O1	94.38 (17)	C16—C17—C18—C19	−1.6 (2)
C2—C1—C8—C9	−83.76 (17)	C17—C18—C19—C20	0.8 (2)
C2—C3—C4—C5	0.8 (2)	C18—O2—C21—C22	178.44 (13)
C3—C2—C7—C6	−2.4 (2)	C18—C19—C20—C15	1.4 (2)
C3—C4—C5—C6	−1.6 (2)	C20—C15—C16—C17	2.0 (2)
C4—C5—C6—C7	0.4 (2)	C21—O2—C18—C17	−0.7 (2)
C5—C6—C7—C2	1.7 (2)	C21—O2—C18—C19	179.29 (14)
C7—C2—C3—C4	1.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O1	0.95	2.56	3.068 (2)	114
C12—H12···O1^{i}	0.95	2.41	3.279 (2)	151
C22—H22*A*···O1^{ii}	0.98	2.55	3.462 (2)	155

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