

2-(2-Chlorobenzoyl)-1-(3,4-dimethoxyphenyl)-3-iodoquinolin-4(1*H*)-one

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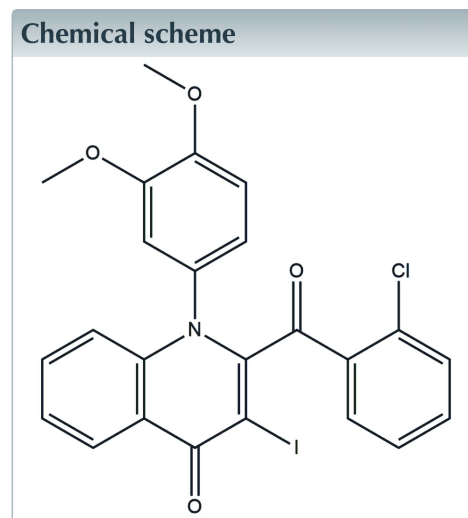
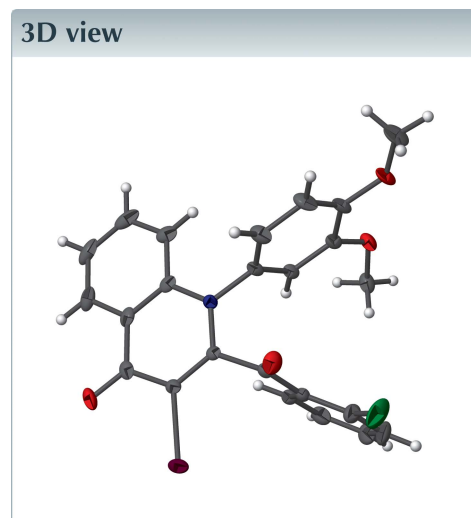
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Keywords: crystal structure; quinolinyl derivative; C—H···O hydrogen bonding; π -stacking.

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

In the title compound $C_{24}H_{17}ClINO_4$, the iodoquinolinyl moiety (r.m.s. deviation = 0.044 Å) makes dihedral angles of 87.44 (10) and 88.64 (10)° with the chloro- and methoxy-substituted benzene rings, respectively. The methoxy groups are present in synperiplanar and antiperiplanar conformations with respect to the benzene ring they are bound to, as indicated by the C—C—O—C torsion angle values of -16.2 (3) and 177.6 (2)°, respectively. The crystal structure features relatively strong methoxybenzene—C—H···O(quinolinyl) hydrogen bonds, leading to helical supramolecular chains along the *a*-axis direction. Additional C—H···O interactions along with π -stacking [inter-centroid distance = 3.6070 (16) Å between quinolinyl-NC₅ and C₆ rings] consolidate the three-dimensional molecular packing.



Structure description

Quinolones and their derivatives have contributed substantially to the evolution of antimicrobial agents. The development of antibiotic quinolone begun in 1962 with the discovery of nalidixic acid which was used to treat urinary tract infections (Leshner *et al.*, 1962). Many diversely substituted 4-quinolones have been extensively investigated as anti-tumour (Nakamura *et al.*, 2005), anti-viral (Santos *et al.*, 2009), anti-diabetic (Edmont *et al.*, 2000), anti-trypanosomal (Wube *et al.*, 2011) and anti-malarial agents (Vinayaka *et al.*, 2014). As part of our studies in this area, the title compound was synthesized to study its crystal structure.

In the title compound, Fig. 1, the mean plane of the iodoquinoline moiety makes dihedral angles of 88.64 (10) and 87.44 (10)° with benzene rings (C2–C7) and (C19–C24), respectively. The iodine and chlorine atoms are almost coplanar with the iodoquinoline

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C1—H0 <i>A</i> C···O2 ⁱ	0.96	2.53	3.357 (3)	145
C4—H4···O3 ⁱⁱ	0.93	2.37	3.185 (3)	147
C20—H9···O3 ⁱⁱ	0.93	2.55	3.263 (3)	134

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

and benzene (C19–C24) rings, with atoms I1 and Cl1 deviating from the respective mean planes by 0.109 (3) and 0.020 (1) Å, respectively. The methoxy groups are present in synperiplanar and antiperiplanar conformations with respect to the (C2–C7) ring moiety, as indicated by the torsion angle values of -16.2 (3) (C8–O2–C3–C4) and 177.6 (2)° (C1–O1–C2–C3), respectively.

The crystal structure features relatively strong methoxy-benzene-C–H···O(quinoliny) hydrogen bonds (Table 1), leading to helical supramolecular chains along the *a*-axis direction. Additional C–H···O interactions along with π -stacking [inter-centroid distance = 3.6070 (16) Å between quinolyl-NC₅ and C₆ rings for symmetry operation $-\frac{1}{2} + x, y, \frac{1}{2} - z$] consolidate the three-dimensional molecular packing.

Synthesis and crystallization

The starting compound 2-(2-chlorobenzoyl)-1-(3,4-trimethoxyphenyl)quinolin-4(1*H*)-one (0.5 g, 1 mmol) was dissolved in acetonitrile (5 ml) followed by the addition of ceric ammonium nitrate (0.11 mmol) and iodine (1.3 mmol). The mixture was stirred at 70°C under an inert atmosphere for 6 h. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to room temperature and treated with an aqueous solution of sodium thiosulfate, then extracted

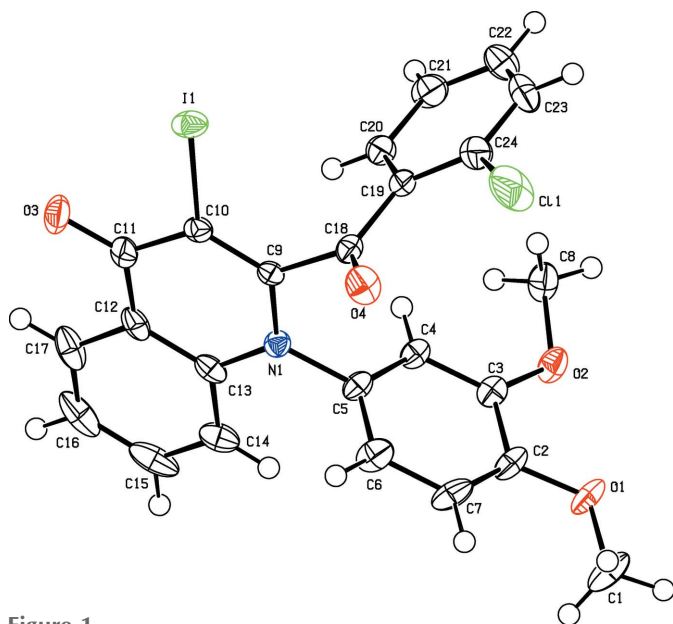


Figure 1
The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₄ H ₁₇ ClINO ₄
<i>M</i> _r	545.74
Crystal system, space group	Orthorhombic, <i>Pbca</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.7884 (19), 16.863 (3), 29.686 (6)
<i>V</i> (Å ³)	4399.4 (15)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.61
Crystal size (mm)	0.28 × 0.25 × 0.22
Data collection	
Diffractometer	Bruker APEXII CCD area-detector
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	56765, 3874, 3593
<i>R</i> _{int}	0.046
(sin θ/λ) _{max} (Å ⁻¹)	0.595
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.024, 0.060, 1.12
No. of reflections	3874
No. of parameters	282
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.59, -0.63

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

with ethyl acetate. The organic layer was dried over anhydrous sodium sulfate and the solvent was removed under reduced pressure to afford the title compound as a crude product, which was purified using silica gel column chromatography. Crystals were obtained by slow evaporation of its ethyl acetate solution.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170182 [https://doi.org/10.1107/S2414314617001821]

2-(2-Chlorobenzoyl)-1-(3,4-dimethoxyphenyl)-3-iodoquinolin-4(1*H*)-one

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2-(2-Chlorobenzoyl)-1-(3,4-dimethoxyphenyl)-3-iodoquinolin-4(1*H*)-one*Crystal data*

$C_{24}H_{17}ClINO_4$

$M_r = 545.74$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 8.7884$ (19) Å

$b = 16.863$ (3) Å

$c = 29.686$ (6) Å

$V = 4399.4$ (15) Å³

$Z = 8$

$F(000) = 2160$

$D_x = 1.648$ Mg m⁻³

Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 3874 reflections

$\theta = 2.5$ – 25.0°

$\mu = 1.61$ mm⁻¹

$T = 296$ K

Block, light-yellow

$0.28 \times 0.25 \times 0.22$ mm

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: Rotating Anode

Graphite monochromator

Detector resolution: 18.4 pixels mm⁻¹

ω and φ scans

56765 measured reflections

3874 independent reflections

3593 reflections with $I > 2\sigma(I)$

$R_{int} = 0.046$

$\theta_{max} = 25.0^\circ$, $\theta_{min} = 2.5^\circ$

$h = -10 \rightarrow 10$

$k = -20 \rightarrow 19$

$l = -35 \rightarrow 35$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.060$

$S = 1.12$

3874 reflections

282 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0219P)^2 + 6.3895P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.004$

$\Delta\rho_{max} = 0.59$ e Å⁻³

$\Delta\rho_{min} = -0.63$ e Å⁻³

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all 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 observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating $-R$ -factor-obs 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
II	-0.39094 (2)	1.04870 (1)	0.21059 (1)	0.0231 (1)
Cl1	-0.27999 (11)	1.03024 (5)	0.03373 (2)	0.0477 (3)
O1	0.1757 (2)	0.74428 (11)	0.01813 (5)	0.0259 (5)
O2	0.29338 (19)	0.86211 (10)	0.06210 (5)	0.0236 (5)
O3	-0.2765 (2)	0.94436 (11)	0.29303 (5)	0.0272 (6)
O4	-0.3203 (2)	0.91957 (11)	0.10683 (6)	0.0261 (6)
N1	-0.1004 (2)	0.84994 (11)	0.17668 (6)	0.0153 (5)
C1	0.1169 (3)	0.67708 (18)	-0.00627 (10)	0.0376 (10)
C2	0.0991 (3)	0.76620 (15)	0.05630 (8)	0.0213 (7)
C3	0.1650 (3)	0.83057 (14)	0.08001 (8)	0.0179 (7)
C4	0.0980 (3)	0.85657 (14)	0.11953 (7)	0.0169 (7)
C5	-0.0345 (3)	0.82028 (14)	0.13488 (8)	0.0180 (7)
C6	-0.1004 (3)	0.75814 (16)	0.11208 (9)	0.0253 (8)
C7	-0.0321 (3)	0.73079 (15)	0.07250 (9)	0.0269 (8)
C8	0.3381 (3)	0.93844 (16)	0.07906 (8)	0.0258 (8)
C9	-0.1894 (2)	0.91661 (13)	0.17572 (7)	0.0134 (6)
C10	-0.2502 (3)	0.94889 (13)	0.21374 (7)	0.0158 (7)
C11	-0.2200 (3)	0.91699 (14)	0.25809 (8)	0.0185 (7)
C12	-0.1132 (3)	0.84990 (15)	0.25812 (8)	0.0195 (7)
C13	-0.0577 (3)	0.81681 (14)	0.21792 (8)	0.0173 (7)
C14	0.0431 (3)	0.75209 (15)	0.21921 (9)	0.0237 (8)
C15	0.0889 (3)	0.72195 (16)	0.26027 (10)	0.0317 (9)
C16	0.0356 (3)	0.75544 (18)	0.30039 (10)	0.0332 (9)
C17	-0.0641 (3)	0.81755 (17)	0.29940 (9)	0.0273 (8)
C18	-0.2210 (3)	0.95053 (13)	0.12885 (7)	0.0168 (7)
C19	-0.1243 (3)	1.01877 (14)	0.11448 (8)	0.0181 (7)
C20	-0.0077 (3)	1.04505 (14)	0.14276 (8)	0.0203 (7)
C21	0.0893 (3)	1.10621 (16)	0.13033 (9)	0.0289 (8)
C22	0.0687 (4)	1.14313 (17)	0.08892 (10)	0.0389 (10)
C23	-0.0457 (4)	1.11858 (17)	0.06040 (9)	0.0404 (10)
C24	-0.1404 (3)	1.05705 (15)	0.07267 (9)	0.0287 (9)
H0AA	0.11530	0.63150	0.01310	0.0560*
H0AB	0.18070	0.66650	-0.03180	0.0560*
H0AC	0.01540	0.68840	-0.01630	0.0560*
H4	0.14130	0.89800	0.13570	0.0200*
H9	0.00530	1.02090	0.17070	0.0240*
H10	0.16710	1.12230	0.14950	0.0350*
H11	0.13240	1.18460	0.08040	0.0470*
H12A	0.25530	0.97510	0.07580	0.0390*

H12B	0.42450	0.95730	0.06240	0.0390*
H12C	0.36450	0.93390	0.11030	0.0390*
H17	0.07860	0.72970	0.19260	0.0280*
H18	0.15560	0.67920	0.26130	0.0380*
H19	0.06820	0.73530	0.32790	0.0400*
H20	-0.10010	0.83870	0.32630	0.0330*
H21	-0.05910	1.14360	0.03280	0.0480*
H23	-0.18900	0.73470	0.12280	0.0300*
H24	-0.07510	0.68850	0.05690	0.0320*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
II	0.0177 (1)	0.0161 (1)	0.0353 (1)	0.0008 (1)	0.0069 (1)	-0.0030 (1)
Cl1	0.0770 (6)	0.0408 (4)	0.0252 (3)	-0.0120 (4)	-0.0219 (4)	0.0116 (3)
O1	0.0287 (10)	0.0306 (10)	0.0183 (8)	0.0073 (8)	-0.0009 (7)	-0.0131 (7)
O2	0.0202 (9)	0.0291 (9)	0.0215 (8)	0.0003 (8)	0.0054 (7)	-0.0056 (7)
O3	0.0298 (11)	0.0336 (11)	0.0182 (9)	-0.0089 (8)	0.0098 (7)	-0.0048 (7)
O4	0.0249 (10)	0.0317 (10)	0.0218 (9)	-0.0061 (8)	-0.0079 (8)	0.0022 (8)
N1	0.0142 (10)	0.0157 (9)	0.0159 (9)	0.0000 (8)	0.0011 (7)	-0.0008 (8)
C1	0.0441 (18)	0.0394 (17)	0.0294 (15)	0.0029 (14)	-0.0004 (13)	-0.0220 (13)
C2	0.0197 (13)	0.0261 (13)	0.0181 (12)	0.0090 (10)	-0.0037 (10)	-0.0087 (10)
C3	0.0138 (12)	0.0216 (12)	0.0182 (11)	0.0042 (10)	-0.0027 (9)	-0.0014 (9)
C4	0.0153 (12)	0.0201 (12)	0.0152 (11)	0.0029 (9)	-0.0041 (9)	-0.0036 (9)
C5	0.0157 (12)	0.0195 (12)	0.0187 (11)	0.0039 (9)	0.0004 (9)	-0.0041 (9)
C6	0.0179 (13)	0.0262 (13)	0.0318 (14)	-0.0028 (11)	0.0021 (11)	-0.0088 (11)
C7	0.0234 (14)	0.0255 (14)	0.0318 (14)	-0.0003 (11)	-0.0036 (11)	-0.0164 (11)
C8	0.0233 (13)	0.0341 (15)	0.0201 (12)	-0.0065 (12)	0.0023 (11)	-0.0030 (11)
C9	0.0122 (11)	0.0122 (10)	0.0158 (11)	-0.0031 (9)	-0.0009 (9)	0.0002 (9)
C10	0.0136 (12)	0.0138 (11)	0.0199 (12)	-0.0024 (9)	0.0014 (9)	-0.0004 (9)
C11	0.0163 (12)	0.0208 (12)	0.0185 (12)	-0.0102 (10)	0.0030 (9)	-0.0013 (10)
C12	0.0171 (12)	0.0217 (12)	0.0198 (12)	-0.0099 (10)	-0.0010 (9)	0.0057 (10)
C13	0.0128 (11)	0.0160 (12)	0.0230 (12)	-0.0069 (10)	-0.0031 (10)	0.0044 (9)
C14	0.0179 (13)	0.0174 (12)	0.0358 (14)	-0.0045 (10)	-0.0044 (11)	0.0030 (10)
C15	0.0202 (13)	0.0206 (13)	0.0544 (19)	-0.0074 (11)	-0.0128 (12)	0.0150 (13)
C16	0.0273 (15)	0.0382 (16)	0.0342 (15)	-0.0153 (13)	-0.0141 (12)	0.0221 (13)
C17	0.0220 (14)	0.0385 (16)	0.0214 (12)	-0.0128 (12)	-0.0035 (11)	0.0110 (11)
C18	0.0172 (12)	0.0184 (12)	0.0149 (11)	0.0029 (10)	0.0005 (9)	-0.0016 (9)
C19	0.0223 (13)	0.0156 (11)	0.0163 (11)	0.0027 (10)	0.0034 (9)	-0.0007 (9)
C20	0.0197 (12)	0.0190 (12)	0.0221 (12)	0.0014 (10)	0.0037 (10)	-0.0001 (10)
C21	0.0255 (14)	0.0256 (14)	0.0355 (15)	-0.0066 (11)	0.0096 (12)	-0.0070 (12)
C22	0.0500 (19)	0.0256 (14)	0.0411 (17)	-0.0143 (14)	0.0201 (15)	0.0021 (13)
C23	0.069 (2)	0.0289 (15)	0.0234 (14)	-0.0103 (15)	0.0088 (15)	0.0075 (12)
C24	0.0431 (17)	0.0231 (14)	0.0199 (13)	-0.0010 (12)	-0.0008 (12)	0.0009 (10)

Geometric parameters (Å, °)

I1—C10	2.091 (2)	C16—C17	1.366 (4)
C11—C24	1.745 (3)	C18—C19	1.493 (3)
O1—C1	1.441 (3)	C19—C20	1.397 (4)
O1—C2	1.369 (3)	C19—C24	1.406 (4)
O2—C3	1.356 (3)	C20—C21	1.388 (4)
O2—C8	1.437 (3)	C21—C22	1.390 (4)
O3—C11	1.239 (3)	C22—C23	1.378 (5)
O4—C18	1.209 (3)	C23—C24	1.379 (4)
N1—C5	1.458 (3)	C1—H0AA	0.9600
N1—C9	1.370 (3)	C1—H0AB	0.9600
N1—C13	1.397 (3)	C1—H0AC	0.9600
C2—C3	1.417 (3)	C4—H4	0.9300
C2—C7	1.385 (4)	C6—H23	0.9300
C3—C4	1.384 (3)	C7—H24	0.9300
C4—C5	1.392 (4)	C8—H12A	0.9600
C5—C6	1.375 (4)	C8—H12B	0.9600
C6—C7	1.398 (4)	C8—H12C	0.9600
C9—C10	1.362 (3)	C14—H17	0.9300
C9—C18	1.530 (3)	C15—H18	0.9300
C10—C11	1.447 (3)	C16—H19	0.9300
C11—C12	1.470 (4)	C17—H20	0.9300
C12—C13	1.405 (3)	C20—H9	0.9300
C12—C17	1.409 (4)	C21—H10	0.9300
C13—C14	1.406 (4)	C22—H11	0.9300
C14—C15	1.381 (4)	C23—H21	0.9300
C15—C16	1.399 (4)		
C1—O1—C2	116.9 (2)	C19—C20—C21	121.8 (2)
C3—O2—C8	116.20 (18)	C20—C21—C22	119.2 (3)
C5—N1—C9	119.39 (18)	C21—C22—C23	120.3 (3)
C5—N1—C13	120.13 (19)	C22—C23—C24	120.3 (3)
C9—N1—C13	119.99 (18)	C11—C24—C19	122.4 (2)
O1—C2—C3	114.6 (2)	C11—C24—C23	116.4 (2)
O1—C2—C7	125.5 (2)	C19—C24—C23	121.2 (2)
C3—C2—C7	119.9 (2)	O1—C1—H0AA	110.00
O2—C3—C2	116.5 (2)	O1—C1—H0AB	109.00
O2—C3—C4	124.2 (2)	O1—C1—H0AC	109.00
C2—C3—C4	119.3 (2)	H0AA—C1—H0AB	109.00
C3—C4—C5	119.6 (2)	H0AA—C1—H0AC	109.00
N1—C5—C4	117.4 (2)	H0AB—C1—H0AC	110.00
N1—C5—C6	120.9 (2)	C3—C4—H4	120.00
C4—C5—C6	121.7 (2)	C5—C4—H4	120.00
C5—C6—C7	119.0 (2)	C5—C6—H23	121.00
C2—C7—C6	120.5 (2)	C7—C6—H23	120.00
N1—C9—C10	122.3 (2)	C2—C7—H24	120.00
N1—C9—C18	115.43 (18)	C6—C7—H24	120.00

C10—C9—C18	122.21 (19)	O2—C8—H12A	110.00
I1—C10—C9	121.11 (16)	O2—C8—H12B	109.00
I1—C10—C11	116.65 (16)	O2—C8—H12C	109.00
C9—C10—C11	122.2 (2)	H12A—C8—H12B	110.00
O3—C11—C10	123.4 (2)	H12A—C8—H12C	109.00
O3—C11—C12	122.8 (2)	H12B—C8—H12C	109.00
C10—C11—C12	113.8 (2)	C13—C14—H17	120.00
C11—C12—C13	121.8 (2)	C15—C14—H17	120.00
C11—C12—C17	119.6 (2)	C14—C15—H18	120.00
C13—C12—C17	118.6 (2)	C16—C15—H18	120.00
N1—C13—C12	119.5 (2)	C15—C16—H19	120.00
N1—C13—C14	120.2 (2)	C17—C16—H19	120.00
C12—C13—C14	120.3 (2)	C12—C17—H20	120.00
C13—C14—C15	119.6 (2)	C16—C17—H20	120.00
C14—C15—C16	120.4 (2)	C19—C20—H9	119.00
C15—C16—C17	120.4 (3)	C21—C20—H9	119.00
C12—C17—C16	120.8 (3)	C20—C21—H10	120.00
O4—C18—C9	117.5 (2)	C22—C21—H10	120.00
O4—C18—C19	126.1 (2)	C21—C22—H11	120.00
C9—C18—C19	116.41 (19)	C23—C22—H11	120.00
C18—C19—C20	119.4 (2)	C22—C23—H21	120.00
C18—C19—C24	123.3 (2)	C24—C23—H21	120.00
C20—C19—C24	117.3 (2)		
C1—O1—C2—C3	177.6 (2)	C10—C9—C18—C19	83.6 (3)
C1—O1—C2—C7	-2.1 (4)	I1—C10—C11—O3	2.2 (3)
C8—O2—C3—C2	164.8 (2)	I1—C10—C11—C12	-176.55 (17)
C8—O2—C3—C4	-16.2 (3)	C9—C10—C11—O3	-178.5 (2)
C9—N1—C5—C4	81.4 (3)	C9—C10—C11—C12	2.8 (3)
C9—N1—C5—C6	-99.5 (3)	O3—C11—C12—C13	176.1 (2)
C13—N1—C5—C4	-90.5 (3)	O3—C11—C12—C17	-4.1 (4)
C13—N1—C5—C6	88.6 (3)	C10—C11—C12—C13	-5.1 (4)
C5—N1—C9—C10	-177.8 (2)	C10—C11—C12—C17	174.7 (2)
C5—N1—C9—C18	4.5 (3)	C11—C12—C13—N1	2.3 (4)
C13—N1—C9—C10	-5.9 (3)	C11—C12—C13—C14	-179.3 (2)
C13—N1—C9—C18	176.4 (2)	C17—C12—C13—N1	-177.6 (2)
C5—N1—C13—C12	175.2 (2)	C17—C12—C13—C14	0.8 (4)
C5—N1—C13—C14	-3.2 (3)	C11—C12—C17—C16	-179.7 (3)
C9—N1—C13—C12	3.3 (3)	C13—C12—C17—C16	0.1 (4)
C9—N1—C13—C14	-175.1 (2)	N1—C13—C14—C15	177.5 (2)
O1—C2—C3—O2	0.3 (3)	C12—C13—C14—C15	-0.9 (4)
O1—C2—C3—C4	-178.9 (2)	C13—C14—C15—C16	0.0 (4)
C7—C2—C3—O2	180.0 (2)	C14—C15—C16—C17	1.0 (4)
C7—C2—C3—C4	0.8 (4)	C15—C16—C17—C12	-1.1 (4)
O1—C2—C7—C6	179.8 (2)	O4—C18—C19—C20	-176.2 (2)
C3—C2—C7—C6	0.1 (4)	O4—C18—C19—C24	1.4 (4)
O2—C3—C4—C5	179.7 (2)	C9—C18—C19—C20	3.2 (3)
C2—C3—C4—C5	-1.3 (4)	C9—C18—C19—C24	-179.2 (2)

C3—C4—C5—N1	180.0 (2)	C18—C19—C20—C21	177.5 (2)
C3—C4—C5—C6	0.9 (4)	C24—C19—C20—C21	-0.3 (4)
N1—C5—C6—C7	-179.0 (2)	C18—C19—C24—C11	2.0 (4)
C4—C5—C6—C7	0.1 (4)	C18—C19—C24—C23	-178.3 (3)
C5—C6—C7—C2	-0.6 (4)	C20—C19—C24—C11	179.58 (19)
N1—C9—C10—I1	-178.10 (15)	C20—C19—C24—C23	-0.7 (4)
N1—C9—C10—C11	2.6 (3)	C19—C20—C21—C22	0.9 (4)
C18—C9—C10—I1	-0.5 (3)	C20—C21—C22—C23	-0.7 (4)
C18—C9—C10—C11	-179.8 (2)	C21—C22—C23—C24	-0.2 (5)
N1—C9—C18—O4	80.7 (3)	C22—C23—C24—C11	-179.4 (2)
N1—C9—C18—C19	-98.7 (2)	C22—C23—C24—C19	0.9 (4)
C10—C9—C18—O4	-97.0 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C1—H0 <i>AC</i> \cdots O2 ⁱ	0.96	2.53	3.357 (3)	145
C4—H4 \cdots O3 ⁱⁱ	0.93	2.37	3.185 (3)	147
C20—H9 \cdots O3 ⁱⁱ	0.93	2.55	3.263 (3)	134

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