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2-Chloro-3-[(2-oxo-2*H*-chromen-6-yl)-amino]naphthalene-1,4-dione

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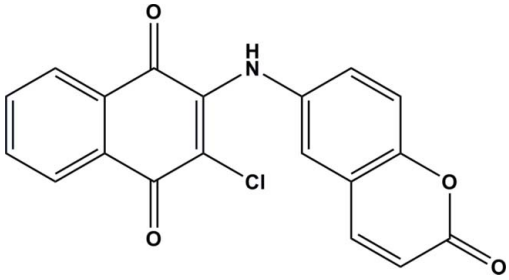
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.065; data-to-parameter ratio = 15.6.

In the title compound, $C_{19}H_{10}ClNO_4$, the dihedral angle between the naphthoquinone and coumarin rings is 48.99 (6)°. In the crystal, molecules are linked by strong N—H···O hydrogen bonds into chains with graph-set motif $C(6)$ along [101]. The packing also features π–π stacking interactions between naphthoquinone and coumarin rings [centroid-to-centroid distances = 3.7679 (12) and 3.6180 (13) Å].

Related literature

For related compounds see: Rózsa *et al.* (1989); Ito *et al.* (1993); Ishikawa *et al.* (1995); Padwal *et al.* (2011). For reference structural data, see: Ibis & Deniz (2012); Resende & Gomez (2012). For graph-set notation of hydrogen bonds, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{19}H_{10}ClNO_4$
M_r = 351.73
Monoclinic, Cc
a = 10.9371 (5) Å
b = 10.4462 (5) Å
c = 13.5104 (7) Å
β = 108.533 (5)°
V = 1463.53 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 150 K
0.23 × 0.13 × 0.07 mm

Data collection

Oxford Xcalibur Gemini Ultra diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.947, T_{max} = 1
15281 measured reflections
3527 independent reflections
2714 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.065
S = 0.91
3527 reflections
226 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1217 Friedel pairs
Absolute structure parameter: −0.07 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.21	3.015 (2)	157

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

This work was supported by the Brazilian agencies Proppi–UFF, FAPERJ, Scholarship Postgraduate Students Agreement Program – PEC-PG, CAPES/CNPq – Brazil and CAPES. The authors thank the X-ray diffraction laboratory LabCri-UFMG for the data collection, Professor Jackson A. L. C. Resende (IQ-UFF), and Professor M. D. Vargas (IQ-UFF) for her help and encouragement.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2446).

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supplementary materials

Acta Cryst. (2013). E**69**, o1317 [doi:10.1107/S1600536813019922]

2-Chloro-3-[(2-oxo-2*H*-chromen-6-yl)amino]naphthalene-1,4-dione

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Comment

There are very few examples in the literature of coumarin–naphthoquinone conjugates, most of them (direct C—C bond) are from natural sources (Rózsa *et al.*, 1989; Ito *et al.*, 1993; Ishikawa *et al.*, 1995; Padwal *et al.*, 2011) and only one synthetic, the coumarin–naphthoquinone hybrid linked through sulfur spacer attached at 7-position of the coumarin ring and 2-position of the naphthoquinone [2-(7-sulphanyl-4-methyl-coumarinyl)-3-(1-ethoxy)-1,4-naphthoquinone; Ibis & Deniz, 2012]. The title compound (I) is the product of the reaction of 2,3-dicloro-1,4-naphtoquionone with 6-amino-coumarin. The average C—C, C—O, C═O and C—N bond distances are in agreement with those observed in *tert*-butyl *N*-{3-[(3-chloro-1,4-dioxo-1,4-dihydronaphthalen2-yl)amino]propyl}carbamate (Resende & Gomez, 2012). The angle between the naphthoquinone and coumarin planes is 48.99 (6)°. The molecular structure is stabilized by one intramolecular N—H···O hydrogen bond. In the crystal, molecules are linked by strong N—H···O hydrogen bonds into chains with graph-set notation *C*(6) along [101] (Bernstein *et al.*, 1995). The packing also features π–π stacking interactions between naphthoquinone and coumarin rings [centroid–centroid distances = 3.7679 (12) and 3.6180 (13) Å]. The dihedral angle between naphthoquinone and coumarin rings is 48.99 (6)°.

Experimental

2,3-Dichloro-1,4-naphthoquinone (681 mg, 3 mmol) was added to a solution of 6-aminocoumarin (579.6 mg, 3.6 mmol) in DMF (10 ml). The mixture was stirred at 60–70°C for 72 h. The solvent was evaporated under reduced pressure and the crude product was purified through recrystallization in hexane, resulting in a red solid. Yield: 833.8 mg, 79%. Single crystals suitable for a study of X-ray diffraction of compound (I) were obtained at 4°C by slow evaporation of an aceto-nitrile–dichloromethane (1:1) solution. m.p. 301°C. Found: C, 64.12; H, 2.91; N, 4.14. Calc. for $C_{19}H_{10}ClNO_4$: C, 64.51; H, 3.42; N, 3.96%. 1H NMR (300 MHz, d6-DMSO): δ 8.16 (d, J = 7.5 Hz, 2H), 8.13 (d, J = 9.6 Hz, 1H), 8.00 (t, J = 7.5 Hz, 1H), 7.94 (t, J = 7.5 Hz, 1H), 7.58–7.52 (m, 2H), 7.48 (d, J = 8.7 Hz, 1H), 6.62 (d, J = 9.6 Hz, 1H). 13 C NMR - APT (d6-DMSO, 75 MHz): δ 180.0, 176.8, 160.0, 150.4, 144.0, 143.3, 135.5, 134.8, 133.4, 131.9, 130.3, 128.0, 126.7, 126.2, 122.7, 118.2, 116.7, 116.0, 114.7. IR (KBr): νC═O (quin.) = 1672, νC═O (ester) = 1720, νC—O (ester) = 1568, 1290, νN—H = 3294, νC—H (arom.) = 3080. UV–Vis [CH_3CN; λ/nm (log ε)]: 277 (4.10), 333 (3.28), 469 (3.10).

Refinement

All C-bound H atoms were placed in calculated idealized positions. The N-bound H atom was placed in the calculated idealized position. All H atoms were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2Ueq using a riding model.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine

structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

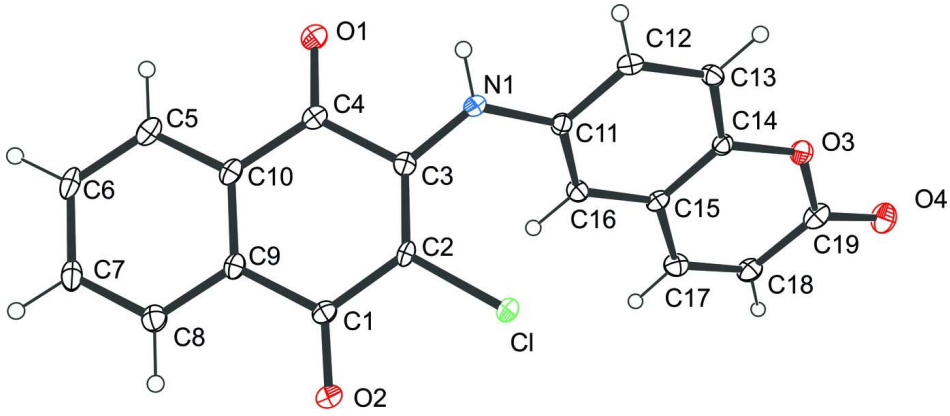

Figure 1

ORTEP representation (Farrugia, 2012) of the molecular structure of compound (I) with the numbering and displacement ellipsoids (at 30% probability level).

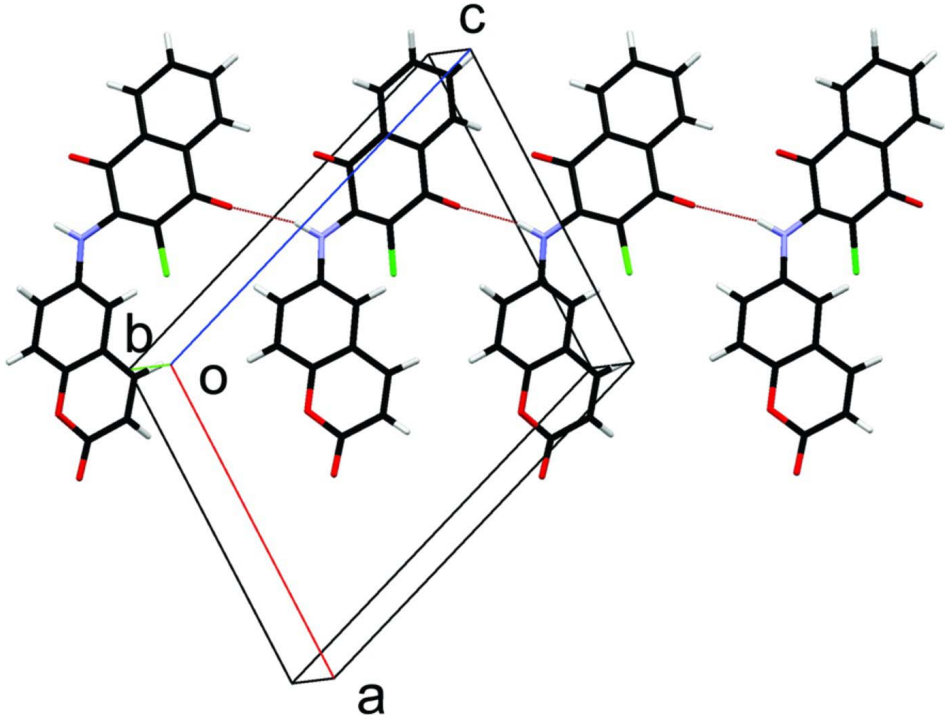

Figure 2

Packing diagram of (I), showing the formation of the *C*(6) chain along [101]. Hydrogen-bonds are shown by dashed lines.

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Crystal data

$C_{19}H_{10}ClNO_4$	a = 10.9371 (5) Å
M_r = 351.73	b = 10.4462 (5) Å
Monoclinic, *Cc*	c = 13.5104 (7) Å
Hall symbol: C -2yc	β = 108.533 (5)°

V = 1463.53 (12) Å^3
Z = 4
F(000) = 720
D_x = 1.596 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5237 reflections

θ = 2.0–29.5°
μ = 0.29 mm^{-1}
T = 150 K
Prism, violet
0.23 × 0.13 × 0.07 mm

Data collection

Oxford Xcalibur Gemini Ultra diffractometer with Atlas detector
Graphite monochromator
Detector resolution: 10.4186 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.947, T_{max} = 1

15281 measured reflections
3527 independent reflections
2714 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 28.5°, θ_{min} = 2.8°
h = −14→14
k = −13→13
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.065
S = 0.91
3527 reflections
226 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.029P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack (1983), 1217 Friedel pairs
Flack parameter: −0.07 (5)

Special details

Experimental. CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.33.55 (release 05-01-2010 CrysAlis171 .NET) (compiled Jan 5 2010,16:28:46) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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 $F^2 > \sigma(F^2)$ 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}
Cl	0.31971 (5)	0.30204 (5)	0.61162 (4)	0.02411 (12)
O4	0.57743 (16)	−0.02583 (15)	0.22630 (13)	0.0366 (4)
O3	0.39509 (13)	0.03816 (14)	0.24617 (11)	0.0246 (4)
O1	−0.11020 (14)	0.09274 (14)	0.55900 (12)	0.0292 (4)
O2	0.31861 (14)	0.29316 (15)	0.82346 (11)	0.0279 (4)
N1	0.07529 (16)	0.14446 (17)	0.48249 (13)	0.0208 (4)
H1	−0.0048	0.1431	0.4453	0.025*

C2	0.20172 (19)	0.23128 (19)	0.65296 (15)	0.0182 (5)
C3	0.09915 (19)	0.17092 (18)	0.58553 (15)	0.0179 (5)
C14	0.3192 (2)	0.0628 (2)	0.30908 (16)	0.0197 (5)
C9	0.11248 (18)	0.2050 (2)	0.80240 (15)	0.0182 (4)
C1	0.2201 (2)	0.2472 (2)	0.76414 (17)	0.0187 (4)
C11	0.16331 (19)	0.11893 (19)	0.42803 (15)	0.0183 (4)
C10	−0.00065 (19)	0.1522 (2)	0.73331 (16)	0.0192 (5)
C13	0.2008 (2)	0.1182 (2)	0.26179 (16)	0.0214 (5)
H13	0.173	0.1363	0.1891	0.026*
C4	−0.0132 (2)	0.13481 (18)	0.62218 (16)	0.0191 (5)
C12	0.1236 (2)	0.14658 (19)	0.32122 (16)	0.0211 (5)
H12	0.042	0.1856	0.2895	0.025*
C15	0.36188 (19)	0.03463 (19)	0.41469 (17)	0.0195 (5)
C16	0.28168 (19)	0.06194 (19)	0.47438 (16)	0.0202 (5)
H16	0.3085	0.0414	0.5466	0.024*
C19	0.5182 (2)	−0.0122 (2)	0.28635 (19)	0.0269 (5)
C18	0.5609 (2)	−0.0425 (2)	0.39665 (18)	0.0258 (5)
H18	0.6438	−0.0795	0.4265	0.031*
C8	0.1236 (2)	0.2211 (2)	0.90669 (17)	0.0240 (5)
H8	0.1993	0.258	0.9536	0.029*
C5	−0.1001 (2)	0.1138 (2)	0.76989 (17)	0.0243 (5)
H5	−0.1765	0.0775	0.7235	0.029*
C6	−0.0869 (2)	0.1289 (2)	0.87452 (18)	0.0265 (5)
H6	−0.1543	0.1017	0.9	0.032*
C7	0.0230 (2)	0.1829 (2)	0.94223 (17)	0.0264 (5)
H7	0.0301	0.1942	1.0136	0.032*
C17	0.4889 (2)	−0.0209 (2)	0.45813 (18)	0.0249 (5)
H17	0.5209	−0.0419	0.5302	0.03*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0214 (2)	0.0303 (3)	0.0225 (2)	−0.0092 (3)	0.0095 (2)	−0.0010 (3)
O4	0.0313 (10)	0.0461 (11)	0.0399 (10)	0.0050 (8)	0.0221 (8)	−0.0034 (8)
O3	0.0222 (8)	0.0287 (9)	0.0246 (9)	0.0013 (7)	0.0101 (7)	−0.0018 (6)
O1	0.0234 (9)	0.0360 (10)	0.0286 (9)	−0.0082 (7)	0.0091 (7)	−0.0020 (7)
O2	0.0187 (8)	0.0391 (10)	0.0252 (8)	−0.0062 (7)	0.0060 (7)	−0.0032 (7)
N1	0.0147 (9)	0.0263 (10)	0.0214 (10)	−0.0009 (7)	0.0055 (8)	−0.0011 (7)
C2	0.0175 (11)	0.0185 (12)	0.0225 (12)	−0.0010 (8)	0.0120 (9)	0.0029 (8)
C3	0.0188 (11)	0.0156 (11)	0.0196 (11)	0.0036 (9)	0.0065 (9)	0.0045 (8)
C14	0.0191 (11)	0.0205 (11)	0.0206 (11)	−0.0041 (9)	0.0079 (9)	−0.0025 (9)
C9	0.0186 (11)	0.0159 (10)	0.0226 (11)	0.0040 (9)	0.0099 (9)	0.0033 (9)
C1	0.0152 (10)	0.0172 (11)	0.0231 (11)	0.0033 (8)	0.0053 (9)	0.0011 (8)
C11	0.0190 (10)	0.0176 (11)	0.0199 (11)	−0.0042 (9)	0.0085 (9)	−0.0047 (9)
C10	0.0170 (11)	0.0149 (11)	0.0279 (12)	0.0057 (8)	0.0103 (9)	0.0041 (9)
C13	0.0230 (11)	0.0235 (12)	0.0165 (11)	−0.0028 (9)	0.0045 (9)	−0.0022 (9)
C4	0.0177 (11)	0.0140 (11)	0.0253 (12)	0.0014 (9)	0.0066 (10)	0.0015 (9)
C12	0.0166 (10)	0.0204 (12)	0.0235 (12)	−0.0001 (9)	0.0027 (9)	−0.0007 (9)
C15	0.0160 (11)	0.0161 (11)	0.0261 (12)	−0.0014 (8)	0.0065 (9)	−0.0005 (8)
C16	0.0210 (11)	0.0207 (12)	0.0186 (11)	0.0007 (9)	0.0060 (9)	−0.0004 (8)

C19	0.0231 (12)	0.0208 (12)	0.0390 (14)	0.0007 (10)	0.0127 (11)	−0.0014 (10)
C18	0.0183 (12)	0.0252 (13)	0.0328 (13)	0.0053 (9)	0.0067 (10)	0.0037 (10)
C8	0.0224 (12)	0.0268 (13)	0.0231 (12)	0.0055 (9)	0.0076 (10)	0.0029 (9)
C5	0.0201 (11)	0.0201 (12)	0.0360 (14)	0.0017 (9)	0.0135 (10)	0.0020 (10)
C6	0.0232 (12)	0.0298 (14)	0.0338 (14)	0.0067 (10)	0.0194 (11)	0.0070 (10)
C7	0.0270 (12)	0.0339 (15)	0.0230 (12)	0.0098 (11)	0.0146 (10)	0.0059 (10)
C17	0.0245 (13)	0.0222 (12)	0.0262 (12)	0.0014 (10)	0.0054 (11)	0.0028 (10)

Geometric parameters (Å, º)

Cl—C2	1.7268 (19)	C10—C5	1.389 (3)
O4—C19	1.197 (2)	C10—C4	1.475 (3)
O3—C19	1.385 (3)	C13—C12	1.370 (3)
O3—C14	1.387 (2)	C13—H13	0.95
O1—C4	1.213 (2)	C12—H12	0.95
O2—C1	1.219 (3)	C15—C16	1.397 (3)
N1—C3	1.361 (2)	C15—C17	1.446 (3)
N1—C11	1.411 (2)	C16—H16	0.95
N1—H1	0.86	C19—C18	1.448 (3)
C2—C3	1.355 (3)	C18—C17	1.333 (3)
C2—C1	1.460 (3)	C18—H18	0.95
C3—C4	1.511 (3)	C8—C7	1.391 (3)
C14—C13	1.376 (3)	C8—H8	0.95
C14—C15	1.385 (3)	C5—C6	1.384 (3)
C9—C8	1.386 (3)	C5—H5	0.95
C9—C10	1.404 (3)	C6—C7	1.379 (3)
C9—C1	1.494 (3)	C6—H6	0.95
C11—C16	1.381 (3)	C7—H7	0.95
C11—C12	1.399 (3)	C17—H17	0.95
C19—O3—C14	121.75 (17)	C13—C12—C11	120.85 (19)
C3—N1—C11	129.15 (18)	C13—C12—H12	119.6
C3—N1—H1	115.4	C11—C12—H12	119.6
C11—N1—H1	115.4	C14—C15—C16	118.94 (18)
C3—C2—C1	123.94 (18)	C14—C15—C17	117.96 (18)
C3—C2—Cl	121.72 (15)	C16—C15—C17	123.1 (2)
C1—C2—Cl	114.29 (15)	C11—C16—C15	119.77 (19)
C2—C3—N1	129.12 (18)	C11—C16—H16	120.1
C2—C3—C4	118.78 (17)	C15—C16—H16	120.1
N1—C3—C4	111.90 (17)	O4—C19—O3	116.6 (2)
C13—C14—C15	121.78 (18)	O4—C19—C18	127.2 (2)
C13—C14—O3	116.84 (18)	O3—C19—C18	116.22 (18)
C15—C14—O3	121.37 (18)	C17—C18—C19	122.9 (2)
C8—C9—C10	119.83 (18)	C17—C18—H18	118.6
C8—C9—C1	119.46 (18)	C19—C18—H18	118.6
C10—C9—C1	120.69 (17)	C9—C8—C7	119.5 (2)
O2—C1—C2	121.67 (19)	C9—C8—H8	120.2
O2—C1—C9	121.19 (19)	C7—C8—H8	120.2
C2—C1—C9	117.14 (18)	C6—C5—C10	119.4 (2)
C16—C11—C12	119.73 (18)	C6—C5—H5	120.3

C16—C11—N1	122.81 (18)	C10—C5—H5	120.3
C12—C11—N1	117.36 (18)	C7—C6—C5	120.7 (2)
C5—C10—C9	120.07 (19)	C7—C6—H6	119.7
C5—C10—C4	119.79 (19)	C5—C6—H6	119.7
C9—C10—C4	120.13 (18)	C6—C7—C8	120.4 (2)
C12—C13—C14	118.92 (19)	C6—C7—H7	119.8
C12—C13—H13	120.5	C8—C7—H7	119.8
C14—C13—H13	120.5	C18—C17—C15	119.8 (2)
O1—C4—C10	122.55 (18)	C18—C17—H17	120.1
O1—C4—C3	118.71 (18)	C15—C17—H17	120.1
C10—C4—C3	118.74 (18)		

C1—C2—C3—N1	−176.13 (19)	N1—C3—C4—O1	−2.7 (3)
Cl—C2—C3—N1	6.5 (3)	C2—C3—C4—C10	−7.3 (3)
C1—C2—C3—C4	9.5 (3)	N1—C3—C4—C10	177.40 (17)
Cl—C2—C3—C4	−167.80 (14)	C14—C13—C12—C11	−0.6 (3)
C11—N1—C3—C2	30.9 (3)	C16—C11—C12—C13	−0.2 (3)
C11—N1—C3—C4	−154.41 (19)	N1—C11—C12—C13	−176.49 (18)
C19—O3—C14—C13	177.18 (19)	C13—C14—C15—C16	0.7 (3)
C19—O3—C14—C15	−1.9 (3)	O3—C14—C15—C16	179.77 (18)
C3—C2—C1—O2	174.1 (2)	C13—C14—C15—C17	−178.7 (2)
Cl—C2—C1—O2	−8.4 (3)	O3—C14—C15—C17	0.4 (3)
C3—C2—C1—C9	−6.0 (3)	C12—C11—C16—C15	1.2 (3)
Cl—C2—C1—C9	171.51 (14)	N1—C11—C16—C15	177.35 (18)
C8—C9—C1—O2	1.6 (3)	C14—C15—C16—C11	−1.5 (3)
C10—C9—C1—O2	179.98 (19)	C17—C15—C16—C11	177.8 (2)
C8—C9—C1—C2	−178.30 (18)	C14—O3—C19—O4	−177.49 (19)
C10—C9—C1—C2	0.1 (3)	C14—O3—C19—C18	2.5 (3)
C3—N1—C11—C16	29.8 (3)	O4—C19—C18—C17	178.2 (2)
C3—N1—C11—C12	−154.0 (2)	O3—C19—C18—C17	−1.8 (3)
C8—C9—C10—C5	−1.4 (3)	C10—C9—C8—C7	1.0 (3)
C1—C9—C10—C5	−179.75 (18)	C1—C9—C8—C7	179.39 (19)
C8—C9—C10—C4	179.97 (18)	C9—C10—C5—C6	0.5 (3)
C1—C9—C10—C4	1.6 (3)	C4—C10—C5—C6	179.15 (19)
C15—C14—C13—C12	0.4 (3)	C10—C5—C6—C7	0.8 (3)
O3—C14—C13—C12	−178.74 (18)	C5—C6—C7—C8	−1.2 (3)
C5—C10—C4—O1	3.3 (3)	C9—C8—C7—C6	0.3 (3)
C9—C10—C4—O1	−178.1 (2)	C19—C18—C17—C15	0.4 (3)
C5—C10—C4—C3	−176.81 (17)	C14—C15—C17—C18	0.4 (3)
C9—C10—C4—C3	1.9 (3)	C16—C15—C17—C18	−179.0 (2)
C2—C3—C4—O1	172.59 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.21	3.015 (2)	157

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