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Crystal structure of 2-amino-7-hydroxy-4-(4-hydroxyphenyl)-4*H*-chromene-3-carbonitrile

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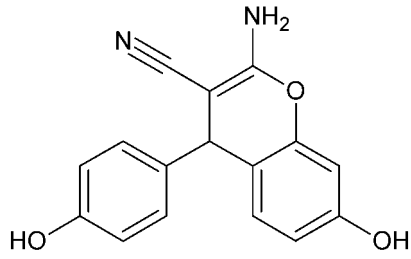
In the title compound, $C_{16}H_{12}N_2O_3$, the chromene ring system is nearly planar [maximum deviation from the mean plane = 0.057 (1) Å], and is almost perpendicular to the benzene ring, with a dihedral angle of 85.29 (5)°. In the crystal, molecules are linked by classical N—H···O, O—H···O and O—H···N hydrogen bonds, and weak C—H···O hydrogen bonds, forming a three-dimensional supramolecular network. Furthermore, a weak π–π stacking interaction is observed; the centroid-to-centroid distance is 3.7260 (7) Å.

Keywords: crystal structure; chromene; hydrogen bonding,.

CCDC reference: 1410244

1. Related literature

For the synthesis and biological activity of molecules having the 2-amino-7-hydroxy-4-(4-hydroxyphenyl)-4*H*-chromene unit, see: Mohr *et al.* (1975); Bianchi & Tava (1987); Khafagy *et al.* (2002); Hiramoto *et al.* (1997); Skommer *et al.* (2006); Gourdeau *et al.* (2004); Anderson *et al.* (2005); Wang *et al.* (2000).



2. Experimental

2.1. Crystal data

$C_{16}H_{12}N_2O_3$
M_r = 280.28
Monoclinic, $C2/c$
a = 18.3084 (13) Å
b = 6.0743 (4) Å
c = 24.5339 (17) Å
β = 106.471 (2)°
V = 2616.5 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 K
0.25 × 0.10 × 0.03 mm

2.2. Data collection

Rigaku AFC12 (Right) diffractometer
Absorption correction: multi-scan (*CrystalClear-SM*; Rigaku, 2012)
T_{min} = 0.830, T_{max} = 1.000
13649 measured reflections
2986 independent reflections
2540 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.091
S = 1.06
2986 reflections
206 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O2^{i}	0.88 (1)	2.16 (1)	3.0316 (14)	169 (2)
N1—H2*N*···O2^{ii}	0.90 (2)	2.51 (2)	3.2052 (15)	135 (1)
O2—H2*O*···O3^{iii}	0.89 (2)	1.81 (2)	2.6875 (13)	168 (2)
O3—H3*O*···N2^{iv}	0.87 (1)	1.89 (1)	2.7550 (14)	174 (2)
C8—H8···O1^{i}	0.95	2.47	3.4011 (14)	165

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

Data collection: *CrystalClear-SM* (Rigaku, 2012); cell refinement: *CrystalClear-SM*; data reduction: *CrystalClear-SM*; 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); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5857).

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supporting information

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S1. Comment

Heterocycles containing the chromene moiety show interesting biological activities such as antitumor (Mohr *et al.*, 1975), sex pheromone (Bianchi & Tava, 1987), antimicrobial (Khafagy *et al.*, 2002), and mutagenicity (Hiramoto *et al.*, 1997). Interestingly, 2-amino-4*H*-chromene derivatives arises from their potential application in the treatment of human inflammatory TNFa-mediated diseases, such as psoriatic arthritis and rheumatoid and in cancer therapy (Skommer *et al.*, 2006; Gourdeau *et al.*, 2004; Anderson *et al.*, 2005; Wang *et al.*, 2000). Such facts inspired us to synthesize and determine the crystal structure of the title compound in this study.

As shown in Fig. 1, the 4*H*-chromene ring system (O1/C1–C9) of the title compound is almost planar with the puckering parameters of Q(2) = 0.0759 (12) Å and φ(2) = 155.5 (9) °. It makes a dihedral angle of 85.29 (5)° with the C11–C16 phenyl ring.

In the crystal structure, N—H···O, O—H···O, O—H···N and C—H···O hydrogen bonds link the adjacent molecules, forming the three dimensional network (Table 1, Fig. 2). In addition, a weak π-π stacking interaction [*Cg*1···*Cg*1 = 3.7260 (7) Å]; where *Cg*1 is the centroid of the O1/C1–C4/C9 ring of the 4*H*-chromene ring system (O1/C1–C9)] are observed.

S2. Experimental

A mixture of 1 mmol (180 mg) of 4-hydroxybenzylidene-malononitrile and 1 mmol (110 mg) of resorcinol was refluxed in 10 ml e thanol for 3 h in the presence of few catalytic drops of pipredine. The mixture was cooled at ambient temperature and the resulting solid was filtered off, dried under vacuum and recrytallized from ethanol to furnish white crystals in a good quality suitable for X-ray diffraction. Mp 523 K.

S3. Refinement

The H atoms of the OH and NH_2 groups were located in a difference Fourier map and were refined freely [O2—H2O = 0.893 (17) Å, O3—H3O = 0.866 (14) Å, N1—H1N = 0.881 (13) Å and N1—H2N = 0.895 (17) Å]. The H atoms attached to the C atoms were positioned geometrically, with C—H = 0.95 Å and C—H = 1.00 Å for aromatic and methine H, respectively and H atoms were constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

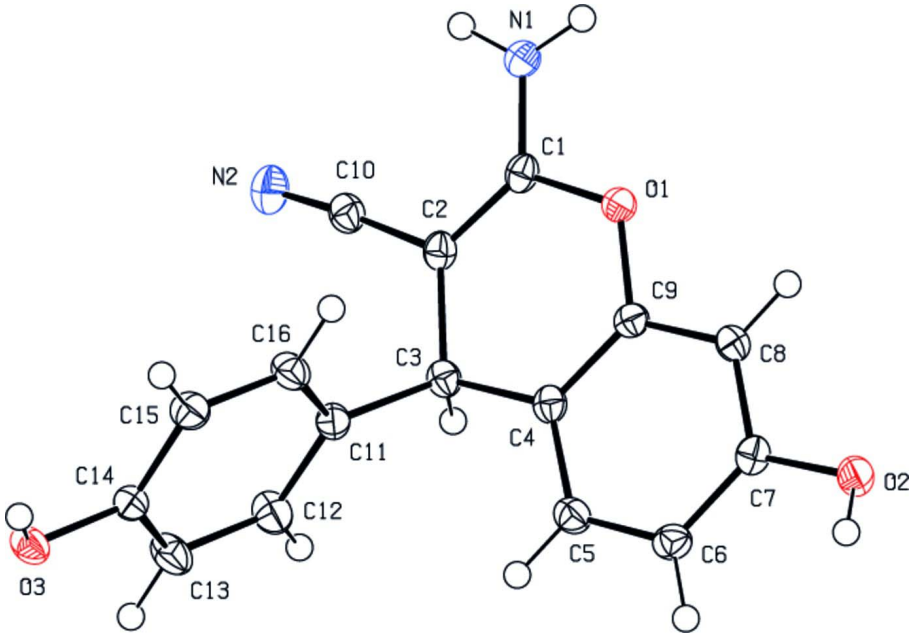

Figure 1

View of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

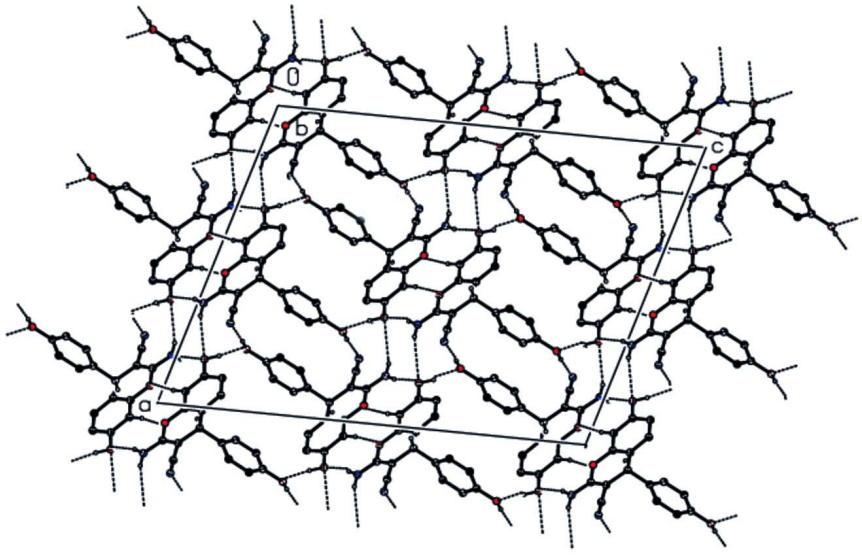

Figure 2

The packing diagram of the title compound viewed down the *b* axis.

2-Amino-7-hydroxy-4-(4-hydroxyphenyl)-4*H*-chromene-3-carbonitrile

Crystal data

$C_{16}H_{12}N_2O_3$
M_r = 280.28

Monoclinic, *C*2/*c*
Hall symbol: -C 2yc

a = 18.3084 (13) Å
b = 6.0743 (4) Å
c = 24.5339 (17) Å
β = 106.471 (2)°
V = 2616.5 (3) Å^3
Z = 8
F(000) = 1168
D_x = 1.423 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 14157 reflections
θ = 2.3–27.5°
μ = 0.10 mm^{-1}
T = 100 K
Blade, brown
0.25 × 0.10 × 0.03 mm

Data collection

Rigaku AFC12 (Right) diffractometer
Radiation source: Rotating Anode
Detector resolution: 28.5714 pixels mm^{-1}
profile data from ω–scans
Absorption correction: multi-scan (*CrystalClear-SM*; Rigaku, 2012)
T_{min} = 0.830, T_{max} = 1.000

13649 measured reflections
2986 independent reflections
2540 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −23→18
k = −7→7
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.091
S = 1.06
2986 reflections
206 parameters
4 restraints

Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2 + 1.7337P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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 e.s.d.'s 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 goodnesses 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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.05989 (4)	0.30160 (13)	0.03455 (3)	0.0187 (2)
O2	−0.15605 (5)	−0.03145 (14)	0.06613 (4)	0.0226 (3)
O3	0.20866 (5)	0.79736 (15)	0.35127 (3)	0.0213 (3)
N1	0.16338 (6)	0.41872 (18)	0.01319 (4)	0.0207 (3)
N2	0.21498 (6)	0.93998 (18)	0.09021 (5)	0.0268 (3)
C1	0.11540 (6)	0.45728 (19)	0.04464 (5)	0.0173 (3)
C2	0.11794 (6)	0.62821 (19)	0.08107 (5)	0.0178 (3)
C3	0.06229 (6)	0.66058 (19)	0.11588 (5)	0.0174 (3)
C4	0.00672 (6)	0.46994 (19)	0.10543 (5)	0.0170 (3)
C5	−0.04921 (6)	0.4552 (2)	0.13396 (5)	0.0192 (3)
C6	−0.10354 (6)	0.2906 (2)	0.12215 (5)	0.0196 (3)

C7	−0.10248 (6)	0.13336 (19)	0.08098 (5)	0.0180 (3)
C8	−0.04727 (6)	0.14161 (19)	0.05235 (5)	0.0172 (3)
C9	0.00636 (6)	0.30919 (19)	0.06543 (5)	0.0164 (3)
C10	0.17293 (7)	0.7951 (2)	0.08532 (5)	0.0200 (3)
C11	0.10251 (6)	0.69419 (19)	0.17886 (5)	0.0178 (3)
C12	0.08736 (7)	0.8801 (2)	0.20677 (5)	0.0235 (3)
C13	0.12262 (7)	0.9120 (2)	0.26446 (5)	0.0250 (3)
C14	0.17396 (6)	0.7573 (2)	0.29446 (5)	0.0182 (3)
C15	0.19056 (7)	0.5711 (2)	0.26720 (5)	0.0206 (3)
C16	0.15444 (7)	0.5408 (2)	0.20975 (5)	0.0210 (3)
H1N	0.1546 (9)	0.304 (2)	−0.0097 (6)	0.034 (4)*
H2N	0.2042 (8)	0.505 (3)	0.0173 (7)	0.034 (4)*
H2O	−0.1713 (10)	−0.071 (3)	0.0962 (7)	0.049 (5)*
H3	0.03240	0.79710	0.10170	0.0210*
H3O	0.2327 (9)	0.681 (2)	0.3673 (7)	0.040 (5)*
H5	−0.04990	0.56130	0.16230	0.0230*
H6	−0.14130	0.28470	0.14190	0.0240*
H8	−0.04620	0.03470	0.02430	0.0210*
H12	0.05240	0.98710	0.18620	0.0280*
H13	0.11150	1.03930	0.28310	0.0300*
H15	0.22620	0.46570	0.28770	0.0250*
H16	0.16540	0.41290	0.19120	0.0250*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0184 (4)	0.0189 (4)	0.0203 (4)	−0.0043 (3)	0.0080 (3)	−0.0035 (3)
O2	0.0241 (4)	0.0258 (5)	0.0199 (4)	−0.0092 (3)	0.0096 (3)	−0.0028 (3)
O3	0.0241 (4)	0.0233 (5)	0.0150 (4)	0.0059 (3)	0.0030 (3)	−0.0014 (3)
N1	0.0188 (5)	0.0219 (5)	0.0228 (5)	−0.0046 (4)	0.0081 (4)	−0.0032 (4)
N2	0.0253 (5)	0.0250 (6)	0.0279 (6)	−0.0066 (4)	0.0039 (4)	−0.0015 (4)
C1	0.0157 (5)	0.0183 (6)	0.0164 (5)	−0.0015 (4)	0.0019 (4)	0.0028 (4)
C2	0.0177 (5)	0.0186 (6)	0.0157 (5)	−0.0021 (4)	0.0026 (4)	0.0009 (4)
C3	0.0188 (5)	0.0162 (5)	0.0161 (5)	0.0007 (4)	0.0031 (4)	0.0001 (4)
C4	0.0168 (5)	0.0172 (6)	0.0153 (5)	0.0011 (4)	0.0016 (4)	0.0015 (4)
C5	0.0206 (5)	0.0203 (6)	0.0164 (5)	0.0021 (4)	0.0047 (4)	−0.0009 (4)
C6	0.0186 (5)	0.0234 (6)	0.0176 (5)	0.0013 (4)	0.0064 (4)	0.0021 (4)
C7	0.0174 (5)	0.0182 (6)	0.0173 (5)	−0.0020 (4)	0.0032 (4)	0.0024 (4)
C8	0.0192 (5)	0.0168 (5)	0.0151 (5)	0.0001 (4)	0.0040 (4)	−0.0002 (4)
C9	0.0153 (5)	0.0188 (6)	0.0149 (5)	0.0010 (4)	0.0040 (4)	0.0021 (4)
C10	0.0208 (6)	0.0212 (6)	0.0165 (5)	0.0004 (5)	0.0030 (4)	0.0000 (4)
C11	0.0176 (5)	0.0187 (6)	0.0166 (5)	−0.0017 (4)	0.0042 (4)	−0.0009 (4)
C12	0.0258 (6)	0.0205 (6)	0.0213 (6)	0.0055 (5)	0.0022 (5)	−0.0009 (5)
C13	0.0299 (6)	0.0215 (6)	0.0217 (6)	0.0065 (5)	0.0044 (5)	−0.0048 (5)
C14	0.0177 (5)	0.0213 (6)	0.0158 (5)	−0.0009 (4)	0.0052 (4)	−0.0013 (4)
C15	0.0203 (5)	0.0209 (6)	0.0194 (6)	0.0049 (4)	0.0039 (4)	0.0012 (5)
C16	0.0235 (6)	0.0191 (6)	0.0198 (6)	0.0034 (4)	0.0053 (5)	−0.0028 (4)

Geometric parameters (Å, º)

O1—C1	1.3586 (14)	C6—C7	1.3943 (17)
O1—C9	1.3992 (14)	C7—C8	1.3857 (16)
O2—C7	1.3763 (15)	C8—C9	1.3873 (16)
O3—C14	1.3796 (14)	C11—C12	1.3888 (17)
N1—C1	1.3440 (16)	C11—C16	1.3921 (17)
N2—C10	1.1529 (17)	C12—C13	1.3926 (17)
O2—H2O	0.893 (17)	C13—C14	1.3842 (17)
O3—H3O	0.866 (14)	C14—C15	1.3907 (17)
N1—H1N	0.881 (13)	C15—C16	1.3890 (17)
C1—C2	1.3622 (16)	C3—H3	1.0000
N1—H2N	0.895 (17)	C5—H5	0.9500
C2—C3	1.5164 (16)	C6—H6	0.9500
C2—C10	1.4116 (17)	C8—H8	0.9500
C3—C11	1.5252 (17)	C12—H12	0.9500
C3—C4	1.5146 (16)	C13—H13	0.9500
C4—C9	1.3831 (16)	C15—H15	0.9500
C4—C5	1.3975 (16)	C16—H16	0.9500
C5—C6	1.3819 (17)		
C1—O1—C9	118.75 (9)	C3—C11—C16	121.40 (10)
C7—O2—H2O	110.1 (12)	C12—C11—C16	118.48 (11)
C14—O3—H3O	110.1 (10)	C3—C11—C12	120.12 (10)
O1—C1—N1	110.55 (10)	C11—C12—C13	120.96 (11)
C1—N1—H1N	118.2 (11)	C12—C13—C14	119.68 (11)
C1—N1—H2N	119.6 (11)	O3—C14—C13	117.79 (11)
H1N—N1—H2N	122.1 (15)	C13—C14—C15	120.29 (11)
O1—C1—C2	122.33 (10)	O3—C14—C15	121.90 (11)
N1—C1—C2	127.11 (11)	C14—C15—C16	119.32 (11)
C3—C2—C10	116.38 (10)	C11—C16—C15	121.26 (11)
C1—C2—C3	124.40 (10)	C2—C3—H3	107.00
C1—C2—C10	119.13 (11)	C4—C3—H3	107.00
C4—C3—C11	112.46 (10)	C11—C3—H3	108.00
C2—C3—C11	112.30 (10)	C4—C5—H5	119.00
C2—C3—C4	109.38 (9)	C6—C5—H5	119.00
C3—C4—C5	121.11 (10)	C5—C6—H6	120.00
C5—C4—C9	116.96 (11)	C7—C6—H6	120.00
C3—C4—C9	121.85 (10)	C7—C8—H8	121.00
C4—C5—C6	121.83 (11)	C9—C8—H8	121.00
C5—C6—C7	119.37 (11)	C11—C12—H12	120.00
O2—C7—C8	117.36 (10)	C13—C12—H12	120.00
C6—C7—C8	120.29 (11)	C12—C13—H13	120.00
O2—C7—C6	122.33 (10)	C14—C13—H13	120.00
C7—C8—C9	118.65 (11)	C14—C15—H15	120.00
O1—C9—C4	122.98 (10)	C16—C15—H15	120.00
O1—C9—C8	114.15 (10)	C11—C16—H16	119.00
C4—C9—C8	122.88 (11)	C15—C16—H16	119.00

N2—C10—C2	175.64 (14)		
C9—O1—C1—N1	177.24 (9)	C5—C4—C9—O1	−178.77 (10)
C9—O1—C1—C2	−4.25 (16)	C5—C4—C9—C8	1.38 (18)
C1—O1—C9—C8	−179.32 (10)	C3—C4—C9—C8	−175.44 (11)
C1—O1—C9—C4	0.81 (16)	C3—C4—C5—C6	175.56 (11)
N1—C1—C2—C3	−179.28 (11)	C4—C5—C6—C7	0.50 (18)
N1—C1—C2—C10	4.29 (19)	C5—C6—C7—C8	0.26 (18)
O1—C1—C2—C10	−173.96 (10)	C5—C6—C7—O2	−178.29 (11)
O1—C1—C2—C3	2.47 (18)	O2—C7—C8—C9	178.43 (10)
C10—C2—C3—C4	178.86 (10)	C6—C7—C8—C9	−0.19 (18)
C1—C2—C3—C4	2.34 (16)	C7—C8—C9—C4	−0.67 (18)
C1—C2—C3—C11	127.93 (12)	C7—C8—C9—O1	179.46 (10)
C10—C2—C3—C11	−55.55 (14)	C3—C11—C12—C13	178.99 (11)
C2—C3—C4—C9	−5.55 (15)	C16—C11—C12—C13	−0.61 (19)
C11—C3—C4—C5	52.26 (15)	C3—C11—C16—C15	−179.53 (11)
C2—C3—C11—C12	124.45 (12)	C12—C11—C16—C15	0.07 (19)
C2—C3—C11—C16	−55.96 (15)	C11—C12—C13—C14	0.48 (19)
C11—C3—C4—C9	−131.05 (12)	C12—C13—C14—O3	178.81 (11)
C2—C3—C4—C5	177.75 (11)	C12—C13—C14—C15	0.21 (19)
C4—C3—C11—C16	67.94 (14)	O3—C14—C15—C16	−179.28 (11)
C4—C3—C11—C12	−111.66 (12)	C13—C14—C15—C16	−0.74 (19)
C9—C4—C5—C6	−1.29 (17)	C14—C15—C16—C11	0.60 (19)
C3—C4—C9—O1	4.41 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O2^{i}	0.88 (1)	2.16 (1)	3.0316 (14)	169 (2)
N1—H2*N*···O2^{ii}	0.90 (2)	2.51 (2)	3.2052 (15)	135 (1)
O2—H2*O*···O3^{iii}	0.89 (2)	1.81 (2)	2.6875 (13)	168 (2)
O3—H3*O*···N2^{iv}	0.87 (1)	1.89 (1)	2.7550 (14)	174 (2)
C8—H8···O1^{i}	0.95	2.47	3.4011 (14)	165

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