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10-Acetyl-2,3,6,7-tetrahydro-1*H*,5*H*,-11*H*-1-benzopyrano[6,7,8-*ij*]quinolizin-11-one

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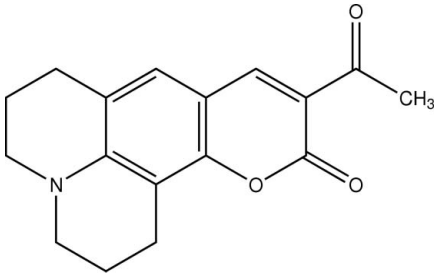
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.163; data-to-parameter ratio = 11.6.

The title compound, $C_{17}H_{17}NO_3$, crystallizes with four independent molecules (*A*, *B*, *C* and *D*) in the asymmetric unit. The independent molecules exist as pseudo-inversion-related pairs (*A*/*B* and *C*/*D*). The *A*/*B* set form sheets parallel to the *bc* plane, and the *C*/*D* set stack alternately in sheets, oblique to the *ac* plane along the *b* axis. The crystal packing is stabilized by an extensive array of C—H···O intermolecular hydrogen-bonding interactions, linking the inversion-related pairs in inversion-related stacks, as well as by π–π stacking interactions between the pyrano rings [*A*/*B* and *C*/*D*; 3.4738 (15) and 3.6424 (16) Å] and benzo rings [*A*/*A*, *B*/*B*, *C*/*C* and *D*/*D*; 3.6142 (15), 3.6152 (16), 3.6442 (16) and 3.6682 (16) Å] and between the pyrano and benzo rings [*D*/*D*; 3.9704 (16) Å] of the independent molecules. The two six-membered rings within the quinolizine group of the *A*/*B* and *C*/*D* molecules adopt envelope and half-chair conformations, respectively.

Related literature

For related structures, see: Honda *et al.* (1996*a*,*b*); Gridunova *et al.* (1992); Yip *et al.* (1996). For related background, see: Pawar & Mulwad (2004); Lin *et al.* (2006); Urano *et al.* (1995); Zhang *et al.* (2003); Aggarwal *et al.* (1996). For related literature, see: Allen (2002); Antonov & Hohla (1983); Bruno *et al.* (2004); Cremer & Pople (1975).



Experimental

Crystal data

$C_{17}H_{17}NO_3$
M_r = 283.32
Monoclinic, $C2/c$
a = 29.6874 (8) Å
b = 16.7851 (5) Å
c = 23.3089 (6) Å
β = 110.4640 (1)°
V = 10882.0 (5) Å^3
Z = 32
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 K
0.24 × 0.18 × 0.17 mm

Data collection

Bruker APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.978, T_{max} = 0.984
60969 measured reflections
9577 independent reflections
5127 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.163
S = 1.08
9577 reflections
829 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4*B*—H4*D*···O3*A*^{i}	0.99	2.57	3.410 (3)	143
C4*D*—H4*H*···O1*B*^{ii}	0.99	2.52	3.407 (3)	149
C7*C*—H7*F*···O3*A*^{iii}	0.99	2.39	3.368 (4)	170
C7*D*—H7*G*···O3*D*^{iv}	0.99	2.42	3.393 (3)	169
C12*A*—H12*A*···O1*D*^{v}	0.95	2.47	3.361 (3)	156
C12*C*—H12*C*···O1*A*^{i}	0.95	2.40	3.273 (3)	152
C12*D*—H12*D*···O1*B*^{vi}	0.95	2.44	3.302 (3)	152

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *WinGX* (Farrugia, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2474).

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supplementary materials

Acta Cryst. (2007). E**63**, o3848-o3849 [**doi:10.1107/S1600536807039621**]

10-Acetyl-2,3,6,7-tetrahydro-1*H*,5*H*,11*H*-1-benzopyrano[6,7,8-*ij*]quinolizin-11-one

J. P. Jasinski, J. M. Jasinski and D. J. Crosby

Comment

The title compound, $C_{17}H_{17}NO_3$, also known as Coumarin 521 (Exiton, Ohio, USA) and Coumarin 334 (Kodak, New York, USA) contains the benzopyrone (or coumarin) structural unit that is important in a wide range of biological activities. This nucleus is the basis of various compounds possessing anticoagulant and anti-inflammatory activities. Coumarin derivatives are known as bioactive compounds with weakly toxic, anticarcinogenic, anticoagulant and antibiotic activities. Also, Coumarin 334 posseses special applications towards improving laser dye stability under Eximer-Laser pumping in the visible and UV regions (Antonov & Hohla, 1983). Synthesis and investigation of new substituted coumarin derivatives make possible new ways for scientific and technical applications. In continuation of our work on crystal structures of organic laser dye compounds and in view of the importance of the title compound, we report here its crystal structure.

A perspective view of molecule A of the title compound is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.28, November 2006 update, January, 2007; Bruno *et al.*, 2004); MOGUL, Version 1.1; Allen, 2002).

The four independent molecules exist as pseudo inversion-related pairs (A/B and C/D). The two six-membered rings within the quinolizin group [N1—C6—C3 and N1—C7—C11] form a distorted envelope within in the A/B molecules and distorted half-chair in the C/D molecules, respectively, with Cremer & Pople (1975) puckering parameters Q, θ and φ of [A = 0.455 (3) & 0.484 (3), B = 0.448 (3) & 0.487 (3), C = 0.449 (3) & 9.480 (3), D = 0.450 (3) & 0.479 (3)] Å], [A = 56.1 (4) & 55.7 (4), B = 56.2 (4) & 56.0 (4), C = 49.8 (4), D = 129.1 (4)]° [A = 49.8 (4) & 128.9 (4), B = 124.5 (5) & 129.2 (4), C = 111.8 (5), D = 299.2 (5)]°. For an ideal envelope conformation, θ and φ are 54.7° and (60*n*)°, and for an ideal half chair conformation θ and φ are 50.8° and (60*n* + 30)°, respectively.

The A/B set of these molecules form sheets parallel to the *bc* plane and the C/D set of molecules stack alternately in sheets, oblique to the *ac* plane along the *b* axis (Fig. 2). The crystal packing is stabilized by an extensive array of C—H···O intermolecular hydrogen-bonding interactions linking the inversion-related pairs in inversion related stacks (Fig. 3) as well as by π-π stacking interactions between the pyrano rings (A/B and C/D) and benzo rings (A/A, B/B, C/C and D/D) and between the pyrano and benzo rings (D/D) of the independent molecules (Fig. 4). The distances in the stack are (*Cg* = centre of gravity): *Cg*(O2A,C1A,C15A—C13A,C2A)··· *Cg*(O2B,C1B,C15B—C13B,C2B) 3.4738 (15) Å, *Cg*(O2C,C1C,C15C—C13C,C2C)···*Cg*(O2D,C1D,C15D—C13D,C2D) 3.6424 (16) Å, *Cg*(C2A,C3A,C10A—C13A)···*Cg*(C2A,C3A,C10A—C13A) 3.6142 (15) Å, *Cg*(C2B,C3B,C10B—C13B)···*Cg*(C2B,C3B,C10B—C13B) 3.6152 (16) Å, *Cg*(C2C,C3C,C10C—C13C)···*Cg*(C2C,C3C,C10C—C13C) 3.6442 (16) Å, *Cg*(C2D,C3D,C10D—C13D)···*Cg*(C2D,C3D,C10D—C13D) 3.6682 (16) Å, *Cg*(O2D,C1D,C15D-13D,C2D)···*Cg*(C2D,C3D,C10D—C13D) 3.9704 (16) Å.

Experimental

Orange crystals of (1), $C_{17}H_{17}NO_3$, (Exciton, Ohio, USA) were grown by the slow evaporation technique from an ethanol solution.

Refinement

The H atoms were included in the riding model approximation with C—H = 0.98–0.99 Å, and with U_{iso}(H) = 0.69–2.93U_{eq}(C).

Figures

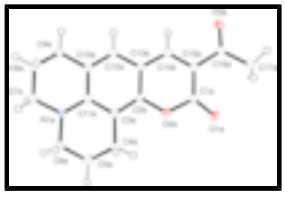


Fig. 1. Molecular structure of molecule A for $C_{17}H_{17}NO_3$, (I), showing the atom labeling and 50% probability displacement ellipsoids.

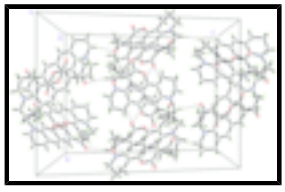


Fig. 2. Packing diagram of $C_{17}H_{17}NO_3$ viewed down the *a* axis. Dashed lines indicate C—H···O hydrogen bonds.

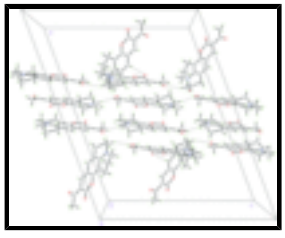


Fig. 3. Packing diagram of $C_{17}H_{17}NO_3$ viewed down the *b* axis. Dashed lines indicate C—H···O hydrogen bonds.

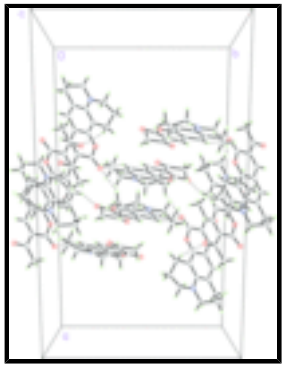


Fig. 4. Packing diagram of $C_{17}H_{17}NO_3$ viewed down the *c* axis. Dashed lines indicate C—H···O hydrogen bonds.

10-Acetyl-2,3,6,7-tetrahydro-1H,5*H*,11*H*-1-benzopyrano[6,7,8-ij]quinolizin-11-one

Crystal data

$C_{17}H_{17}NO_3$	F_{000} = 4800
M_r = 283.32	D_x = 1.383 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 6523 reflections
a = 29.6874 (8) Å	θ = 2.6–28.3º
b = 16.7851 (5) Å	μ = 0.10 mm^{-1}
c = 23.3089 (6) Å	*T* = 100 K
β = 110.4640 (1)º	Prism, colorless
V = 10882.0 (5) Å^3	0.24 × 0.18 × 0.17 mm
Z = 32	

Data collection

Bruker APEX II CCD area-detector diffractometer	9577 independent reflections
Radiation source: fine-focus sealed tube	5127 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.070
T = 100 K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	*h* = −33→35
T_{min} = 0.978, T_{max} = 0.984	*k* = −19→19
60969 measured reflections	*l* = −27→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained
$wR(F^2)$ = 0.163	$w = 1/[\sigma^2(F_o^2) + (0.0825P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max}$ = 0.001
9577 reflections	$\Delta\rho_{max}$ = 0.60 e Å^{-3}
829 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
C1A	0.86253 (9)	0.48634 (15)	−0.04969 (12)	0.0181 (6)
O1A	0.82826 (6)	0.53135 (11)	−0.06384 (9)	0.0293 (5)
O2A	0.89908 (6)	0.50559 (10)	0.00535 (8)	0.0177 (4)
C2A	0.94247 (9)	0.46585 (16)	0.02683 (12)	0.0145 (6)
C3A	0.97562 (9)	0.49217 (15)	0.08114 (11)	0.0161 (6)
C4A	0.96476 (9)	0.56010 (16)	0.11640 (12)	0.0211 (6)
H4A	0.9477	0.5397	0.1430	0.062 (11)*
H4B	0.9436	0.5990	0.0875	0.027 (8)*
C5A	1.01113 (10)	0.60111 (17)	0.15547 (14)	0.0287 (7)
H5A	1.0250	0.6303	0.1286	0.045 (11)*
H5B	1.0040	0.6402	0.1829	0.041 (9)*
C6A	1.04724 (11)	0.54078 (19)	0.19341 (14)	0.0279 (8)
H6A	1.0784	0.5678	0.2138	0.049 (10)*
H6B	1.0360	0.5197	0.2258	0.048 (11)*
N1A	1.05443 (9)	0.47440 (16)	0.15706 (11)	0.0168 (6)
C7A	1.09979 (9)	0.43148 (16)	0.18500 (13)	0.0236 (7)
H7A	1.1081	0.4307	0.2300	0.038 (9)*
H7B	1.1257	0.4603	0.1760	0.030 (8)*
C8A	1.09734 (11)	0.34637 (19)	0.16177 (14)	0.0220 (8)
H8A	1.1298	0.3221	0.1772	0.023 (7)*
H8B	1.0758	0.3144	0.1770	0.024 (8)*
C9A	1.07847 (10)	0.3464 (2)	0.09245 (14)	0.0178 (7)
H9A	1.1016	0.3740	0.0773	0.022 (7)*
H9B	1.0750	0.2908	0.0772	0.015 (7)*

C10A	1.03044 (9)	0.38793 (15)	0.06866 (12)	0.0171 (6)
C11A	1.02053 (9)	0.45266 (15)	0.10281 (12)	0.0160 (6)
C12A	0.99542 (9)	0.36300 (15)	0.01624 (12)	0.0172 (6)
H12A	1.0016	0.3188	−0.0054	0.018 (7)*
C13A	0.95006 (10)	0.40107 (17)	−0.00692 (13)	0.0155 (7)
C14A	0.91318 (9)	0.37836 (15)	−0.06029 (12)	0.0174 (6)
H14A	0.9181	0.3335	−0.0822	0.023 (7)*
C15A	0.87001 (9)	0.41787 (15)	−0.08270 (12)	0.0166 (6)
C16A	0.83342 (11)	0.39017 (19)	−0.14014 (14)	0.0161 (7)
O3A	0.84256 (7)	0.33284 (14)	−0.16681 (10)	0.0237 (6)
C17A	0.78566 (9)	0.43212 (17)	−0.16712 (13)	0.0239 (7)
H17A	0.7641	0.4002	−0.2008	0.024 (7)*
H17B	0.7905	0.4845	−0.1826	0.042 (10)*
H17C	0.7713	0.4389	−0.1355	0.043 (9)*
C1B	0.11370 (9)	0.26290 (15)	0.45055 (12)	0.0183 (6)
O1B	0.07960 (7)	0.21787 (11)	0.43609 (9)	0.0292 (5)
O2B	0.14987 (6)	0.24414 (10)	0.50562 (8)	0.0180 (4)
C2B	0.19319 (10)	0.28407 (16)	0.52708 (13)	0.0155 (6)
C3B	0.22630 (9)	0.25714 (15)	0.58141 (12)	0.0154 (6)
C4B	0.21540 (9)	0.18841 (16)	0.61643 (12)	0.0203 (6)
H4C	0.1941	0.1498	0.5873	0.031 (8)*
H4D	0.1984	0.2084	0.6432	0.030 (8)*
C5B	0.26158 (10)	0.14711 (16)	0.65505 (13)	0.0239 (7)
H5C	0.2544	0.1076	0.6822	0.024 (7)*
H5D	0.2753	0.1182	0.6279	0.023 (8)*
C6B	0.29781 (11)	0.20628 (19)	0.69328 (14)	0.0267 (8)
H6C	0.2871	0.2262	0.7264	0.035 (9)*
H6D	0.3290	0.1790	0.7127	0.033 (8)*
N1B	0.30471 (9)	0.27432 (16)	0.65762 (11)	0.0179 (6)
C7B	0.35028 (9)	0.31734 (16)	0.68639 (13)	0.0231 (6)
H7C	0.3763	0.2890	0.6774	0.024 (7)*
H7D	0.3584	0.3174	0.7314	0.041 (9)*
C8B	0.34788 (11)	0.4027 (2)	0.66400 (14)	0.0223 (8)
H8C	0.3261	0.4342	0.6792	0.029 (8)*
H8D	0.3803	0.4271	0.6799	0.029 (8)*
C9B	0.32941 (10)	0.4034 (2)	0.59472 (14)	0.0195 (8)
H9C	0.3527	0.3760	0.5798	0.014 (7)*
H9D	0.3261	0.4591	0.5798	0.037 (9)*
C10B	0.28118 (9)	0.36194 (15)	0.56986 (12)	0.0167 (6)
C11B	0.27137 (9)	0.29707 (15)	0.60385 (12)	0.0164 (6)
C12B	0.24623 (9)	0.38724 (15)	0.51737 (12)	0.0173 (6)
H12B	0.2525	0.4318	0.4961	0.019 (7)*
C13B	0.20109 (10)	0.34902 (17)	0.49384 (13)	0.0169 (7)
C14B	0.16408 (9)	0.37156 (15)	0.44012 (12)	0.0173 (6)
H14B	0.1689	0.4165	0.4181	0.019 (7)*
C15B	0.12110 (9)	0.33144 (15)	0.41786 (12)	0.0185 (6)
C16B	0.08427 (11)	0.3592 (2)	0.35943 (14)	0.0194 (8)
O3B	0.09384 (8)	0.41360 (14)	0.33067 (10)	0.0267 (6)
C17B	0.03597 (10)	0.31972 (17)	0.33530 (13)	0.0251 (7)

H17D	0.0242	0.3101	0.3691	0.029 (8)*
H17E	0.0388	0.2689	0.3162	0.027 (9)*
H17F	0.0133	0.3544	0.3049	0.044 (9)*
C1C	0.19562 (9)	0.92745 (16)	0.55231 (12)	0.0169 (6)
O1C	0.20649 (7)	0.99583 (11)	0.56698 (8)	0.0242 (5)
O2C	0.20187 (6)	0.90352 (11)	0.49804 (8)	0.0176 (4)
C2C	0.19387 (9)	0.82699 (16)	0.47556 (13)	0.0135 (6)
C3C	0.20219 (9)	0.81210 (15)	0.42181 (12)	0.0157 (6)
C4C	0.21869 (10)	0.87708 (16)	0.38877 (12)	0.0205 (6)
H4E	0.2541	0.8828	0.4070	0.021 (7)*
H4F	0.2040	0.9284	0.3936	0.029 (8)*
C5C	0.20459 (11)	0.85758 (18)	0.32132 (13)	0.0269 (7)
H5E	0.1693	0.8631	0.3013	0.031 (8)*
H5F	0.2201	0.8959	0.3018	0.045 (9)*
C6C	0.21928 (11)	0.77443 (19)	0.31194 (14)	0.0242 (7)
H6E	0.2076	0.7622	0.2676	0.020 (8)*
H6F	0.2548	0.7707	0.3275	0.032 (8)*
N1C	0.19976 (9)	0.71595 (16)	0.34359 (11)	0.0180 (6)
C7C	0.19415 (10)	0.63494 (16)	0.31891 (13)	0.0233 (6)
H7E	0.2256	0.6074	0.3340	0.030 (8)*
H7F	0.1835	0.6374	0.2737	0.023 (7)*
C8C	0.15780 (11)	0.5877 (2)	0.33744 (14)	0.0232 (8)
H8E	0.1563	0.5323	0.3224	0.028 (8)*
H8F	0.1255	0.6119	0.3190	0.028 (8)*
C9C	0.17271 (11)	0.58799 (19)	0.40678 (14)	0.0186 (8)
H9E	0.1477	0.5613	0.4189	0.022 (7)*
H9F	0.2031	0.5580	0.4249	0.017 (7)*
C10C	0.17952 (9)	0.67196 (15)	0.43084 (12)	0.0172 (6)
C11C	0.19435 (8)	0.73313 (15)	0.39824 (11)	0.0157 (6)
C12C	0.17093 (9)	0.69114 (15)	0.48301 (11)	0.0162 (6)
H12C	0.1599	0.6510	0.5036	0.027 (8)*
C13C	0.17802 (9)	0.76872 (17)	0.50708 (13)	0.0147 (6)
C14C	0.17005 (9)	0.79158 (15)	0.56072 (11)	0.0167 (6)
H14C	0.1587	0.7526	0.5819	0.016 (7)*
C15C	0.17788 (9)	0.86735 (15)	0.58401 (12)	0.0163 (6)
C16C	0.16927 (10)	0.8852 (2)	0.64185 (14)	0.0166 (7)
O3C	0.15682 (8)	0.83118 (14)	0.66819 (10)	0.0293 (6)
C17C	0.17655 (10)	0.96703 (16)	0.66879 (12)	0.0221 (6)
H17G	0.1656	0.9686	0.7039	0.019 (7)*
H17H	0.1580	1.0054	0.6378	0.028 (8)*
H17I	0.2108	0.9808	0.6823	0.031 (9)*
C1D	0.05356 (9)	0.82343 (15)	0.45000 (12)	0.0156 (6)
O1D	0.04216 (7)	0.75545 (11)	0.43507 (9)	0.0238 (5)
O2D	0.04696 (6)	0.84777 (11)	0.50384 (8)	0.0173 (4)
C2D	0.05539 (9)	0.92410 (16)	0.52645 (13)	0.0144 (6)
C3D	0.04677 (9)	0.93951 (15)	0.58010 (12)	0.0164 (6)
C4D	0.02934 (10)	0.87487 (16)	0.61212 (12)	0.0209 (6)
H4G	0.0439	0.8234	0.6075	0.019 (7)*
H4H	−0.0060	0.8697	0.5931	0.032 (8)*

C5D	0.04274 (11)	0.89429 (17)	0.67948 (13)	0.0253 (7)
H5G	0.0264	0.8566	0.6984	0.041 (9)*
H5H	0.0779	0.8878	0.7002	0.028 (8)*
C6D	0.02859 (11)	0.97813 (18)	0.68830 (14)	0.0239 (7)
H6G	−0.0069	0.9828	0.6718	0.038 (9)*
H6H	0.0396	0.9904	0.7326	0.036 (9)*
N1D	0.04937 (9)	1.03572 (16)	0.65767 (11)	0.0181 (6)
C7D	0.05565 (10)	1.11663 (16)	0.68283 (13)	0.0233 (7)
H7G	0.0657	1.1139	0.7280	0.027 (8)*
H7H	0.0246	1.1452	0.6673	0.036 (9)*
C8D	0.09298 (11)	1.1625 (2)	0.66545 (14)	0.0220 (8)
H8G	0.0950	1.2179	0.6807	0.033 (8)*
H8H	0.1249	1.1373	0.6844	0.023 (8)*
C9D	0.07894 (11)	1.16259 (19)	0.59634 (14)	0.0177 (7)
H9G	0.0491	1.1938	0.5779	0.037 (9)*
H9H	0.1046	1.1883	0.5850	0.026 (8)*
C10D	0.07115 (9)	1.07886 (15)	0.57157 (12)	0.0160 (6)
C11D	0.05522 (8)	1.01819 (15)	0.60354 (11)	0.0151 (6)
C12D	0.07993 (8)	1.05915 (15)	0.51995 (11)	0.0158 (6)
H12D	0.0915	1.0991	0.4997	0.011 (6)*
C13D	0.07251 (10)	0.98180 (17)	0.49536 (13)	0.0161 (6)
C14D	0.08076 (9)	0.95862 (15)	0.44224 (11)	0.0155 (6)
H14D	0.0928	0.9971	0.4213	0.016 (7)*
C15D	0.07227 (9)	0.88257 (15)	0.41891 (12)	0.0171 (6)
C16D	0.08162 (10)	0.8646 (2)	0.36167 (14)	0.0152 (7)
O3D	0.09468 (8)	0.91850 (13)	0.33578 (10)	0.0226 (6)
C17D	0.07449 (10)	0.78164 (15)	0.33540 (12)	0.0215 (6)
H17J	0.0893	0.7775	0.3039	0.017 (7)*
H17K	0.0400	0.7703	0.3171	0.026 (9)*
H17L	0.0896	0.7431	0.3681	0.032 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.0144 (14)	0.0181 (14)	0.0199 (15)	0.0002 (12)	0.0038 (12)	−0.0006 (12)
O1A	0.0185 (11)	0.0242 (11)	0.0366 (13)	0.0096 (9)	−0.0011 (9)	−0.0076 (9)
O2A	0.0155 (10)	0.0161 (10)	0.0192 (10)	0.0038 (8)	0.0032 (8)	−0.0017 (8)
C2A	0.0138 (15)	0.0132 (15)	0.0192 (16)	0.0017 (12)	0.0092 (13)	0.0033 (12)
C3A	0.0187 (14)	0.0136 (14)	0.0165 (14)	0.0002 (11)	0.0069 (12)	0.0011 (11)
C4A	0.0209 (15)	0.0166 (14)	0.0235 (16)	0.0009 (12)	0.0050 (13)	−0.0056 (12)
C5A	0.0318 (18)	0.0244 (17)	0.0279 (18)	0.0047 (14)	0.0079 (15)	−0.0087 (14)
C6A	0.0292 (19)	0.0250 (19)	0.0221 (17)	0.0073 (15)	−0.0003 (15)	−0.0063 (14)
N1A	0.0141 (13)	0.0197 (15)	0.0125 (14)	0.0028 (11)	−0.0006 (11)	−0.0005 (11)
C7A	0.0195 (15)	0.0270 (16)	0.0195 (16)	0.0051 (12)	0.0008 (13)	0.0013 (12)
C8A	0.0202 (17)	0.0244 (19)	0.0190 (18)	0.0070 (14)	0.0037 (14)	0.0047 (14)
C9A	0.0141 (17)	0.0166 (18)	0.0213 (18)	0.0039 (14)	0.0045 (14)	0.0024 (14)
C10A	0.0163 (14)	0.0145 (14)	0.0222 (15)	0.0034 (11)	0.0089 (12)	0.0043 (11)
C11A	0.0174 (14)	0.0150 (14)	0.0160 (15)	−0.0019 (11)	0.0063 (12)	0.0041 (11)

C12A	0.0197 (15)	0.0148 (14)	0.0176 (15)	0.0028 (11)	0.0073 (12)	0.0020 (11)
C13A	0.0170 (15)	0.0165 (17)	0.0150 (16)	0.0010 (13)	0.0080 (13)	0.0009 (13)
C14A	0.0224 (15)	0.0148 (14)	0.0179 (15)	0.0019 (11)	0.0106 (12)	0.0018 (11)
C15A	0.0171 (14)	0.0162 (14)	0.0167 (15)	−0.0003 (11)	0.0062 (12)	0.0025 (11)
C16A	0.0190 (18)	0.0153 (18)	0.0149 (17)	−0.0026 (14)	0.0068 (14)	0.0009 (14)
O3A	0.0244 (13)	0.0241 (14)	0.0191 (13)	0.0012 (11)	0.0032 (11)	−0.0056 (11)
C17A	0.0195 (15)	0.0275 (17)	0.0220 (16)	−0.0031 (13)	0.0036 (13)	−0.0007 (13)
C1B	0.0159 (14)	0.0163 (14)	0.0207 (15)	0.0019 (12)	0.0039 (12)	−0.0009 (12)
O1B	0.0207 (11)	0.0251 (11)	0.0335 (12)	−0.0078 (9)	−0.0011 (9)	0.0075 (9)
O2B	0.0141 (10)	0.0176 (10)	0.0197 (10)	−0.0037 (8)	0.0024 (8)	0.0023 (8)
C2B	0.0155 (15)	0.0123 (15)	0.0218 (17)	−0.0014 (12)	0.0103 (13)	−0.0020 (12)
C3B	0.0160 (14)	0.0142 (14)	0.0175 (15)	−0.0010 (11)	0.0079 (12)	−0.0010 (11)
C4B	0.0189 (15)	0.0178 (14)	0.0234 (16)	−0.0019 (12)	0.0065 (13)	0.0034 (12)
C5B	0.0225 (16)	0.0212 (16)	0.0256 (17)	0.0020 (13)	0.0054 (14)	0.0057 (13)
C6B	0.0258 (18)	0.0283 (19)	0.0212 (17)	−0.0045 (15)	0.0020 (14)	0.0076 (14)
N1B	0.0147 (13)	0.0188 (14)	0.0166 (14)	−0.0048 (11)	0.0009 (11)	0.0001 (11)
C7B	0.0160 (14)	0.0262 (16)	0.0232 (17)	−0.0047 (12)	0.0021 (12)	−0.0033 (13)
C8B	0.0161 (17)	0.0253 (19)	0.0235 (18)	−0.0053 (14)	0.0045 (14)	−0.0053 (15)
C9B	0.0191 (18)	0.0172 (18)	0.0249 (19)	−0.0043 (14)	0.0110 (15)	−0.0015 (14)
C10B	0.0184 (14)	0.0149 (14)	0.0182 (15)	−0.0016 (11)	0.0083 (12)	−0.0038 (11)
C11B	0.0173 (14)	0.0146 (14)	0.0189 (15)	0.0005 (11)	0.0083 (12)	−0.0032 (11)
C12B	0.0208 (15)	0.0138 (14)	0.0205 (15)	−0.0029 (11)	0.0114 (12)	−0.0003 (12)
C13B	0.0185 (15)	0.0169 (17)	0.0166 (16)	0.0019 (13)	0.0077 (13)	0.0010 (13)
C14B	0.0212 (15)	0.0131 (13)	0.0198 (15)	0.0021 (11)	0.0099 (12)	0.0015 (11)
C15B	0.0180 (14)	0.0190 (15)	0.0193 (15)	0.0005 (11)	0.0075 (12)	−0.0019 (12)
C16B	0.0206 (18)	0.022 (2)	0.0174 (18)	0.0036 (15)	0.0089 (15)	−0.0028 (15)
O3B	0.0289 (14)	0.0291 (15)	0.0217 (13)	−0.0008 (11)	0.0081 (11)	0.0092 (11)
C17B	0.0223 (16)	0.0308 (17)	0.0201 (16)	0.0029 (13)	0.0047 (13)	−0.0003 (13)
C1C	0.0148 (14)	0.0205 (15)	0.0152 (15)	−0.0003 (11)	0.0047 (11)	0.0002 (11)
O1C	0.0326 (12)	0.0152 (11)	0.0281 (11)	−0.0073 (9)	0.0148 (9)	−0.0044 (9)
O2C	0.0191 (10)	0.0159 (10)	0.0167 (10)	−0.0048 (8)	0.0050 (8)	−0.0007 (8)
C2C	0.0077 (13)	0.0127 (15)	0.0146 (16)	−0.0015 (11)	−0.0030 (11)	0.0012 (12)
C3C	0.0116 (13)	0.0169 (14)	0.0159 (14)	−0.0017 (11)	0.0012 (11)	0.0037 (11)
C4C	0.0233 (16)	0.0187 (16)	0.0202 (15)	−0.0045 (12)	0.0083 (13)	0.0009 (12)
C5C	0.0302 (18)	0.0309 (18)	0.0204 (16)	−0.0018 (14)	0.0099 (14)	0.0051 (14)
C6C	0.0235 (18)	0.0313 (19)	0.0189 (17)	−0.0038 (14)	0.0090 (14)	0.0003 (14)
N1C	0.0176 (14)	0.0194 (15)	0.0167 (15)	−0.0016 (11)	0.0057 (12)	−0.0011 (11)
C7C	0.0273 (16)	0.0219 (15)	0.0187 (16)	0.0016 (13)	0.0054 (13)	−0.0035 (12)
C8C	0.0209 (18)	0.0204 (19)	0.0229 (19)	−0.0020 (14)	0.0010 (14)	−0.0054 (14)
C9C	0.0159 (17)	0.0163 (18)	0.0216 (18)	−0.0029 (14)	0.0040 (14)	−0.0001 (14)
C10C	0.0099 (13)	0.0173 (14)	0.0209 (15)	0.0014 (11)	0.0009 (11)	0.0021 (11)
C11C	0.0087 (13)	0.0207 (14)	0.0142 (14)	0.0007 (11)	−0.0003 (11)	−0.0002 (11)
C12C	0.0116 (13)	0.0166 (14)	0.0178 (15)	−0.0003 (11)	0.0021 (12)	0.0031 (11)
C13C	0.0077 (14)	0.0165 (15)	0.0164 (15)	−0.0001 (12)	−0.0002 (12)	0.0033 (12)
C14C	0.0139 (13)	0.0195 (15)	0.0164 (15)	−0.0012 (11)	0.0050 (12)	0.0035 (11)
C15C	0.0129 (13)	0.0178 (14)	0.0165 (14)	−0.0003 (11)	0.0031 (11)	0.0033 (11)
C16C	0.0153 (17)	0.0185 (19)	0.0156 (17)	0.0003 (14)	0.0049 (14)	0.0023 (14)
O3C	0.0418 (16)	0.0254 (15)	0.0278 (15)	−0.0047 (12)	0.0210 (13)	0.0019 (11)
C17C	0.0205 (15)	0.0259 (16)	0.0203 (16)	0.0000 (12)	0.0077 (13)	−0.0023 (12)

C1D	0.0124 (13)	0.0191 (15)	0.0141 (14)	−0.0005 (11)	0.0029 (11)	0.0015 (11)
O1D	0.0320 (12)	0.0172 (11)	0.0267 (11)	−0.0076 (9)	0.0159 (9)	−0.0047 (8)
O2D	0.0195 (10)	0.0153 (10)	0.0178 (10)	−0.0030 (8)	0.0072 (8)	−0.0008 (8)
C2D	0.0089 (13)	0.0146 (15)	0.0169 (16)	−0.0005 (11)	0.0009 (12)	0.0023 (12)
C3D	0.0107 (13)	0.0189 (14)	0.0165 (15)	0.0001 (11)	0.0010 (11)	0.0020 (11)
C4D	0.0222 (16)	0.0195 (15)	0.0207 (16)	−0.0038 (12)	0.0070 (13)	0.0015 (12)
C5D	0.0312 (18)	0.0251 (17)	0.0222 (17)	0.0000 (14)	0.0123 (14)	0.0052 (13)
C6D	0.0267 (18)	0.0284 (18)	0.0180 (17)	−0.0047 (14)	0.0094 (14)	−0.0001 (13)
N1D	0.0181 (14)	0.0206 (15)	0.0147 (14)	−0.0012 (11)	0.0047 (11)	−0.0003 (11)
C7D	0.0278 (16)	0.0230 (16)	0.0173 (16)	−0.0026 (13)	0.0057 (13)	−0.0061 (12)
C8D	0.0224 (18)	0.0206 (19)	0.0201 (18)	−0.0054 (14)	0.0038 (14)	−0.0068 (14)
C9D	0.0138 (17)	0.0160 (18)	0.0212 (18)	−0.0012 (14)	0.0036 (14)	0.0006 (14)
C10D	0.0093 (13)	0.0169 (14)	0.0187 (15)	0.0010 (11)	0.0011 (11)	0.0021 (11)
C11D	0.0080 (13)	0.0205 (14)	0.0140 (14)	0.0021 (11)	0.0004 (11)	0.0019 (11)
C12D	0.0120 (13)	0.0158 (14)	0.0185 (15)	−0.0009 (11)	0.0039 (11)	0.0053 (12)
C13D	0.0104 (15)	0.0179 (16)	0.0173 (16)	0.0032 (12)	0.0017 (12)	0.0040 (12)
C14D	0.0117 (13)	0.0182 (14)	0.0147 (14)	−0.0027 (11)	0.0023 (11)	0.0034 (11)
C15D	0.0118 (13)	0.0206 (15)	0.0165 (15)	−0.0024 (11)	0.0019 (11)	0.0003 (11)
C16D	0.0092 (16)	0.0194 (19)	0.0141 (17)	0.0013 (14)	0.0005 (13)	0.0022 (14)
O3D	0.0305 (14)	0.0203 (14)	0.0207 (13)	−0.0046 (11)	0.0134 (11)	0.0004 (10)
C17D	0.0214 (16)	0.0216 (15)	0.0215 (16)	0.0005 (12)	0.0075 (13)	−0.0008 (12)

Geometric parameters (Å, °)

C1A—O1A	1.217 (3)	C1C—O1C	1.209 (3)
C1A—O2A	1.398 (3)	C1C—O2C	1.400 (3)
C1A—C15A	1.443 (4)	C1C—C15C	1.454 (3)
O2A—C2A	1.380 (3)	O2C—C2C	1.376 (3)
C2A—C3A	1.377 (4)	C2C—C3C	1.382 (4)
C2A—C13A	1.406 (4)	C2C—C13C	1.400 (4)
C3A—C11A	1.415 (3)	C3C—C11C	1.422 (4)
C3A—C4A	1.505 (3)	C3C—C4C	1.512 (3)
C4A—C5A	1.524 (4)	C4C—C5C	1.515 (4)
C4A—H4A	0.9900	C4C—H4E	0.9900
C4A—H4B	0.9900	C4C—H4F	0.9900
C5A—C6A	1.514 (4)	C5C—C6C	1.501 (4)
C5A—H5A	0.9900	C5C—H5E	0.9900
C5A—H5B	0.9900	C5C—H5F	0.9900
C6A—N1A	1.460 (4)	C6C—N1C	1.464 (4)
C6A—H6A	0.9900	C6C—H6E	0.9900
C6A—H6B	0.9900	C6C—H6F	0.9900
N1A—C11A	1.362 (3)	N1C—C11C	1.369 (3)
N1A—C7A	1.464 (3)	N1C—C7C	1.463 (4)
C7A—C8A	1.520 (4)	C7C—C8C	1.518 (4)
C7A—H7A	0.9900	C7C—H7E	0.9900
C7A—H7B	0.9900	C7C—H7F	0.9900
C8A—C9A	1.514 (4)	C8C—C9C	1.519 (4)
C8A—H8A	0.9900	C8C—H8E	0.9900
C8A—H8B	0.9900	C8C—H8F	0.9900

C9A—C10A	1.508 (4)	C9C—C10C	1.504 (4)
C9A—H9A	0.9900	C9C—H9E	0.9900
C9A—H9B	0.9900	C9C—H9F	0.9900
C10A—C12A	1.364 (4)	C10C—C12C	1.366 (4)
C10A—C11A	1.437 (3)	C10C—C11C	1.435 (4)
C12A—C13A	1.416 (4)	C12C—C13C	1.404 (4)
C12A—H12A	0.9500	C12C—H12C	0.9500
C13A—C14A	1.393 (4)	C13C—C14C	1.405 (4)
C14A—C15A	1.374 (3)	C14C—C15C	1.370 (4)
C14A—H14A	0.9500	C14C—H14C	0.9500
C15A—C16A	1.474 (4)	C15C—C16C	1.488 (4)
C16A—O3A	1.226 (4)	C16C—O3C	1.222 (4)
C16A—C17A	1.509 (4)	C16C—C17C	1.495 (4)
C17A—H17A	0.9800	C17C—H17G	0.9800
C17A—H17B	0.9800	C17C—H17H	0.9800
C17A—H17C	0.9800	C17C—H17I	0.9800
C1B—O1B	1.213 (3)	C1D—O1D	1.206 (3)
C1B—O2B	1.391 (3)	C1D—O2D	1.397 (3)
C1B—C15B	1.439 (4)	C1D—C15D	1.449 (3)
O2B—C2B	1.380 (3)	O2D—C2D	1.375 (3)
C2B—C3B	1.380 (4)	C2D—C3D	1.386 (4)
C2B—C13B	1.404 (4)	C2D—C13D	1.407 (4)
C3B—C11B	1.422 (3)	C3D—C11D	1.418 (4)
C3B—C4B	1.512 (3)	C3D—C4D	1.507 (4)
C4B—C5B	1.519 (4)	C4D—C5D	1.514 (4)
C4B—H4C	0.9900	C4D—H4G	0.9900
C4B—H4D	0.9900	C4D—H4H	0.9900
C5B—C6B	1.506 (4)	C5D—C6D	1.503 (4)
C5B—H5C	0.9900	C5D—H5G	0.9900
C5B—H5D	0.9900	C5D—H5H	0.9900
C6B—N1B	1.468 (4)	C6D—N1D	1.460 (4)
C6B—H6C	0.9900	C6D—H6G	0.9900
C6B—H6D	0.9900	C6D—H6H	0.9900
N1B—C11B	1.352 (4)	N1D—C11D	1.365 (3)
N1B—C7B	1.472 (3)	N1D—C7D	1.465 (4)
C7B—C8B	1.518 (4)	C7D—C8D	1.516 (4)
C7B—H7C	0.9900	C7D—H7G	0.9900
C7B—H7D	0.9900	C7D—H7H	0.9900
C8B—C9B	1.513 (4)	C8D—C9D	1.516 (4)
C8B—H8C	0.9900	C8D—H8G	0.9900
C8B—H8D	0.9900	C8D—H8H	0.9900
C9B—C10B	1.513 (4)	C9D—C10D	1.506 (4)
C9B—H9C	0.9900	C9D—H9G	0.9900
C9B—H9D	0.9900	C9D—H9H	0.9900
C10B—C12B	1.366 (4)	C10D—C12D	1.358 (3)
C10B—C11B	1.435 (3)	C10D—C11D	1.436 (3)
C12B—C13B	1.412 (4)	C12D—C13D	1.405 (4)
C12B—H12B	0.9500	C12D—H12D	0.9500
C13B—C14B	1.399 (4)	C13D—C14D	1.399 (4)

C14B—C15B	1.374 (4)	C14D—C15D	1.376 (4)
C14B—H14B	0.9500	C14D—H14D	0.9500
C15B—C16B	1.492 (4)	C15D—C16D	1.486 (4)
C16B—O3B	1.224 (4)	C16D—O3D	1.223 (4)
C16B—C17B	1.499 (4)	C16D—C17D	1.506 (4)
C17B—H17D	0.9800	C17D—H17J	0.9800
C17B—H17E	0.9800	C17D—H17K	0.9800
C17B—H17F	0.9800	C17D—H17L	0.9800
O1A—C1A—O2A	114.4 (2)	O1C—C1C—O2C	114.9 (2)
O1A—C1A—C15A	128.3 (2)	O1C—C1C—C15C	128.6 (2)
O2A—C1A—C15A	117.3 (2)	O2C—C1C—C15C	116.5 (2)
C2A—O2A—C1A	123.2 (2)	C2C—O2C—C1C	123.5 (2)
C3A—C2A—O2A	117.1 (2)	O2C—C2C—C3C	116.9 (2)
C3A—C2A—C13A	124.1 (3)	O2C—C2C—C13C	119.8 (2)
O2A—C2A—C13A	118.9 (2)	C3C—C2C—C13C	123.3 (3)
C2A—C3A—C11A	117.3 (2)	C2C—C3C—C11C	117.5 (2)
C2A—C3A—C4A	121.6 (2)	C2C—C3C—C4C	121.6 (2)
C11A—C3A—C4A	121.0 (2)	C11C—C3C—C4C	120.9 (2)
C3A—C4A—C5A	110.3 (2)	C3C—C4C—C5C	110.6 (2)
C3A—C4A—H4A	109.6	C3C—C4C—H4E	109.5
C5A—C4A—H4A	109.6	C5C—C4C—H4E	109.5
C3A—C4A—H4B	109.6	C3C—C4C—H4F	109.5
C5A—C4A—H4B	109.6	C5C—C4C—H4F	109.5
H4A—C4A—H4B	108.1	H4E—C4C—H4F	108.1
C6A—C5A—C4A	110.7 (2)	C6C—C5C—C4C	111.3 (2)
C6A—C5A—H5A	109.5	C6C—C5C—H5E	109.4
C4A—C5A—H5A	109.5	C4C—C5C—H5E	109.4
C6A—C5A—H5B	109.5	C6C—C5C—H5F	109.4
C4A—C5A—H5B	109.5	C4C—C5C—H5F	109.4
H5A—C5A—H5B	108.1	H5E—C5C—H5F	108.0
N1A—C6A—C5A	112.9 (2)	N1C—C6C—C5C	111.3 (2)
N1A—C6A—H6A	109.0	N1C—C6C—H6E	109.4
C5A—C6A—H6A	109.0	C5C—C6C—H6E	109.4
N1A—C6A—H6B	109.0	N1C—C6C—H6F	109.4
C5A—C6A—H6B	109.0	C5C—C6C—H6F	109.4
H6A—C6A—H6B	107.8	H6E—C6C—H6F	108.0
C11A—N1A—C6A	122.2 (2)	C11C—N1C—C7C	121.8 (2)
C11A—N1A—C7A	123.2 (2)	C11C—N1C—C6C	121.6 (3)
C6A—N1A—C7A	114.6 (2)	C7C—N1C—C6C	115.8 (2)
N1A—C7A—C8A	112.5 (2)	N1C—C7C—C8C	111.6 (2)
N1A—C7A—H7A	109.1	N1C—C7C—H7E	109.3
C8A—C7A—H7A	109.1	C8C—C7C—H7E	109.3
N1A—C7A—H7B	109.1	N1C—C7C—H7F	109.3
C8A—C7A—H7B	109.1	C8C—C7C—H7F	109.3
H7A—C7A—H7B	107.8	H7E—C7C—H7F	108.0
C9A—C8A—C7A	109.5 (3)	C7C—C8C—C9C	109.2 (2)
C9A—C8A—H8A	109.8	C7C—C8C—H8E	109.8
C7A—C8A—H8A	109.8	C9C—C8C—H8E	109.8
C9A—C8A—H8B	109.8	C7C—C8C—H8F	109.8

C7A—C8A—H8B	109.8	C9C—C8C—H8F	109.8
H8A—C8A—H8B	108.2	H8E—C8C—H8F	108.3
C10A—C9A—C8A	110.0 (2)	C10C—C9C—C8C	110.5 (3)
C10A—C9A—H9A	109.7	C10C—C9C—H9E	109.6
C8A—C9A—H9A	109.7	C8C—C9C—H9E	109.5
C10A—C9A—H9B	109.7	C10C—C9C—H9F	109.6
C8A—C9A—H9B	109.7	C8C—C9C—H9F	109.6
H9A—C9A—H9B	108.2	H9E—C9C—H9F	108.1
C12A—C10A—C11A	119.2 (2)	C12C—C10C—C11C	119.4 (2)
C12A—C10A—C9A	120.9 (2)	C12C—C10C—C9C	120.7 (2)
C11A—C10A—C9A	119.8 (2)	C11C—C10C—C9C	120.0 (2)
N1A—C11A—C3A	120.3 (2)	N1C—C11C—C3C	119.9 (2)
N1A—C11A—C10A	119.3 (2)	N1C—C11C—C10C	120.0 (2)
C3A—C11A—C10A	120.4 (2)	C3C—C11C—C10C	120.1 (2)
C10A—C12A—C13A	121.9 (2)	C10C—C12C—C13C	121.7 (2)
C10A—C12A—H12A	119.0	C10C—C12C—H12C	119.1
C13A—C12A—H12A	119.0	C13C—C12C—H12C	119.1
C14A—C13A—C2A	118.8 (3)	C2C—C13C—C12C	118.0 (2)
C14A—C13A—C12A	124.3 (3)	C2C—C13C—C14C	117.9 (3)
C2A—C13A—C12A	116.9 (3)	C12C—C13C—C14C	124.1 (2)
C15A—C14A—C13A	123.0 (3)	C15C—C14C—C13C	123.2 (2)
C15A—C14A—H14A	118.5	C15C—C14C—H14C	118.4
C13A—C14A—H14A	118.5	C13C—C14C—H14C	118.4
C14A—C15A—C1A	118.6 (2)	C14C—C15C—C1C	119.0 (2)
C14A—C15A—C16A	119.1 (2)	C14C—C15C—C16C	119.1 (2)
C1A—C15A—C16A	122.3 (2)	C1C—C15C—C16C	121.9 (2)
O3A—C16A—C15A	119.0 (3)	O3C—C16C—C15C	119.0 (3)
O3A—C16A—C17A	119.8 (3)	O3C—C16C—C17C	119.7 (3)
C15A—C16A—C17A	121.2 (3)	C15C—C16C—C17C	121.3 (3)
C16A—C17A—H17A	109.5	C16C—C17C—H17G	109.5
C16A—C17A—H17B	109.5	C16C—C17C—H17H	109.5
H17A—C17A—H17B	109.5	H17G—C17C—H17H	109.5
C16A—C17A—H17C	109.5	C16C—C17C—H17I	109.5
H17A—C17A—H17C	109.5	H17G—C17C—H17I	109.5
H17B—C17A—H17C	109.5	H17H—C17C—H17I	109.5
O1B—C1B—O2B	114.5 (2)	O1D—C1D—O2D	115.0 (2)
O1B—C1B—C15B	128.2 (3)	O1D—C1D—C15D	128.4 (2)
O2B—C1B—C15B	117.3 (2)	O2D—C1D—C15D	116.6 (2)
C2B—O2B—C1B	123.1 (2)	C2D—O2D—C1D	123.6 (2)
O2B—C2B—C3B	116.6 (2)	O2D—C2D—C3D	117.0 (2)
O2B—C2B—C13B	119.4 (3)	O2D—C2D—C13D	119.6 (2)
C3B—C2B—C13B	123.9 (3)	C3D—C2D—C13D	123.4 (3)
C2B—C3B—C11B	117.4 (2)	C2D—C3D—C11D	117.3 (2)
C2B—C3B—C4B	121.8 (2)	C2D—C3D—C4D	121.1 (2)
C11B—C3B—C4B	120.8 (2)	C11D—C3D—C4D	121.7 (2)
C3B—C4B—C5B	110.4 (2)	C3D—C4D—C5D	110.3 (2)
C3B—C4B—H4C	109.6	C3D—C4D—H4G	109.6
C5B—C4B—H4C	109.6	C5D—C4D—H4G	109.6
C3B—C4B—H4D	109.6	C3D—C4D—H4H	109.6

C5B—C4B—H4D	109.6	C5D—C4D—H4H	109.6
H4C—C4B—H4D	108.1	H4G—C4D—H4H	108.1
C6B—C5B—C4B	111.1 (2)	C6D—C5D—C4D	111.0 (2)
C6B—C5B—H5C	109.4	C6D—C5D—H5G	109.4
C4B—C5B—H5C	109.4	C4D—C5D—H5G	109.4
C6B—C5B—H5D	109.4	C6D—C5D—H5H	109.4
C4B—C5B—H5D	109.4	C4D—C5D—H5H	109.4
H5C—C5B—H5D	108.0	H5G—C5D—H5H	108.0
N1B—C6B—C5B	113.0 (2)	N1D—C6D—C5D	111.5 (2)
N1B—C6B—H6C	109.0	N1D—C6D—H6G	109.3
C5B—C6B—H6C	109.0	C5D—C6D—H6G	109.3
N1B—C6B—H6D	109.0	N1D—C6D—H6H	109.3
C5B—C6B—H6D	109.0	C5D—C6D—H6H	109.3
H6C—C6B—H6D	107.8	H6G—C6D—H6H	108.0
C11B—N1B—C6B	122.9 (2)	C11D—N1D—C6D	121.4 (3)
C11B—N1B—C7B	122.8 (2)	C11D—N1D—C7D	122.0 (2)
C6B—N1B—C7B	114.3 (2)	C6D—N1D—C7D	115.7 (2)
N1B—C7B—C8B	112.4 (2)	N1D—C7D—C8D	111.5 (2)
N1B—C7B—H7C	109.1	N1D—C7D—H7G	109.3
C8B—C7B—H7C	109.1	C8D—C7D—H7G	109.3
N1B—C7B—H7D	109.1	N1D—C7D—H7H	109.3
C8B—C7B—H7D	109.1	C8D—C7D—H7H	109.3
H7C—C7B—H7D	107.9	H7G—C7D—H7H	108.0
C9B—C8B—C7B	109.3 (3)	C9D—C8D—C7D	109.2 (2)
C9B—C8B—H8C	109.8	C9D—C8D—H8G	109.8
C7B—C8B—H8C	109.8	C7D—C8D—H8G	109.8
C9B—C8B—H8D	109.8	C9D—C8D—H8H	109.8
C7B—C8B—H8D	109.8	C7D—C8D—H8H	109.8
H8C—C8B—H8D	108.3	H8G—C8D—H8H	108.3
C8B—C9B—C10B	110.3 (2)	C10D—C9D—C8D	110.8 (3)
C8B—C9B—H9C	109.6	C10D—C9D—H9G	109.5
C10B—C9B—H9C	109.6	C8D—C9D—H9G	109.5
C8B—C9B—H9D	109.6	C10D—C9D—H9H	109.5
C10B—C9B—H9D	109.6	C8D—C9D—H9H	109.5
H9C—C9B—H9D	108.1	H9G—C9D—H9H	108.1
C12B—C10B—C11B	119.5 (2)	C12D—C10D—C11D	119.1 (2)
C12B—C10B—C9B	121.4 (2)	C12D—C10D—C9D	121.0 (2)
C11B—C10B—C9B	119.0 (2)	C11D—C10D—C9D	119.8 (2)
N1B—C11B—C3B	119.8 (2)	N1D—C11D—C3D	119.6 (2)
N1B—C11B—C10B	120.1 (2)	N1D—C11D—C10D	119.9 (2)
C3B—C11B—C10B	120.1 (2)	C3D—C11D—C10D	120.4 (2)
C10B—C12B—C13B	121.8 (2)	C10D—C12D—C13D	122.4 (2)
C10B—C12B—H12B	119.1	C10D—C12D—H12D	118.8
C13B—C12B—H12B	119.1	C13D—C12D—H12D	118.8
C14B—C13B—C2B	118.3 (3)	C14D—C13D—C12D	124.5 (3)
C14B—C13B—C12B	124.5 (3)	C14D—C13D—C2D	118.1 (3)
C2B—C13B—C12B	117.2 (3)	C12D—C13D—C2D	117.4 (2)
C15B—C14B—C13B	122.7 (3)	C15D—C14D—C13D	122.9 (2)
C15B—C14B—H14B	118.6	C15D—C14D—H14D	118.5

C13B—C14B—H14B	118.6	C13D—C14D—H14D	118.5
C14B—C15B—C1B	119.0 (2)	C14D—C15D—C1D	119.1 (2)
C14B—C15B—C16B	118.6 (3)	C14D—C15D—C16D	118.5 (2)
C1B—C15B—C16B	122.3 (2)	C1D—C15D—C16D	122.3 (2)
O3B—C16B—C15B	119.8 (3)	O3D—C16D—C15D	118.9 (3)
O3B—C16B—C17B	119.9 (3)	O3D—C16D—C17D	120.5 (3)
C15B—C16B—C17B	120.3 (3)	C15D—C16D—C17D	120.6 (3)
C16B—C17B—H17D	109.5	C16D—C17D—H17J	109.5
C16B—C17B—H17E	109.5	C16D—C17D—H17K	109.5
H17D—C17B—H17E	109.5	H17J—C17D—H17K	109.5
C16B—C17B—H17F	109.5	C16D—C17D—H17L	109.5
H17D—C17B—H17F	109.5	H17J—C17D—H17L	109.5
H17E—C17B—H17F	109.5	H17K—C17D—H17L	109.5
O1A—C1A—O2A—C2A	−174.6 (2)	O1C—C1C—O2C—C2C	176.5 (2)
C15A—C1A—O2A—C2A	4.5 (3)	C15C—C1C—O2C—C2C	−2.5 (3)
C1A—O2A—C2A—C3A	178.7 (2)	C1C—O2C—C2C—C3C	−179.2 (2)
C1A—O2A—C2A—C13A	−2.2 (4)	C1C—O2C—C2C—C13C	0.9 (4)
O2A—C2A—C3A—C11A	−178.8 (2)	O2C—C2C—C3C—C11C	179.6 (2)
C13A—C2A—C3A—C11A	2.1 (4)	C13C—C2C—C3C—C11C	−0.4 (4)
O2A—C2A—C3A—C4A	1.3 (4)	O2C—C2C—C3C—C4C	−0.8 (4)
C13A—C2A—C3A—C4A	−177.8 (2)	C13C—C2C—C3C—C4C	179.2 (3)
C2A—C3A—C4A—C5A	−154.1 (3)	C2C—C3C—C4C—C5C	−155.2 (2)
C11A—C3A—C4A—C5A	26.0 (3)	C11C—C3C—C4C—C5C	24.4 (3)
C3A—C4A—C5A—C6A	−50.8 (3)	C3C—C4C—C5C—C6C	−49.9 (3)
C4A—C5A—C6A—N1A	50.8 (3)	C4C—C5C—C6C—N1C	55.2 (3)
C5A—C6A—N1A—C11A	−24.0 (4)	C5C—C6C—N1C—C11C	−34.2 (4)
C5A—C6A—N1A—C7A	158.6 (3)	C5C—C6C—N1C—C7C	155.7 (3)
C11A—N1A—C7A—C8A	−21.6 (4)	C11C—N1C—C7C—C8C	31.3 (4)
C6A—N1A—C7A—C8A	155.8 (3)	C6C—N1C—C7C—C8C	−158.6 (3)
N1A—C7A—C8A—C9A	51.5 (3)	N1C—C7C—C8C—C9C	−55.9 (3)
C7A—C8A—C9A—C10A	−55.9 (3)	C7C—C8C—C9C—C10C	54.4 (3)
C8A—C9A—C10A—C12A	−145.2 (3)	C8C—C9C—C10C—C12C	149.5 (3)
C8A—C9A—C10A—C11A	32.2 (4)	C8C—C9C—C10C—C11C	−29.4 (4)
C6A—N1A—C11A—C3A	−3.0 (4)	C7C—N1C—C11C—C3C	177.2 (2)
C7A—N1A—C11A—C3A	174.1 (2)	C6C—N1C—C11C—C3C	7.7 (4)
C6A—N1A—C11A—C10A	178.5 (2)	C7C—N1C—C11C—C10C	−4.4 (4)
C7A—N1A—C11A—C10A	−4.3 (4)	C6C—N1C—C11C—C10C	−173.9 (2)
C2A—C3A—C11A—N1A	−178.3 (2)	C2C—C3C—C11C—N1C	176.8 (2)
C4A—C3A—C11A—N1A	1.6 (4)	C4C—C3C—C11C—N1C	−2.8 (4)
C2A—C3A—C11A—C10A	0.2 (4)	C2C—C3C—C11C—C10C	−1.5 (4)
C4A—C3A—C11A—C10A	−179.9 (2)	C4C—C3C—C11C—C10C	178.9 (2)
C12A—C10A—C11A—N1A	176.0 (2)	C12C—C10C—C11C—N1C	−175.3 (2)
C9A—C10A—C11A—N1A	−1.5 (4)	C9C—C10C—C11C—N1C	3.5 (4)
C12A—C10A—C11A—C3A	−2.4 (4)	C12C—C10C—C11C—C3C	3.0 (4)
C9A—C10A—C11A—C3A	−179.9 (2)	C9C—C10C—C11C—C3C	−178.1 (2)
C11A—C10A—C12A—C13A	2.5 (4)	C11C—C10C—C12C—C13C	−2.5 (4)
C9A—C10A—C12A—C13A	180.0 (2)	C9C—C10C—C12C—C13C	178.6 (3)
C3A—C2A—C13A—C14A	177.9 (3)	O2C—C2C—C13C—C12C	−179.1 (2)
O2A—C2A—C13A—C14A	−1.2 (4)	C3C—C2C—C13C—C12C	0.9 (4)

C3A—C2A—C13A—C12A	−2.0 (4)	O2C—C2C—C13C—C14C	1.1 (4)
O2A—C2A—C13A—C12A	178.9 (2)	C3C—C2C—C13C—C14C	−178.9 (2)
C10A—C12A—C13A—C14A	179.7 (2)	C10C—C12C—C13C—C2C	0.6 (4)
C10A—C12A—C13A—C2A	−0.4 (4)	C10C—C12C—C13C—C14C	−179.6 (2)
C2A—C13A—C14A—C15A	2.0 (4)	C2C—C13C—C14C—C15C	−1.2 (4)
C12A—C13A—C14A—C15A	−178.0 (2)	C12C—C13C—C14C—C15C	179.0 (3)
C13A—C14A—C15A—C1A	0.3 (4)	C13C—C14C—C15C—C1C	−0.4 (4)
C13A—C14A—C15A—C16A	179.0 (2)	C13C—C14C—C15C—C16C	−178.8 (2)
O1A—C1A—C15A—C14A	175.5 (3)	O1C—C1C—C15C—C14C	−176.6 (3)
O2A—C1A—C15A—C14A	−3.5 (3)	O2C—C1C—C15C—C14C	2.2 (4)
O1A—C1A—C15A—C16A	−3.1 (4)	O1C—C1C—C15C—C16C	1.7 (4)
O2A—C1A—C15A—C16A	177.9 (2)	O2C—C1C—C15C—C16C	−179.5 (2)
C14A—C15A—C16A—O3A	−0.6 (4)	C14C—C15C—C16C—O3C	2.2 (4)
C1A—C15A—C16A—O3A	178.0 (3)	C1C—C15C—C16C—O3C	−176.1 (3)
C14A—C15A—C16A—C17A	−179.2 (2)	C14C—C15C—C16C—C17C	−179.1 (3)
C1A—C15A—C16A—C17A	−0.6 (4)	C1C—C15C—C16C—C17C	2.6 (4)
O1B—C1B—O2B—C2B	174.2 (2)	O1D—C1D—O2D—C2D	−176.4 (2)
C15B—C1B—O2B—C2B	−5.2 (3)	C15D—C1D—O2D—C2D	2.7 (3)
C1B—O2B—C2B—C3B	−177.9 (2)	C1D—O2D—C2D—C3D	179.4 (2)
C1B—O2B—C2B—C13B	2.8 (4)	C1D—O2D—C2D—C13D	−1.3 (4)
O2B—C2B—C3B—C11B	179.3 (2)	O2D—C2D—C3D—C11D	−179.8 (2)
C13B—C2B—C3B—C11B	−1.4 (4)	C13D—C2D—C3D—C11D	0.9 (4)
O2B—C2B—C3B—C4B	−1.2 (4)	O2D—C2D—C3D—C4D	0.5 (4)
C13B—C2B—C3B—C4B	178.1 (2)	C13D—C2D—C3D—C4D	−178.8 (3)
C2B—C3B—C4B—C5B	153.9 (2)	C2D—C3D—C4D—C5D	155.7 (2)
C11B—C3B—C4B—C5B	−26.6 (3)	C11D—C3D—C4D—C5D	−24.0 (3)
C3B—C4B—C5B—C6B	50.8 (3)	C3D—C4D—C5D—C6D	49.4 (3)
C4B—C5B—C6B—N1B	−49.7 (3)	C4D—C5D—C6D—N1D	−55.4 (3)
C5B—C6B—N1B—C11B	22.6 (4)	C5D—C6D—N1D—C11D	34.8 (4)
C5B—C6B—N1B—C7B	−159.3 (2)	C5D—C6D—N1D—C7D	−155.2 (3)
C11B—N1B—C7B—C8B	21.5 (4)	C11D—N1D—C7D—C8D	−31.4 (4)
C6B—N1B—C7B—C8B	−156.5 (3)	C6D—N1D—C7D—C8D	158.7 (3)
N1B—C7B—C8B—C9B	−51.7 (3)	N1D—C7D—C8D—C9D	55.8 (3)
C7B—C8B—C9B—C10B	56.2 (3)	C7D—C8D—C9D—C10D	−54.2 (3)
C8B—C9B—C10B—C12B	145.0 (3)	C8D—C9D—C10D—C12D	−149.7 (3)
C8B—C9B—C10B—C11B	−32.1 (4)	C8D—C9D—C10D—C11D	28.9 (3)
C6B—N1B—C11B—C3B	3.5 (4)	C6D—N1D—C11D—C3D	−8.1 (4)
C7B—N1B—C11B—C3B	−174.3 (2)	C7D—N1D—C11D—C3D	−177.4 (2)
C6B—N1B—C11B—C10B	−177.2 (2)	C6D—N1D—C11D—C10D	173.6 (2)
C7B—N1B—C11B—C10B	4.9 (4)	C7D—N1D—C11D—C10D	4.3 (4)
C2B—C3B—C11B—N1B	178.5 (2)	C2D—C3D—C11D—N1D	−177.1 (2)
C4B—C3B—C11B—N1B	−1.1 (4)	C4D—C3D—C11D—N1D	2.6 (4)
C2B—C3B—C11B—C10B	−0.8 (4)	C2D—C3D—C11D—C10D	1.2 (4)
C4B—C3B—C11B—C10B	179.7 (2)	C4D—C3D—C11D—C10D	−179.1 (2)
C12B—C10B—C11B—N1B	−176.4 (2)	C12D—C10D—C11D—N1D	175.6 (2)
C9B—C10B—C11B—N1B	0.8 (4)	C9D—C10D—C11D—N1D	−3.0 (4)
C12B—C10B—C11B—C3B	2.9 (4)	C12D—C10D—C11D—C3D	−2.7 (4)
C9B—C10B—C11B—C3B	−180.0 (2)	C9D—C10D—C11D—C3D	178.7 (2)
C11B—C10B—C12B—C13B	−2.9 (4)	C11D—C10D—C12D—C13D	2.1 (4)

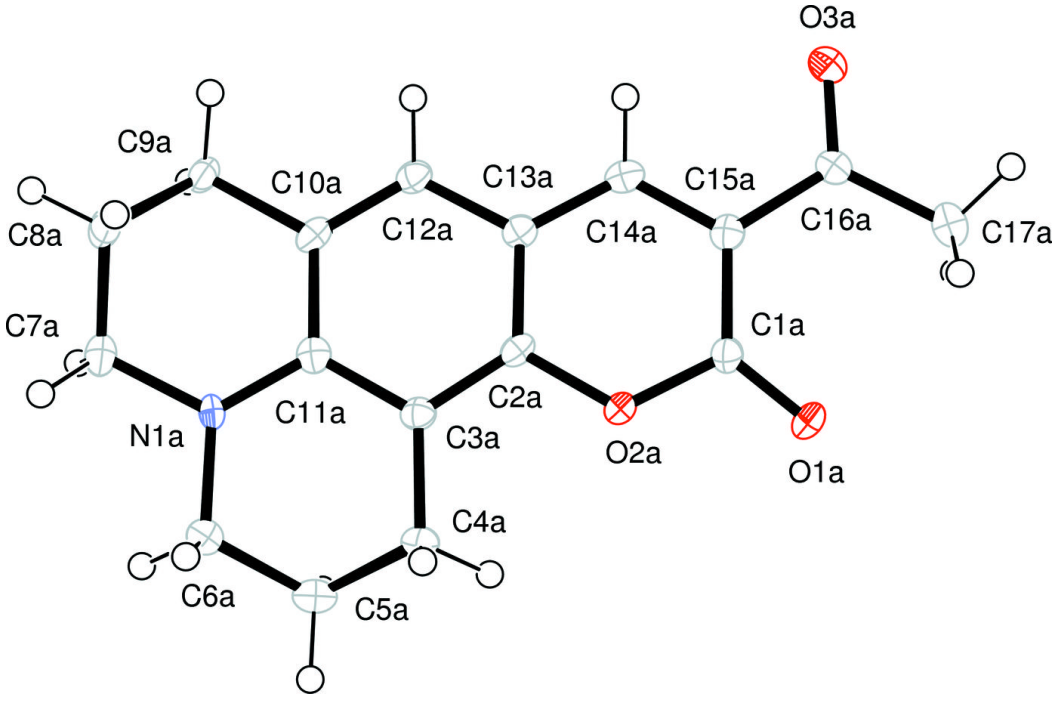
C9B—C10B—C12B—C13B	−179.9 (2)	C9D—C10D—C12D—C13D	−179.3 (2)
O2B—C2B—C13B—C14B	0.8 (4)	C10D—C12D—C13D—C14D	179.7 (3)
C3B—C2B—C13B—C14B	−178.4 (3)	C10D—C12D—C13D—C2D	−0.1 (4)
O2B—C2B—C13B—C12B	−179.3 (2)	O2D—C2D—C13D—C14D	−0.5 (4)
C3B—C2B—C13B—C12B	1.5 (4)	C3D—C2D—C13D—C14D	178.7 (2)
C10B—C12B—C13B—C14B	−179.4 (2)	O2D—C2D—C13D—C12D	179.2 (2)
C10B—C12B—C13B—C2B	0.8 (4)	C3D—C2D—C13D—C12D	−1.5 (4)
C2B—C13B—C14B—C15B	−1.9 (4)	C12D—C13D—C14D—C15D	−178.8 (3)
C12B—C13B—C14B—C15B	178.2 (2)	C2D—C13D—C14D—C15D	0.9 (4)
C13B—C14B—C15B—C1B	−0.6 (4)	C13D—C14D—C15D—C1D	0.5 (4)
C13B—C14B—C15B—C16B	−178.7 (2)	C13D—C14D—C15D—C16D	179.1 (2)
O1B—C1B—C15B—C14B	−175.4 (3)	O1D—C1D—C15D—C14D	176.7 (3)
O2B—C1B—C15B—C14B	4.0 (4)	O2D—C1D—C15D—C14D	−2.2 (3)
O1B—C1B—C15B—C16B	2.7 (4)	O1D—C1D—C15D—C16D	−1.9 (4)
O2B—C1B—C15B—C16B	−177.9 (2)	O2D—C1D—C15D—C16D	179.2 (2)
C14B—C15B—C16B—O3B	4.2 (4)	C14D—C15D—C16D—O3D	−2.9 (4)
C1B—C15B—C16B—O3B	−173.8 (3)	C1D—C15D—C16D—O3D	175.7 (3)
C14B—C15B—C16B—C17B	−176.8 (2)	C14D—C15D—C16D—C17D	177.9 (2)
C1B—C15B—C16B—C17B	5.1 (4)	C1D—C15D—C16D—C17D	−3.5 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4B—H4D···O3A^{i}	0.99	2.57	3.410 (3)	143
C4D—H4H···O1B^{ii}	0.99	2.52	3.407 (3)	149
C7C—H7F···O3A^{iii}	0.99	2.39	3.368 (4)	170
C7D—H7G···O3D^{iv}	0.99	2.42	3.393 (3)	169
C12A—H12A···O1D^{v}	0.95	2.47	3.361 (3)	156
C12C—H12C···O1A^{i}	0.95	2.40	3.273 (3)	152
C12D—H12D···O1B^{vi}	0.95	2.44	3.302 (3)	152

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

Fig. 1


O3a
C9a
C10a
C13a
C15a
C16a
C17a
C8a
C12a
C14a
C7a
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N1a
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O2a
O1a
C4a
C6a
C5a

Fig. 2

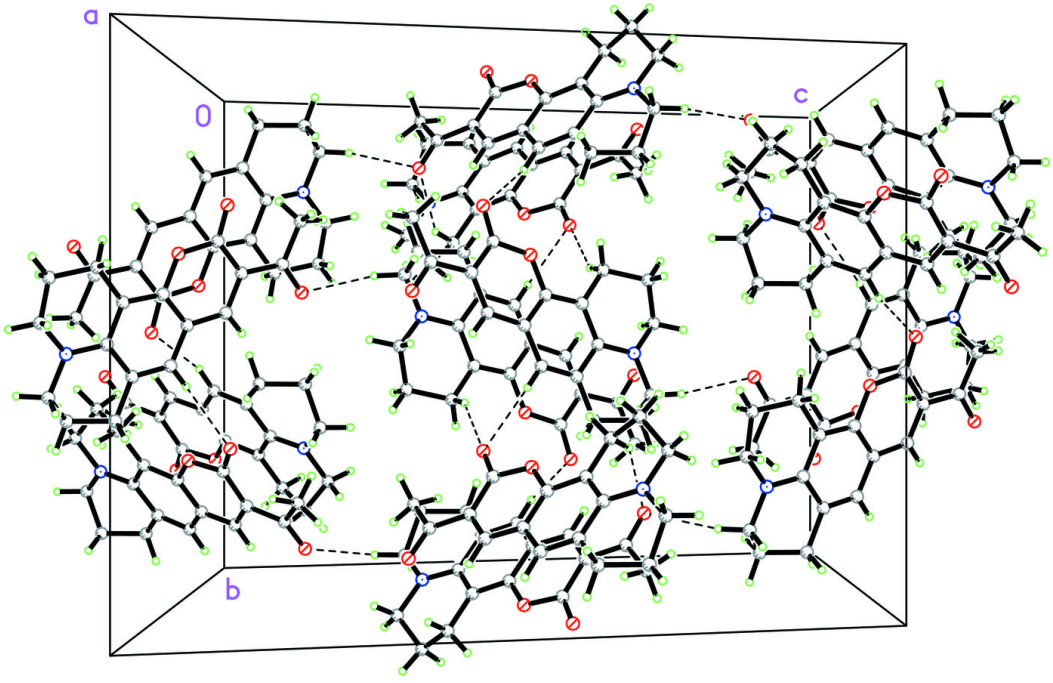

Fig. 3

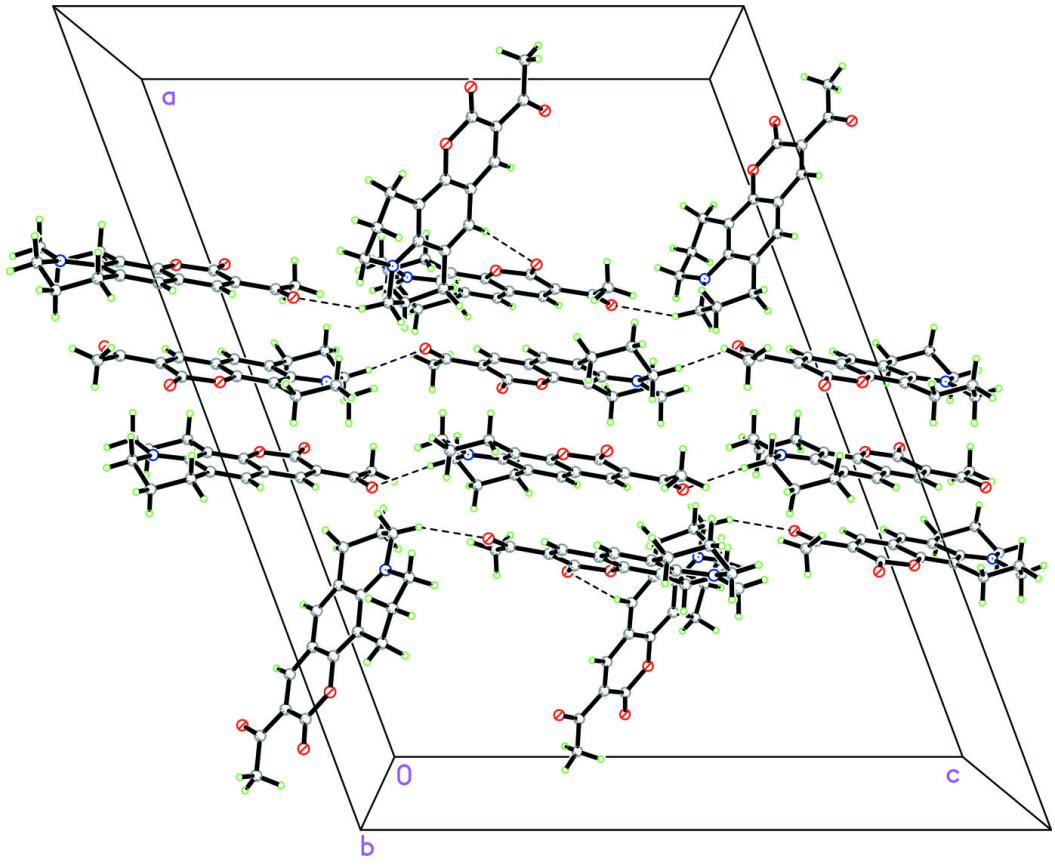

Fig. 4