Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(1′*S*,12′*R*,13′*S*,17′*S*)-15′,15′-Dimethyl-1,2-dihydro-11′,14′,16′,18′-tetraoxa-7′-azaspiro[indole-3,8′-pentacyclo-[10.6.0.0^{2,9}.0^{3,7}.0^{13,17}]octadecane]-2,10′-dione

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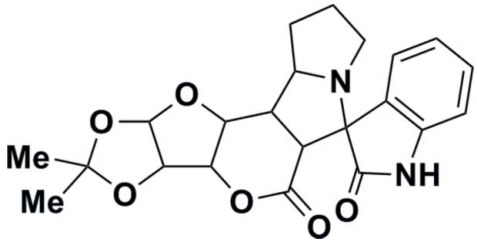
Received 11 February 2013; accepted 25 February 2013

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.090; data-to-parameter ratio = 14.6.

In the title compound, $C_{22}H_{24}N_2O_6$, the indole ring has a twist conformation and the tetrahydro-2*H*-pyran-2-one ring a half-chair conformation. One of the pyrrolidine rings adopts an envelope conformation on the N atom, while the other has a twist conformation; the 'butterfly' angle between their mean planes is 62.98 (11)°. The dioxolane ring adopts a twist conformation and the tetrahydrofuran ring has an envelope conformation on the C atom in the fused tetrahydro-2*H*-pyran-2-one ring adjacent to the O atom of the tetrahydrofuran ring. The 'butterfly' angle between the mean planes of these two five-membered rings is 69.14 (10)°. In the crystal, molecules are linked by N—H···O hydrogen bonds, forming chains along the *a* axis.

Related literature

For the biological activity of indole derivatives, see: Stevenson *et al.* (2000); Rajeswaran *et al.* (1999); Amal Raj *et al.* (2003). For a related structure, see: Jagadeesan *et al.* (2012).



Experimental

Crystal data

$C_{22}H_{24}N_2O_6$
M_r = 412.43
Orthorhombic, $P2_12_12_1$
a = 9.2737 (5) Å
b = 11.6543 (8) Å
c = 18.8489 (14) Å
V = 2037.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.30 × 0.30 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2008)
T_{min} = 0.922, T_{max} = 0.947
21465 measured reflections
4717 independent reflections
3800 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.090
S = 1.04
4717 reflections
324 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.06	2.8849 (19)	161

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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: *SHELXL97* and *PLATON* (Spek, 2009).

SA and VS thank the UGC, India, for financial support. The authors thank Dr Babu Varghese, Senior Scientific Officer, SAIF, IIT, Chennai, India, for the X-ray intensity data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2563).

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supporting information

Acta Cryst. (2013). E**69**, o466 [doi:10.1107/S1600536813005436]

(1′*S*,12′*R*,13′*S*,17′*S*)-15′,15′-Dimethyl-1,2-dihydro-11′,14′,16′,18′-tetraoxa-7′-azaspiro[indole-3,8′-pentacyclo[10.6.0.0^{2,9}.0^{3,7}.0^{13,17}]octadecane]-2,10′-dione

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S1. Comment

Indole compounds can be used as bioactive drugs (Stevenson *et al.*, 2000) and have also been proven to display high aldose reductase inhibitory activity (Rajeswaran *et al.*, 1999), and antimicrobial and antifungal activities (Amal Raj *et al.*, 2003).

The molecular structure of the title compound is shown in Fig. 1. The indole ring is essentially planar with the maximum deviation from planarity being 0.123 (2) Å for atom C7. Atom O1 deviates from the mean plane of the indole ring by 0.2095 (13) Å. The tetrahydro-2H-pyran-2-one ring (O3/C13-C17) has a half-chair conformation.

The five-membered pyrrolidine ring (N2/C9-C12) adopts an envelope conformation with atom N2 as the flap; it is 0.5267 (12) Å out of the mean plane formed by the other ring atoms. The other pyrrolidine ring (N2/C6/C12-C14) has a twist conformation on bond N2-C12; the "butter-fly" angle between their mean planes is 62.98 (11)°.

The dioxolane ring (O5/O6/C18-C20) adopts a twist conformation on bond O6-C20. The tetrahydrofuran ring (O4/C16-C19) adopts an envelope conformation with atom C17 deviating from the mean plane of the remaining ring atoms by 0.6286 (17) Å; the "butter-fly" angle between the ring mean planes is 69.14 (10) °.

In the crystal, molecules are linked via N-H···O hydrogen bonds forming chains propagating along the a axis direction (Table 1 and Fig. 2).

The title compound exhibits structural similarities with a related structure (Jagadeesan *et al.*, 2012).

S2. Experimental

A solution of 5,6-Dideoxy-l,2-*O*-isopropylidene-a-*D*-*xylo*-hept-5-enofuranurono-7,3-lactone (300 mg, 1.5 mmol), sarcosine (125 mg, 1.5 mmol) and isatin (210 mg, 1.5 mmol) were refluxed in dry toluene under a N_2 atmosphere for 6–8 h at 383 K using a Dean-Stark apparatus. After the completion of the reaction as indicated by TLC, toluene was evaporated under reduced pressure. The crude product was washed with water and extracted with dichloromethane (4 × 20mL). The combined organic layers were dried ($MgSO_4$) and filtered, concentrated in vacuum. The crude product was purified by column chromatography using hexane:EtOAc (7:3) mixture as eluent. On slow evaporation of the solvents colourless block-like crystals were obtained.

S3. Refinement

The methine and methylene H atoms were included in calculated positions freely refined. The remainder of the H atoms were included in calculated positions and allowed to ride on their parent atom: C—H = 0.93 - 0.96 Å, N-H = 0.86 Å, with U_{iso} = 1.5U_{eq}(C-methyl), and = 1.2U_{eq}(C,N) for other H atoms.

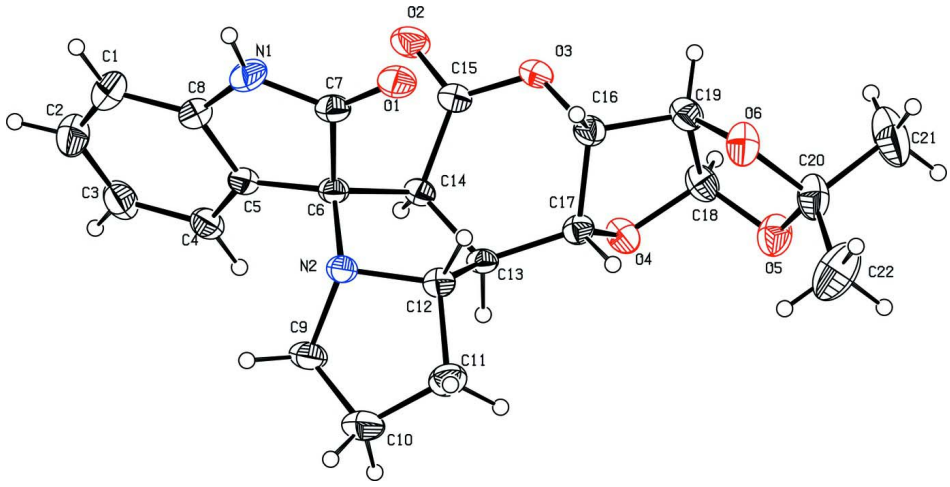

Figure 1

View of the molecular structure of the title molecule, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

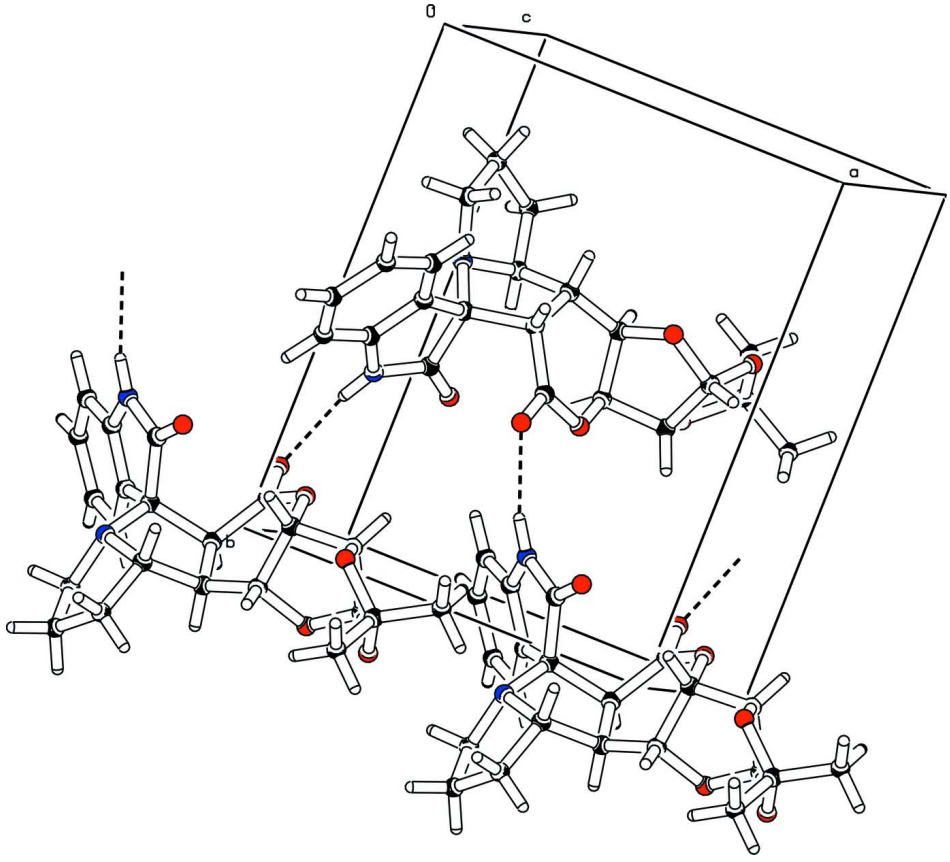

Figure 2

A view along the c axis of the crystal packing of the title compound, showing the N-H···O hydrogen bonds (dashed lines; see Table 1 for details).

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Crystal data

$C_{22}H_{24}N_2O_6$
M_r = 412.43
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 9.2737 (5) Å
b = 11.6543 (8) Å
c = 18.8489 (14) Å
V = 2037.2 (2) Å^3
Z = 4
$F(000)$ = 872
D_x = 1.345 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8834 reflections
θ = 2.1–31.2°
μ = 0.10 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker 2008)
T_{min} = 0.922, T_{max} = 0.947
21465 measured reflections
4717 independent reflections
3800 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 27.6°, θ_{min} = 2.1°
h = −6→12
k = −15→14
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.090
S = 1.04
4717 reflections
324 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.1058P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0043 (7)

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 $F^2 > \sigma(F^2)$ 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}
H9A	0.090 (2)	0.2846 (19)	0.0396 (11)	0.064 (6)*
H11A	0.384 (2)	0.2235 (18)	0.1817 (11)	0.059 (6)*

H11B	0.251 (2)	0.278 (2)	0.2138 (12)	0.078 (7)*
H10B	0.242 (3)	0.136 (3)	0.1028 (15)	0.109 (10)*
H10A	0.115 (4)	0.178 (4)	0.1375 (19)	0.162 (15)*
H12	0.3470 (19)	0.4460 (16)	0.1690 (10)	0.044 (5)*
H9B	0.251 (2)	0.2576 (16)	0.0170 (10)	0.051 (5)*
H17	0.6125 (17)	0.3803 (14)	0.1785 (9)	0.031 (4)*
H16	0.5679 (19)	0.5796 (16)	0.1708 (10)	0.041 (5)*
H14	0.4660 (17)	0.4184 (14)	−0.0175 (9)	0.034 (4)*
H18	0.929 (2)	0.4543 (16)	0.0878 (10)	0.049 (5)*
H13	0.4947 (16)	0.3027 (15)	0.0749 (8)	0.030 (4)*
H19	0.8300 (18)	0.6200 (17)	0.1434 (9)	0.042 (5)*
O4	0.74044 (11)	0.37954 (10)	0.09447 (6)	0.0428 (3)
O1	0.30443 (14)	0.64064 (10)	0.11353 (7)	0.0494 (3)
C13	0.48045 (16)	0.37792 (13)	0.08903 (9)	0.0321 (3)
O2	0.51578 (14)	0.62812 (10)	−0.03068 (7)	0.0553 (4)
N2	0.22433 (13)	0.39789 (11)	0.08173 (7)	0.0343 (3)
O3	0.62164 (13)	0.59996 (10)	0.07089 (7)	0.0458 (3)
O6	0.79932 (13)	0.52782 (12)	0.23306 (6)	0.0519 (3)
O5	0.91693 (13)	0.38056 (12)	0.18080 (7)	0.0553 (4)
N1	0.14101 (17)	0.64572 (13)	0.02193 (9)	0.0517 (4)
H1	0.0942	0.7067	0.0334	0.062*
C14	0.44834 (16)	0.45548 (13)	0.02581 (9)	0.0321 (3)
C17	0.61096 (16)	0.41353 (14)	0.13092 (9)	0.0346 (3)
C5	0.20045 (16)	0.48417 (13)	−0.03945 (9)	0.0364 (4)
C12	0.33988 (16)	0.37913 (14)	0.13385 (9)	0.0353 (4)
C7	0.24724 (18)	0.59935 (14)	0.06148 (9)	0.0392 (4)
C11	0.3016 (2)	0.26639 (17)	0.17006 (12)	0.0498 (5)
C16	0.63188 (18)	0.54190 (14)	0.13806 (9)	0.0382 (4)
C8	0.11618 (19)	0.58297 (15)	−0.03980 (10)	0.0465 (4)
C4	0.20154 (18)	0.41338 (15)	−0.09800 (9)	0.0435 (4)
H4	0.2601	0.3486	−0.0991	0.052*
C6	0.28163 (15)	0.47975 (12)	0.02961 (8)	0.0329 (3)
C15	0.53006 (18)	0.56665 (14)	0.02019 (9)	0.0386 (4)
C9	0.1869 (2)	0.28246 (15)	0.05469 (11)	0.0471 (4)
C19	0.78866 (19)	0.54907 (17)	0.15952 (10)	0.0439 (4)
C20	0.91327 (19)	0.4474 (2)	0.24389 (11)	0.0555 (5)
C1	0.0264 (2)	0.6093 (2)	−0.09595 (12)	0.0644 (6)
H1A	−0.0322	0.6740	−0.0951	0.077*
C3	0.1137 (2)	0.44023 (19)	−0.15530 (10)	0.0558 (5)
H3	0.1136	0.3933	−0.1952	0.067*
C18	0.85583 (18)	0.44176 (16)	0.12504 (10)	0.0437 (4)
C2	0.0269 (2)	0.5360 (2)	−0.15326 (12)	0.0688 (6)
H2	−0.0330	0.5516	−0.1916	0.083*
C10	0.2036 (3)	0.2056 (2)	0.11837 (16)	0.0706 (7)
C21	1.0539 (2)	0.5104 (3)	0.25265 (17)	0.0961 (10)
H21B	1.1302	0.4561	0.2602	0.144*
H21C	1.0476	0.5610	0.2927	0.144*
H21A	1.0736	0.5542	0.2106	0.144*

C22	0.8736 (3)	0.3709 (3)	0.30471 (13)	0.0978 (10)
H22A	0.9498	0.3167	0.3128	0.147*
H22C	0.7862	0.3306	0.2937	0.147*
H22B	0.8595	0.4165	0.3466	0.147*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0336 (5)	0.0432 (6)	0.0518 (7)	0.0007 (5)	0.0049 (5)	−0.0152 (6)
O1	0.0596 (7)	0.0338 (6)	0.0546 (8)	0.0031 (5)	−0.0002 (6)	−0.0115 (6)
C13	0.0352 (7)	0.0216 (8)	0.0394 (9)	0.0007 (6)	0.0028 (6)	−0.0012 (7)
O2	0.0696 (8)	0.0466 (7)	0.0496 (8)	−0.0215 (6)	−0.0061 (6)	0.0149 (6)
N2	0.0331 (6)	0.0280 (6)	0.0419 (7)	−0.0016 (5)	0.0016 (5)	0.0005 (6)
O3	0.0509 (7)	0.0329 (6)	0.0535 (7)	−0.0120 (6)	−0.0089 (6)	0.0030 (6)
O6	0.0454 (7)	0.0664 (9)	0.0441 (7)	0.0126 (6)	−0.0043 (5)	−0.0161 (6)
O5	0.0511 (7)	0.0602 (9)	0.0545 (8)	0.0143 (6)	−0.0071 (6)	−0.0121 (7)
N1	0.0562 (9)	0.0333 (8)	0.0657 (10)	0.0160 (7)	−0.0051 (8)	−0.0021 (8)
C14	0.0336 (7)	0.0280 (8)	0.0346 (8)	−0.0032 (6)	0.0036 (6)	−0.0044 (7)
C17	0.0335 (8)	0.0327 (8)	0.0375 (9)	0.0038 (6)	0.0040 (7)	−0.0002 (7)
C5	0.0356 (8)	0.0292 (8)	0.0444 (9)	−0.0045 (6)	−0.0007 (7)	0.0028 (7)
C12	0.0367 (8)	0.0330 (8)	0.0362 (9)	0.0007 (7)	0.0041 (6)	0.0002 (7)
C7	0.0423 (8)	0.0278 (8)	0.0474 (10)	0.0007 (7)	0.0057 (8)	−0.0012 (7)
C11	0.0486 (10)	0.0453 (11)	0.0554 (12)	−0.0017 (9)	0.0066 (9)	0.0142 (9)
C16	0.0405 (8)	0.0339 (9)	0.0402 (9)	−0.0007 (7)	−0.0011 (7)	−0.0050 (7)
C8	0.0477 (9)	0.0358 (9)	0.0559 (11)	0.0019 (8)	−0.0069 (9)	0.0064 (9)
C4	0.0430 (9)	0.0398 (9)	0.0478 (10)	−0.0094 (8)	−0.0006 (8)	−0.0002 (8)
C6	0.0336 (7)	0.0245 (7)	0.0404 (9)	−0.0003 (6)	0.0016 (6)	−0.0007 (7)
C15	0.0412 (8)	0.0328 (8)	0.0418 (9)	−0.0052 (7)	0.0030 (7)	0.0011 (8)
C9	0.0533 (11)	0.0297 (9)	0.0584 (12)	−0.0073 (8)	0.0010 (10)	−0.0008 (8)
C19	0.0434 (9)	0.0417 (10)	0.0466 (10)	−0.0042 (8)	−0.0017 (8)	−0.0079 (8)
C20	0.0406 (9)	0.0743 (14)	0.0518 (11)	0.0117 (9)	−0.0063 (8)	−0.0156 (11)
C1	0.0631 (12)	0.0561 (12)	0.0740 (15)	0.0123 (11)	−0.0187 (11)	0.0104 (11)
C3	0.0543 (11)	0.0626 (13)	0.0504 (11)	−0.0167 (10)	−0.0088 (9)	−0.0014 (10)
C18	0.0340 (8)	0.0526 (11)	0.0445 (10)	−0.0053 (7)	0.0061 (8)	−0.0099 (9)
C2	0.0627 (13)	0.0754 (15)	0.0684 (15)	−0.0042 (12)	−0.0246 (11)	0.0161 (13)
C10	0.0868 (17)	0.0419 (12)	0.0830 (17)	−0.0201 (12)	−0.0164 (14)	0.0179 (12)
C21	0.0457 (12)	0.119 (2)	0.123 (2)	0.0087 (14)	−0.0179 (13)	−0.057 (2)
C22	0.108 (2)	0.126 (3)	0.0594 (15)	0.040 (2)	−0.0009 (14)	0.0199 (17)

Geometric parameters (Å, º)

O4—C18	1.415 (2)	C7—C6	1.551 (2)
O4—C17	1.4390 (18)	C11—C10	1.509 (3)
O1—C7	1.215 (2)	C11—H11A	0.94 (2)
C13—C17	1.503 (2)	C11—H11B	0.96 (2)
C13—C14	1.525 (2)	C16—C19	1.511 (2)
C13—C12	1.553 (2)	C16—H16	0.962 (19)
C13—H13	0.925 (17)	C8—C1	1.381 (3)

O2—C15	1.204 (2)	C4—C3	1.388 (3)
N2—C6	1.469 (2)	C4—H4	0.9300
N2—C12	1.470 (2)	C9—C10	1.506 (3)
N2—C9	1.480 (2)	C9—H9A	0.95 (2)
O3—C15	1.336 (2)	C9—H9B	0.97 (2)
O3—C16	1.439 (2)	C19—C18	1.541 (2)
O6—C19	1.411 (2)	C19—H19	0.961 (19)
O6—C20	1.427 (2)	C20—C22	1.498 (3)
O5—C18	1.391 (2)	C20—C21	1.505 (3)
O5—C20	1.422 (2)	C1—C2	1.377 (3)
N1—C7	1.348 (2)	C1—H1A	0.9300
N1—C8	1.393 (2)	C3—C2	1.376 (3)
N1—H1	0.8600	C3—H3	0.9300
C14—C15	1.505 (2)	C18—H18	0.985 (19)
C14—C6	1.573 (2)	C2—H2	0.9300
C14—H14	0.938 (17)	C10—H10B	0.93 (3)
C17—C16	1.515 (2)	C10—H10A	0.95 (4)
C17—H17	0.977 (17)	C21—H21B	0.9600
C5—C4	1.378 (2)	C21—H21C	0.9600
C5—C8	1.392 (2)	C21—H21A	0.9600
C5—C6	1.505 (2)	C22—H22A	0.9600
C12—C11	1.523 (2)	C22—H22C	0.9600
C12—H12	1.026 (19)	C22—H22B	0.9600

C18—O4—C17	107.19 (11)	N2—C6—C7	104.49 (12)
C17—C13—C14	113.82 (13)	C5—C6—C7	101.62 (13)
C17—C13—C12	112.80 (14)	N2—C6—C14	105.62 (12)
C14—C13—C12	104.82 (12)	C5—C6—C14	117.28 (13)
C17—C13—H13	107.3 (10)	C7—C6—C14	112.42 (12)
C14—C13—H13	111.4 (10)	O2—C15—O3	117.81 (14)
C12—C13—H13	106.6 (10)	O2—C15—C14	120.85 (15)
C6—N2—C12	106.25 (11)	O3—C15—C14	121.33 (15)
C6—N2—C9	116.41 (13)	N2—C9—C10	104.02 (17)
C12—N2—C9	105.42 (13)	N2—C9—H9A	107.6 (14)
C15—O3—C16	122.32 (12)	C10—C9—H9A	110.7 (13)
C19—O6—C20	107.92 (14)	N2—C9—H9B	112.2 (11)
C18—O5—C20	109.96 (15)	C10—C9—H9B	110.0 (11)
C7—N1—C8	111.83 (14)	H9A—C9—H9B	112.0 (17)
C7—N1—H1	124.1	O6—C19—C16	108.69 (15)
C8—N1—H1	124.1	O6—C19—C18	104.10 (15)
C15—C14—C13	117.84 (13)	C16—C19—C18	103.36 (14)
C15—C14—C6	110.08 (13)	O6—C19—H19	115.7 (10)
C13—C14—C6	105.24 (12)	C16—C19—H19	110.3 (10)
C15—C14—H14	104.3 (10)	C18—C19—H19	113.9 (10)
C13—C14—H14	111.9 (10)	O5—C20—O6	104.94 (14)
C6—C14—H14	107.1 (10)	O5—C20—C22	108.7 (2)
O4—C17—C13	110.19 (13)	O6—C20—C22	108.59 (17)
O4—C17—C16	101.97 (13)	O5—C20—C21	109.76 (17)

C13—C17—C16	114.99 (14)	O6—C20—C21	109.69 (19)
O4—C17—H17	108.4 (9)	C22—C20—C21	114.7 (2)
C13—C17—H17	112.6 (9)	C2—C1—C8	117.46 (19)
C16—C17—H17	108.0 (10)	C2—C1—H1A	121.3
C4—C5—C8	119.72 (15)	C8—C1—H1A	121.3
C4—C5—C6	131.97 (14)	C2—C3—C4	120.3 (2)
C8—C5—C6	108.26 (14)	C2—C3—H3	119.9
N2—C12—C11	104.95 (14)	C4—C3—H3	119.9
N2—C12—C13	104.46 (12)	O5—C18—O4	110.66 (15)
C11—C12—C13	115.57 (14)	O5—C18—C19	105.19 (14)
N2—C12—H12	111.5 (10)	O4—C18—C19	106.37 (13)
C11—C12—H12	112.4 (10)	O5—C18—H18	109.7 (11)
C13—C12—H12	107.7 (10)	O4—C18—H18	107.7 (11)
O1—C7—N1	127.35 (15)	C19—C18—H18	117.2 (11)
O1—C7—C6	125.38 (15)	C3—C2—C1	121.80 (19)
N1—C7—C6	107.24 (14)	C3—C2—H2	119.1
C10—C11—C12	104.84 (17)	C1—C2—H2	119.1
C10—C11—H11A	113.1 (13)	C9—C10—C11	107.29 (16)
C12—C11—H11A	111.9 (13)	C9—C10—H10B	107.9 (18)
C10—C11—H11B	108.9 (14)	C11—C10—H10B	112.7 (19)
C12—C11—H11B	112.5 (15)	C9—C10—H10A	114 (2)
H11A—C11—H11B	105.7 (18)	C11—C10—H10A	116 (2)
O3—C16—C19	105.85 (14)	H10B—C10—H10A	99 (3)
O3—C16—C17	112.20 (14)	C20—C21—H21B	109.5
C19—C16—C17	101.63 (14)	C20—C21—H21C	109.5
O3—C16—H16	108.0 (11)	H21B—C21—H21C	109.5
C19—C16—H16	113.4 (10)	C20—C21—H21A	109.5
C17—C16—H16	115.4 (11)	H21B—C21—H21A	109.5
C1—C8—C5	121.73 (18)	H21C—C21—H21A	109.5
C1—C8—N1	128.53 (18)	C20—C22—H22A	109.5
C5—C8—N1	109.73 (15)	C20—C22—H22C	109.5
C5—C4—C3	118.93 (17)	H22A—C22—H22C	109.5
C5—C4—H4	120.5	C20—C22—H22B	109.5
C3—C4—H4	120.5	H22A—C22—H22B	109.5
N2—C6—C5	114.83 (12)	H22C—C22—H22B	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.06	2.8849 (19)	161

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