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4-[4-(Diethylamino)phenyl]-*N*-methyl-3-nitro-4*H*-chromen-2-amine

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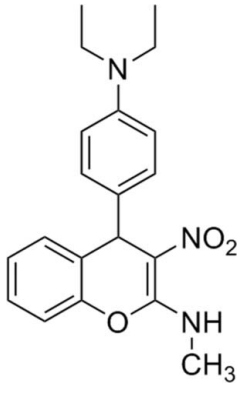
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.162; data-to-parameter ratio = 14.3.

In the title compound, $C_{20}H_{23}N_3O_3$, the dihydropyran ring adopts half-chair conformation. The chromene system makes a dihedral angle of 87.35 (5)° with the adjacent benzene ring. An intramolecular N—H···O hydrogen bond generates an S(6) motif, which stabilizes the molecular conformation. In the crystal, weak intermolecular C—H···O hydrogen bonds contribute to the stabilization of the packing.

Related literature

For the biological importance of 4*H*-chromene derivatives, see: Cai (2007, 2008); Cai *et al.* (2006); Gabor (1988); Brooks (1998); Valenti *et al.* (1993); Hyana & Saimoto (1987); Afantitis *et al.* (2006); Tang *et al.* (2007). For the structures of 4*H*-chromene derivatives, see: Muthukumaran *et al.* (2011); Gayathri *et al.* (2006); Bhaskaran *et al.* (2006). For ring puckering analysis, see: Cremer & Pople (1975) and for hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{20}H_{23}N_3O_3$
M_r = 353.41
Triclinic, $P\overline{1}$
a = 8.9199 (11) Å
b = 10.4333 (12) Å
c = 11.6697 (8) Å
α = 65.100 (9)°
β = 82.388 (8)°
γ = 69.513 (11)°
V = 922.63 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.45 × 0.35 × 0.35 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.923, T_{max} = 1.000
17119 measured reflections
3242 independent reflections
2625 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.162
S = 1.05
3242 reflections
226 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	1.96	2.596 (2)	129
C5—H5···O3^{i}	0.93	2.52	3.325 (3)	144

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; 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, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5141).

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supporting information

Acta Cryst. (2011). E**67**, o1395–o1396 [doi:10.1107/S1600536811017338]

4-[4-(Diethylamino)phenyl]-*N*-methyl-3-nitro-4*H*-chromen-2-amine

J. Muthukumaran, A. Parthiban, P. Manivel, H. Surya Prakash Rao and R. Krishna

S1. Comment

4*H*-chromenes and their derivatives possess various biological and pharmacological properties such as anti-viral, anti-fungal, anti-inflammatory, antidiabetic, cardionthonic, anti-anaphylactic and anti-cancer activity (Cai, 2008; Cai, 2007; Cai *et al.*, 2006; Gabor,1988; Brooks,1998; Valenti *et al.*, 1993; Hyana & Saimoto, 1987; Tang *et al.*, 2007). 4-aryl-4*H*-chromenes are a new series of apoptosis inducers, which exhibit potent anticancer activity (Afantitis *et al.*, 2006). Considering the importance of 4-aryl-4*H*-chromene derivatives, a single-crystal X-ray diffraction study on the title compound was carried out and analyzed.

Some 4*H*-chromene derivatives are already reported in the literature (Muthukumaran *et al.*, 2011; Gayathri *et al.*, 2006; Bhaskaran *et al.*, 2006). The molecular structure of the title compound is shown in Fig. 1. From the puckering analysis (Cremer & Pople, 1975), the fused dihydropyran ring (O1/C1/C6/C7/C8/C9) of 4*H*-chromene system is very similar to half chair (H form) conformation with puckering parameters of Q = 0.253 (2) Å, θ = 103.2 (5) ° and Φ = 7.0 (5) °. In the title compound, the 4*H*-chromene system makes a dihedral angle of 87.35 (5)° with the adjacent phenyl ring. The intramolecular N1—H1···O2 interaction generates a graph-set motif S (6) (Bernstein *et al.*, 1995) (Fig. 2) with a *D*···*A* bond distance of 2.596 (2) Å. The crystal packing (Fig. 3) is stabilized by weak intermolecular C—H···O interactions.

S2. Experimental

To a vigorously stirred solution of *N*-methyl-*N*-[3-nitro-4-(methylsulfanyl)-4*H*-2-chromenyl]amine (0.5 g, 2 mmol) in ethanol (15 ml), *N*, *N*-diethylaminobenzene (0.33 g, 2.2 mmol) was added and the resulting solution was refluxed for 12 h by which time the reaction was complete (TLC; hexane: EtOAc, 6:4). The reaction mixture was cooled to room temperature and kept aside for 3 h. The solid, which separated was filtered to obtain 0.59 g of *N*2-methyl-4-[4-(diethyl-amino)phenyl]-3-nitro-4*H*-2-chromenamine in 92% yield as colorless solid; mp 201 °C. R_f 0.4 (hexane: EtOAc, 6:4). A sample suitable for single crystal X-ray analysis was obtained by recrystallization from a mixture of dichloromethane and hexane (3:1).

S3. Refinement

All hydrogen atoms were placed in calculated positions, with N—H=0.86 and C—H=0.93 and included in the final cycles of refinement using a riding model with U_{iso}(H) = 1.2 U_{eq}(C).

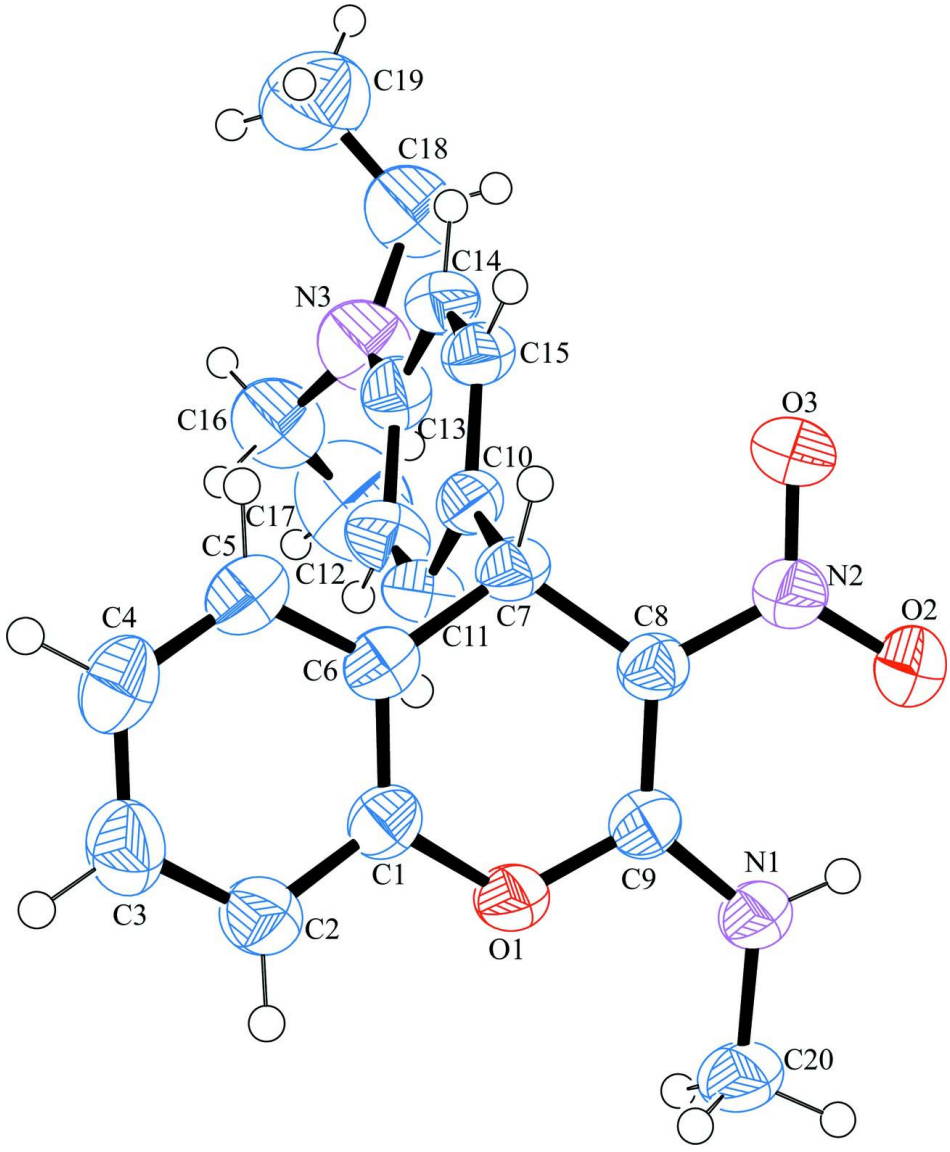

Figure 1

The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level.

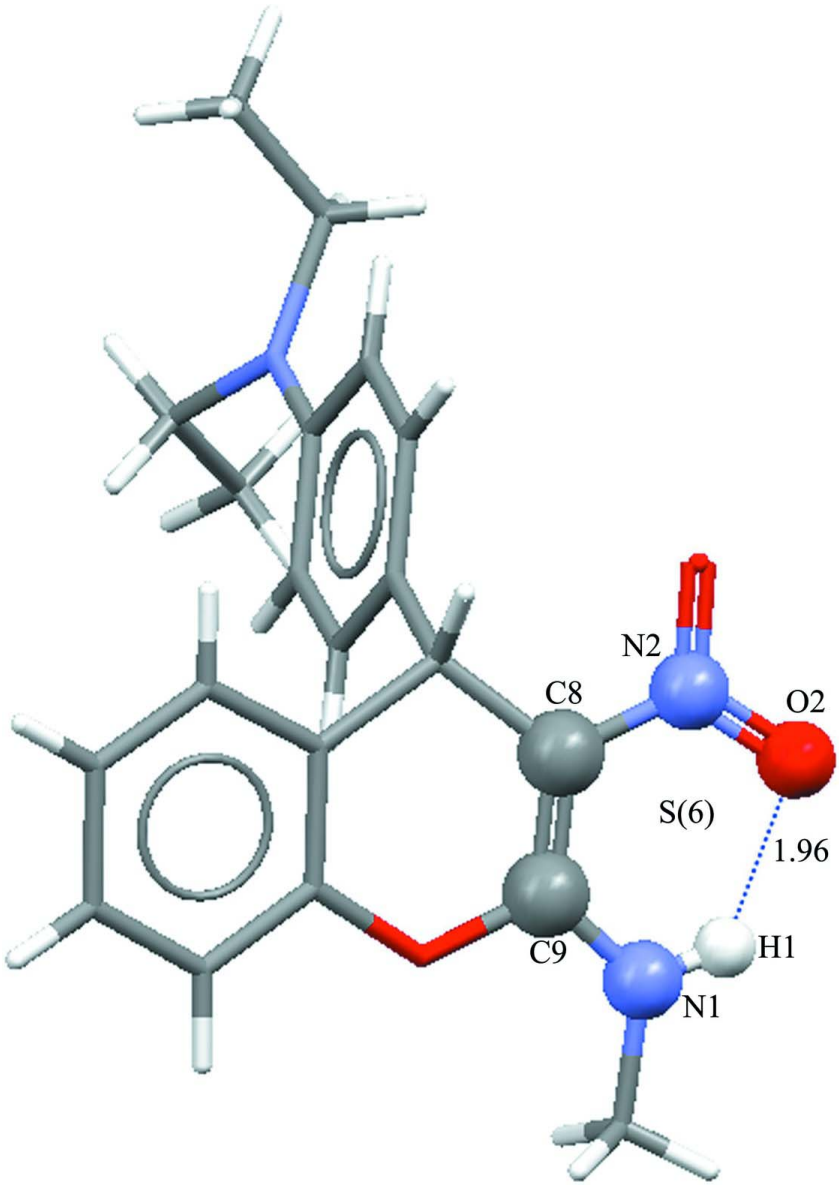

Figure 2

A view of intramolecular motif *S* (6) formed by N—H···O interaction in Compound (I). The motif forming atoms are shown in ball and stick model and the Hydrogen bond are shown in blue dashed lines.

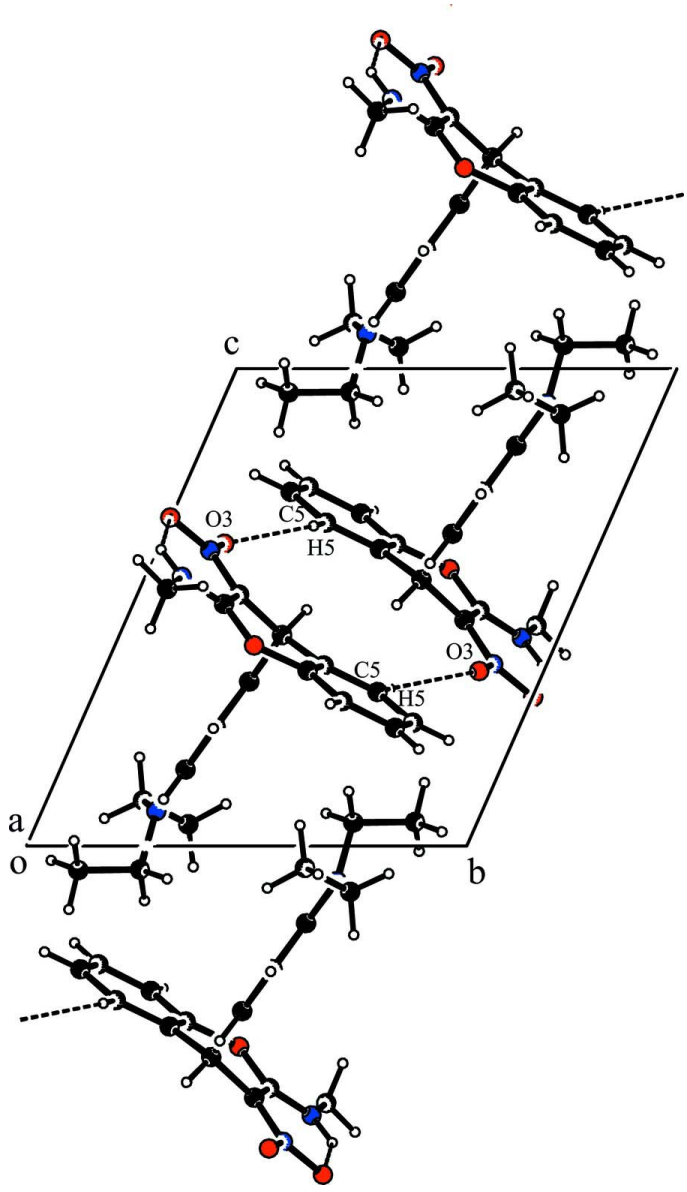

Figure 3

The crystal packing of (I) showing intermolecular interactions as dashed lines.

4-[4-(Diethylamino)phenyl]-*N*-methyl-3-nitro-4*H*-chromen-2-amine

Crystal data

$C_{20}H_{23}N_3O_3$
M_r = 353.41
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.9199 (11) Å
b = 10.4333 (12) Å
c = 11.6697 (8) Å
α = 65.100 (9)°
β = 82.388 (8)°
γ = 69.513 (11)°
V = 922.63 (19) Å^3
Z = 2
F(000) = 376
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8151 reflections
θ = 2.7–29.3°
μ = 0.09 mm^{-1}

T = 293 K
Block, yellow

0.45 × 0.35 × 0.35 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 15.9821 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.923, T_{max} = 1.000

17119 measured reflections
3242 independent reflections
2625 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 25.0°, θ_{min} = 2.7°
h = −10→10
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.162
S = 1.05
3242 reflections
226 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 0.5254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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}
O1	0.42869 (17)	0.68371 (16)	0.57975 (15)	0.0483 (4)
N1	0.3634 (2)	0.9167 (2)	0.43607 (18)	0.0466 (5)
H1	0.3882	0.9910	0.3790	0.056*
N2	0.6967 (2)	0.8783 (2)	0.38082 (17)	0.0474 (5)
C8	0.6437 (2)	0.7689 (2)	0.47334 (19)	0.0395 (5)
C7	0.7689 (2)	0.6305 (2)	0.55805 (19)	0.0391 (5)
H7	0.8571	0.6001	0.5053	0.047*
O3	0.84395 (19)	0.8532 (2)	0.36670 (17)	0.0620 (5)
C9	0.4810 (2)	0.7932 (2)	0.4932 (2)	0.0397 (5)
O2	0.5993 (2)	1.00198 (19)	0.31188 (17)	0.0658 (5)
C6	0.6982 (2)	0.5058 (2)	0.6218 (2)	0.0399 (5)
C10	0.8361 (2)	0.6586 (2)	0.65559 (19)	0.0385 (5)
C15	0.9923 (2)	0.6551 (2)	0.6541 (2)	0.0425 (5)
H15	1.0599	0.6340	0.5919	0.051*

C1	0.5350 (3)	0.5370 (2)	0.6324 (2)	0.0424 (5)
C13	0.9558 (3)	0.7122 (3)	0.8384 (2)	0.0491 (6)
C5	0.7938 (3)	0.3569 (3)	0.6773 (2)	0.0484 (6)
H5	0.9044	0.3321	0.6705	0.058*
C11	0.7400 (3)	0.6897 (3)	0.7504 (2)	0.0482 (5)
H11	0.6339	0.6932	0.7536	0.058*
C14	1.0514 (3)	0.6821 (3)	0.7422 (2)	0.0478 (5)
H14	1.1570	0.6802	0.7373	0.057*
C12	0.7968 (3)	0.7153 (3)	0.8397 (2)	0.0544 (6)
H12	0.7288	0.7351	0.9022	0.065*
C20	0.1945 (3)	0.9377 (3)	0.4617 (3)	0.0563 (6)
H20A	0.1681	0.8589	0.4560	0.084*
H20B	0.1316	1.0323	0.4009	0.084*
H20C	0.1724	0.9357	0.5451	0.084*
N3	1.0125 (3)	0.7401 (3)	0.9267 (2)	0.0778 (5)
C2	0.4655 (3)	0.4275 (3)	0.6966 (2)	0.0527 (6)
H2	0.3548	0.4520	0.7021	0.063*
C3	0.5633 (3)	0.2813 (3)	0.7523 (3)	0.0602 (7)
H3	0.5187	0.2061	0.7971	0.072*
C4	0.7278 (3)	0.2458 (3)	0.7418 (2)	0.0584 (6)
H4	0.7935	0.1467	0.7784	0.070*
C18	1.1609 (4)	0.7810 (4)	0.9042 (3)	0.0778 (5)
H18A	1.1720	0.8322	0.8140	0.093*
H18B	1.1496	0.8506	0.9421	0.093*
C16	0.9352 (4)	0.7188 (4)	1.0492 (3)	0.0778 (5)
H16A	0.8790	0.6478	1.0685	0.093*
H16B	1.0165	0.6772	1.1144	0.093*
C17	0.8226 (6)	0.8584 (5)	1.0503 (5)	0.1329 (17)
H17A	0.8774	0.9296	1.0298	0.199*
H17B	0.7774	0.8405	1.1327	0.199*
H17C	0.7387	0.8971	0.9890	0.199*
C19	1.3069 (5)	0.6543 (5)	0.9545 (4)	0.1141 (14)
H19A	1.2959	0.6005	1.0433	0.171*
H19B	1.3960	0.6901	0.9411	0.171*
H19C	1.3248	0.5891	0.9120	0.171*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0341 (8)	0.0406 (8)	0.0607 (10)	−0.0087 (6)	0.0025 (7)	−0.0150 (7)
N1	0.0364 (9)	0.0393 (10)	0.0554 (11)	−0.0078 (8)	−0.0005 (8)	−0.0145 (9)
N2	0.0400 (10)	0.0525 (11)	0.0445 (11)	−0.0133 (9)	0.0030 (8)	−0.0168 (9)
C8	0.0367 (11)	0.0437 (11)	0.0381 (11)	−0.0115 (9)	0.0013 (9)	−0.0179 (9)
C7	0.0316 (10)	0.0437 (11)	0.0406 (11)	−0.0070 (8)	0.0014 (8)	−0.0202 (9)
O3	0.0406 (9)	0.0702 (11)	0.0623 (11)	−0.0191 (8)	0.0105 (8)	−0.0170 (9)
C9	0.0386 (11)	0.0401 (11)	0.0411 (11)	−0.0103 (9)	−0.0002 (9)	−0.0187 (9)
O2	0.0520 (10)	0.0530 (10)	0.0628 (11)	−0.0111 (8)	−0.0009 (8)	−0.0005 (9)
C6	0.0407 (11)	0.0436 (12)	0.0386 (11)	−0.0100 (9)	−0.0032 (9)	−0.0214 (9)

C10	0.0361 (10)	0.0386 (11)	0.0383 (11)	−0.0094 (8)	−0.0008 (8)	−0.0150 (9)
C15	0.0344 (11)	0.0470 (12)	0.0442 (12)	−0.0094 (9)	0.0013 (9)	−0.0199 (10)
C1	0.0418 (11)	0.0393 (11)	0.0451 (12)	−0.0090 (9)	−0.0023 (9)	−0.0186 (10)
C13	0.0539 (13)	0.0516 (13)	0.0449 (13)	−0.0201 (11)	−0.0051 (10)	−0.0184 (11)
C5	0.0455 (12)	0.0486 (13)	0.0494 (13)	−0.0057 (10)	−0.0061 (10)	−0.0241 (11)
C11	0.0381 (11)	0.0626 (14)	0.0517 (13)	−0.0198 (10)	0.0060 (10)	−0.0292 (11)
C14	0.0371 (11)	0.0543 (13)	0.0515 (13)	−0.0157 (10)	−0.0025 (10)	−0.0192 (11)
C12	0.0543 (14)	0.0726 (16)	0.0496 (14)	−0.0261 (12)	0.0123 (11)	−0.0359 (13)
C20	0.0363 (12)	0.0499 (13)	0.0732 (17)	−0.0054 (10)	0.0002 (11)	−0.0229 (12)
N3	0.0905 (12)	0.1014 (13)	0.0670 (10)	−0.0482 (10)	−0.0023 (9)	−0.0428 (10)
C2	0.0494 (13)	0.0516 (14)	0.0595 (15)	−0.0204 (11)	0.0012 (11)	−0.0216 (12)
C3	0.0729 (17)	0.0459 (14)	0.0617 (16)	−0.0251 (12)	−0.0033 (13)	−0.0158 (12)
C4	0.0681 (17)	0.0405 (13)	0.0597 (15)	−0.0073 (11)	−0.0104 (12)	−0.0191 (11)
C18	0.0905 (12)	0.1014 (13)	0.0670 (10)	−0.0482 (10)	−0.0023 (9)	−0.0428 (10)
C16	0.0905 (12)	0.1014 (13)	0.0670 (10)	−0.0482 (10)	−0.0023 (9)	−0.0428 (10)
C17	0.172 (5)	0.129 (4)	0.145 (4)	−0.071 (3)	0.028 (3)	−0.088 (3)
C19	0.094 (3)	0.151 (4)	0.098 (3)	−0.039 (3)	−0.022 (2)	−0.044 (3)

Geometric parameters (Å, º)

O1—C9	1.349 (3)	C11—C12	1.373 (3)
O1—C1	1.402 (2)	C11—H11	0.9300
N1—C9	1.312 (3)	C14—H14	0.9300
N1—C20	1.453 (3)	C12—H12	0.9300
N1—H1	0.8600	C20—H20A	0.9600
N2—O3	1.249 (2)	C20—H20B	0.9600
N2—O2	1.262 (2)	C20—H20C	0.9600
N2—C8	1.377 (3)	N3—C16	1.465 (4)
C8—C9	1.388 (3)	N3—C18	1.487 (4)
C8—C7	1.507 (3)	C2—C3	1.376 (3)
C7—C6	1.510 (3)	C2—H2	0.9300
C7—C10	1.525 (3)	C3—C4	1.384 (4)
C7—H7	0.9800	C3—H3	0.9300
O3—N2	1.249 (2)	C4—H4	0.9300
O2—N2	1.262 (2)	C18—C19	1.460 (5)
C6—C1	1.377 (3)	C18—H18A	0.9700
C6—C5	1.390 (3)	C18—H18B	0.9700
C10—C15	1.380 (3)	C16—C17	1.455 (5)
C10—C11	1.385 (3)	C16—H16A	0.9700
C15—C14	1.380 (3)	C16—H16B	0.9700
C15—H15	0.9300	C17—H17A	0.9600
C1—C2	1.380 (3)	C17—H17B	0.9600
C13—N3	1.378 (3)	C17—H17C	0.9600
C13—C14	1.393 (3)	C19—H19A	0.9600
C13—C12	1.406 (3)	C19—H19B	0.9600
C5—C4	1.372 (4)	C19—H19C	0.9600
C5—H5	0.9300		

C9—O1—C1	119.79 (16)	C11—C12—H12	119.4
C9—N1—C20	125.1 (2)	C13—C12—H12	119.4
C9—N1—H1	117.5	N1—C20—H20A	109.5
C20—N1—H1	117.5	N1—C20—H20B	109.5
O3—N2—O2	120.32 (18)	H20A—C20—H20B	109.5
O3—N2—O2	120.32 (18)	N1—C20—H20C	109.5
O3—N2—C8	118.58 (18)	H20A—C20—H20C	109.5
O2—N2—C8	121.10 (18)	H20B—C20—H20C	109.5
N2—C8—C9	120.35 (19)	C13—N3—C16	120.7 (2)
N2—C8—C7	117.15 (17)	C13—N3—C18	120.8 (2)
C9—C8—C7	122.25 (19)	C16—N3—C18	118.3 (2)
C6—C7—C8	109.37 (17)	C3—C2—C1	118.6 (2)
C6—C7—C10	110.83 (17)	C3—C2—H2	120.7
C8—C7—C10	111.95 (17)	C1—C2—H2	120.7
C6—C7—H7	108.2	C2—C3—C4	120.2 (2)
C10—C7—H7	108.2	C2—C3—H3	119.9
N1—C9—O1	112.50 (18)	C4—C3—H3	119.9
N1—C9—C8	127.1 (2)	C5—C4—C3	119.9 (2)
O1—C9—C8	120.41 (18)	C5—C4—H4	120.0
C1—C6—C5	117.4 (2)	C3—C4—H4	120.0
C1—C6—C7	120.57 (18)	C19—C18—N3	114.4 (3)
C5—C6—C7	121.92 (19)	C19—C18—H18A	108.7
C15—C10—C11	117.06 (19)	N3—C18—H18A	108.7
C15—C10—C7	122.49 (18)	C19—C18—H18B	108.7
C11—C10—C7	120.45 (18)	N3—C18—H18B	108.7
C14—C15—C10	122.0 (2)	H18A—C18—H18B	107.6
C14—C15—H15	119.0	C17—C16—N3	112.0 (3)
C10—C15—H15	119.0	C17—C16—H16A	109.2
C6—C1—C2	122.6 (2)	N3—C16—H16A	109.2
C6—C1—O1	121.69 (19)	C17—C16—H16B	109.2
C2—C1—O1	115.70 (19)	N3—C16—H16B	109.2
N3—C13—C14	122.1 (2)	H16A—C16—H16B	107.9
N3—C13—C12	121.4 (2)	C16—C17—H17A	109.5
C14—C13—C12	116.5 (2)	C16—C17—H17B	109.5
C4—C5—C6	121.2 (2)	H17A—C17—H17B	109.5
C4—C5—H5	119.4	C16—C17—H17C	109.5
C6—C5—H5	119.4	H17A—C17—H17C	109.5
C12—C11—C10	121.9 (2)	H17B—C17—H17C	109.5
C12—C11—H11	119.0	C18—C19—H19A	109.5
C10—C11—H11	119.0	C18—C19—H19B	109.5
C15—C14—C13	121.3 (2)	H19A—C19—H19B	109.5
C15—C14—H14	119.3	C18—C19—H19C	109.5
C13—C14—H14	119.3	H19A—C19—H19C	109.5
C11—C12—C13	121.2 (2)	H19B—C19—H19C	109.5

O3—N2—C8—N2	0 (17)	C8—C7—C6—C5	162.23 (19)
O2—N2—C8—N2	0 (100)	C10—C7—C6—C5	−73.9 (2)
O2—N2—C8—N2	0 (100)	C6—C7—C10—C15	124.8 (2)

N2—N2—C8—C9	0.00 (11)	C8—C7—C10—C15	−112.8 (2)
O3—N2—C8—C9	179.15 (19)	C6—C7—C10—C11	−55.4 (3)
O2—N2—C8—C9	−0.4 (3)	C8—C7—C10—C11	67.0 (3)
O2—N2—C8—C9	−0.4 (3)	C11—C10—C15—C14	−0.4 (3)
N2—N2—C8—C7	0.00 (19)	C7—C10—C15—C14	179.4 (2)
O3—N2—C8—C7	4.7 (3)	C5—C6—C1—C2	1.0 (3)
O2—N2—C8—C7	−174.88 (19)	C7—C6—C1—C2	−175.9 (2)
O2—N2—C8—C7	−174.88 (19)	C5—C6—C1—O1	179.92 (18)
N2—C8—C7—C6	−161.30 (17)	C7—C6—C1—O1	3.0 (3)
N2—C8—C7—C6	−161.30 (17)	C9—O1—C1—C6	15.4 (3)
C9—C8—C7—C6	24.4 (3)	C9—O1—C1—C2	−165.57 (19)
N2—C8—C7—C10	75.5 (2)	C1—C6—C5—C4	−1.0 (3)
N2—C8—C7—C10	75.5 (2)	C7—C6—C5—C4	175.8 (2)
C9—C8—C7—C10	−98.9 (2)	C15—C10—C11—C12	−0.3 (3)
O2—N2—O3—N2	0 (39)	C7—C10—C11—C12	179.9 (2)
O2—N2—O3—N2	0 (39)	C10—C15—C14—C13	1.0 (3)
C8—N2—O3—N2	0 (100)	N3—C13—C14—C15	−179.6 (2)
C20—N1—C9—O1	0.6 (3)	C12—C13—C14—C15	−0.8 (3)
C20—N1—C9—C8	−178.9 (2)	C10—C11—C12—C13	0.4 (4)
C1—O1—C9—N1	168.16 (18)	N3—C13—C12—C11	179.0 (2)
C1—O1—C9—C8	−12.3 (3)	C14—C13—C12—C11	0.1 (4)
N2—C8—C9—N1	−3.7 (3)	C14—C13—N3—C16	−158.1 (3)
N2—C8—C9—N1	−3.7 (3)	C12—C13—N3—C16	23.1 (4)
C7—C8—C9—N1	170.5 (2)	C14—C13—N3—C18	17.1 (4)
N2—C8—C9—O1	176.92 (18)	C12—C13—N3—C18	−161.7 (3)
N2—C8—C9—O1	176.92 (18)	C6—C1—C2—C3	0.0 (4)
C7—C8—C9—O1	−8.9 (3)	O1—C1—C2—C3	−179.0 (2)
N2—N2—O2—O2	0.0	C1—C2—C3—C4	−1.0 (4)
O3—N2—O2—O2	0.0 (2)	C6—C5—C4—C3	0.1 (4)
C8—N2—O2—O2	0.00 (11)	C2—C3—C4—C5	1.0 (4)
O3—N2—O2—N2	0 (10)	C13—N3—C18—C19	−92.4 (4)
O2—N2—O2—N2	0 (100)	C16—N3—C18—C19	82.9 (4)
C8—N2—O2—N2	0 (100)	C13—N3—C16—C17	−97.1 (4)
C8—C7—C6—C1	−21.0 (3)	C18—N3—C16—C17	87.6 (4)
C10—C7—C6—C1	102.9 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	1.96	2.596 (2)	129
C5—H5···O3^{i}	0.93	2.52	3.325 (3)	144

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