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4-Nitrophenyl naphthalene-1-sulfonate

Jasmine P. Vennila,[a] Helen P. Kavitha,[b] D. John Thiruvadigal,[c] B. R. Venkatraman[d] and V. Manivannan[e]*

[a]Department of Physics, Panimalar Institute of Technology, Chennai 600 095, India, [b]Department of Chemistry, SRM University, Ramapuram, Chennai 600 089, India, [c]Department of Physics, SRM University, Kattankulathur Campus, Chennai, India, [d]Department of Chemistry, Periyar E.V.R. College, Tiruchirappalli 620 023, India, and [e]Department of Physics, Presidency College, Chennai 600 005, India
Correspondence e-mail: manivan_1999@yahoo.com

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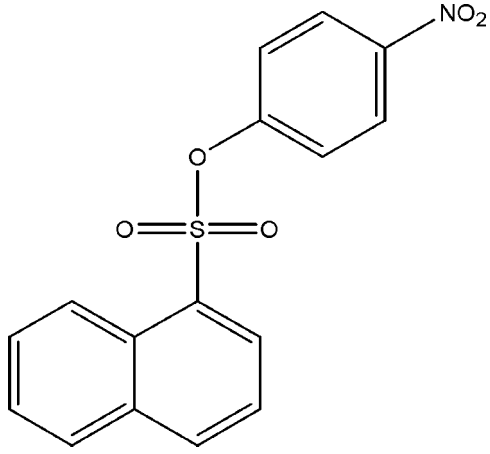
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.160; data-to-parameter ratio = 13.5.

In the crystal structure of the title compound, $C_{16}H_{11}NO_5S$, the plane of the naphthalene ring system forms a dihedral angle of 63.39 (8)° with the benzene ring. The nitro group makes a dihedral angle of 10.73 (16)° with the benzene ring. Weak intra- and intermolecular C—H···O interactions are observed.

Related literature

For related literature, see: Manivannan *et al.* (2005); Vennila *et al.* (2008); Yachi *et al.* (1989).



Experimental

Crystal data

$C_{16}H_{11}NO_5S$
M_r = 329.32
Monoclinic, $P2_1/n$
a = 13.4407 (8) Å
b = 6.2990 (3) Å
c = 18.2556 (12) Å
β = 106.296 (2)°
V = 1483.48 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 295 (2) K
0.28 × 0.20 × 0.16 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.935, T_{max} = 0.962
14281 measured reflections
2801 independent reflections
1935 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.160
S = 1.08
2801 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 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
C8—H8···O2	0.93	2.43	2.829 (5)	106
C16—H16···O3	0.93	2.46	3.058 (4)	122
C5—H5···O2^{i}	0.93	2.48	3.179 (3)	132
C15—H15···O4^{ii}	0.93	2.47	3.340 (5)	155

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

Data collection: *APEX2* and *SAINT* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge the Sophisticated Analytical Instrument Facility, Indian Institute of Technology, Chennai, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2328).

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supporting information

Acta Cryst. (2008). E**64**, o1848 [doi:10.1107/S1600536808027396]

4-Nitrophenyl naphthalene-1-sulfonate

Jasmine P. Vennila, Helen P. Kavitha, D. John Thiruvadigal, B. R. Venkatraman and V. Manivannan

S1. Comment

The merging of lipids can be monitored using a derivative of *para*-toluene sulfonate (Yachi *et al.*, 1989). The geometric parameters of the title molecule, (I) (Fig. 1), agree well with the reported structures (Manivannan *et al.* 2005; Vennila *et al.* 2008)

The plane of the benzene ring forms a dihedral angle of 63.39 (8)° with the naphthalene ring system. The torsion angles O2—S1—C7—C8 and O3—S1—C7—C12 [0.1 (3) ° and 45.8 (2)°, respectively] indicate the *syn* conformation of sulfonyl moiety. The molecular structure is stabilized by weak intramolecular C—H···O interactions and the crystal packing is stabilized by weak intermolecular C—H···O interactions (Fig. 2).

S2. Experimental

1-Naphthalene sulfonyl chloride (2.5 mmol) dissolved in acetone (4 ml) was added dropwise to 4-nitrophenol (2.5 mmol) in aqueous NaOH (4 ml, 5%) with constant shaking. The precipitated compound (1.8 mmol, yield 72%) was recrystallized from ethanol to get diffraction quality pale yellow crystals.

S3. Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C).

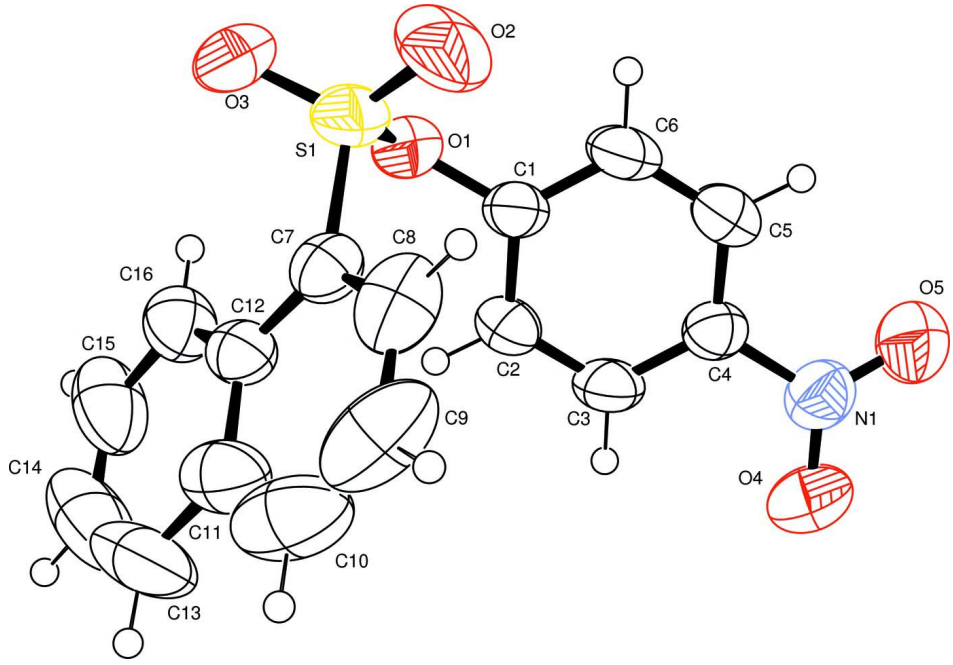

Figure 1

The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

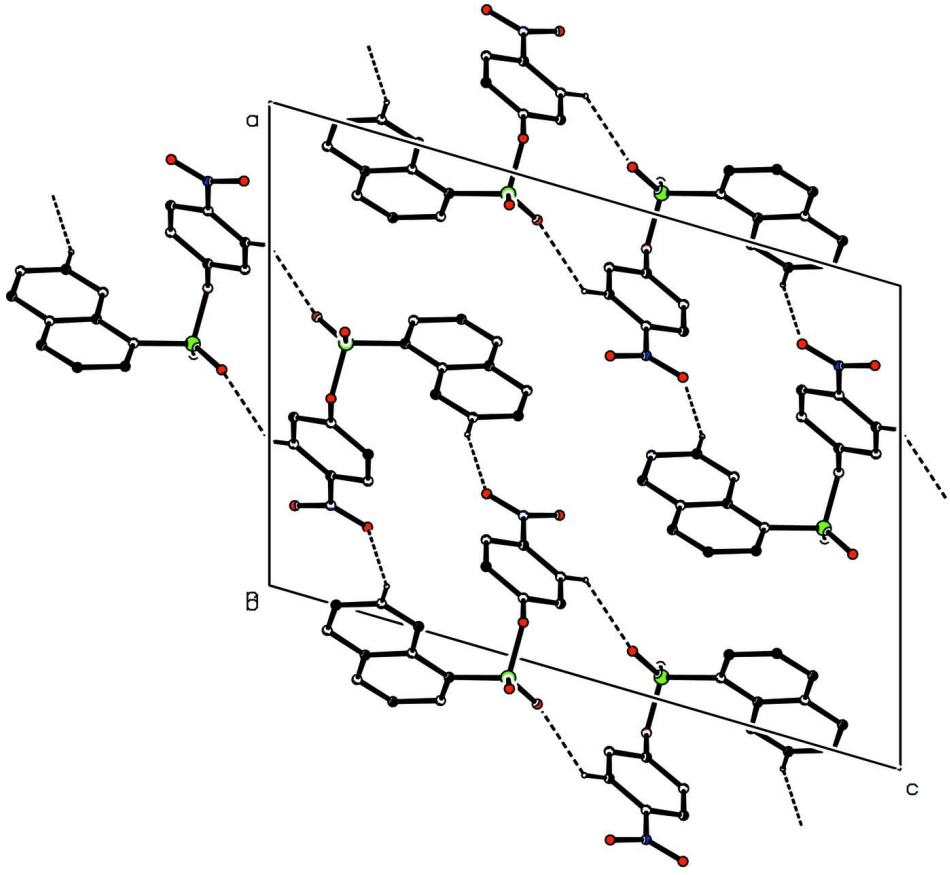

Figure 2

The packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

4-Nitrophenyl naphthalene-1-sulfonate

Crystal data

$C_{16}H_{11}NO_5S$
$M_r = 329.32$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 13.4407\ (8)$ Å
$b = 6.2990\ (3)$ Å
$c = 18.2556\ (12)$ Å
$\beta = 106.296\ (2)°$
$V = 1483.48\ (15)$ Å^3
$Z = 4$
$F(000) = 680$
$D_x = 1.474$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4818 reflections
$\theta = 2.2–25.4°$
$\mu = 0.24$ mm^{-1}
$T = 295$ K
Block, yellow
0.28 × 0.20 × 0.16 mm

Data collection

Bruker Kappa APEX2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.935$, $T_{max} = 0.962$
14281 measured reflections
2801 independent reflections
1935 reflections with $I > 2\sigma(I)$

R_{int} = 0.041
θ_{max} = 25.7°, θ_{min} = 1.7°
h = −16→16
k = −7→5
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.160
S = 1.08
2801 reflections
208 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0801P)^2 + 0.4092P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.54713 (6)	0.94373 (13)	0.12153 (4)	0.0704 (3)
C1	0.37278 (18)	0.7401 (4)	0.09748 (13)	0.0528 (6)
C2	0.3303 (2)	0.7033 (4)	0.15655 (14)	0.0598 (6)
H2	0.3391	0.8008	0.1961	0.072*
C3	0.2749 (2)	0.5218 (4)	0.15633 (15)	0.0613 (7)
H3	0.2454	0.4937	0.1957	0.074*
C4	0.26342 (18)	0.3817 (4)	0.09726 (14)	0.0537 (6)
C5	0.3065 (2)	0.4177 (4)	0.03838 (15)	0.0654 (7)
H5	0.2979	0.3198	−0.0010	0.079*
C6	0.3621 (2)	0.5999 (4)	0.03865 (15)	0.0673 (7)
H6	0.3921	0.6277	−0.0005	0.081*
C7	0.58144 (18)	0.8465 (4)	0.21516 (15)	0.0576 (6)
C8	0.6346 (2)	0.6587 (5)	0.2287 (2)	0.0839 (9)
H8	0.6500	0.5851	0.1891	0.101*
C9	0.6658 (3)	0.5785 (7)	0.3043 (4)	0.1117 (16)
H9	0.7032	0.4525	0.3147	0.134*
C10	0.6415 (3)	0.6838 (9)	0.3611 (3)	0.1157 (15)
H10	0.6627	0.6289	0.4103	0.139*
C11	0.5863 (2)	0.8702 (6)	0.34821 (18)	0.0846 (10)
C12	0.55403 (18)	0.9590 (4)	0.27417 (14)	0.0577 (6)
C13	0.5581 (4)	0.9799 (11)	0.4083 (2)	0.1245 (18)
H13	0.5799	0.9270	0.4579	0.149*
C14	0.5005 (4)	1.1579 (11)	0.3943 (3)	0.137 (2)
H14	0.4815	1.2248	0.4337	0.165*
C15	0.4701 (3)	1.2404 (7)	0.3225 (3)	0.1029 (12)
H15	0.4312	1.3647	0.3139	0.124*
C16	0.4949 (2)	1.1465 (5)	0.26351 (18)	0.0725 (8)
H16	0.4725	1.2067	0.2151	0.087*
O1	0.42304 (14)	0.9358 (3)	0.09765 (10)	0.0644 (5)
O2	0.58335 (18)	0.7992 (4)	0.07547 (14)	0.1056 (8)
O3	0.56871 (18)	1.1638 (4)	0.11968 (12)	0.0901 (7)

O4	0.1795 (2)	0.1450 (4)	0.15547 (16)	0.1094 (9)
O5	0.1800 (2)	0.0787 (4)	0.04028 (14)	0.0949 (7)
N1	0.20241 (18)	0.1888 (4)	0.09722 (15)	0.0705 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0768 (5)	0.0848 (6)	0.0604 (5)	−0.0147 (4)	0.0373 (4)	−0.0034 (3)
C1	0.0608 (14)	0.0552 (14)	0.0448 (12)	0.0025 (11)	0.0187 (10)	0.0049 (11)
C2	0.0746 (16)	0.0619 (16)	0.0507 (14)	0.0009 (12)	0.0304 (12)	−0.0052 (12)
C3	0.0741 (16)	0.0690 (17)	0.0507 (15)	0.0013 (13)	0.0337 (12)	0.0051 (12)
C4	0.0581 (14)	0.0527 (14)	0.0511 (14)	0.0055 (11)	0.0168 (11)	0.0068 (11)
C5	0.0781 (17)	0.0737 (18)	0.0491 (14)	−0.0039 (14)	0.0254 (13)	−0.0083 (12)
C6	0.0809 (18)	0.085 (2)	0.0436 (14)	−0.0105 (15)	0.0306 (13)	−0.0030 (13)
C7	0.0517 (13)	0.0586 (15)	0.0676 (16)	−0.0013 (12)	0.0252 (12)	0.0026 (12)
C8	0.0627 (16)	0.0708 (19)	0.124 (3)	0.0023 (15)	0.0362 (18)	−0.0020 (19)
C9	0.065 (2)	0.092 (3)	0.167 (5)	0.0121 (17)	0.014 (2)	0.057 (3)
C10	0.080 (2)	0.154 (4)	0.098 (3)	−0.011 (3)	0.001 (2)	0.056 (3)
C11	0.0654 (18)	0.120 (3)	0.0612 (19)	−0.0228 (19)	0.0052 (14)	0.0139 (18)
C12	0.0504 (13)	0.0711 (17)	0.0525 (15)	−0.0091 (12)	0.0158 (11)	0.0008 (12)
C13	0.101 (3)	0.224 (6)	0.0479 (19)	−0.057 (3)	0.0186 (19)	−0.009 (3)
C14	0.119 (4)	0.214 (6)	0.096 (4)	−0.058 (4)	0.058 (3)	−0.076 (4)
C15	0.095 (2)	0.116 (3)	0.112 (3)	−0.019 (2)	0.052 (2)	−0.053 (2)
C16	0.0740 (18)	0.0747 (19)	0.0751 (19)	−0.0021 (15)	0.0312 (15)	−0.0112 (15)
O1	0.0746 (12)	0.0641 (12)	0.0561 (11)	−0.0065 (9)	0.0206 (9)	0.0071 (8)
O2	0.1001 (16)	0.145 (2)	0.0946 (16)	−0.0191 (15)	0.0642 (14)	−0.0393 (15)
O3	0.1088 (17)	0.0895 (15)	0.0763 (14)	−0.0348 (12)	0.0328 (12)	0.0139 (11)
O4	0.151 (2)	0.0943 (17)	0.1024 (19)	−0.0314 (15)	0.0678 (18)	0.0109 (14)
O5	0.1127 (19)	0.0819 (16)	0.0837 (17)	−0.0223 (12)	0.0167 (13)	−0.0090 (12)
N1	0.0763 (15)	0.0610 (15)	0.0735 (17)	0.0015 (11)	0.0196 (13)	0.0074 (13)

Geometric parameters (Å, º)

S1—O2	1.415 (2)	C8—C9	1.418 (6)
S1—O3	1.419 (2)	C8—H8	0.9300
S1—O1	1.602 (2)	C9—C10	1.346 (6)
S1—C7	1.751 (3)	C9—H9	0.9300
C1—C6	1.367 (4)	C10—C11	1.374 (6)
C1—C2	1.374 (3)	C10—H10	0.9300
C1—O1	1.405 (3)	C11—C12	1.414 (4)
C2—C3	1.364 (4)	C11—C13	1.435 (6)
C2—H2	0.9300	C12—C16	1.406 (4)
C3—C4	1.368 (4)	C13—C14	1.345 (7)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.375 (4)	C14—C15	1.361 (7)
C4—N1	1.466 (3)	C14—H14	0.9300
C5—C6	1.369 (4)	C15—C16	1.350 (4)
C5—H5	0.9300	C15—H15	0.9300

C6—H6	0.9300	C16—H16	0.9300
C7—C8	1.368 (4)	O4—N1	1.218 (3)
C7—C12	1.422 (4)	O5—N1	1.215 (3)

O2—S1—O3	120.53 (15)	C9—C8—H8	120.6
O2—S1—O1	108.88 (12)	C10—C9—C8	120.3 (4)
O3—S1—O1	103.19 (12)	C10—C9—H9	119.9
O2—S1—C7	108.34 (15)	C8—C9—H9	119.9
O3—S1—C7	111.42 (13)	C9—C10—C11	121.7 (4)
O1—S1—C7	102.92 (10)	C9—C10—H10	119.1
C6—C1—C2	122.2 (2)	C11—C10—H10	119.1
C6—C1—O1	120.9 (2)	C10—C11—C12	120.5 (4)
C2—C1—O1	116.9 (2)	C10—C11—C13	121.8 (4)
C3—C2—C1	119.1 (2)	C12—C11—C13	117.7 (4)
C3—C2—H2	120.5	C16—C12—C11	118.3 (3)
C1—C2—H2	120.5	C16—C12—C7	124.8 (2)
C2—C3—C4	118.9 (2)	C11—C12—C7	116.9 (3)
C2—C3—H3	120.5	C14—C13—C11	121.1 (4)
C4—C3—H3	120.5	C14—C13—H13	119.5
C3—C4—C5	122.1 (2)	C11—C13—H13	119.5
C3—C4—N1	118.3 (2)	C13—C14—C15	120.3 (4)
C5—C4—N1	119.6 (2)	C13—C14—H14	119.9
C6—C5—C4	119.0 (2)	C15—C14—H14	119.9
C6—C5—H5	120.5	C16—C15—C14	121.7 (4)
C4—C5—H5	120.5	C16—C15—H15	119.1
C1—C6—C5	118.8 (2)	C14—C15—H15	119.1
C1—C6—H6	120.6	C15—C16—C12	120.9 (3)
C5—C6—H6	120.6	C15—C16—H16	119.5
C8—C7—C12	121.8 (3)	C12—C16—H16	119.5
C8—C7—S1	117.4 (2)	C1—O1—S1	119.41 (15)
C12—C7—S1	120.8 (2)	O5—N1—O4	123.7 (3)
C7—C8—C9	118.8 (4)	O5—N1—C4	118.6 (2)
C7—C8—H8	120.6	O4—N1—C4	117.7 (3)

C6—C1—C2—C3	−0.5 (4)	C13—C11—C12—C16	−1.2 (4)
O1—C1—C2—C3	175.8 (2)	C10—C11—C12—C7	0.1 (4)
C1—C2—C3—C4	0.1 (4)	C13—C11—C12—C7	−179.1 (3)
C2—C3—C4—C5	0.4 (4)	C8—C7—C12—C16	−176.5 (3)
C2—C3—C4—N1	−179.1 (2)	S1—C7—C12—C16	3.0 (3)
C3—C4—C5—C6	−0.3 (4)	C8—C7—C12—C11	1.3 (4)
N1—C4—C5—C6	179.1 (2)	S1—C7—C12—C11	−179.13 (19)
C2—C1—C6—C5	0.5 (4)	C10—C11—C13—C14	−177.4 (4)
O1—C1—C6—C5	−175.6 (2)	C12—C11—C13—C14	1.8 (6)
C4—C5—C6—C1	−0.1 (4)	C11—C13—C14—C15	−1.7 (7)
O2—S1—C7—C8	0.1 (3)	C13—C14—C15—C16	0.9 (7)
O3—S1—C7—C8	−134.7 (2)	C14—C15—C16—C12	−0.3 (5)
O1—S1—C7—C8	115.3 (2)	C11—C12—C16—C15	0.5 (4)
O2—S1—C7—C12	−179.42 (19)	C7—C12—C16—C15	178.3 (3)

O3—S1—C7—C12	45.8 (2)	C6—C1—O1—S1	−78.7 (3)
O1—S1—C7—C12	−64.2 (2)	C2—C1—O1—S1	104.9 (2)
C12—C7—C8—C9	−2.0 (4)	O2—S1—O1—C1	54.4 (2)
S1—C7—C8—C9	178.4 (2)	O3—S1—O1—C1	−176.40 (18)
C7—C8—C9—C10	1.3 (5)	C7—S1—O1—C1	−60.4 (2)
C8—C9—C10—C11	0.1 (6)	C3—C4—N1—O5	170.0 (3)
C9—C10—C11—C12	−0.8 (5)	C5—C4—N1—O5	−9.4 (4)
C9—C10—C11—C13	178.4 (4)	C3—C4—N1—O4	−12.0 (4)
C10—C11—C12—C16	178.0 (3)	C5—C4—N1—O4	168.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2	0.93	2.43	2.829 (5)	106
C16—H16···O3	0.93	2.46	3.058 (4)	122
C5—H5···O2^{i}	0.93	2.48	3.179 (3)	132
C15—H15···O4^{ii}	0.93	2.47	3.340 (5)	155

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+1/2, *y*+3/2, −*z*+1/2.