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(*E*)-1-Nitro-4-(2-nitroethenyl)benzene

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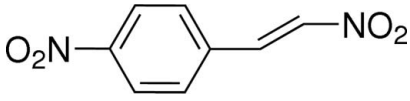
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.090; data-to-parameter ratio = 7.6.

The asymmetric unit of the title compound, $C_8H_6N_2O_4$, consists of two independent molecules with similar geometries, each adopting a *trans* configuration about the olefinic double bond. The two molecules are both almost planar (r.m.s. deviations = 0.034 and 0.035 Å) and form a dihedral angle of 83.62 (2)°. Short N···O contacts [2.834 (3)–2.861 (3) Å] are observed between the nitro groups of neighbouring molecules, with the O atom located directly atop the *p* orbital of the N atom. In the crystal, the molecules are linked into a three-dimensional network by the N···O interactions and by C—H···O hydrogen bonds.

Related literature

For general background to β-nitroolefins, see: Barrett & Graboski (1986). For the synthesis, see: Valdes *et al.* (2007).



Experimental

Crystal data

$C_8H_6N_2O_4$
M_r = 194.15
Orthorhombic, $Pna2_1$
a = 15.847 (4) Å
b = 4.9991 (11) Å
c = 20.495 (5) Å
V = 1623.6 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 93 K
0.43 × 0.17 × 0.17 mm

Data collection

Rigaku AFC10/Saturn724+ diffractometer
Absorption correction: none
12157 measured reflections
1921 independent reflections
1821 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.13
1921 reflections
253 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O5^{i}	0.95	2.57	3.389 (3)	144
C5—H5···O6^{ii}	0.95	2.43	3.234 (3)	143
C6—H6···O7^{iii}	0.95	2.56	3.469 (3)	160
C7—H7···O5^{i}	0.95	2.45	3.304 (3)	150
C10—H10···O4^{iv}	0.95	2.41	3.352 (3)	174
C11—H11···O1^{v}	0.95	2.44	3.243 (3)	142
C14—H14···O2^{vi}	0.95	2.57	3.381 (3)	144
C15—H15···O2^{vi}	0.95	2.44	3.296 (3)	150

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2942).

References

Barrett, A. G. M. & Graboski, G. G. (1986). *Chem. Rev.* **86**, 751–762.
Rigaku (2004). *RAPID-AUTO*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Valdes, A. C., Pina-Luis, G. & Rivero, I. A. (2007). *J. Mex. Chem. Soc.* **51**, 87–95.

supporting information

Acta Cryst. (2009). E**65**, o2809 [https://doi.org/10.1107/S1600536809042561]

(*E*)-1-Nitro-4-(2-nitroethenyl)benzene

Lin-Hai Jing

S1. Comment

β-Nitroolefins are a class of useful and versatile building blocks in organic synthesis (Barrett & Graboski, 1986). The author reports here, the crystal structure of the title compound.

The asymmetric unit of the title compound consists of two crystallographically independent molecules (Fig. 1) each of which adopts a *trans* configuration about the olefinic double bond. All atoms in each independent molecule are almost coplanar. The N2/O3/O4 and C1-C6 (r.m.s. deviation 0.001 Å) planes form a dihedral angle of 1.4 (4)°. The dihedral angle between the C1-C6 and N1/O1/O2/C7/C8 (r.m.s. deviation 0.031 Å) planes is 2.9 (1)°. The N4/O7/O8 and C9-C14 (r.m.s. deviation 0.004 Å) planes form a dihedral angle of 2.9 (4)°. The dihedral angle between the C9-C14 and N3/O5/O6/C15/C16 (r.m.s. deviation 0.028 Å) planes is 2.9 (1)°. The crystal packing is stabilized by C—H···O hydrogen bonds (Table 1) and N···O short contacts.

S2. Experimental

The title compound was synthesized according to the method reported in the literature (Valdes *et al.*, 2007). Yellow single crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution.

S3. Refinement

All H atoms were placed in calculated positions, with C-H = 0.95 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering, Friedel pairs were merged prior to the final refinement.

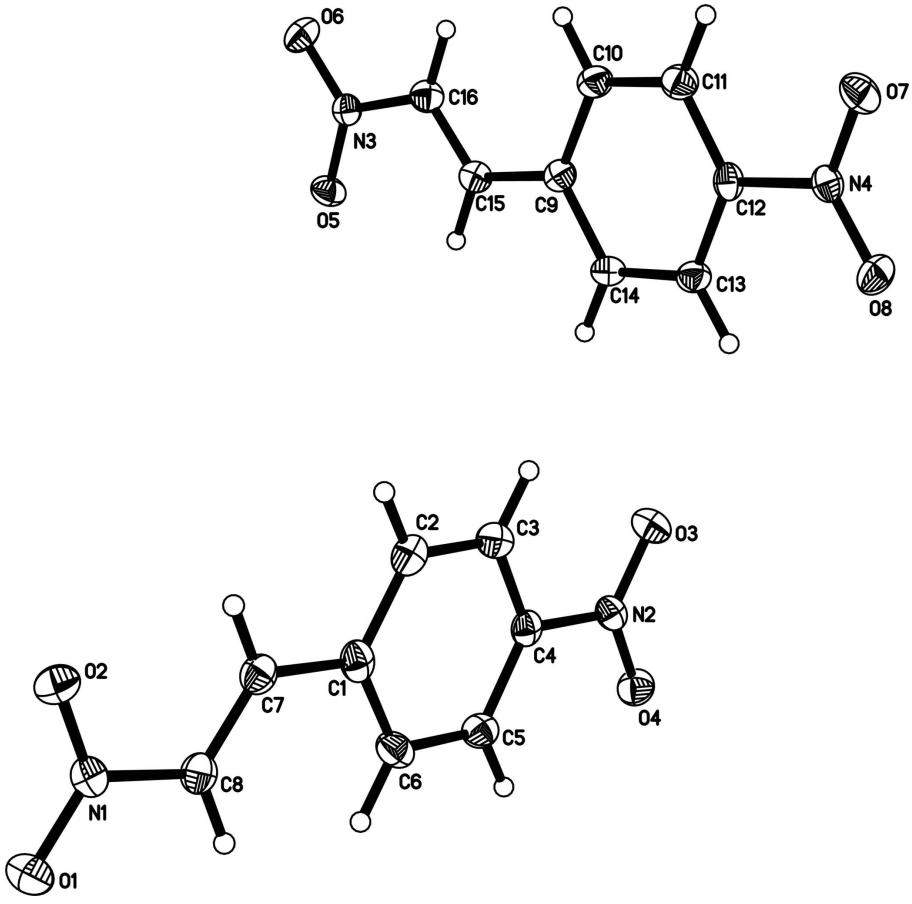

Figure 1

The asymmetric unit of the title compound showing the atomic numbering. Displacement ellipsoids are drawn at the 50% probability level.

(*E*)-1-Nitro-4-(2-nitroethenyl)benzene

Crystal data

$C_8H_6N_2O_4$
M_r = 194.15
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
a = 15.847 (4) Å
b = 4.9991 (11) Å
c = 20.495 (5) Å
V = 1623.6 (7) Å^3
Z = 8
$F(000)$ = 800
D_x = 1.588 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5000 reflections
θ = 3.3–27.5°
μ = 0.13 mm^{-1}
T = 93 K
Prism, yellow
0.43 × 0.17 × 0.17 mm

Data collection

Rigaku AFC10/Saturn724+ diffractometer
Radiation source: Rotating Anode
Graphite monochromator
Detector resolution: 28.5714 pixels mm^{-1}
multi–scan
12157 measured reflections
1921 independent reflections
1821 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −20→20
k = −6→6
l = −20→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.090$
$S = 1.13$
1921 reflections
253 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.0124P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ 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	0.00934 (11)	−0.2104 (4)	0.37970 (9)	0.0256 (4)
O2	0.03415 (11)	−0.1404 (4)	0.27702 (8)	0.0227 (4)
O3	0.40990 (11)	1.2126 (4)	0.30965 (8)	0.0231 (4)
O4	0.39197 (11)	1.1786 (3)	0.41409 (8)	0.0227 (4)
N1	0.04305 (12)	−0.0847 (4)	0.33513 (10)	0.0181 (4)
N2	0.37733 (12)	1.1093 (4)	0.35767 (10)	0.0172 (4)
C1	0.20144 (14)	0.4859 (5)	0.32540 (12)	0.0201 (5)
C2	0.24209 (16)	0.6078 (5)	0.27306 (12)	0.0212 (5)
H2	0.2299	0.5506	0.2299	0.025*
C3	0.29987 (15)	0.8108 (5)	0.28293 (12)	0.0194 (5)
H3	0.3273	0.8938	0.2470	0.023*
C4	0.31691 (14)	0.8909 (5)	0.34625 (11)	0.0170 (5)
C5	0.27766 (15)	0.7755 (5)	0.39972 (12)	0.0195 (5)
H5	0.2901	0.8348	0.4427	0.023*
C6	0.21957 (15)	0.5709 (5)	0.38928 (12)	0.0214 (5)
H6	0.1922	0.4887	0.4253	0.026*
C7	0.14131 (14)	0.2682 (5)	0.31123 (13)	0.0200 (5)
H7	0.1345	0.2178	0.2669	0.024*
C8	0.09642 (15)	0.1380 (5)	0.35480 (12)	0.0198 (5)
H8	0.0988	0.1896	0.3994	0.024*
O5	0.69565 (11)	0.3595 (4)	0.15876 (8)	0.0214 (4)
O6	0.72313 (10)	0.2899 (4)	0.05672 (9)	0.0234 (4)
O7	0.33698 (11)	1.6608 (4)	0.01863 (8)	0.0239 (4)
O8	0.31958 (11)	1.7112 (3)	0.12274 (9)	0.0222 (4)
N3	0.68809 (12)	0.4151 (4)	0.10092 (10)	0.0167 (4)

N4	0.35187 (12)	1.6000 (4)	0.07547 (10)	0.0167 (4)
C9	0.52828 (13)	0.9813 (5)	0.11027 (11)	0.0170 (5)
C10	0.51094 (15)	1.0658 (5)	0.04660 (12)	0.0203 (5)
H10	0.5396	0.9851	0.0110	0.024*
C11	0.45240 (14)	1.2658 (5)	0.03503 (12)	0.0204 (5)
H11	0.4398	1.3216	−0.0082	0.024*
C12	0.41275 (14)	1.3822 (5)	0.08803 (11)	0.0167 (5)
C13	0.42840 (15)	1.3075 (5)	0.15165 (12)	0.0184 (5)
H13	0.4004	1.3928	0.1870	0.022*
C14	0.48642 (15)	1.1037 (5)	0.16264 (12)	0.0173 (5)
H14	0.4978	1.0470	0.2060	0.021*
C15	0.58824 (14)	0.7649 (5)	0.12470 (12)	0.0175 (5)
H15	0.5946	0.7135	0.1691	0.021*
C16	0.63421 (15)	0.6356 (5)	0.08075 (11)	0.0191 (5)
H16	0.6320	0.6871	0.0362	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0256 (9)	0.0291 (9)	0.0220 (9)	−0.0036 (8)	0.0025 (7)	0.0041 (8)
O2	0.0238 (9)	0.0263 (10)	0.0180 (9)	0.0004 (7)	0.0000 (7)	−0.0033 (8)
O3	0.0225 (8)	0.0260 (9)	0.0209 (8)	−0.0040 (8)	0.0013 (7)	0.0046 (7)
O4	0.0261 (10)	0.0234 (9)	0.0186 (8)	−0.0004 (7)	−0.0041 (7)	−0.0025 (7)
N1	0.0155 (10)	0.0182 (10)	0.0204 (10)	−0.0008 (8)	−0.0018 (8)	0.0016 (8)
N2	0.0149 (9)	0.0170 (9)	0.0198 (9)	0.0004 (8)	−0.0016 (8)	0.0031 (8)
C1	0.0159 (11)	0.0164 (11)	0.0279 (14)	0.0038 (10)	−0.0002 (9)	0.0024 (10)
C2	0.0216 (12)	0.0197 (11)	0.0224 (12)	0.0023 (10)	−0.0031 (10)	−0.0033 (9)
C3	0.0171 (11)	0.0220 (12)	0.0191 (12)	0.0024 (9)	−0.0008 (9)	0.0019 (10)
C4	0.0131 (10)	0.0152 (10)	0.0228 (12)	0.0038 (9)	0.0001 (9)	0.0005 (10)
C5	0.0210 (11)	0.0217 (13)	0.0159 (12)	0.0028 (11)	−0.0022 (9)	0.0007 (9)
C6	0.0210 (11)	0.0216 (12)	0.0217 (12)	0.0017 (10)	0.0021 (10)	0.0060 (10)
C7	0.0199 (11)	0.0186 (12)	0.0215 (11)	0.0032 (11)	−0.0011 (10)	−0.0011 (10)
C8	0.0199 (12)	0.0184 (11)	0.0210 (11)	−0.0013 (9)	−0.0021 (9)	−0.0019 (9)
O5	0.0235 (9)	0.0239 (9)	0.0167 (8)	0.0021 (7)	−0.0017 (7)	0.0045 (7)
O6	0.0237 (9)	0.0237 (9)	0.0230 (9)	0.0051 (7)	−0.0005 (7)	−0.0066 (8)
O7	0.0249 (9)	0.0249 (10)	0.0218 (9)	0.0030 (7)	−0.0035 (7)	0.0067 (8)
O8	0.0210 (8)	0.0215 (8)	0.0241 (9)	0.0057 (7)	0.0001 (7)	−0.0039 (7)
N3	0.0147 (9)	0.0161 (9)	0.0193 (10)	−0.0008 (8)	−0.0003 (8)	0.0003 (8)
N4	0.0156 (9)	0.0149 (9)	0.0194 (10)	−0.0017 (8)	−0.0019 (7)	0.0014 (8)
C9	0.0149 (10)	0.0178 (11)	0.0184 (12)	−0.0025 (9)	0.0007 (9)	−0.0020 (9)
C10	0.0216 (12)	0.0212 (12)	0.0182 (11)	0.0032 (10)	0.0029 (9)	−0.0007 (10)
C11	0.0213 (11)	0.0220 (12)	0.0179 (12)	0.0006 (11)	−0.0023 (9)	0.0002 (9)
C12	0.0135 (10)	0.0143 (10)	0.0222 (12)	0.0017 (9)	−0.0020 (9)	0.0011 (9)
C13	0.0180 (12)	0.0195 (10)	0.0176 (11)	−0.0009 (9)	0.0032 (9)	−0.0006 (10)
C14	0.0168 (11)	0.0206 (11)	0.0146 (11)	−0.0001 (10)	0.0005 (9)	0.0000 (9)
C15	0.0157 (10)	0.0195 (12)	0.0172 (11)	−0.0007 (10)	−0.0014 (9)	0.0005 (9)
C16	0.0181 (11)	0.0210 (12)	0.0182 (11)	0.0009 (9)	−0.0015 (9)	0.0008 (9)

Geometric parameters (Å, º)

O1—N1	1.231 (3)	O5—N3	1.223 (3)
O2—N1	1.231 (3)	O6—N3	1.233 (3)
O3—N2	1.225 (3)	O7—N4	1.227 (3)
O4—N2	1.229 (3)	O8—N4	1.229 (3)
N1—C8	1.455 (3)	N3—C16	1.455 (3)
N2—C4	1.471 (3)	N4—C12	1.477 (3)
C1—C2	1.392 (3)	C9—C10	1.399 (3)
C1—C6	1.406 (3)	C9—C14	1.402 (3)
C1—C7	1.476 (3)	C9—C15	1.470 (3)
C2—C3	1.382 (3)	C10—C11	1.385 (3)
C2—H2	0.95	C10—H10	0.95
C3—C4	1.385 (3)	C11—C12	1.383 (3)
C3—H3	0.95	C11—H11	0.95
C4—C5	1.386 (3)	C12—C13	1.379 (3)
C5—C6	1.392 (4)	C13—C14	1.391 (3)
C5—H5	0.95	C13—H13	0.95
C6—H6	0.95	C14—H14	0.95
C7—C8	1.314 (4)	C15—C16	1.327 (3)
C7—H7	0.95	C15—H15	0.95
C8—H8	0.95	C16—H16	0.95
O2—N1—O1	123.6 (2)	O5—N3—O6	123.5 (2)
O2—N1—C8	120.5 (2)	O5—N3—C16	120.3 (2)
O1—N1—C8	115.9 (2)	O6—N3—C16	116.11 (19)
O3—N2—O4	123.9 (2)	O7—N4—O8	123.8 (2)
O3—N2—C4	117.33 (19)	O7—N4—C12	118.28 (19)
O4—N2—C4	118.79 (19)	O8—N4—C12	117.89 (19)
C2—C1—C6	119.4 (2)	C10—C9—C14	119.3 (2)
C2—C1—C7	118.0 (2)	C10—C9—C15	122.5 (2)
C6—C1—C7	122.6 (2)	C14—C9—C15	118.2 (2)
C3—C2—C1	121.0 (2)	C11—C10—C9	120.6 (2)
C3—C2—H2	119.5	C11—C10—H10	119.7
C1—C2—H2	119.5	C9—C10—H10	119.7
C2—C3—C4	118.6 (2)	C12—C11—C10	118.3 (2)
C2—C3—H3	120.7	C12—C11—H11	120.9
C4—C3—H3	120.7	C10—C11—H11	120.9
C3—C4—C5	122.2 (2)	C13—C12—C11	123.2 (2)
C3—C4—N2	119.4 (2)	C13—C12—N4	118.8 (2)
C5—C4—N2	118.4 (2)	C11—C12—N4	118.0 (2)
C4—C5—C6	118.7 (2)	C12—C13—C14	118.1 (2)
C4—C5—H5	120.6	C12—C13—H13	121.0
C6—C5—H5	120.6	C14—C13—H13	121.0
C5—C6—C1	120.0 (2)	C13—C14—C9	120.6 (2)
C5—C6—H6	120.0	C13—C14—H14	119.7
C1—C6—H6	120.0	C9—C14—H14	119.7
C8—C7—C1	125.5 (2)	C16—C15—C9	125.2 (2)

C8—C7—H7	117.2	C16—C15—H15	117.4
C1—C7—H7	117.2	C9—C15—H15	117.4
C7—C8—N1	120.3 (2)	C15—C16—N3	119.9 (2)
C7—C8—H8	119.8	C15—C16—H16	120.0
N1—C8—H8	119.8	N3—C16—H16	120.0
C6—C1—C2—C3	0.0 (4)	C14—C9—C10—C11	−0.8 (4)
C7—C1—C2—C3	−179.2 (2)	C15—C9—C10—C11	178.3 (2)
C1—C2—C3—C4	0.2 (4)	C9—C10—C11—C12	1.0 (4)
C2—C3—C4—C5	−0.4 (4)	C10—C11—C12—C13	−0.4 (4)
C2—C3—C4—N2	−179.1 (2)	C10—C11—C12—N4	178.6 (2)
O3—N2—C4—C3	0.4 (3)	O7—N4—C12—C13	−178.4 (2)
O4—N2—C4—C3	−180.0 (2)	O8—N4—C12—C13	2.2 (3)
O3—N2—C4—C5	−178.4 (2)	O7—N4—C12—C11	2.6 (3)
O4—N2—C4—C5	1.2 (3)	O8—N4—C12—C11	−176.8 (2)
C3—C4—C5—C6	0.4 (4)	C11—C12—C13—C14	−0.5 (4)
N2—C4—C5—C6	179.2 (2)	N4—C12—C13—C14	−179.5 (2)
C4—C5—C6—C1	−0.3 (4)	C12—C13—C14—C9	0.8 (3)
C2—C1—C6—C5	0.1 (4)	C10—C9—C14—C13	−0.2 (3)
C7—C1—C6—C5	179.3 (2)	C15—C9—C14—C13	−179.3 (2)
C2—C1—C7—C8	−178.2 (2)	C10—C9—C15—C16	2.9 (4)
C6—C1—C7—C8	2.6 (4)	C14—C9—C15—C16	−178.0 (2)
C1—C7—C8—N1	−176.1 (2)	C9—C15—C16—N3	−176.7 (2)
O2—N1—C8—C7	−5.7 (3)	O5—N3—C16—C15	−4.9 (3)
O1—N1—C8—C7	173.6 (2)	O6—N3—C16—C15	173.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O5^{i}	0.95	2.57	3.389 (3)	144
C5—H5···O6^{ii}	0.95	2.43	3.234 (3)	143
C6—H6···O7^{iii}	0.95	2.56	3.469 (3)	160
C7—H7···O5^{i}	0.95	2.45	3.304 (3)	150
C10—H10···O4^{iv}	0.95	2.41	3.352 (3)	174
C11—H11···O1^{v}	0.95	2.44	3.243 (3)	142
C14—H14···O2^{vi}	0.95	2.57	3.381 (3)	144
C15—H15···O2^{vi}	0.95	2.44	3.296 (3)	150

Symmetry codes: (i) $x-1/2, -y+1/2, z$; (ii) $-x+1, -y+1, z+1/2$; (iii) $-x+1/2, y-3/2, z+1/2$; (iv) $-x+1, -y+2, z-1/2$; (v) $-x+1/2, y+3/2, z-1/2$; (vi) $x+1/2, -y+1/2, z$.