Title

Dimethyl 2,2′-dinitrobiphenyl-4,4′-dicarboxylate

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Dimethyl 2,2′-dinitrobiphenyl-4,4′-dicarboxylate

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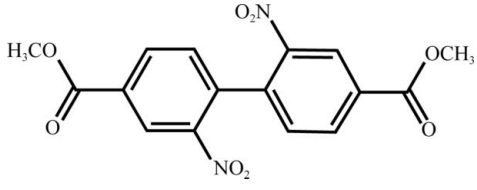
Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.096; data-to-parameter ratio = 11.8.

The title compound, $C_{16}H_{12}N_2O_8$, exhibits two near-planar aromatic ester groups with aryl–ester dihedral angles of 2.1 (2) and 4.2 (3)°. The dihedral angle between the aromatic rings is 58.0 (1)°. The two nitro groups are tilted slightly from the plane of the aromatic rings, making dihedral angles of 14.1 (1) and 8.2 (2)°. In the crystal, molecules are connected by weak C—H···O interactions, forming a three-dimensional network.

Related literature

For the synthesis of the title compound, see: Ol'khovik *et al.* (2008). For the structure of 2,2′-dinitrobiphenyl-4,4′-dicarboxylic acid, see: Wu *et al.* (2010). For metal-organic frameworks and coordination polymers featuring this linker, see: Qu (2007); Li, Zhou *et al.* (2011); Li, Li *et al.* (2011); Li, Zhang *et al.* (2011); Zhang, Ma *et al.* (2011); Zhang, Jing *et al.* (2011); Li, Yang *et al.* (2012); Zhang, Li *et al.* (2012).



Experimental

Crystal data

$C_{16}H_{12}N_2O_8$
M_r = 360.28
Triclinic, $P\overline{1}$
a = 8.0520 (5) Å
b = 10.4193 (7) Å
c = 10.5310 (11) Å
α = 108.423 (4)°
β = 95.142 (4)°
γ = 111.617 (3)°
V = 757.71 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 90 K
0.28 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.965, T_{max} = 0.981
9906 measured reflections
2787 independent reflections
2297 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.096
S = 1.02
2787 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 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
C16—H16A···O3^{i}	0.98	2.50	3.253 (2)	134
C1—H1C···O2^{ii}	0.98	2.57	3.5214 (19)	164
C14—H14A···O2^{iii}	0.95	2.47	3.2399 (19)	138
C8—H8A···O3^{iv}	0.95	2.41	3.3239 (19)	162

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: FF2126).

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supplementary materials

Acta Cryst. (2014). E**70**, o305 [doi:10.1107/S1600536814003067]

Dimethyl 2,2′-dinitrobiphenyl-4,4′-dicarboxylate

Ryan L. Lehane, James A. Golen, Arnold L. Rheingold and David R. Manke

1. Comment

Biphenyl-4,4′-dicarboxylate and its derivatives are widely used in metal-organic frameworks (MOFs) as linkers. One of the many advantages of MOFs is the ability to incorporate different functional groups within their pores. As a part of our efforts in this field, we prepared the previously reported dimethyl 2,2′-dinitrobiphenyl-4,4′-dicarboxylate (Ol'khovik *et al.* 2008) and report its structure herein.

The molecular structure of the title compound is shown in Figure 1. The structure demonstrates two near planar aromatic ester groups with aryl-ester dihedral angles of 2.1 (2)° and 4.2 (3)°. The two aromatic rings demonstrate a dihedral angle of 58.0 (1)°. The nitro groups are skewed slightly with aryl-nitro dihedral angles of 8.2 (2)° and 14.1 (1)°. No π-π interactions were noted between the aromatic rings. The packing for the title compound is shown in Figure 2.

2. Experimental

The compound was prepared by literature procedure (Ol'khovik *et al.* 2008). Crystals suitable for single-crystal X-ray analysis were grown by slow evaporation of an ethanol solution.

3. Refinement

All non-hydrogen atoms refined anisotropically by full matrix least squares on F^2. All hydrogen atoms were placed in calculated positions and then refined with riding model with C—H lengths of 0.95 Å for (CH) and 0.98 Å for (CH_3) and with isotropic displacement parameters set to 1.20 and 1.50 times U_{eq} of the parent C atom.

Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

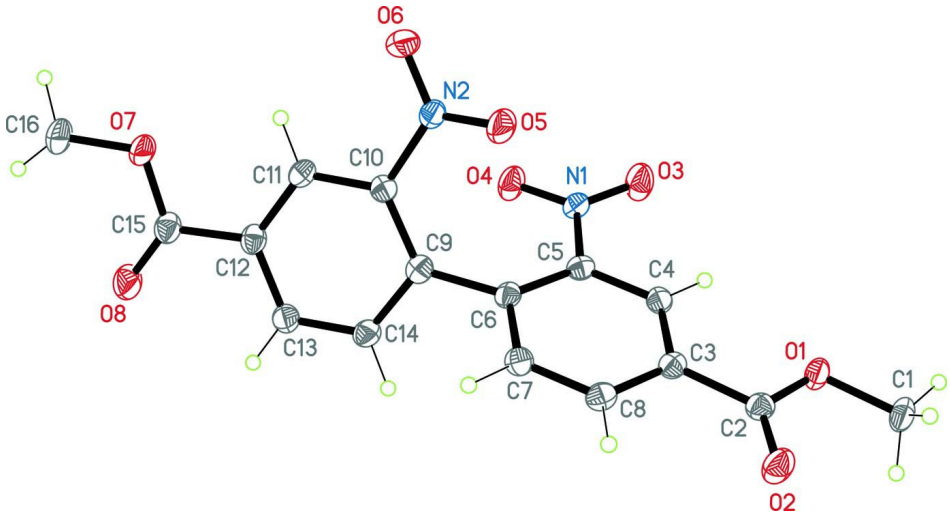

Figure 1

Molecular structure of the title compound, showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as spheres of arbitrary radius.

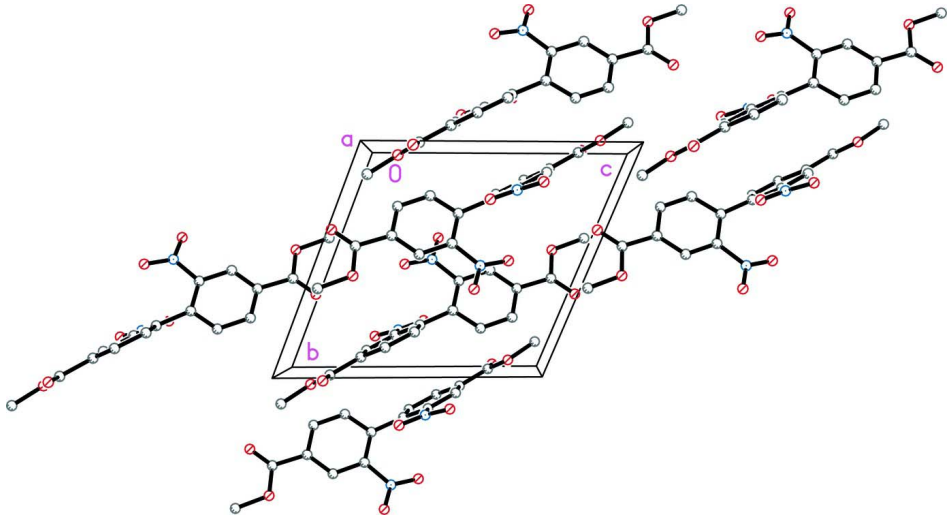

Figure 2

Molecular packing of the title compound.

Dimethyl 2,2′-dinitrobiphenyl-4,4′-dicarboxylate

Crystal data

$C_{16}H_{12}N_2O_8$
$M_r = 360.28$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.0520$ (5) Å
$b = 10.4193$ (7) Å
$c = 10.5310$ (11) Å
$\alpha = 108.423$ (4)°
$\beta = 95.142$ (4)°
$\gamma = 111.617$ (3)°
$V = 757.71$ (11) Å^3
$Z = 2$
$F(000) = 372$
$D_x = 1.579$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5153 reflections
$\theta = 2.8$–25.4°
$\mu = 0.13$ mm^{-1}
$T = 90$ K
BLOCK, yellow
0.28 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.965, T_{max} = 0.981
9906 measured reflections
2787 independent reflections
2297 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.4°, θ_{min} = 2.8°
h = −9→9
k = −12→12
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.096
S = 1.02
2787 reflections
237 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
$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 0.234P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.28379 (14)	−0.04398 (11)	0.86338 (10)	0.0223 (3)
O2	0.02811 (15)	−0.01405 (13)	0.81152 (11)	0.0283 (3)
O3	0.80395 (15)	0.15657 (14)	0.70622 (13)	0.0350 (3)
O4	0.80373 (15)	0.23016 (13)	0.53753 (11)	0.0283 (3)
O5	0.72326 (16)	0.49239 (12)	0.69694 (11)	0.0327 (3)
O6	0.93059 (15)	0.61445 (13)	0.61157 (11)	0.0323 (3)
O7	0.80462 (15)	0.55730 (12)	0.14341 (11)	0.0292 (3)
O8	0.56913 (17)	0.35679 (13)	−0.01199 (11)	0.0355 (3)
N1	0.72907 (16)	0.18850 (13)	0.62186 (13)	0.0196 (3)
N2	0.78359 (17)	0.51402 (14)	0.59936 (12)	0.0206 (3)
C1	0.1936 (2)	−0.12748 (18)	0.94307 (16)	0.0253 (4)
H1A	0.2829	−0.1467	0.9949	0.038*
H1B	0.0943	−0.2224	0.8810	0.038*
H1C	0.1427	−0.0698	1.0072	0.038*
C2	0.1814 (2)	0.00368 (16)	0.79992 (15)	0.0199 (3)
C3	0.2780 (2)	0.07985 (15)	0.71294 (14)	0.0181 (3)
C4	0.4574 (2)	0.10299 (15)	0.70668 (14)	0.0182 (3)

H4A	0.5234	0.0717	0.7606	0.022*
C5	0.53980 (19)	0.17125 (15)	0.62247 (15)	0.0179 (3)
C6	0.4489 (2)	0.21904 (15)	0.53960 (15)	0.0181 (3)
C7	0.2683 (2)	0.19281 (16)	0.54750 (15)	0.0199 (3)
H7A	0.2004	0.2214	0.4919	0.024*
C8	0.1845 (2)	0.12668 (16)	0.63336 (15)	0.0201 (3)
H8A	0.0622	0.1132	0.6379	0.024*
C9	0.5175 (2)	0.28358 (16)	0.43647 (15)	0.0186 (3)
C10	0.6699 (2)	0.41620 (16)	0.45972 (15)	0.0187 (3)
C11	0.7209 (2)	0.46404 (16)	0.35496 (15)	0.0196 (3)
H11A	0.8284	0.5524	0.3740	0.024*
C12	0.6138 (2)	0.38191 (16)	0.22211 (15)	0.0208 (3)
C13	0.4585 (2)	0.25263 (17)	0.19660 (16)	0.0232 (3)
H13A	0.3833	0.1967	0.1060	0.028*
C14	0.4123 (2)	0.20443 (16)	0.30184 (15)	0.0217 (3)
H14A	0.3060	0.1149	0.2819	0.026*
C15	0.6575 (2)	0.42811 (17)	0.10439 (16)	0.0239 (4)
C16	0.8490 (3)	0.6119 (2)	0.03466 (17)	0.0354 (4)
H16A	0.9564	0.7083	0.0729	0.053*
H16B	0.7443	0.6240	−0.0062	0.053*
H16C	0.8765	0.5404	−0.0362	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0235 (6)	0.0248 (6)	0.0241 (6)	0.0100 (5)	0.0094 (4)	0.0154 (5)
O2	0.0227 (6)	0.0362 (7)	0.0344 (7)	0.0134 (5)	0.0140 (5)	0.0205 (5)
O3	0.0253 (6)	0.0526 (8)	0.0442 (7)	0.0200 (6)	0.0117 (5)	0.0348 (6)
O4	0.0251 (6)	0.0383 (7)	0.0328 (6)	0.0153 (5)	0.0158 (5)	0.0230 (6)
O5	0.0419 (7)	0.0275 (6)	0.0197 (6)	0.0035 (5)	0.0098 (5)	0.0099 (5)
O6	0.0255 (6)	0.0306 (6)	0.0274 (6)	−0.0018 (5)	0.0033 (5)	0.0109 (5)
O7	0.0336 (7)	0.0274 (6)	0.0213 (6)	0.0032 (5)	0.0068 (5)	0.0140 (5)
O8	0.0512 (8)	0.0268 (6)	0.0189 (6)	0.0071 (6)	0.0035 (5)	0.0088 (5)
N1	0.0185 (7)	0.0177 (6)	0.0228 (7)	0.0066 (5)	0.0056 (5)	0.0087 (5)
N2	0.0227 (7)	0.0186 (6)	0.0208 (7)	0.0072 (6)	0.0059 (5)	0.0095 (5)
C1	0.0312 (9)	0.0242 (8)	0.0245 (8)	0.0097 (7)	0.0113 (7)	0.0149 (7)
C2	0.0200 (8)	0.0174 (7)	0.0190 (8)	0.0060 (6)	0.0042 (6)	0.0050 (6)
C3	0.0196 (8)	0.0153 (7)	0.0173 (7)	0.0064 (6)	0.0051 (6)	0.0042 (6)
C4	0.0207 (8)	0.0158 (7)	0.0170 (7)	0.0074 (6)	0.0029 (6)	0.0057 (6)
C5	0.0168 (7)	0.0160 (7)	0.0194 (7)	0.0065 (6)	0.0050 (6)	0.0049 (6)
C6	0.0213 (8)	0.0130 (7)	0.0173 (7)	0.0054 (6)	0.0044 (6)	0.0045 (6)
C7	0.0195 (8)	0.0194 (8)	0.0228 (8)	0.0094 (6)	0.0041 (6)	0.0090 (6)
C8	0.0184 (8)	0.0191 (8)	0.0223 (8)	0.0080 (6)	0.0066 (6)	0.0065 (6)
C9	0.0198 (8)	0.0174 (7)	0.0223 (8)	0.0106 (6)	0.0069 (6)	0.0083 (6)
C10	0.0200 (8)	0.0180 (7)	0.0183 (8)	0.0086 (6)	0.0042 (6)	0.0062 (6)
C11	0.0210 (8)	0.0160 (7)	0.0233 (8)	0.0078 (6)	0.0069 (6)	0.0087 (6)
C12	0.0263 (8)	0.0187 (8)	0.0203 (8)	0.0113 (7)	0.0069 (6)	0.0083 (6)
C13	0.0272 (8)	0.0191 (8)	0.0203 (8)	0.0074 (7)	0.0021 (6)	0.0073 (6)
C14	0.0218 (8)	0.0173 (7)	0.0248 (8)	0.0068 (6)	0.0040 (6)	0.0087 (6)
C15	0.0309 (9)	0.0197 (8)	0.0223 (9)	0.0111 (7)	0.0069 (7)	0.0089 (7)

C16	0.0409 (10)	0.0378 (10)	0.0272 (9)	0.0071 (8)	0.0099 (8)	0.0225 (8)

Geometric parameters (Å, º)

O1—C2	1.3363 (18)	C5—C6	1.405 (2)
O1—C1	1.4469 (17)	C6—C7	1.393 (2)
O2—C2	1.2024 (18)	C6—C9	1.494 (2)
O3—N1	1.2256 (16)	C7—C8	1.381 (2)
O4—N1	1.2188 (16)	C7—H7A	0.9500
O5—N2	1.2239 (16)	C8—H8A	0.9500
O6—N2	1.2197 (16)	C9—C14	1.392 (2)
O7—C15	1.3315 (19)	C9—C10	1.399 (2)
O7—C16	1.4486 (18)	C10—C11	1.383 (2)
O8—C15	1.1995 (19)	C11—C12	1.384 (2)
N1—C5	1.4682 (18)	C11—H11A	0.9500
N2—C10	1.4708 (19)	C12—C13	1.385 (2)
C1—H1A	0.9800	C12—C15	1.491 (2)
C1—H1B	0.9800	C13—C14	1.381 (2)
C1—H1C	0.9800	C13—H13A	0.9500
C2—C3	1.485 (2)	C14—H14A	0.9500
C3—C8	1.387 (2)	C16—H16A	0.9800
C3—C4	1.385 (2)	C16—H16B	0.9800
C4—C5	1.374 (2)	C16—H16C	0.9800
C4—H4A	0.9500		
C2—O1—C1	115.18 (11)	C6—C7—H7A	118.9
C15—O7—C16	115.00 (12)	C3—C8—C7	120.31 (14)
O4—N1—O3	122.78 (12)	C3—C8—H8A	119.8
O4—N1—C5	119.80 (12)	C7—C8—H8A	119.8
O3—N1—C5	117.40 (12)	C14—C9—C10	116.34 (13)
O6—N2—O5	123.65 (13)	C14—C9—C6	115.67 (13)
O6—N2—C10	118.19 (12)	C10—C9—C6	127.94 (13)
O5—N2—C10	118.13 (12)	C11—C10—C9	122.64 (13)
O1—C1—H1A	109.5	C11—C10—N2	116.29 (13)
O1—C1—H1B	109.5	C9—C10—N2	121.07 (13)
H1A—C1—H1B	109.5	C12—C11—C10	119.37 (14)
O1—C1—H1C	109.5	C12—C11—H11A	120.3
H1A—C1—H1C	109.5	C10—C11—H11A	120.3
H1B—C1—H1C	109.5	C11—C12—C13	119.30 (14)
O2—C2—O1	123.67 (14)	C11—C12—C15	122.49 (14)
O2—C2—C3	124.01 (14)	C13—C12—C15	118.20 (14)
O1—C2—C3	112.32 (12)	C14—C13—C12	120.55 (14)
C8—C3—C4	118.93 (13)	C14—C13—H13A	119.7
C8—C3—C2	118.95 (13)	C12—C13—H13A	119.7
C4—C3—C2	122.11 (13)	C13—C14—C9	121.72 (14)
C5—C4—C3	120.01 (14)	C13—C14—H14A	119.1
C5—C4—H4A	120.0	C9—C14—H14A	119.1
C3—C4—H4A	120.0	O8—C15—O7	124.10 (14)
C4—C5—C6	122.65 (13)	O8—C15—C12	123.56 (14)
C4—C5—N1	115.70 (13)	O7—C15—C12	112.33 (13)

C6—C5—N1	121.64 (13)	O7—C16—H16A	109.5
C7—C6—C5	115.81 (13)	O7—C16—H16B	109.5
C7—C6—C9	116.20 (13)	H16A—C16—H16B	109.5
C5—C6—C9	127.81 (13)	O7—C16—H16C	109.5
C8—C7—C6	122.27 (14)	H16A—C16—H16C	109.5
C8—C7—H7A	118.9	H16B—C16—H16C	109.5
C1—O1—C2—O2	3.3 (2)	C7—C6—C9—C10	122.53 (16)
C1—O1—C2—C3	−176.29 (11)	C5—C6—C9—C10	−62.6 (2)
O2—C2—C3—C8	−3.9 (2)	C14—C9—C10—C11	−3.2 (2)
O1—C2—C3—C8	175.74 (12)	C6—C9—C10—C11	179.48 (14)
O2—C2—C3—C4	177.44 (14)	C14—C9—C10—N2	175.83 (13)
O1—C2—C3—C4	−2.96 (19)	C6—C9—C10—N2	−1.5 (2)
C8—C3—C4—C5	−0.1 (2)	O6—N2—C10—C11	−12.78 (19)
C2—C3—C4—C5	178.64 (13)	O5—N2—C10—C11	165.42 (13)
C3—C4—C5—C6	−0.5 (2)	O6—N2—C10—C9	168.14 (13)
C3—C4—C5—N1	−179.15 (12)	O5—N2—C10—C9	−13.7 (2)
O4—N1—C5—C4	170.63 (13)	C9—C10—C11—C12	2.8 (2)
O3—N1—C5—C4	−7.86 (19)	N2—C10—C11—C12	−176.24 (13)
O4—N1—C5—C6	−8.1 (2)	C10—C11—C12—C13	−0.6 (2)
O3—N1—C5—C6	173.45 (13)	C10—C11—C12—C15	178.61 (13)
C4—C5—C6—C7	−0.1 (2)	C11—C12—C13—C14	−1.1 (2)
N1—C5—C6—C7	178.50 (12)	C15—C12—C13—C14	179.67 (13)
C4—C5—C6—C9	−174.94 (13)	C12—C13—C14—C9	0.6 (2)
N1—C5—C6—C9	3.7 (2)	C10—C9—C14—C13	1.4 (2)
C5—C6—C7—C8	1.2 (2)	C6—C9—C14—C13	179.09 (13)
C9—C6—C7—C8	176.70 (13)	C16—O7—C15—O8	2.6 (2)
C4—C3—C8—C7	1.2 (2)	C16—O7—C15—C12	−177.15 (13)
C2—C3—C8—C7	−177.57 (13)	C11—C12—C15—O8	178.12 (15)
C6—C7—C8—C3	−1.8 (2)	C13—C12—C15—O8	−2.7 (2)
C7—C6—C9—C14	−54.82 (18)	C11—C12—C15—O7	−2.1 (2)
C5—C6—C9—C14	120.00 (16)	C13—C12—C15—O7	177.07 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16*A*···O3^{i}	0.98	2.50	3.253 (2)	134
C1—H1*C*···O2^{ii}	0.98	2.57	3.5214 (19)	164
C14—H14*A*···O2^{iii}	0.95	2.47	3.2399 (19)	138
C8—H8*A*···O3^{iv}	0.95	2.41	3.3239 (19)	162

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