

Crystal structure of (3*E*)-3-(2,4-dinitrophenoxymethyl)-4-phenylbut-3-en-2-oneIgnez Caracelli,^{a*} Stella H. Maganhi,^a Paulo J. S. Moran,^b Bruno R. S. de Paula,^b Felix N. Delling^c and Edward R. T. Tiekink^d

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Received 15 August 2014; accepted 19 August 2014

Edited by P. C. Healy, Griffith University, Australia

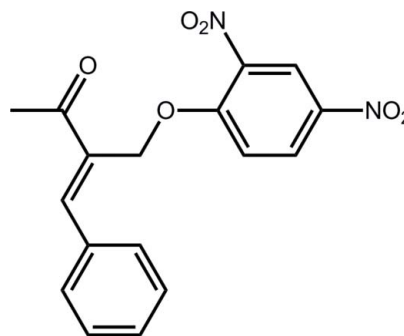
In the title compound, C₁₇H₁₄N₂O₆, the conformation about the C=C double bond [1.345 (2) Å] is *E*, with the ketone moiety almost coplanar [C–C–C–C torsion angle = 9.5 (2)°] along with the phenyl ring [C–C–C–C = 5.9 (2)°]. The aromatic rings are almost perpendicular to each other [dihedral angle = 86.66 (7)°]. The 4-nitro moiety is approximately coplanar with the benzene ring to which it is attached [O–N–C–C = 4.2 (2)°], whereas the one in the *ortho* position is twisted [O–N–C–C = 138.28 (13)°]. The molecules associate *via* C–H...O interactions, involving both O atoms from the 2-nitro group, to form a helical supramolecular chain along [010]. Nitro–nitro N...O interactions [2.8461 (19) Å] connect the chains into layers that stack along [001].

Keywords: crystal structure; hydrogen bonding; N...O interactions.

CCDC reference: 1020026

1. Related literature

For background to biotransformations mediated by *Saccharomyces cerevisiae*, see: Rodrigues *et al.* (2004); de Paula *et al.* (2013). For a related structure, see: Zukerman-Schpector *et al.* (2014). For interactions between nitro groups, see: Daszkiewicz (2013).



2. Experimental

2.1. Crystal data

C₁₇H₁₄N₂O₆
M_r = 342.30
Monoclinic, *P*2₁/*c*
a = 12.8459 (6) Å
b = 7.6983 (4) Å
c = 19.4283 (8) Å
b = 122.254 (2)°
V = 1624.82 (14) Å³
Z = 4
Mo Kα radiation
μ = 0.11 mm⁻¹
T = 290 K
0.66 × 0.45 × 0.28 mm

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
*T*_{min} = 0.699, *T*_{max} = 0.745
10435 measured reflections
2957 independent reflections
2630 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.019

2.3. Refinement

R[*F*² > 2σ(*F*²)] = 0.037
wR(*F*²) = 0.101
S = 1.04
2957 reflections
228 parameters
H-atom parameters constrained
Δρ_{max} = 0.20 e Å⁻³
Δρ_{min} = -0.21 e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C6–H6...O5 ⁱ	0.93	2.41	3.1375 (18)	135
C16–H16...O6 ⁱⁱ	0.93	2.58	3.292 (3)	134

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *QMol* (Gans & Shalloway, 2001) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *MarvinSketch* (ChemAxon, 2010) and *pubCIF* (Westrip, 2010).

Acknowledgements

We thank Professor Regina H. A. Santos from IQSC-USP for the data collection. The Brazilian agencies CNPq (306121/2013-1 to IC), CAPES (808/2009 to IC) and FAPESP (2012/22524-9 to SHM) are acknowledged for financial support.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5406).

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supporting information

Acta Cryst. (2014). E70, o1051–o1052 [doi:10.1107/S1600536814018819]

Crystal structure of (3*E*)-3-(2,4-dinitrophenoxymethyl)-4-phenylbut-3-en-2-one

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S1. Structural commentary

In the context of the study of biotransformation reactions mediated by *Saccharomyces cerevisiae*, such as the bio-reduction of α -haloketones and enones (Rodrigues *et al.*, 2004), the title compound, (3*E*)-3-(2,4-dinitrophenoxymethyl)-4-phenylbut-3-en-2-one, (I), as well as its 4-nitrophenylmethyl analogue, i.e. (3*E*)-3-(4-nitrophenoxymethyl)-4-phenylbut-3-en-2-one, (II), (Zukerman-Schpector *et al.* 2014), were synthesised to be used as substrates in order to compare their behaviour with that of the 3-halomethyl-4-phenyl-3-buten-2-ones analogues (de Paula *et al.*, 2013). Herein, the crystal structure determination and spectroscopic details of (I) are described.

In (I), the conformation about the C=C double bond [1.345 (2) Å] is *E*. The ketone moiety almost co-planar [C11–C8–C9–C10 torsion angle = 9.5 (2) °] with the double bond but the phenyl ring is twisted [C8–C11–C12–C17 = -150.23 (16)°]. The aromatic rings are almost perpendicular to each other [dihedral angle = 86.66 (7)°]. The *p*-nitro moiety is approximately co-planar with the benzene ring to which it is attached [O3–N1–C4–C5 = -175.29 (14) °] while the one in the *o*-position is twisted [O5–N2–C2–C3 = -40.76 (17)°].

Fig. 2 shows an overlay diagram of (I) and the inverted molecule of (II) (Zukerman-Schpector *et al.* 2014). Clearly, the two molecules adopt very similar conformations.

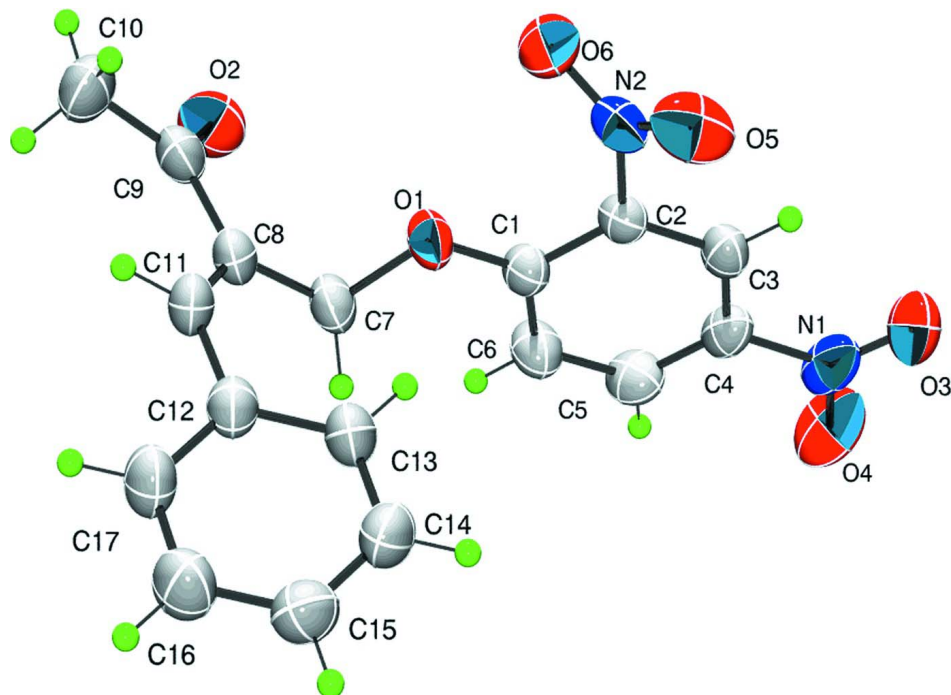
In the crystal packing, molecules associate *via* C—H \cdots O interactions, whereby the O atoms of the *o*-nitro group interact with H derived from a benzene or a phenyl ring, leading to a supramolecular helical chain along [0 1 0]; Fig. 2. There are also N \cdots O5 interactions [2.8461 (19) Å], i.e. nitro \cdots nitro interactions (Daszkiewicz, 2013), that link the chains into a layer. Layers stack along [0 0 1] without specific intermolecular interactions between them, Fig. 3.

S2. Synthesis and crystallization

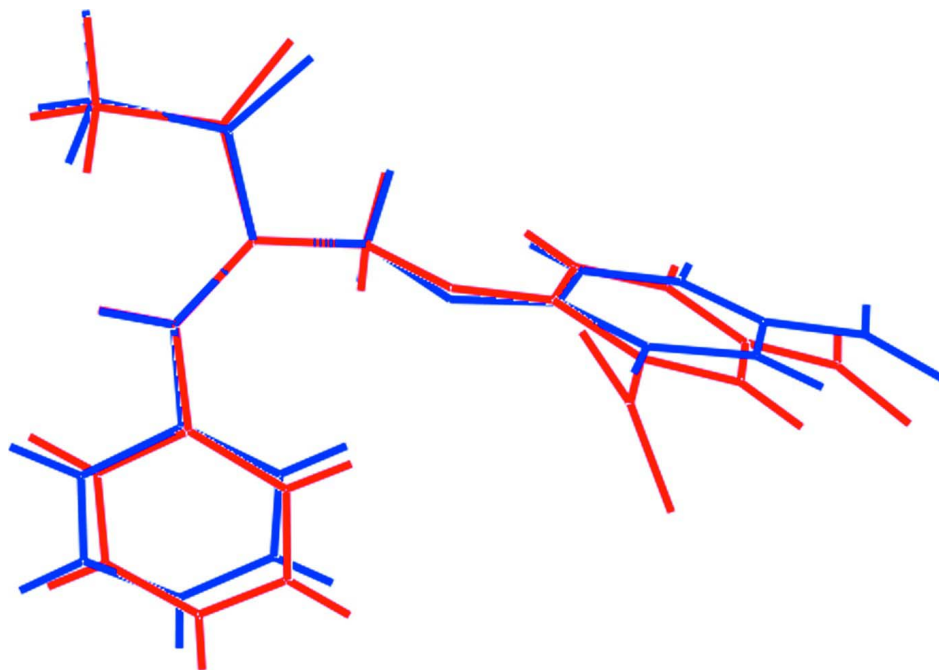
Potassium carbonate (232 mg, 2.4 mmol) and 2,4-dinitrophenol (368 mg, 2 mmol) were added to a solution of 4-nitrophenol (1.53 g, 11 mmol) and 3-bromomethyl-4-phenyl-3-buten-2-one (478 mg, 2 mmol) in dry acetone (4 mL). The reaction mixture was stirred for 16 hours and filtered. The solvent was evaporated and the residue was purified by column chromatography (hexane/EtOAc, 80:20) to afford the product as a colourless solid in 75% yield. The product was recrystallized by slow evaporation of a 2:1 dichloromethane/hexane mixture. *M.pt.*: 442.2–442.8 K. ¹H NMR (CD₂Cl₂, 400 MHz): δ 2.52 (3H, s), 5.12 (2H, s), 7.41 (d, 1H, *J* = 9.2 Hz), 7.43–7.56 (5H, m), 7.99 (1H, s), 8.42 (dd, 1H, *J* = 2.8, 9.2 Hz), 8.72 (d, 1H, *J* = 2.8 Hz). ¹³C NMR (CD₂Cl₂, 150 MHz): δ 26.2, 64.7, 116.1, 122.3, 129.5, 129.7, 130.2, 130.8, 134.5, 134.6, 139.8, 140.9, 148.1, 157.0, 198.4.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 to 0.97 Å) and were included in the refinement in the riding model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}(\text{methyl-C})$.

**Figure 1**

The molecular structure of the title showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

**Figure 2**

Overlay diagram of (I), red image, with inverted (II), blue image, drawn so that the C=C—C(phenyl) atoms are overlapped.

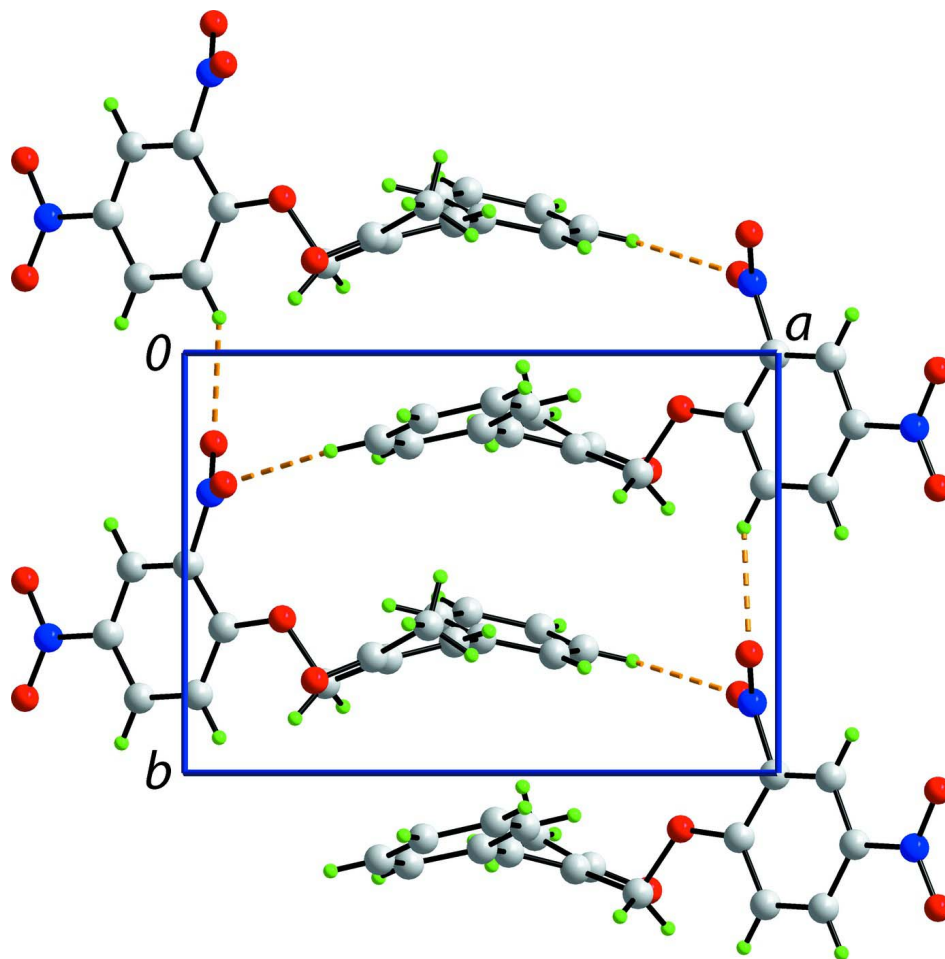
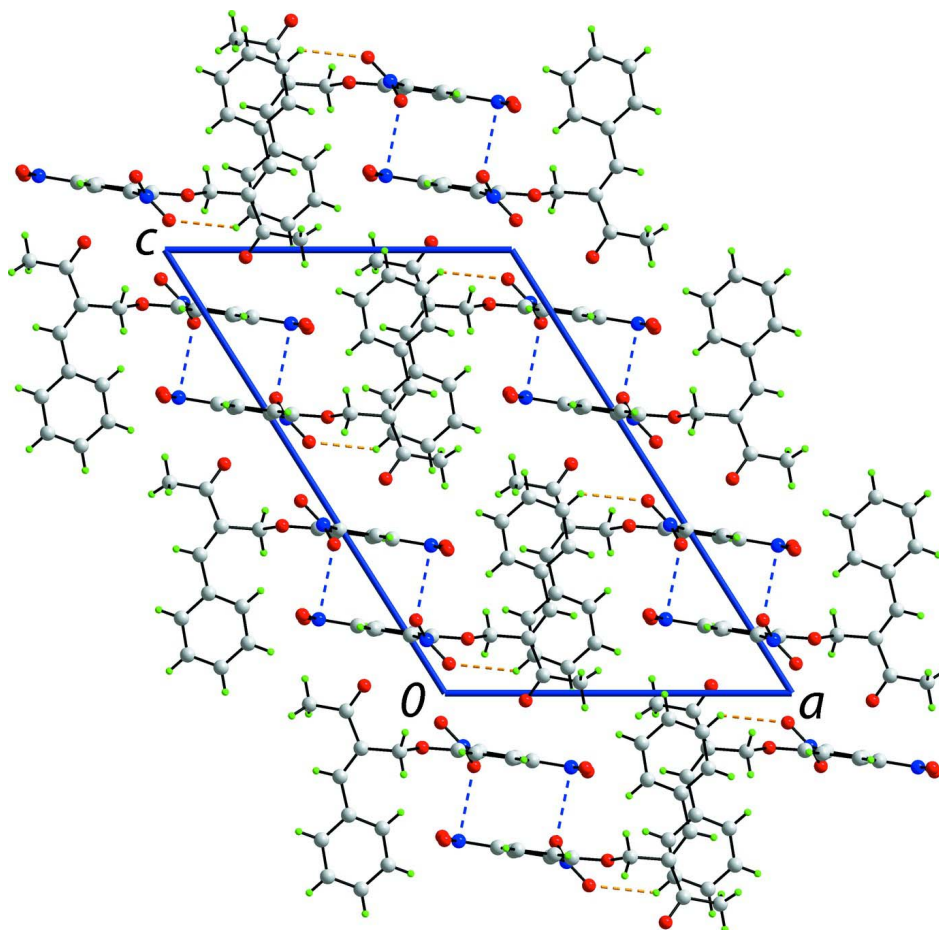


Figure 3

A view of helical supramolecular chain along $[0\ 1\ 0]$. The C—H \cdots O contacts are shown as orange dashed lines.

**Figure 4**

A view of unit-cell contents in projection down the b axis. The C—H...O and N...O contacts are shown as orange and blue dashed lines, respectively.

(3E)-3-(2,4-Dinitrophenoxymethyl)-4-phenylbut-3-en-2-one

Crystal data

$C_{17}H_{14}N_2O_6$
 $M_r = 342.30$
 Monoclinic, $P2_1/c$
 Hall symbol: -P 2ybc
 $a = 12.8459$ (6) Å
 $b = 7.6983$ (4) Å
 $c = 19.4283$ (8) Å
 $\beta = 122.254$ (2)°
 $V = 1624.82$ (14) Å³
 $Z = 4$

$F(000) = 712$
 $D_x = 1.399$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 6161 reflections
 $\theta = 2.9$ – 25.3 °
 $\mu = 0.11$ mm⁻¹
 $T = 290$ K
 Irregular, colourless
 $0.66 \times 0.45 \times 0.28$ mm

Data collection

Bruker Kappa APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω and φ scans

Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.699$, $T_{\max} = 0.745$
 10435 measured reflections
 2957 independent reflections

2630 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$
 $\theta_{\text{max}} = 25.3^\circ$, $\theta_{\text{min}} = 1.9^\circ$

$h = -10 \rightarrow 15$
 $k = -7 \rightarrow 9$
 $l = -23 \rightarrow 19$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.101$
 $S = 1.04$
 2957 reflections
 228 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
 $w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.4196P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.20 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0323 (19)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.93401 (11)	0.15407 (17)	0.37127 (8)	0.0384 (3)
C2	0.99377 (11)	0.00425 (16)	0.36899 (7)	0.0364 (3)
C3	1.08837 (11)	0.01022 (18)	0.35523 (8)	0.0409 (3)
H3	1.1239	-0.0912	0.3510	0.049*
C4	1.12866 (12)	0.17061 (19)	0.34788 (8)	0.0436 (3)
C5	1.07599 (14)	0.3221 (2)	0.35327 (9)	0.0509 (4)
H5	1.1062	0.4292	0.3496	0.061*
C6	0.97836 (14)	0.31403 (18)	0.36410 (10)	0.0494 (4)
H6	0.9418	0.4161	0.3666	0.059*
C7	0.76361 (13)	0.28733 (18)	0.36901 (10)	0.0463 (3)
H7A	0.7331	0.3422	0.3167	0.056*
H7B	0.8140	0.3705	0.4115	0.056*
C8	0.65850 (12)	0.22873 (19)	0.37591 (9)	0.0437 (3)
C9	0.68382 (13)	0.2244 (2)	0.46004 (9)	0.0503 (4)
C10	0.58981 (16)	0.1491 (3)	0.47503 (11)	0.0656 (5)
H10A	0.6229	0.1458	0.5325	0.098*
H10B	0.5694	0.0334	0.4534	0.098*
H10C	0.5171	0.2199	0.4488	0.098*
C11	0.54588 (13)	0.18897 (19)	0.31208 (9)	0.0464 (3)
H11	0.4877	0.1628	0.3251	0.056*

C12	0.50092 (13)	0.18058 (18)	0.22527 (9)	0.0447 (3)
C13	0.57329 (14)	0.1286 (2)	0.19522 (9)	0.0502 (4)
H13	0.6557	0.1012	0.2312	0.060*
C14	0.52360 (15)	0.1174 (2)	0.11257 (10)	0.0568 (4)
H14	0.5729	0.0830	0.0933	0.068*
C15	0.40169 (16)	0.1568 (2)	0.05828 (10)	0.0596 (4)
H15	0.3690	0.1496	0.0026	0.071*
C16	0.32823 (15)	0.2069 (2)	0.08653 (10)	0.0613 (4)
H16	0.2458	0.2337	0.0500	0.074*
C17	0.37725 (14)	0.2172 (2)	0.16927 (10)	0.0539 (4)
H17	0.3268	0.2492	0.1880	0.065*
N1	1.22919 (11)	0.1784 (2)	0.33327 (8)	0.0572 (4)
N2	0.95589 (10)	-0.16711 (15)	0.38003 (7)	0.0443 (3)
O1	0.83551 (8)	0.13359 (12)	0.37729 (6)	0.0459 (3)
O2	0.78088 (11)	0.27977 (19)	0.51669 (7)	0.0716 (4)
O3	1.26869 (11)	0.0420 (2)	0.32347 (8)	0.0767 (4)
O4	1.26880 (12)	0.32170 (19)	0.33128 (9)	0.0825 (4)
O5	0.95090 (13)	-0.28306 (15)	0.33557 (8)	0.0716 (4)
O6	0.93475 (11)	-0.18635 (15)	0.43354 (8)	0.0673 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0332 (6)	0.0384 (7)	0.0442 (7)	-0.0002 (5)	0.0209 (6)	0.0030 (5)
C2	0.0316 (6)	0.0352 (7)	0.0391 (6)	-0.0014 (5)	0.0167 (5)	0.0027 (5)
C3	0.0341 (6)	0.0469 (8)	0.0400 (7)	0.0039 (6)	0.0187 (6)	0.0018 (6)
C4	0.0338 (6)	0.0564 (9)	0.0412 (7)	-0.0039 (6)	0.0204 (6)	0.0042 (6)
C5	0.0478 (8)	0.0461 (8)	0.0605 (9)	-0.0090 (6)	0.0301 (7)	0.0067 (7)
C6	0.0496 (8)	0.0357 (7)	0.0681 (10)	0.0009 (6)	0.0349 (8)	0.0041 (7)
C7	0.0426 (7)	0.0407 (8)	0.0599 (9)	0.0080 (6)	0.0302 (7)	0.0032 (6)
C8	0.0405 (7)	0.0443 (8)	0.0518 (8)	0.0104 (6)	0.0284 (6)	0.0041 (6)
C9	0.0443 (8)	0.0550 (9)	0.0509 (8)	0.0158 (7)	0.0248 (7)	0.0081 (7)
C10	0.0647 (10)	0.0875 (13)	0.0582 (10)	0.0071 (9)	0.0419 (9)	0.0055 (9)
C11	0.0418 (7)	0.0524 (8)	0.0542 (8)	0.0061 (6)	0.0318 (7)	0.0013 (6)
C12	0.0436 (7)	0.0443 (8)	0.0517 (8)	0.0024 (6)	0.0291 (7)	0.0003 (6)
C13	0.0470 (8)	0.0546 (9)	0.0541 (8)	0.0103 (7)	0.0304 (7)	0.0040 (7)
C14	0.0668 (10)	0.0592 (10)	0.0597 (9)	0.0106 (8)	0.0440 (8)	0.0052 (8)
C15	0.0666 (10)	0.0640 (11)	0.0492 (9)	0.0053 (8)	0.0317 (8)	0.0051 (7)
C16	0.0463 (8)	0.0755 (12)	0.0553 (9)	0.0049 (8)	0.0226 (7)	0.0018 (8)
C17	0.0418 (7)	0.0650 (10)	0.0591 (9)	0.0018 (7)	0.0298 (7)	-0.0040 (7)
N1	0.0398 (7)	0.0847 (11)	0.0497 (7)	-0.0076 (7)	0.0256 (6)	0.0055 (7)
N2	0.0342 (6)	0.0364 (6)	0.0536 (7)	0.0010 (5)	0.0177 (5)	0.0058 (5)
O1	0.0380 (5)	0.0394 (5)	0.0685 (6)	0.0048 (4)	0.0339 (5)	0.0072 (4)
O2	0.0542 (7)	0.0928 (10)	0.0513 (7)	0.0044 (6)	0.0170 (6)	0.0071 (6)
O3	0.0611 (7)	0.0984 (10)	0.0919 (9)	0.0169 (7)	0.0550 (7)	0.0151 (8)
O4	0.0699 (8)	0.0988 (11)	0.0971 (10)	-0.0359 (7)	0.0567 (8)	-0.0084 (8)
O5	0.0896 (9)	0.0395 (6)	0.0671 (8)	-0.0070 (6)	0.0294 (7)	-0.0080 (5)
O6	0.0747 (8)	0.0542 (7)	0.0984 (9)	0.0033 (6)	0.0632 (8)	0.0199 (6)

Geometric parameters (Å, °)

C1—O1	1.3405 (15)	C10—H10A	0.9600
C1—C6	1.3947 (18)	C10—H10B	0.9600
C1—C2	1.3993 (18)	C10—H10C	0.9600
C2—C3	1.3773 (17)	C11—C12	1.464 (2)
C2—N2	1.4610 (16)	C11—H11	0.9300
C3—C4	1.375 (2)	C12—C17	1.394 (2)
C3—H3	0.9300	C12—C13	1.3945 (19)
C4—C5	1.380 (2)	C13—C14	1.378 (2)
C4—N1	1.4638 (17)	C13—H13	0.9300
C5—C6	1.379 (2)	C14—C15	1.376 (2)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—C16	1.376 (2)
C7—O1	1.4565 (16)	C15—H15	0.9300
C7—C8	1.4959 (19)	C16—C17	1.381 (2)
C7—H7A	0.9700	C16—H16	0.9300
C7—H7B	0.9700	C17—H17	0.9300
C8—C11	1.345 (2)	N1—O4	1.2242 (18)
C8—C9	1.487 (2)	N1—O3	1.2242 (19)
C9—O2	1.2176 (19)	N2—O6	1.2156 (16)
C9—C10	1.502 (2)	N2—O5	1.2198 (16)
O1—C1—C6	124.58 (12)	H10A—C10—H10B	109.5
O1—C1—C2	117.72 (11)	C9—C10—H10C	109.5
C6—C1—C2	117.66 (12)	H10A—C10—H10C	109.5
C3—C2—C1	122.31 (12)	H10B—C10—H10C	109.5
C3—C2—N2	117.14 (11)	C8—C11—C12	129.87 (13)
C1—C2—N2	120.55 (11)	C8—C11—H11	115.1
C4—C3—C2	118.04 (12)	C12—C11—H11	115.1
C4—C3—H3	121.0	C17—C12—C13	117.91 (13)
C2—C3—H3	121.0	C17—C12—C11	118.36 (12)
C3—C4—C5	121.58 (12)	C13—C12—C11	123.63 (13)
C3—C4—N1	118.47 (13)	C14—C13—C12	120.53 (14)
C5—C4—N1	119.95 (13)	C14—C13—H13	119.7
C6—C5—C4	119.75 (13)	C12—C13—H13	119.7
C6—C5—H5	120.1	C15—C14—C13	120.61 (14)
C4—C5—H5	120.1	C15—C14—H14	119.7
C5—C6—C1	120.54 (13)	C13—C14—H14	119.7
C5—C6—H6	119.7	C16—C15—C14	119.88 (15)
C1—C6—H6	119.7	C16—C15—H15	120.1
O1—C7—C8	107.14 (11)	C14—C15—H15	120.1
O1—C7—H7A	110.3	C15—C16—C17	119.79 (15)
C8—C7—H7A	110.3	C15—C16—H16	120.1
O1—C7—H7B	110.3	C17—C16—H16	120.1
C8—C7—H7B	110.3	C16—C17—C12	121.26 (14)
H7A—C7—H7B	108.5	C16—C17—H17	119.4
C11—C8—C9	120.33 (12)	C12—C17—H17	119.4

C11—C8—C7	124.35 (13)	O4—N1—O3	123.64 (13)
C9—C8—C7	115.26 (13)	O4—N1—C4	117.88 (15)
O2—C9—C8	120.24 (14)	O3—N1—C4	118.49 (13)
O2—C9—C10	120.09 (14)	O6—N2—O5	124.41 (13)
C8—C9—C10	119.67 (14)	O6—N2—C2	118.65 (12)
C9—C10—H10A	109.5	O5—N2—C2	116.90 (12)
C9—C10—H10B	109.5	C1—O1—C7	117.86 (10)
O1—C1—C2—C3	173.75 (11)	C8—C11—C12—C17	-150.23 (16)
C6—C1—C2—C3	-3.9 (2)	C8—C11—C12—C13	33.5 (2)
O1—C1—C2—N2	-5.24 (18)	C17—C12—C13—C14	1.2 (2)
C6—C1—C2—N2	177.08 (12)	C11—C12—C13—C14	177.53 (15)
C1—C2—C3—C4	3.50 (19)	C12—C13—C14—C15	-0.2 (3)
N2—C2—C3—C4	-177.48 (11)	C13—C14—C15—C16	-0.4 (3)
C2—C3—C4—C5	-0.6 (2)	C14—C15—C16—C17	-0.1 (3)
C2—C3—C4—N1	179.98 (11)	C15—C16—C17—C12	1.1 (3)
C3—C4—C5—C6	-1.8 (2)	C13—C12—C17—C16	-1.7 (2)
N1—C4—C5—C6	177.66 (13)	C11—C12—C17—C16	-178.17 (15)
C4—C5—C6—C1	1.3 (2)	C3—C4—N1—O4	-176.08 (13)
O1—C1—C6—C5	-176.05 (13)	C5—C4—N1—O4	4.5 (2)
C2—C1—C6—C5	1.5 (2)	C3—C4—N1—O3	4.2 (2)
O1—C7—C8—C11	-94.16 (16)	C5—C4—N1—O3	-175.29 (14)
O1—C7—C8—C9	88.75 (14)	C3—C2—N2—O6	137.34 (13)
C11—C8—C9—O2	-171.36 (15)	C1—C2—N2—O6	-43.62 (17)
C7—C8—C9—O2	5.9 (2)	C3—C2—N2—O5	-40.76 (17)
C11—C8—C9—C10	9.5 (2)	C1—C2—N2—O5	138.28 (13)
C7—C8—C9—C10	-173.26 (13)	C6—C1—O1—C7	5.4 (2)
C9—C8—C11—C12	-178.44 (14)	C2—C1—O1—C7	-172.16 (12)
C7—C8—C11—C12	4.6 (2)	C8—C7—O1—C1	178.57 (11)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6—H6 \cdots O5 ⁱ	0.93	2.41	3.1375 (18)	135
C16—H16 \cdots O6 ⁱⁱ	0.93	2.58	3.292 (3)	134

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