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2-Aminobenzoxazole–oxalic acid (2/1)

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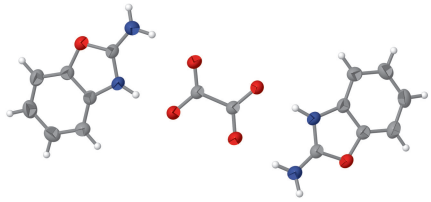
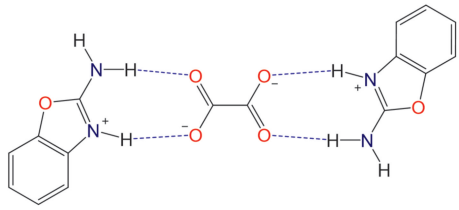
In the title compound, $2C_7H_7N_2O^+\cdot C_2O_4^{2-}$, proton transfer from oxalic acid to the N atom of the heterocycle has occurred to form a 2:1 molecular salt. In the extended structure, N—H···O hydrogen bonds link the components into [100] chains, which feature $R_2^2(8)$ and $R_4^4(14)$ loops.

3D view



Chemical scheme



Structure description

2-Aminobenzoxazole has gained significant attention in the field of organic chemistry due to its diverse range of applications and properties. This heterocyclic compound exhibits intriguing structural features and has demonstrated potential utility in the development of pharmaceuticals and agrochemicals and in materials science (Hwang *et al.*, 2006; Potashman *et al.*, 2007). With its aromatic and nitrogen-containing structural motifs, 2-aminobenzoxazole has emerged as a key scaffold for the synthesis of biologically active molecules and advanced materials. Herein, we report on the crystal structure analysis of a new 2-aminobenzoxazole–oxalic acid molecular salt.

The title organic salt crystallizes in the monoclinic space group $P2_1/n$. The molecular structure of the organic salt is shown in Fig. 1. The geometric parameters of the arene and oxazole rings are similar to standard values and to those in other related structures (Ashurov *et al.*, 2011, 2015; Wang *et al.*, 2016). In the oxalate (OXL) part of the organic salt, two hydrogen atoms are transferred to the nitrogen of the oxazole fragments, as in other 2-aminobenzoxazole (2ABO) structures (Nandy *et al.*, 2016; Razzoqova *et al.*, 2022, 2023). As a result, the 2ABO and OXL ions form two closed eight-membered rings with an $R_2^2(8)$ graph-set notation (Etter *et al.*, 1990). This represents a 1:2 acid-base association (Calva *et al.*, 2011), with the first ring formed by N1—H1···O4 and N2—H2*B*···O3 hydrogen bonds and the second by N4—H4*B*···O6 and N3—H3*A*···O5 hydrogen bonds (Table 1). N2—H2*A*···O4 and N4—H4*A*···O5 hydrogen bonds further link the

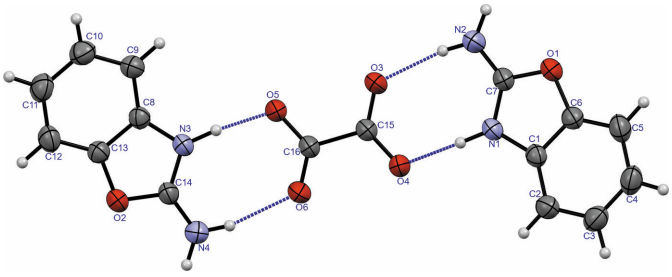


Figure 1
The organic salt structure of 2ABO and OXL. Displacement ellipsoids are drawn at the 50% probability level and N—H···O hydrogen bonds are shown as dashed lines.

components into [100] chains, thereby forming a 14-membered ring with an $R_4^4(14)$ graph-set motif (Fig. 2) (Etter *et al.*, 1990). The chains are shown in Fig. 3.

The identification of the co-crystal as a salt is based on the successful refinement of the relevant H atoms using X-ray data. The proton transfer is further supported by the C—O distances [O4—C15 = 1.266 (2) Å, O3—C15 = 1.234 (2) Å, O5—C16 = 1.272 (2) Å and O6—C16 = 1.222 (2) Å] with differences between the bond lengths within each group of 0.032 and 0.050 Å; these differences differ from those for O—C distances in deprotonated carboxyl groups. In non-

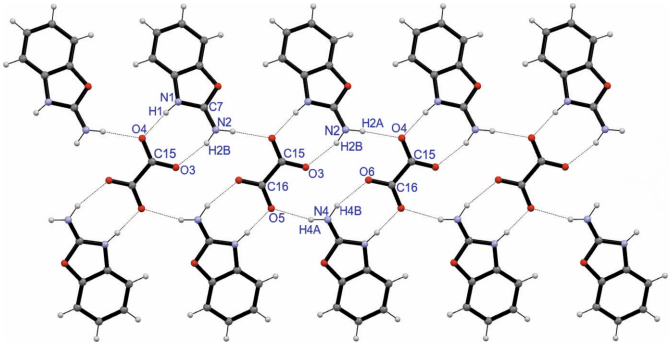


Figure 2
The crystal structure of the organic salt structure of 2ABO and OXL viewed along the *c* axis.

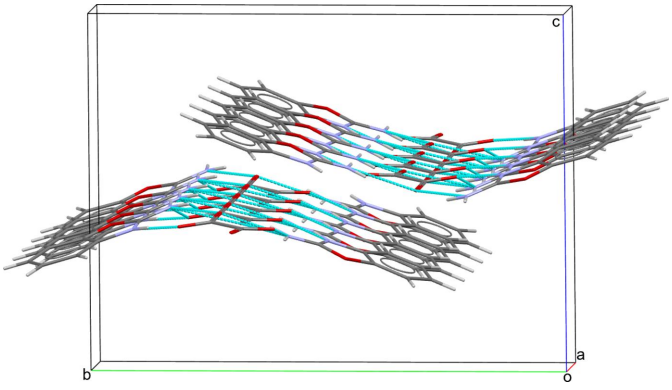


Figure 3
A fragment of a [100] chain in the extended structure of the title compound with hydrogen bonds shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4	0.88 (1)	1.78 (1)	2.650 (2)	176 (3)
N2—H2*A*···O4^{i}	0.87 (1)	2.00 (1)	2.863 (2)	174 (3)
N2—H2*B*···O3	0.86 (1)	1.94 (1)	2.770 (2)	164 (2)
C2—H2···O1^{ii}	0.93	2.65	3.522 (2)	157
N3—H3*A*···O5	0.88 (1)	1.71 (1)	2.577 (2)	173 (3)
N4—H4*A*···O5^{ii}	0.87 (1)	2.06 (1)	2.918 (2)	172 (2)
N4—H4*B*···O6	0.86 (1)	2.02 (1)	2.851 (2)	163 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_7H_7N_2O^+\cdot C_2O_4^{2-}$
M_r	358.31
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, *b*, *c* (Å)	6.5080 (2), 17.6943 (7), 13.6264 (5)
β (°)	100.200 (4)
V (Å^3)	1544.34 (10)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.03
Crystal size (mm)	0.17 × 0.14 × 0.12
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix3000
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2020)
T_{min}, T_{max}	0.157, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2960, 2960, 2288
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.132, 1.04
No. of reflections	2960
No. of parameters	259
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.20

Computer programs: *CrysAlis PRO* (Rigaku OD, 2020), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

deprotonated oxalic acid, these differences are greater (Sasaki *et al.*, 2020). The mean planes of the carboxylic fragments in the OXL ion are turned by 10.13 (4)° from each other. In the crystal, the 2BAO and OXL ions are not coplanar, the 2ABO ions being inclined to the OXL ions by 18.81 (3) and 16.00 (5)°. The dihedral angle between the 2ABO ions is 37.52 (2)°.

Synthesis and crystallization

A 2:1 stoichiometric ratio of 2-aminobenzoxazole (0.268 g, 2.0 mmol) and oxalic acid (0.090 g, 1.0 mmol) was dissolved and mixed well in distilled water (5 ml). The mixture was stirred at room temperature for 30 minutes. The solution was then transferred to a vial with small holes in the cover to allow

for evaporation. After about 3 weeks, cube-like single crystals of the title salt suitable for data collection were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2024). **9**, x240033 [https://doi.org/10.1107/S2414314624000336]

2-Aminobenzoxazole–oxalic acid (2/1)

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Bis(2-aminobenzoxazol-3-ium) oxalate

Crystal data

$2C_7H_7N_2O^+\cdot C_2O_4^{2-}$
M_r = 358.31
Monoclinic, $P2_1/n$
a = 6.5080 (2) Å
b = 17.6943 (7) Å
c = 13.6264 (5) Å
β = 100.200 (4)°
V = 1544.34 (10) Å^3
Z = 4
$F(000)$ = 744
D_x = 1.541 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 2449 reflections
θ = 4.1–70.3°
μ = 1.03 mm^{-1}
T = 293 K
Needle, light yellow
0.17 × 0.14 × 0.12 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix3000 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2020)
T_{min} = 0.157, T_{max} = 1.000
2960 measured reflections
2960 independent reflections
2288 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 71.4°, θ_{min} = 4.1°
h = −8→7
k = −20→21
l = −13→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.132
S = 1.03
2960 reflections
259 parameters
6 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0724P)^2 + 0.1538P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

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

Refinement. The hydrogen atoms of amino groups and protonated nitrogen atoms of oxzole groups were located in difference - Fourier maps and refined with restrained distances of 0.85±(1) Å. The H atoms of the benzene ring were calculated geometrically with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.1212 (2)	0.44529 (8)	0.33805 (10)	0.0428 (3)
N1	0.4453 (2)	0.48755 (9)	0.38019 (11)	0.0381 (4)
H1	0.545 (3)	0.5203 (13)	0.3995 (19)	0.082 (9)*
C1	0.4597 (3)	0.41299 (11)	0.34764 (13)	0.0366 (4)
O2	1.3397 (2)	0.94256 (8)	0.42539 (10)	0.0410 (3)
N2	0.1639 (3)	0.56637 (11)	0.39934 (16)	0.0521 (5)
H2A	0.0351 (19)	0.5701 (15)	0.4069 (18)	0.069 (8)*
H2B	0.252 (3)	0.6021 (11)	0.4168 (18)	0.069 (8)*
C2	0.6255 (3)	0.36637 (12)	0.34088 (15)	0.0439 (5)
H2	0.762934	0.382283	0.360114	0.053*
O3	0.4839 (2)	0.67161 (8)	0.42640 (12)	0.0540 (4)
N3	1.0284 (2)	0.88951 (9)	0.42134 (12)	0.0381 (4)
H3A	0.927 (3)	0.8578 (14)	0.427 (2)	0.090 (10)*
C3	0.5769 (4)	0.29442 (12)	0.30389 (16)	0.0518 (5)
H3	0.685094	0.261048	0.299092	0.062*
O4	0.7441 (2)	0.58949 (7)	0.42948 (10)	0.0432 (3)
N4	1.3345 (3)	0.81860 (10)	0.47545 (14)	0.0470 (4)
H4A	1.4629 (19)	0.8123 (15)	0.4680 (17)	0.061 (7)*
H4B	1.258 (3)	0.7797 (10)	0.4805 (18)	0.064 (8)*
C4	0.3719 (4)	0.27030 (13)	0.27364 (17)	0.0533 (6)
H4	0.346243	0.222044	0.247253	0.064*
O5	0.7522 (2)	0.78759 (8)	0.43539 (12)	0.0517 (4)
C5	0.2049 (3)	0.31731 (12)	0.28231 (16)	0.0497 (5)
H5	0.066961	0.301904	0.263314	0.060*
O6	1.0164 (2)	0.70685 (9)	0.46759 (14)	0.0624 (5)
C6	0.2561 (3)	0.38746 (11)	0.32045 (13)	0.0394 (4)
C7	0.2444 (3)	0.50366 (11)	0.37490 (13)	0.0383 (4)
C8	0.9941 (3)	0.96341 (10)	0.38748 (13)	0.0350 (4)
C9	0.8136 (3)	1.00364 (12)	0.35338 (13)	0.0420 (4)
H9	0.682079	0.982192	0.350086	0.050*
C10	0.8389 (3)	1.07772 (13)	0.32431 (15)	0.0490 (5)
H10	0.720945	1.106402	0.300336	0.059*
C11	1.0345 (4)	1.11046 (13)	0.32983 (16)	0.0531 (5)
H11	1.044476	1.160508	0.310364	0.064*
C12	1.2147 (3)	1.06995 (12)	0.36377 (16)	0.0483 (5)
H12	1.346707	1.091225	0.368116	0.058*
C13	1.1870 (3)	0.99662 (11)	0.39057 (13)	0.0377 (4)
C14	1.2326 (3)	0.87935 (11)	0.44171 (13)	0.0372 (4)
C15	0.6703 (3)	0.65540 (10)	0.43310 (13)	0.0354 (4)
C16	0.8301 (3)	0.72137 (11)	0.44698 (14)	0.0379 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0305 (7)	0.0392 (7)	0.0574 (8)	−0.0051 (5)	0.0037 (5)	−0.0028 (6)
N1	0.0284 (8)	0.0363 (9)	0.0492 (8)	−0.0048 (6)	0.0058 (6)	−0.0030 (7)
C1	0.0356 (10)	0.0348 (10)	0.0396 (9)	−0.0046 (8)	0.0071 (7)	0.0037 (7)
O2	0.0322 (7)	0.0382 (7)	0.0536 (8)	−0.0047 (5)	0.0098 (5)	0.0007 (6)
N2	0.0331 (9)	0.0404 (10)	0.0844 (13)	−0.0023 (8)	0.0144 (9)	−0.0085 (9)
C2	0.0377 (11)	0.0428 (11)	0.0523 (11)	0.0007 (8)	0.0110 (8)	0.0039 (9)
O3	0.0292 (7)	0.0391 (8)	0.0945 (11)	−0.0031 (6)	0.0131 (7)	−0.0047 (8)
N3	0.0298 (8)	0.0342 (9)	0.0515 (9)	−0.0049 (7)	0.0101 (6)	−0.0018 (7)
C3	0.0567 (14)	0.0396 (11)	0.0626 (13)	0.0058 (10)	0.0202 (10)	0.0046 (10)
O4	0.0327 (7)	0.0323 (7)	0.0645 (8)	−0.0021 (5)	0.0086 (6)	−0.0027 (6)
N4	0.0360 (10)	0.0392 (10)	0.0663 (11)	0.0014 (8)	0.0102 (8)	0.0037 (8)
C4	0.0648 (15)	0.0344 (11)	0.0637 (13)	−0.0072 (10)	0.0199 (11)	−0.0045 (10)
O5	0.0324 (7)	0.0332 (7)	0.0900 (11)	−0.0013 (6)	0.0120 (7)	0.0054 (7)
C5	0.0486 (12)	0.0430 (12)	0.0579 (12)	−0.0135 (9)	0.0105 (9)	−0.0027 (9)
O6	0.0291 (8)	0.0397 (9)	0.1155 (14)	−0.0015 (6)	0.0047 (8)	0.0032 (8)
C6	0.0351 (10)	0.0378 (10)	0.0451 (10)	−0.0019 (8)	0.0063 (7)	0.0037 (8)
C7	0.0328 (9)	0.0344 (10)	0.0477 (10)	−0.0039 (7)	0.0066 (7)	0.0009 (8)
C8	0.0355 (10)	0.0337 (10)	0.0367 (8)	−0.0029 (7)	0.0093 (7)	−0.0032 (7)
C9	0.0353 (10)	0.0433 (11)	0.0476 (10)	0.0004 (8)	0.0082 (8)	−0.0014 (9)
C10	0.0491 (12)	0.0459 (12)	0.0525 (11)	0.0074 (9)	0.0102 (9)	0.0043 (9)
C11	0.0620 (14)	0.0383 (12)	0.0616 (13)	−0.0022 (10)	0.0180 (10)	0.0085 (10)
C12	0.0476 (12)	0.0418 (12)	0.0576 (12)	−0.0100 (9)	0.0154 (9)	0.0013 (9)
C13	0.0361 (10)	0.0357 (10)	0.0423 (9)	−0.0014 (8)	0.0098 (7)	−0.0029 (8)
C14	0.0330 (10)	0.0340 (10)	0.0453 (9)	−0.0050 (7)	0.0090 (7)	−0.0041 (8)
C15	0.0304 (9)	0.0343 (10)	0.0420 (9)	−0.0025 (7)	0.0079 (7)	0.0009 (8)
C16	0.0305 (9)	0.0336 (10)	0.0498 (10)	−0.0033 (7)	0.0077 (7)	0.0007 (8)

Geometric parameters (Å, º)

O1—C6	1.397 (2)	N4—H4A	0.866 (10)
O1—C7	1.349 (2)	N4—H4B	0.858 (10)
N1—H1	0.876 (10)	N4—C14	1.303 (3)
N1—C1	1.400 (3)	C4—H4	0.9300
N1—C7	1.328 (2)	C4—C5	1.390 (3)
C1—C2	1.374 (3)	O5—C16	1.276 (2)
C1—C6	1.386 (3)	C5—H5	0.9300
O2—C13	1.400 (2)	C5—C6	1.364 (3)
O2—C14	1.357 (2)	O6—C16	1.222 (2)
N2—H2A	0.865 (10)	C8—C9	1.382 (3)
N2—H2B	0.857 (10)	C8—C13	1.380 (3)
N2—C7	1.296 (3)	C9—H9	0.9300
C2—H2	0.9300	C9—C10	1.388 (3)
C2—C3	1.385 (3)	C10—H10	0.9300
O3—C15	1.234 (2)	C10—C11	1.388 (3)
N3—H3A	0.877 (10)	C11—H11	0.9300

N3—C8	1.391 (2)	C11—C12	1.382 (3)
N3—C14	1.321 (2)	C12—H12	0.9300
C3—H3	0.9300	C12—C13	1.369 (3)
C3—C4	1.392 (3)	C15—C16	1.553 (3)
O4—C15	1.266 (2)		

C7—O1—C6	105.93 (14)	C5—C6—C1	123.77 (19)
C1—N1—H1	129 (2)	N1—C7—O1	111.77 (16)
C7—N1—H1	123 (2)	N2—C7—O1	120.69 (17)
C7—N1—C1	107.77 (15)	N2—C7—N1	127.53 (18)
C2—C1—N1	133.15 (18)	C9—C8—N3	132.26 (18)
C2—C1—C6	120.73 (18)	C13—C8—N3	107.36 (16)
C6—C1—N1	106.12 (16)	C13—C8—C9	120.37 (18)
C14—O2—C13	105.31 (14)	C8—C9—H9	121.8
H2A—N2—H2B	122 (3)	C8—C9—C10	116.46 (19)
C7—N2—H2A	122.7 (18)	C10—C9—H9	121.8
C7—N2—H2B	115.0 (19)	C9—C10—H10	118.9
C1—C2—H2	121.8	C9—C10—C11	122.2 (2)
C1—C2—C3	116.40 (19)	C11—C10—H10	118.9
C3—C2—H2	121.8	C10—C11—H11	119.4
C8—N3—H3A	123 (2)	C12—C11—C10	121.1 (2)
C14—N3—H3A	129 (2)	C12—C11—H11	119.4
C14—N3—C8	107.10 (15)	C11—C12—H12	122.1
C2—C3—H3	118.8	C13—C12—C11	115.9 (2)
C2—C3—C4	122.3 (2)	C13—C12—H12	122.1
C4—C3—H3	118.8	C8—C13—O2	107.87 (16)
H4A—N4—H4B	119 (2)	C12—C13—O2	128.21 (18)
C14—N4—H4A	120.4 (17)	C12—C13—C8	123.92 (19)
C14—N4—H4B	115.1 (18)	N3—C14—O2	112.34 (16)
C3—C4—H4	119.5	N4—C14—O2	119.57 (17)
C5—C4—C3	120.9 (2)	N4—C14—N3	128.08 (18)
C5—C4—H4	119.5	O3—C15—O4	125.89 (17)
C4—C5—H5	122.1	O3—C15—C16	117.56 (16)
C6—C5—C4	115.8 (2)	O4—C15—C16	116.55 (16)
C6—C5—H5	122.1	O5—C16—C15	115.62 (16)
C1—C6—O1	108.39 (16)	O6—C16—O5	125.33 (18)
C5—C6—O1	127.84 (18)	O6—C16—C15	119.06 (17)

N1—C1—C2—C3	−179.9 (2)	C6—C1—C2—C3	1.4 (3)
N1—C1—C6—O1	−1.0 (2)	C7—O1—C6—C1	0.03 (19)
N1—C1—C6—C5	178.36 (18)	C7—O1—C6—C5	−179.3 (2)
C1—N1—C7—O1	−1.8 (2)	C7—N1—C1—C2	−177.2 (2)
C1—N1—C7—N2	179.0 (2)	C7—N1—C1—C6	1.7 (2)
C1—C2—C3—C4	0.9 (3)	C8—N3—C14—O2	1.1 (2)
C2—C1—C6—O1	178.00 (16)	C8—N3—C14—N4	179.93 (19)
C2—C1—C6—C5	−2.6 (3)	C8—C9—C10—C11	−0.6 (3)
C2—C3—C4—C5	−2.0 (3)	C9—C8—C13—O2	−178.45 (16)
O3—C15—C16—O5	−10.1 (3)	C9—C8—C13—C12	1.8 (3)

O3—C15—C16—O6	169.97 (19)	C9—C10—C11—C12	0.8 (3)
N3—C8—C9—C10	−179.46 (19)	C10—C11—C12—C13	0.3 (3)
N3—C8—C13—O2	0.65 (19)	C11—C12—C13—O2	178.73 (18)
N3—C8—C13—C12	−179.10 (18)	C11—C12—C13—C8	−1.6 (3)
C3—C4—C5—C6	0.9 (3)	C13—O2—C14—N3	−0.71 (19)
O4—C15—C16—O5	169.79 (17)	C13—O2—C14—N4	−179.63 (17)
O4—C15—C16—O6	−10.2 (3)	C13—C8—C9—C10	−0.6 (3)
C4—C5—C6—O1	−179.32 (18)	C14—O2—C13—C8	0.00 (18)
C4—C5—C6—C1	1.4 (3)	C14—O2—C13—C12	179.74 (19)
C6—O1—C7—N1	1.1 (2)	C14—N3—C8—C9	177.88 (19)
C6—O1—C7—N2	−179.66 (18)	C14—N3—C8—C13	−1.07 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4	0.88 (1)	1.78 (1)	2.650 (2)	176 (3)
N2—H2*A*···O4^{i}	0.87 (1)	2.00 (1)	2.863 (2)	174 (3)
N2—H2*B*···O3	0.86 (1)	1.94 (1)	2.770 (2)	164 (2)
C2—H2···O1^{ii}	0.93	2.65	3.522 (2)	157
N3—H3*A*···O5	0.88 (1)	1.71 (1)	2.577 (2)	173 (3)
N4—H4*A*···O5^{ii}	0.87 (1)	2.06 (1)	2.918 (2)	172 (2)
N4—H4*B*···O6	0.86 (1)	2.02 (1)	2.851 (2)	163 (2)

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