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# *N*,*N*′-Bis(2-hydroxyethyl)-*N*,*N*′-[ethylenedioxybis(*o*-phenylenemethylene)]-diammonium fumarate tetrahydrate

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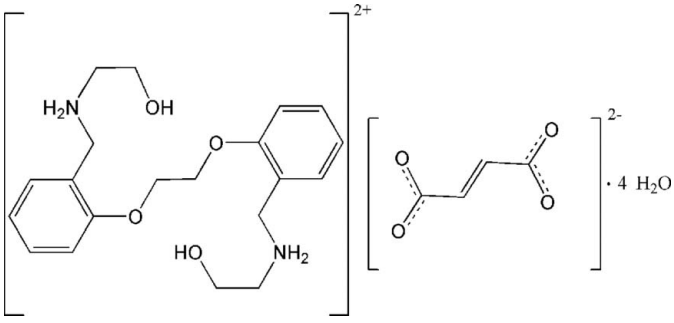
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.045; $wR$ factor = 0.128; data-to-parameter ratio = 16.2.

The reaction of 1,2-bis{2-[(2-hydroxyethyl)aminomethyl]-phenoxy}ethane and fumaric acid in a mixed solution in ethanol–water (1:1 *v*/*v*) yields the title compound, $C_{20}H_{30}N_2O_4^{2+}\cdot C_4H_2O_4^{2-}\cdot 4H_2O$. In the crystal structure, the anions, cations and water molecules are connected via O—H···O and N—H···O hydrogen bonds into a three-dimensional network. The fumarate anion and the *N*,*N*′-bis(2-hydroxyethyl)-*N*,*N*′-[ethylenedioxybis(*o*-phenylenemethylene)]diammonium cation are located on centers of inversion, whereas the two crystallographically independent water molecules occupy general positions.

## Related literature

For a related structure, see: Wang & Wei (2005). For background to the synthesis, see: Armstrong & Lindoy (1975).




## Experimental

### Crystal data

$C_{20}H_{30}N_2O_4^{2+}\cdot C_4H_2O_4^{2-}\cdot 4H_2O$
$M_r$ = 548.58
Triclinic, $P\overline{1}$
$a$ = 7.585 (7) Å
$b$ = 8.623 (6) Å
$c$ = 11.515 (7) Å
$\alpha$ = 104.64 (2)°
$\beta$ = 96.77 (3)°
$\gamma$ = 104.29 (3)°
$V$ = 693.0 (9) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 293 (2) K
0.41 × 0.34 × 0.28 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.952, $T_{max}$ = 0.983
6826 measured reflections
3128 independent reflections
2394 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.128
$S$ = 1.11
3128 reflections
193 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.68 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* |
|---|---|---|---|---|
| O1*W*—H1*C*···O2*W* | 0.85 (3) | 1.97 (3) | 2.792 (3) | 164 (3) |
| O2*W*—H2*C*···O2 | 0.85 (3) | 1.97 (3) | 2.828 (3) | 176 (3) |
| N5—H5*B*···O2 | 0.950 (19) | 1.811 (19) | 2.749 (2) | 168.6 (16) |
| O1*W*—H1*D*···O3$^{i}$ | 0.91 (3) | 1.96 (3) | 2.830 (3) | 159 (3) |
| O2*W*—H2*D*···O4$^{ii}$ | 0.86 (3) | 2.01 (3) | 2.867 (3) | 175 (3) |
| N5—H5*A*···O1*W*$^{iii}$ | 0.900 (19) | 2.125 (19) | 2.925 (3) | 147.6 (15) |

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2116).

## References

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# supporting information

*Acta Cryst.* (2008). E**64**, o2162 [doi:10.1107/S1600536808033746]

## *N*,*N*′-Bis(2-hydroxyethyl)-*N*,*N*′-[ethylenedioxybis(*o*-phenylenemethylene)]di-ammonium fumarate tetrahydrate

**Hong-Ye Bai, Hai-Yan Liu and Jian-Fang Ma**

### S1. Comment

Currently, many groups are investigating crystal structures of cocrystals containing organic acids and organic bases, which are based on hydrogen bonding (Wang & Wei, 2005). In this context, the crystal structure of the title compound is presented.

The crystal structure consists of one N,N′-bis(2-hydroxyethyl)-N,N′-[ethylenedioxybis(o-phenylenemethylene)]di-ammonium cation and one fumarate anion located on centers of inversion and two crystallographically independent water molecules that occupy general positions (Fig. 1). In the crystal structure, different O—H···O and N—H···O hydrogen bonds link the components of the title compound into a three-dimensional network (Table 1 and Fig. 2).

### S2. Experimental

All chemicals were obtained from commercial sources and used without further purification except for *L* (*L* is 1,2-bis-{2-[(2-hydroxyethyl)aminomethyl]phenoxy}ethane). 1,4-bis(2-formylphenyl)-1,4-dioxabutuane, which was prepared according to the literature (Armstrong & Lindoy, 1975). 2-aminoethanol (1.22 g, 2.0 mol) in 50 ml of methanol were added slowly to a stirred boiling solution of 1,4-bis(2′-formylphenyl)-1,4-dioxabutuane (2.70 g, 1 mol) in 100 ml of methanol. The mixed solution was refluxed for 1 h, filtered off and cooled to room temperature. 1.52 g $NaBH_4$ were added slowly to the filtrate and stirred for a further 2 h. The solvent was evaporated and 100 ml water of were added. After extraction with chloroform the solvent was evaporated, which led to a white solid of *L*. Crystals of the title compound were obtained by dissolving *L* (0.180 g, 1 mmol) and fumaric acid (0.116 g, 1 mmol) in a mixture of ethanol and water (1:1), followed by slow evaporation of the solvents.

### S3. Refinement

The C—H H atoms were positioned with idealized geometry and treated as riding atoms with distances C—H = 0.97 ($CH_2$) and 0.93 Å (CH).90 Å and $U_{iso}$ = 1.2$U_{eq}$(C). The H atoms bonded to N atoms and O atoms were located in a difference Fourier map and were refined with varying coordinates isotropic with $U_{iso}$(H) = 1.5$U_{eq}$ of the parent atom.

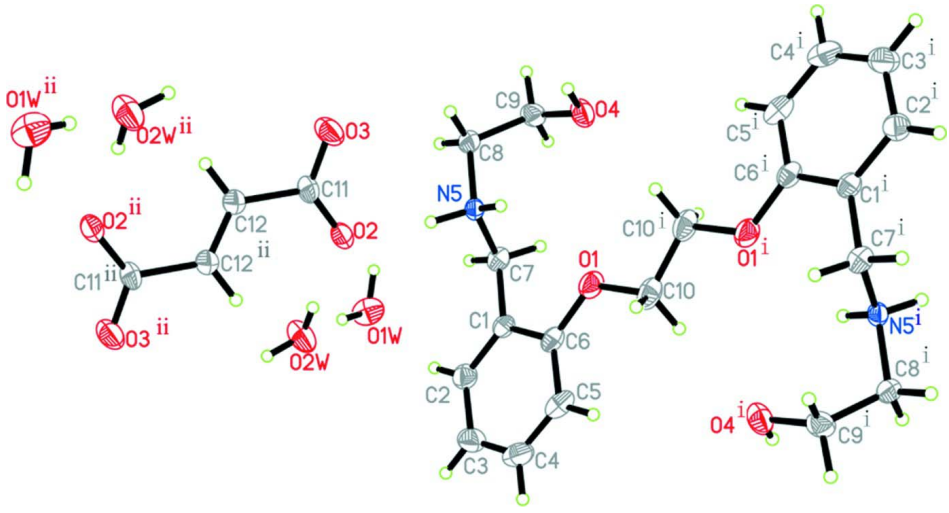


**Figure 1**

Crystal structure of the title compound with labelling and displacement ellipsoids drawn at the 30% probability level (for the H atoms spheres of arbitrary size are used). Symmetry codes: (i) -*x* + 2, -*y* + 1, -*z* + 1; (ii) -*x* + 1, -*y*, -*z* + 2.

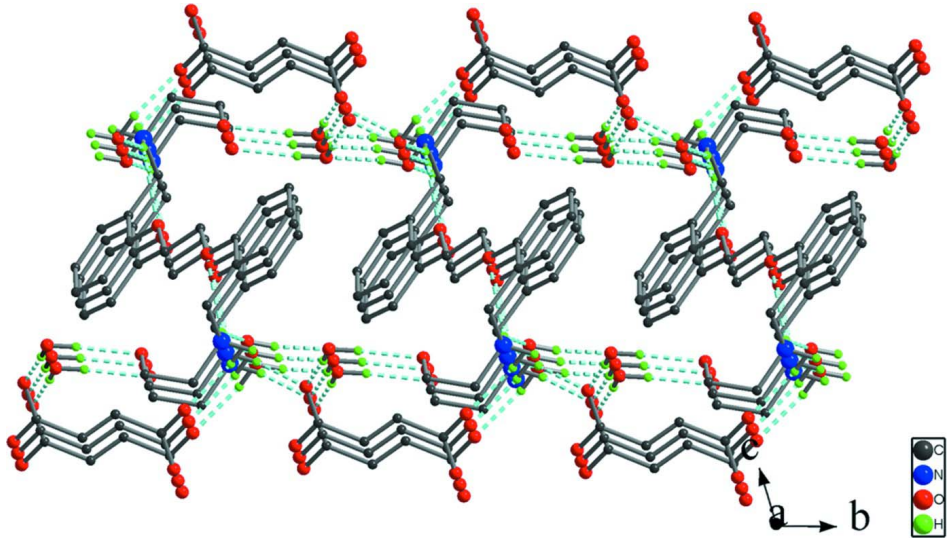


**Figure 2**

Crystal structure of the title compound with hydrogen bonding indicated by dashed lines. For clarity, H atoms not involved in hydrogen bonding are omitted.

### N,N′-Bis(2-hydroxyethyl)-N,N′-[ethylenedioxybis(o-phenylenemethylene)]diammonium fumarate tetrahydrate

*Crystal data*

$C_{20}H_{30}N_2O_4^{2+}\cdot C_4H_2O_4^{2-}\cdot 4H_2O$
$M_r = 548.58$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
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$\alpha = 104.64\ (2)°$
$\beta = 96.77\ (3)°$
$\gamma = 104.29\ (3)°$
$V = 693.0\ (9)$ Å$^3$
$Z = 1$
$F(000) = 294$
$D_x = 1.315$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 3128 reflections

$\theta$ = 3.1–27.4°
$\mu$ = 0.11 mm$^{-1}$
$T$ = 293 K

Block, colourless
0.41 × 0.34 × 0.28 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.952, $T_{max}$ = 0.983

6826 measured reflections
3128 independent reflections
2394 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018
$\theta_{max}$ = 27.4°, $\theta_{min}$ = 3.1°
$h$ = −9→9
$k$ = −11→10
$l$ = −14→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.128
$S$ = 1.11
3128 reflections
193 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 0.1182P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.68 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.4884 (2) | 0.33265 (18) | 0.58122 (12) | 0.0353 (3) |
| C2 | 0.3124 (2) | 0.2213 (2) | 0.54836 (15) | 0.0470 (4) |
| H2 | 0.2257 | 0.2368 | 0.5977 | 0.056* |
| C3 | 0.2632 (3) | 0.0871 (2) | 0.44313 (17) | 0.0582 (5) |
| H3 | 0.1438 | 0.0140 | 0.4212 | 0.070* |
| C4 | 0.3923 (3) | 0.0628 (2) | 0.37144 (15) | 0.0576 (5) |
| H4 | 0.3599 | −0.0284 | 0.3015 | 0.069* |
| C5 | 0.5695 (3) | 0.1718 (2) | 0.40173 (14) | 0.0507 (4) |
| H5 | 0.6560 | 0.1539 | 0.3528 | 0.061* |
| C6 | 0.6173 (2) | 0.3083 (2) | 0.50592 (12) | 0.0388 (3) |
| C7 | 0.5438 (2) | 0.48184 (19) | 0.69256 (13) | 0.0381 (3) |
| H7A | 0.5907 | 0.5822 | 0.6688 | 0.046* |

| | | | | |
|---|---|---|---|---|
| H7B | 0.4355 | 0.4914 | 0.7277 | 0.046* |
| C8 | 0.7528 (2) | 0.61530 (18) | 0.90008 (13) | 0.0406 (3) |
| H8A | 0.8408 | 0.5931 | 0.9574 | 0.049* |
| H8B | 0.6472 | 0.6266 | 0.9380 | 0.049* |
| C9 | 0.8425 (2) | 0.77871 (19) | 0.87634 (15) | 0.0471 (4) |
| H9A | 0.7507 | 0.8081 | 0.8269 | 0.056* |
| H9B | 0.8863 | 0.8665 | 0.9536 | 0.056* |
| C10 | 0.9210 (2) | 0.4234 (2) | 0.46928 (15) | 0.0532 (4) |
| H10A | 0.8711 | 0.4244 | 0.3880 | 0.064* |
| H10B | 0.9610 | 0.3235 | 0.4623 | 0.064* |
| C11 | 0.6218 (2) | 0.21555 (18) | 0.97927 (15) | 0.0403 (3) |
| C12 | 0.5574 (2) | 0.07174 (19) | 1.03092 (14) | 0.0431 (4) |
| H12 | 0.6033 | 0.0873 | 1.1129 | 0.052* |
| O1 | 0.78557 (15) | 0.42777 (16) | 0.54483 (10) | 0.0503 (3) |
| O2 | 0.52895 (15) | 0.21994 (13) | 0.88286 (10) | 0.0485 (3) |
| O3 | 0.76640 (19) | 0.32235 (16) | 1.03867 (13) | 0.0684 (4) |
| O1W | 0.0354 (2) | 0.3790 (2) | 0.77573 (13) | 0.0646 (4) |
| H1C | 0.050 (4) | 0.289 (4) | 0.787 (2) | 0.097* |
| H1D | 0.122 (4) | 0.462 (4) | 0.836 (3) | 0.097* |
| O2W | 0.1427 (2) | 0.09631 (18) | 0.79075 (15) | 0.0672 (4) |
| H2C | 0.260 (5) | 0.129 (4) | 0.818 (3) | 0.101* |
| H2D | 0.101 (4) | −0.004 (4) | 0.795 (3) | 0.101* |
| O4 | 0.99312 (17) | 0.76942 (15) | 0.81566 (12) | 0.0521 (3) |
| H4A | 1.073 (3) | 0.739 (3) | 0.860 (2) | 0.078* |
| N5 | 0.68936 (17) | 0.46959 (14) | 0.78706 (10) | 0.0310 (3) |
| H5A | 0.792 (3) | 0.458 (2) | 0.7581 (16) | 0.046* |
| H5B | 0.638 (2) | 0.374 (2) | 0.8117 (15) | 0.046* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0385 (8) | 0.0408 (8) | 0.0311 (6) | 0.0160 (6) | 0.0048 (5) | 0.0145 (6) |
| C2 | 0.0411 (9) | 0.0564 (10) | 0.0431 (8) | 0.0116 (7) | 0.0047 (7) | 0.0178 (7) |
| C3 | 0.0580 (11) | 0.0534 (10) | 0.0505 (10) | 0.0022 (9) | −0.0066 (8) | 0.0145 (8) |
| C4 | 0.0831 (14) | 0.0453 (9) | 0.0381 (8) | 0.0208 (9) | −0.0048 (8) | 0.0062 (7) |
| C5 | 0.0675 (12) | 0.0614 (10) | 0.0326 (7) | 0.0346 (9) | 0.0104 (7) | 0.0139 (7) |
| C6 | 0.0426 (8) | 0.0501 (9) | 0.0309 (7) | 0.0206 (7) | 0.0070 (6) | 0.0172 (6) |
| C7 | 0.0407 (8) | 0.0432 (8) | 0.0363 (7) | 0.0194 (6) | 0.0082 (6) | 0.0142 (6) |
| C8 | 0.0494 (9) | 0.0363 (8) | 0.0324 (7) | 0.0077 (7) | 0.0096 (6) | 0.0077 (6) |
| C9 | 0.0546 (10) | 0.0323 (8) | 0.0485 (8) | 0.0073 (7) | 0.0042 (7) | 0.0095 (7) |
| C10 | 0.0455 (9) | 0.0832 (13) | 0.0438 (9) | 0.0271 (9) | 0.0210 (7) | 0.0269 (9) |
| C11 | 0.0413 (8) | 0.0330 (7) | 0.0523 (9) | 0.0105 (6) | 0.0112 (7) | 0.0213 (7) |
| C12 | 0.0460 (9) | 0.0398 (8) | 0.0414 (8) | 0.0063 (6) | 0.0036 (6) | 0.0166 (6) |
| O1 | 0.0404 (6) | 0.0728 (8) | 0.0381 (6) | 0.0139 (6) | 0.0152 (5) | 0.0156 (5) |
| O2 | 0.0438 (6) | 0.0429 (6) | 0.0542 (7) | −0.0019 (5) | 0.0034 (5) | 0.0230 (5) |
| O3 | 0.0600 (8) | 0.0487 (7) | 0.0848 (10) | −0.0074 (6) | −0.0187 (7) | 0.0361 (7) |
| O1W | 0.0677 (9) | 0.0684 (9) | 0.0612 (8) | 0.0352 (8) | 0.0032 (6) | 0.0141 (7) |
| O2W | 0.0480 (8) | 0.0537 (8) | 0.1011 (11) | 0.0065 (6) | −0.0001 (7) | 0.0393 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O4 | 0.0433 (7) | 0.0515 (7) | 0.0639 (7) | 0.0049 (5) | 0.0056 (5) | 0.0319 (6) |
| N5 | 0.0327 (6) | 0.0306 (6) | 0.0313 (6) | 0.0079 (5) | 0.0087 (5) | 0.0122 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.383 (2) | C9—O4 | 1.416 (2) |
| C1—C6 | 1.400 (2) | C9—H9A | 0.9700 |
| C1—C7 | 1.499 (2) | C9—H9B | 0.9700 |
| C2—C3 | 1.385 (3) | C10—O1 | 1.424 (2) |
| C2—H2 | 0.9300 | C10—C10$^{i}$ | 1.492 (4) |
| C3—C4 | 1.374 (3) | C10—H10A | 0.9700 |
| C3—H3 | 0.9300 | C10—H10B | 0.9700 |
| C4—C5 | 1.383 (3) | C11—O3 | 1.235 (2) |
| C4—H4 | 0.9300 | C11—O2 | 1.257 (2) |
| C5—C6 | 1.389 (2) | C11—C12 | 1.508 (2) |
| C5—H5 | 0.9300 | C12—C12$^{ii}$ | 1.293 (3) |
| C6—O1 | 1.369 (2) | C12—H12 | 0.9300 |
| C7—N5 | 1.499 (2) | O1W—H1C | 0.85 (3) |
| C7—H7A | 0.9700 | O1W—H1D | 0.91 (3) |
| C7—H7B | 0.9700 | O2W—H2C | 0.85 (3) |
| C8—N5 | 1.494 (2) | O2W—H2D | 0.86 (3) |
| C8—C9 | 1.513 (2) | O4—H4A | 0.88 (3) |
| C8—H8A | 0.9700 | N5—H5A | 0.900 (19) |
| C8—H8B | 0.9700 | N5—H5B | 0.950 (19) |
| | | | |
| C2—C1—C6 | 118.93 (15) | H8A—C8—H8B | 107.7 |
| C2—C1—C7 | 122.15 (14) | O4—C9—C8 | 112.16 (13) |
| C6—C1—C7 | 118.89 (14) | O4—C9—H9A | 109.2 |
| C1—C2—C3 | 120.98 (17) | C8—C9—H9A | 109.2 |
| C1—C2—H2 | 119.5 | O4—C9—H9B | 109.2 |
| C3—C2—H2 | 119.5 | C8—C9—H9B | 109.2 |
| C4—C3—C2 | 119.45 (18) | H9A—C9—H9B | 107.9 |
| C4—C3—H3 | 120.3 | O1—C10—C10$^{i}$ | 105.74 (17) |
| C2—C3—H3 | 120.3 | O1—C10—H10A | 110.6 |
| C3—C4—C5 | 121.00 (17) | C10$^{i}$—C10—H10A | 110.6 |
| C3—C4—H4 | 119.5 | O1—C10—H10B | 110.6 |
| C5—C4—H4 | 119.5 | C10$^{i}$—C10—H10B | 110.6 |
| C4—C5—C6 | 119.42 (17) | H10A—C10—H10B | 108.7 |
| C4—C5—H5 | 120.3 | O3—C11—O2 | 125.21 (14) |
| C6—C5—H5 | 120.3 | O3—C11—C12 | 114.98 (14) |
| O1—C6—C5 | 125.51 (15) | O2—C11—C12 | 119.81 (14) |
| O1—C6—C1 | 114.30 (14) | C12$^{ii}$—C12—C11 | 124.47 (19) |
| C5—C6—C1 | 120.19 (16) | C12$^{ii}$—C12—H12 | 117.8 |
| N5—C7—C1 | 112.04 (12) | C11—C12—H12 | 117.8 |
| N5—C7—H7A | 109.2 | C6—O1—C10 | 118.86 (13) |
| C1—C7—H7A | 109.2 | H1C—O1W—H1D | 104 (2) |
| N5—C7—H7B | 109.2 | H2C—O2W—H2D | 108 (3) |
| C1—C7—H7B | 109.2 | C9—O4—H4A | 108.2 (15) |

| | | | |
|---|---|---|---|
| H7A—C7—H7B | 107.9 | C8—N5—C7 | 114.91 (12) |
| N5—C8—C9 | 113.42 (13) | C8—N5—H5A | 106.3 (11) |
| N5—C8—H8A | 108.9 | C7—N5—H5A | 112.5 (11) |
| C9—C8—H8A | 108.9 | C8—N5—H5B | 106.9 (10) |
| N5—C8—H8B | 108.9 | C7—N5—H5B | 107.6 (10) |
| C9—C8—H8B | 108.9 | H5A—N5—H5B | 108.3 (15) |
| | | | |
| C6—C1—C2—C3 | 0.3 (2) | C2—C1—C7—N5 | 114.29 (16) |
| C7—C1—C2—C3 | 178.16 (14) | C6—C1—C7—N5 | −67.81 (17) |
| C1—C2—C3—C4 | 1.1 (3) | N5—C8—C9—O4 | −55.82 (19) |
| C2—C3—C4—C5 | −1.0 (3) | O3—C11—C12—C12$^{ii}$ | −160.5 (2) |
| C3—C4—C5—C6 | −0.3 (3) | O2—C11—C12—C12$^{ii}$ | 19.9 (3) |
| C4—C5—C6—O1 | −178.31 (14) | C5—C6—O1—C10 | 5.5 (2) |
| C4—C5—C6—C1 | 1.6 (2) | C1—C6—O1—C10 | −174.42 (13) |
| C2—C1—C6—O1 | 178.34 (12) | C10$^{i}$—C10—O1—C6 | 174.87 (16) |
| C7—C1—C6—O1 | 0.37 (18) | C9—C8—N5—C7 | −61.95 (18) |
| C2—C1—C6—C5 | −1.6 (2) | C1—C7—N5—C8 | 179.32 (12) |
| C7—C1—C6—C5 | −179.58 (13) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*C*···O2*W* | 0.85 (3) | 1.97 (3) | 2.792 (3) | 164 (3) |
| O2*W*—H2*C*···O2 | 0.85 (3) | 1.97 (3) | 2.828 (3) | 176 (3) |
| N5—H5*B*···O2 | 0.950 (19) | 1.811 (19) | 2.749 (2) | 168.6 (16) |
| O1*W*—H1*D*···O3$^{iii}$ | 0.91 (3) | 1.96 (3) | 2.830 (3) | 159 (3) |
| O2*W*—H2*D*···O4$^{iv}$ | 0.86 (3) | 2.01 (3) | 2.867 (3) | 175 (3) |
| N5—H5*A*···O1*W*$^{v}$ | 0.900 (19) | 2.125 (19) | 2.925 (3) | 147.6 (15) |

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