# organic compounds

# 3,5-Bis(4-hydroxyphenyl)-4H-1,2,4-triazol-4-amine monohydrate

**Sidik Silong,[a] Mohamad Zaki Ab. Rahman,[a] Mansor Hj Ahmad,[a] Huey Chong Kwong[a] and Seik Weng Ng[b]\***

[a]Department of Chemistry, Universiti Putra Malaysia, 43400 Serdang, Malaysia, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

The triazole ring in the title compound, $C_{14}H_{12}N_4O_2 \cdot H_2O$, makes dihedral angles of 36.9 (1) and 37.3 (1)° with the two benzene rings. Each hydroxy group is a hydrogen-bond donor to a two-coordinate N atom of an adjacent molecule; these O—H⋯N hydrogen bonds generate a layer parallel to the *ab* plane. Adjacent layers are linked by N—-H⋯O and O$_{water}$—H⋯O hydrogen bonds into a three-dimensional network.

## Related literature

For two modifications of 4-amino-3,5-diphenyl-1,2,4-triazole, see: Ikemi *et al.* (2002); Zhang *et al.* (2009). For comparison structures, see: Wang *et al.* (2006); Zachara *et al.* (2004); Bentiss *et al.* (1998).
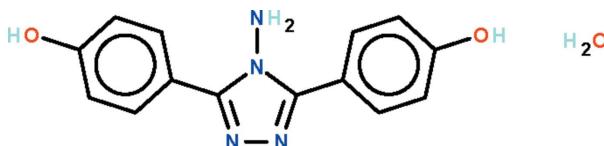
## Experimental

### Crystal data
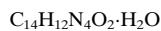
$C_{14}H_{12}N_4O_2 \cdot H_2O$
$M_r = 286.29$
Orthorhombic, $Pca2_1$
$a = 10.6659$ (5) Å
$b = 15.9790$ (8) Å
$c = 7.4632$ (4) Å

$V = 1271.96$ (11) Å$^3$
$Z = 4$
Cu $K\alpha$ radiation
$\mu = 0.90$ mm$^{-1}$
$T = 100$ K
$0.30 \times 0.10 \times 0.05$ mm

### Data collection

Oxford Diffraction Gemini E diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
$T_{min} = 0.773$, $T_{max} = 0.956$

2460 measured reflections
1275 independent reflections
1172 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.097$
$S = 1.05$
1275 reflections
215 parameters
8 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.23$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ e Å$^{-3}$

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| O1—H1o⋯N3[i] | 0.84 (3) | 1.92 (3) | 2.730 (2) | 163 (3) |
| O2—H2o⋯N4[ii] | 0.84 (3) | 2.02 (3) | 2.850 (2) | 168 (4) |
| O1w—H11⋯O2[iii] | 0.85 (3) | 2.19 (3) | 3.020 (3) | 166 (4) |
| N1—H1n⋯O1w | 0.87 (3) | 2.08 (3) | 2.943 (4) | 173 (4) |
| N1—H2n⋯O1[iv] | 0.86 (3) | 2.36 (3) | 3.202 (4) | 164 (3) |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

## References

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# supporting information

## 3,5-Bis(4-hydroxyphenyl)-4*H*-1,2,4-triazol-4-amine monohydrate

**Sidik Silong, Mohamad Zaki Ab. Rahman, Mansor Hj Ahmad, Huey Chong Kwong and Seik Weng Ng**

### S1. Comment

The class of 3,5-bis(*n*-hydroxyphenyl)-4-amino-1,2,4-triazoles represents a class of efficient corrosion inhibitors that are synthesized from *n*-hydroxybenzonitrile, hydrazine and hydrazine sulfate. The pure product is obtained in a number of steps that involve acidification/basification followed by recrystallization, as exemplified by 3,5-bis(4-hydroxyphenyl)-4-amino-1,2,4-triazole (Bentiss *et al.*, 1998). The compound can be synthesized, more conveniently, though a microwave route. The compound is, in fact, a monohydrate (Scheme I, Fig. 1).

### S2. Experimental

4-Hydroxybenzonitrile (3 mmol), hydrazine dihydrochloride (1 mmol) and anhydrous hydrazine (3 mmol) along with *n*-butanol (3 ml) were placed in a microwave synthesizer tube. The tube was irradiated in a CEM Discovery Synthesizer. The magnetron was set to 'normal′ and the temperature to 403 K. The tube was irradiated for 8 minutes. Water (10 ml) was added to dissolve the contents. The solution was set aside for the growth of the faint-yellow crystals, which separated after 3 days.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with $U$(H) set to $1.2U$(C). The amino and water H-atoms were located in a difference Fourier map, and were refined with distance restraints [N–H 0.86 + 0.01 Å and O–H 0.84 + 0.01 Å]; their displacement parameters were freely refined. For the water molecule, the H⋯H distance was restrained to 1.37±0.01 Å. 402 Friedel pairs were merged.
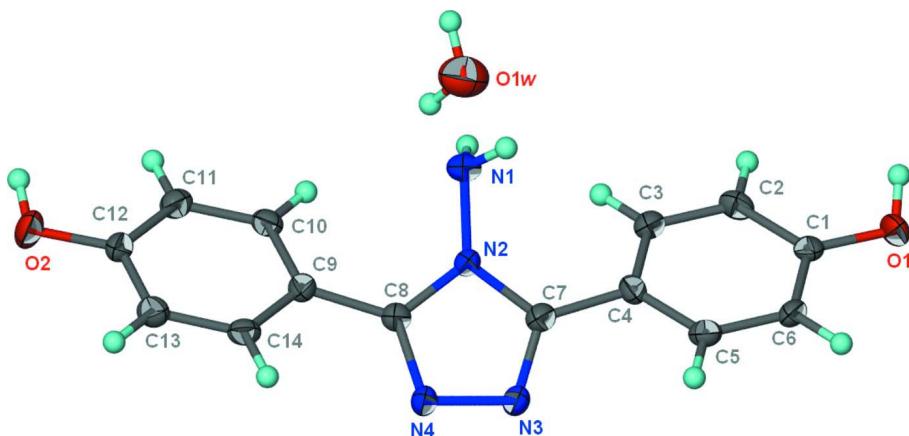
**Figure 1**

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{14}H_{12}N_4O_2 \cdot H_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

**3,5-Bis(4-hydroxyphenyl)-4$H$-1,2,4-triazol-4-amine monohydrate**

*Crystal data*

| | |
|---|---|
| $C_{14}H_{12}N_4O_2 \cdot H_2O$ | $F(000) = 600$ |
| $M_r = 286.29$ | $D_x = 1.495$ Mg m$^{-3}$ |
| Orthorhombic, $Pca2_1$ | Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å |
| Hall symbol: P 2c -2ac | Cell parameters from 1690 reflections |
| $a = 10.6659$ (5) Å | $\theta = 4.1–70.4°$ |
| $b = 15.9790$ (8) Å | $\mu = 0.90$ mm$^{-1}$ |
| $c = 7.4632$ (4) Å | $T = 100$ K |
| $V = 1271.96$ (11) Å$^3$ | Prism, yellow |
| $Z = 4$ | $0.30 \times 0.10 \times 0.05$ mm |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini E diffractometer | 2460 measured reflections |
| Radiation source: fine-focus sealed tube | 1275 independent reflections |
| Graphite monochromator | 1172 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 16.1952 pixels mm$^{-1}$ | $R_{int} = 0.019$ |
| $\omega$ scans | $\theta_{max} = 70.0°$, $\theta_{min} = 5.0°$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010) | $h = -11 \rightarrow 12$ |
| | $k = -14 \rightarrow 19$ |
| $T_{min} = 0.773$, $T_{max} = 0.956$ | $l = -9 \rightarrow 8$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H atoms treated by a mixture of independent and constrained refinement |
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | |
| $wR(F^2) = 0.097$ | |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0762P)^2 + 0.0334P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 1275 reflections | |
| 215 parameters | $(\Delta/\sigma)_{max} = 0.001$ |
| 8 restraints | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{min} = -0.24$ e Å$^{-3}$ |
| Secondary atom site location: difference Fourier map | Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc$^*$=kFc[1+0.001xFc$^2\lambda^3$/sin(2$\theta$)]$^{-1/4}$ |
| | Extinction coefficient: 0.0033 (6) |

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

|  | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 1.05710 (16) | 1.15554 (10) | 0.5001 (3) | 0.0257 (5) |
| O2 | 1.07428 (16) | 0.33922 (9) | 0.5626 (3) | 0.0252 (4) |
| O1W | 0.8047 (2) | 0.76244 (13) | 0.3567 (3) | 0.0375 (5) |
| C1 | 1.0874 (2) | 1.07317 (13) | 0.5123 (3) | 0.0175 (5) |
| C2 | 1.0093 (2) | 1.01053 (14) | 0.4426 (3) | 0.0184 (5) |
| H2 | 0.9335 | 1.0254 | 0.3839 | 0.022* |
| C3 | 1.0424 (2) | 0.92705 (14) | 0.4592 (3) | 0.0175 (5) |
| H3 | 0.9886 | 0.8848 | 0.4135 | 0.021* |
| C4 | 1.1546 (2) | 0.90481 (12) | 0.5428 (3) | 0.0157 (5) |
| C5 | 1.2323 (2) | 0.96757 (13) | 0.6105 (3) | 0.0166 (5) |
| H5 | 1.3087 | 0.9528 | 0.6676 | 0.020* |
| C6 | 1.1993 (2) | 1.05105 (13) | 0.5954 (4) | 0.0173 (5) |
| H6 | 1.2531 | 1.0932 | 0.6418 | 0.021* |
| C7 | 1.19711 (19) | 0.81723 (13) | 0.5495 (4) | 0.0165 (5) |
| C8 | 1.20070 (19) | 0.68071 (13) | 0.5660 (3) | 0.0154 (5) |
| C9 | 1.1602 (2) | 0.59292 (12) | 0.5747 (3) | 0.0156 (5) |
| C10 | 1.0488 (2) | 0.56628 (14) | 0.4941 (3) | 0.0166 (5) |
| H10 | 0.9928 | 0.6063 | 0.4444 | 0.020* |
| C11 | 1.0195 (2) | 0.48188 (13) | 0.4864 (3) | 0.0177 (5) |
| H11A | 0.9448 | 0.4640 | 0.4288 | 0.021* |
| C12 | 1.0998 (2) | 0.42316 (13) | 0.5633 (4) | 0.0176 (5) |
| C13 | 1.2108 (2) | 0.44890 (13) | 0.6442 (3) | 0.0187 (5) |
| H13 | 1.2658 | 0.4089 | 0.6960 | 0.022* |
| C14 | 1.2406 (2) | 0.53350 (13) | 0.6487 (3) | 0.0165 (5) |
| H14 | 1.3167 | 0.5511 | 0.7029 | 0.020* |
| N1 | 0.9975 (2) | 0.74477 (11) | 0.6363 (4) | 0.0212 (5) |
| N2 | 1.1228 (2) | 0.74854 (9) | 0.5740 (3) | 0.0161 (5) |
| N3 | 1.31389 (18) | 0.79302 (10) | 0.5291 (3) | 0.0185 (5) |
| N4 | 1.31642 (18) | 0.70604 (10) | 0.5380 (3) | 0.0188 (5) |
| H1O | 0.9790 (11) | 1.161 (2) | 0.508 (5) | 0.042 (10)* |
| H2O | 0.9976 (14) | 0.331 (3) | 0.542 (7) | 0.082 (16)* |
| H11 | 0.827 (3) | 0.7358 (19) | 0.264 (3) | 0.053 (12)* |
| H12 | 0.7286 (15) | 0.7500 (18) | 0.376 (6) | 0.072 (17)* |
| H1N | 0.945 (3) | 0.7523 (17) | 0.549 (4) | 0.046 (11)* |
| H2N | 0.987 (4) | 0.7803 (18) | 0.722 (4) | 0.055 (11)* |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0173 (8) | 0.0142 (7) | 0.0455 (13) | 0.0051 (6) | 0.0026 (8) | 0.0015 (8) |
| O2 | 0.0207 (8) | 0.0137 (7) | 0.0412 (12) | −0.0040 (6) | −0.0055 (9) | 0.0015 (8) |
| O1W | 0.0296 (11) | 0.0460 (11) | 0.0368 (13) | −0.0008 (9) | 0.0020 (9) | −0.0085 (11) |
| C1 | 0.0144 (11) | 0.0154 (10) | 0.0226 (14) | 0.0001 (8) | 0.0072 (10) | 0.0021 (9) |
| C2 | 0.0144 (10) | 0.0202 (11) | 0.0207 (13) | 0.0038 (8) | −0.0007 (9) | 0.0006 (10) |
| C3 | 0.0147 (11) | 0.0166 (10) | 0.0212 (13) | −0.0018 (8) | 0.0015 (9) | −0.0003 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 0.0166 (10) | 0.0124 (10) | 0.0181 (11) | 0.0013 (8) | 0.0030 (10) | −0.0009 (9) |
| C5 | 0.0129 (10) | 0.0187 (10) | 0.0182 (12) | −0.0002 (8) | 0.0013 (9) | 0.0012 (9) |
| C6 | 0.0147 (10) | 0.0144 (10) | 0.0229 (14) | −0.0039 (8) | 0.0033 (9) | −0.0023 (10) |
| C7 | 0.0154 (10) | 0.0154 (10) | 0.0186 (13) | −0.0014 (8) | 0.0011 (10) | −0.0010 (10) |
| C8 | 0.0149 (10) | 0.0148 (10) | 0.0164 (12) | 0.0001 (8) | 0.0006 (10) | 0.0001 (10) |
| C9 | 0.0157 (10) | 0.0133 (10) | 0.0177 (12) | −0.0008 (8) | 0.0025 (10) | −0.0002 (9) |
| C10 | 0.0136 (11) | 0.0170 (10) | 0.0192 (13) | 0.0021 (8) | 0.0014 (9) | 0.0010 (9) |
| C11 | 0.0159 (10) | 0.0185 (12) | 0.0187 (12) | −0.0021 (8) | 0.0010 (10) | −0.0004 (10) |
| C12 | 0.0158 (11) | 0.0142 (9) | 0.0229 (12) | −0.0018 (8) | 0.0026 (10) | −0.0037 (10) |
| C13 | 0.0168 (11) | 0.0166 (11) | 0.0225 (14) | 0.0019 (8) | 0.0006 (10) | 0.0038 (9) |
| C14 | 0.0114 (9) | 0.0197 (9) | 0.0184 (13) | −0.0007 (9) | 0.0004 (9) | −0.0018 (9) |
| N1 | 0.0135 (11) | 0.0214 (10) | 0.0288 (12) | −0.0006 (7) | 0.0036 (10) | −0.0013 (9) |
| N2 | 0.0129 (9) | 0.0121 (9) | 0.0234 (11) | −0.0013 (6) | 0.0015 (9) | 0.0002 (7) |
| N3 | 0.0144 (9) | 0.0118 (9) | 0.0294 (13) | −0.0011 (6) | −0.0004 (8) | 0.0010 (9) |
| N4 | 0.0148 (9) | 0.0108 (9) | 0.0307 (13) | −0.0007 (6) | 0.0001 (9) | −0.0008 (9) |

## Geometric parameters (Å, º)

| | | | |
|---|---|---|---|
| O1—C1 | 1.359 (3) | C7—N2 | 1.366 (3) |
| O1—H1O | 0.84 (3) | C8—N4 | 1.316 (3) |
| O2—C12 | 1.369 (2) | C8—N2 | 1.367 (3) |
| O2—H2O | 0.84 (3) | C8—C9 | 1.469 (3) |
| O1w—H11 | 0.85 (3) | C9—C14 | 1.393 (3) |
| O1w—H12 | 0.85 (3) | C9—C10 | 1.399 (3) |
| C1—C6 | 1.391 (3) | C10—C11 | 1.385 (3) |
| C1—C2 | 1.402 (3) | C10—H10 | 0.9500 |
| C2—C3 | 1.386 (3) | C11—C12 | 1.393 (3) |
| C2—H2 | 0.9500 | C11—H11A | 0.9500 |
| C3—C4 | 1.395 (3) | C12—C13 | 1.392 (3) |
| C3—H3 | 0.9500 | C13—C14 | 1.389 (3) |
| C4—C5 | 1.396 (3) | C13—H13 | 0.9500 |
| C4—C7 | 1.472 (3) | C14—H14 | 0.9500 |
| C5—C6 | 1.384 (3) | N1—N2 | 1.416 (3) |
| C5—H5 | 0.9500 | N1—H1N | 0.87 (3) |
| C6—H6 | 0.9500 | N1—H2N | 0.86 (3) |
| C7—N3 | 1.313 (3) | N3—N4 | 1.392 (3) |
| | | | |
| C1—O1—H1O | 109 (2) | C14—C9—C10 | 119.06 (19) |
| C12—O2—H2O | 110 (3) | C14—C9—C8 | 119.2 (2) |
| H11—O1W—H12 | 106.8 (17) | C10—C9—C8 | 121.4 (2) |
| O1—C1—C6 | 118.7 (2) | C11—C10—C9 | 120.4 (2) |
| O1—C1—C2 | 121.7 (2) | C11—C10—H10 | 119.8 |
| C6—C1—C2 | 119.60 (19) | C9—C10—H10 | 119.8 |
| C3—C2—C1 | 120.2 (2) | C10—C11—C12 | 120.0 (2) |
| C3—C2—H2 | 119.9 | C10—C11—H11A | 120.0 |
| C1—C2—H2 | 119.9 | C12—C11—H11A | 120.0 |
| C2—C3—C4 | 120.2 (2) | O2—C12—C13 | 117.4 (2) |
| C2—C3—H3 | 119.9 | O2—C12—C11 | 122.4 (2) |

| | | | |
|---|---|---|---|
| C4—C3—H3 | 119.9 | C13—C12—C11 | 120.15 (19) |
| C3—C4—C5 | 119.21 (19) | C14—C13—C12 | 119.5 (2) |
| C3—C4—C7 | 121.4 (2) | C14—C13—H13 | 120.2 |
| C5—C4—C7 | 119.2 (2) | C12—C13—H13 | 120.2 |
| C6—C5—C4 | 120.8 (2) | C13—C14—C9 | 120.9 (2) |
| C6—C5—H5 | 119.6 | C13—C14—H14 | 119.6 |
| C4—C5—H5 | 119.6 | C9—C14—H14 | 119.6 |
| C5—C6—C1 | 119.9 (2) | N2—N1—H1N | 111 (3) |
| C5—C6—H6 | 120.0 | N2—N1—H2N | 110 (3) |
| C1—C6—H6 | 120.0 | H1N—N1—H2N | 112 (3) |
| N3—C7—N2 | 109.22 (19) | C7—N2—C8 | 106.2 (2) |
| N3—C7—C4 | 124.7 (2) | C7—N2—N1 | 128.73 (17) |
| N2—C7—C4 | 126.12 (19) | C8—N2—N1 | 123.65 (17) |
| N4—C8—N2 | 109.47 (19) | C7—N3—N4 | 107.88 (16) |
| N4—C8—C9 | 125.19 (19) | C8—N4—N3 | 107.25 (16) |
| N2—C8—C9 | 125.21 (19) | | |

| | | | |
|---|---|---|---|
| O1—C1—C2—C3 | −179.3 (2) | C10—C11—C12—O2 | 178.7 (2) |
| C6—C1—C2—C3 | 1.1 (4) | C10—C11—C12—C13 | −1.5 (4) |
| C1—C2—C3—C4 | −1.0 (4) | O2—C12—C13—C14 | −179.8 (2) |
| C2—C3—C4—C5 | 0.5 (4) | C11—C12—C13—C14 | 0.4 (4) |
| C2—C3—C4—C7 | −175.0 (2) | C12—C13—C14—C9 | 0.6 (4) |
| C3—C4—C5—C6 | 0.0 (4) | C10—C9—C14—C13 | −0.4 (3) |
| C7—C4—C5—C6 | 175.5 (2) | C8—C9—C14—C13 | −174.0 (2) |
| C4—C5—C6—C1 | 0.1 (4) | N3—C7—N2—C8 | −0.5 (3) |
| O1—C1—C6—C5 | 179.7 (2) | C4—C7—N2—C8 | 178.4 (2) |
| C2—C1—C6—C5 | −0.6 (3) | N3—C7—N2—N1 | 166.0 (2) |
| C3—C4—C7—N3 | 140.3 (3) | C4—C7—N2—N1 | −15.2 (4) |
| C5—C4—C7—N3 | −35.2 (4) | N4—C8—N2—C7 | −0.1 (3) |
| C3—C4—C7—N2 | −38.4 (4) | C9—C8—N2—C7 | −176.1 (2) |
| C5—C4—C7—N2 | 146.2 (3) | N4—C8—N2—N1 | −167.4 (2) |
| N4—C8—C9—C14 | 34.9 (4) | C9—C8—N2—N1 | 16.6 (4) |
| N2—C8—C9—C14 | −149.7 (2) | N2—C7—N3—N4 | 0.8 (3) |
| N4—C8—C9—C10 | −138.5 (3) | C4—C7—N3—N4 | −178.0 (2) |
| N2—C8—C9—C10 | 36.9 (4) | N2—C8—N4—N3 | 0.5 (3) |
| C14—C9—C10—C11 | −0.7 (4) | C9—C8—N4—N3 | 176.6 (2) |
| C8—C9—C10—C11 | 172.7 (2) | C7—N3—N4—C8 | −0.8 (2) |
| C9—C10—C11—C12 | 1.7 (4) | | |

*Hydrogen-bond geometry (Å, °)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| O1—H1o···N3[i] | 0.84 (3) | 1.92 (3) | 2.730 (2) | 163 (3) |
| O2—H2o···N4[ii] | 0.84 (3) | 2.02 (3) | 2.850 (2) | 168 (4) |
| O1w—H11···O2[iii] | 0.85 (3) | 2.19 (3) | 3.020 (3) | 166 (4) |
| O1w—H12···O1[i] | 0.85 (3) | 2.55 (3) | 3.137 (3) | 128 (2) |

| N1—H1n···O1w | 0.87 (3) | 2.08 (3) | 2.943 (4) | 173 (4) |
| N1—H2n···O1$^{iv}$ | 0.86 (3) | 2.36 (3) | 3.202 (4) | 164 (3) |

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