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3,4,5-Trihydroxy-*N*′-(1*H*-indol-3-ylmethylidene)benzohydrazide pentahydrate

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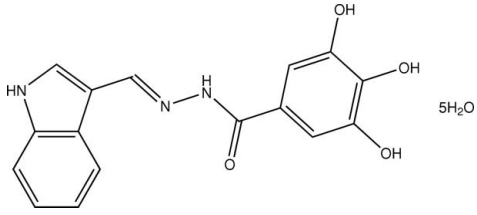
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.115; data-to-parameter ratio = 13.1.

The two aromatic parts of the title compound, $C_{16}H_{13}N_3O_4\cdot5H_2O$, are connected through a conjugated –CH=N–NH–C(O)– fragment, giving an almost planar molecule. The organic molecules and uncoordinated water molecules are linked by N—H···O and O—H···O hydrogen bonds into a three-dimensional network.

Related literature

For the structure of anhydrous *N*′-(1*H*-indol-3-ylmethylidene)-3,4,5-trihydroxybenzohydrazide, see: Khaledi *et al.* (2008).



Experimental

Crystal data

$C_{16}H_{13}N_3O_4\cdot5H_2O$
M_r = 401.37
Triclinic, $P\overline{1}$
a = 7.4379 (2) Å
b = 9.1178 (2) Å
c = 14.1966 (3) Å
α = 103.814 (1)°
β = 103.716 (1)°
γ = 90.613 (2)°
V = 905.95 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 100 (2) K
0.30 × 0.25 × 0.04 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
7524 measured reflections
4096 independent reflections
3285 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.05
4096 reflections
313 parameters
15 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*o*···O4^{i}	0.85 (1)	1.90 (1)	2.740 (2)	174 (2)
O2—H2*o*···O2*w*	0.84 (1)	1.94 (1)	2.697 (2)	149 (2)
O3—H3*o*···O3*w*	0.85 (1)	1.90 (1)	2.724 (2)	164 (2)
N1—H1*n*···O1*w*^{ii}	0.88 (1)	2.11 (1)	2.978 (2)	169 (2)
N3—H3*n*···O4*w*^{iii}	0.88 (1)	2.15 (1)	3.024 (2)	171 (2)
O1*w*—H11···O1	0.85 (1)	1.93 (1)	2.771 (2)	170 (3)
O1*w*—H12···O3*w*^{iv}	0.86 (1)	1.94 (1)	2.760 (2)	161 (3)
O2*w*—H21···O3^{v}	0.84 (1)	2.29 (1)	3.123 (2)	172 (2)
O2*w*—H22···O5*w*	0.85 (1)	1.94 (2)	2.753 (2)	161 (3)
O3*w*—H31···O5*w*^{vi}	0.85 (1)	1.95 (1)	2.796 (2)	172 (3)
O3*w*—H32···O3^{vii}	0.85 (1)	2.06 (1)	2.890 (2)	165 (2)
O4*w*—H41···O1*w*	0.85 (1)	1.97 (1)	2.803 (2)	169 (2)
O4*w*—H42···O4^{viii}	0.84 (1)	2.37 (2)	2.921 (2)	124 (2)
O4*w*—H42···N2^{viii}	0.84 (1)	2.39 (1)	3.211 (2)	166 (2)
O5*w*—H51···O4*w*^{ix}	0.85 (1)	1.97 (1)	2.798 (2)	167 (2)
O5*w*—H52···O2*w*^{x}	0.85 (1)	1.97 (1)	2.810 (2)	168 (3)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2007); 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: *pubCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2335).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
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Khaledi, H., Mohd Ali, H. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o2108.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2008). *publCIF*. In preparation.

supporting information

Acta Cryst. (2008). E**64**, o2481 [doi:10.1107/S1600536808039342]

3,4,5-Trihydroxy-*N*′-(1*H*-indol-3-ylmethylidene)benzohydrazide pentahydrate

Hamid Khaledi, Hapipah Mohd Ali and Seik Weng Ng

S1. Experimental

Indole-3-carbaldehyde (1.0 g, 7 mmol) and 3,4,5-trihydroxybenzoylhydrazine (1.29 g, 7 mmol) were heated in ethanol (60 ml) for 6 h. About 1 ml of acetic acid also added. The solution was set aside for the growth of crystals.

S2. Refinement

Hydrogen atoms were placed at calculated positions (C–H 0.95 Å), and were treated as riding on their parent carbon atoms, with U(H) set to 1.2U_{eq}(C). The nitrogen- and oxygen-bound H atoms were located in a difference Fourier map, and were refined with distance restraints of N–H 0.88±0.01 and O–H 0.84±0.01 Å.

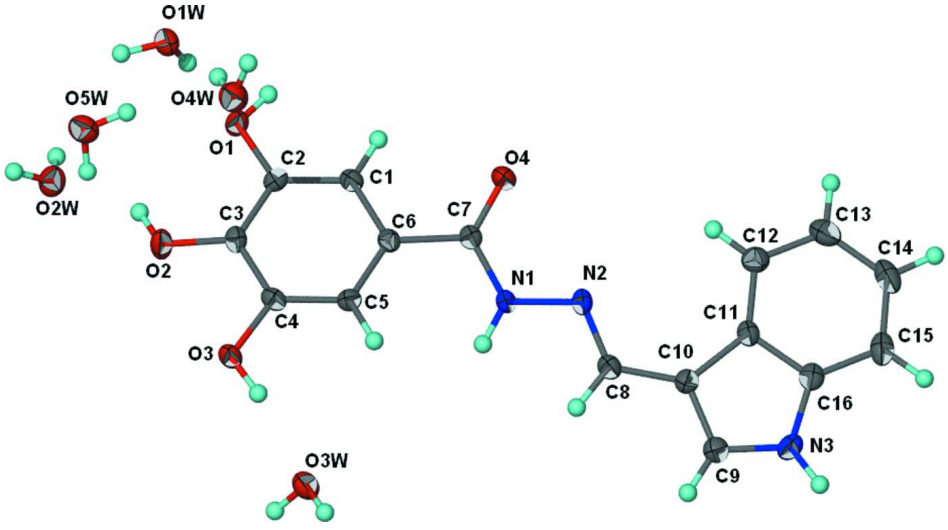

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{16}H_{13}N_3O_4$.5H2O at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

3,4,5-Trihydroxy-*N*′-(1*H*-indol-3-ylmethylidene)benzohydrazide pentahydrate

Crystal data

$C_{16}H_{13}N_3O_4·5H_2O$
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Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.4379 (2) Å
b = 9.1178 (2) Å
c = 14.1966 (3) Å
α = 103.814 (1)°
β = 103.716 (1)°
γ = 90.613 (2)°
V = 905.95 (4) Å^3
Z = 2
F(000) = 424
D_x = 1.471 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2461 reflections

θ = 2.3–28.0°
μ = 0.12 mm^{-1}
T = 100 K

Plate, pale-yellow
0.30 × 0.25 × 0.04 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
7524 measured reflections
4096 independent reflections

3285 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −9→9
k = −11→11
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.05
4096 reflections
313 parameters
15 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
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.1789P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.59471 (16)	0.40029 (12)	0.72041 (8)	0.0184 (2)
O2	0.51512 (17)	0.56940 (13)	0.89648 (8)	0.0217 (3)
O3	0.35915 (16)	0.82334 (12)	0.90287 (8)	0.0180 (2)
O4	0.31349 (16)	0.68239 (12)	0.45992 (8)	0.0197 (3)
O1w	0.35758 (17)	0.17412 (13)	0.73409 (8)	0.0200 (3)
O2w	0.75855 (17)	0.38643 (13)	0.97416 (9)	0.0221 (3)
O3w	0.34432 (17)	1.12598 (13)	0.91713 (8)	0.0213 (3)
O4w	0.01511 (18)	0.30256 (13)	0.69710 (9)	0.0231 (3)
O5w	1.07168 (17)	0.33392 (13)	0.90316 (9)	0.0232 (3)
N1	0.29295 (19)	0.91884 (14)	0.55157 (9)	0.0162 (3)
N2	0.24067 (18)	0.97264 (14)	0.46592 (9)	0.0165 (3)
N3	0.08352 (19)	1.39294 (15)	0.34212 (10)	0.0183 (3)
C1	0.4530 (2)	0.58425 (16)	0.63391 (11)	0.0147 (3)
H1	0.4753	0.5274	0.5729	0.018*
C2	0.5040 (2)	0.53102 (16)	0.71918 (11)	0.0146 (3)
C3	0.4698 (2)	0.61229 (17)	0.80875 (11)	0.0151 (3)
C4	0.3855 (2)	0.74827 (16)	0.81103 (11)	0.0147 (3)
C5	0.3332 (2)	0.80233 (16)	0.72644 (11)	0.0148 (3)
H5	0.2733	0.8942	0.7290	0.018*
C6	0.3693 (2)	0.72070 (16)	0.63685 (10)	0.0140 (3)
C7	0.3236 (2)	0.77172 (16)	0.54225 (11)	0.0144 (3)
C8	0.2179 (2)	1.11562 (17)	0.48486 (11)	0.0168 (3)

H8	0.2354	1.1700	0.5528	0.020*
C9	0.1240 (2)	1.34618 (17)	0.42795 (11)	0.0175 (3)
H9	0.1226	1.4073	0.4921	0.021*
C10	0.1675 (2)	1.19684 (17)	0.40875 (11)	0.0158 (3)
C11	0.1553 (2)	1.14989 (17)	0.30295 (11)	0.0154 (3)
C12	0.1934 (2)	1.01736 (17)	0.23897 (11)	0.0194 (3)
H12A	0.2299	0.9310	0.2632	0.023*
C13	0.1763 (2)	1.01605 (19)	0.13982 (12)	0.0229 (4)
H13	0.2023	0.9275	0.0956	0.028*
C14	0.1213 (2)	1.1422 (2)	0.10270 (12)	0.0241 (4)
H14	0.1093	1.1367	0.0338	0.029*
C15	0.0845 (2)	1.27369 (19)	0.16400 (12)	0.0212 (3)
H15	0.0478	1.3594	0.1390	0.025*
C16	0.1033 (2)	1.27600 (17)	0.26438 (11)	0.0169 (3)
H1o	0.616 (3)	0.370 (2)	0.6634 (10)	0.046 (7)*
H2o	0.584 (3)	0.4971 (18)	0.8974 (16)	0.039 (6)*
H3o	0.333 (3)	0.9129 (14)	0.8998 (16)	0.038 (6)*
H1n	0.314 (3)	0.9850 (17)	0.6102 (9)	0.025 (5)*
H3n	0.052 (3)	1.4844 (15)	0.3374 (17)	0.046 (6)*
H11	0.438 (3)	0.235 (2)	0.7274 (19)	0.060 (8)*
H12	0.380 (4)	0.163 (3)	0.7939 (10)	0.059 (8)*
H21	0.719 (3)	0.336 (2)	1.0090 (16)	0.055 (7)*
H22	0.848 (3)	0.349 (4)	0.952 (2)	0.112 (13)*
H31	0.255 (3)	1.184 (3)	0.915 (2)	0.067 (9)*
H32	0.425 (2)	1.158 (2)	0.9721 (10)	0.037 (6)*
H41	0.117 (2)	0.260 (3)	0.7001 (18)	0.055 (8)*
H42	−0.066 (3)	0.242 (2)	0.6537 (15)	0.063 (8)*
H51	1.039 (3)	0.331 (3)	0.8414 (8)	0.055 (8)*
H52	1.124 (4)	0.4219 (19)	0.932 (2)	0.101 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0248 (6)	0.0168 (5)	0.0172 (6)	0.0079 (5)	0.0091 (5)	0.0068 (4)
O2	0.0281 (7)	0.0247 (6)	0.0164 (6)	0.0119 (5)	0.0081 (5)	0.0099 (5)
O3	0.0241 (6)	0.0179 (6)	0.0123 (5)	0.0060 (5)	0.0060 (4)	0.0026 (4)
O4	0.0282 (6)	0.0169 (5)	0.0131 (5)	0.0037 (5)	0.0051 (5)	0.0021 (4)
O1w	0.0247 (6)	0.0202 (6)	0.0156 (6)	0.0008 (5)	0.0053 (5)	0.0051 (4)
O2w	0.0242 (7)	0.0240 (6)	0.0223 (6)	0.0054 (5)	0.0101 (5)	0.0094 (5)
O3w	0.0235 (6)	0.0233 (6)	0.0155 (6)	0.0042 (5)	0.0031 (5)	0.0032 (4)
O4w	0.0217 (6)	0.0249 (6)	0.0217 (6)	0.0056 (5)	0.0035 (5)	0.0057 (5)
O5w	0.0249 (7)	0.0234 (6)	0.0203 (6)	0.0028 (5)	0.0070 (5)	0.0023 (5)
N1	0.0228 (7)	0.0147 (6)	0.0106 (6)	0.0027 (5)	0.0029 (5)	0.0037 (5)
N2	0.0201 (7)	0.0179 (6)	0.0127 (6)	0.0027 (5)	0.0041 (5)	0.0063 (5)
N3	0.0196 (7)	0.0150 (6)	0.0212 (7)	0.0033 (5)	0.0041 (5)	0.0069 (5)
C1	0.0158 (7)	0.0148 (7)	0.0129 (7)	0.0006 (6)	0.0040 (6)	0.0019 (5)
C2	0.0143 (7)	0.0127 (7)	0.0176 (7)	0.0014 (6)	0.0046 (6)	0.0043 (6)
C3	0.0144 (7)	0.0181 (7)	0.0138 (7)	0.0005 (6)	0.0034 (6)	0.0060 (6)

C4	0.0140 (7)	0.0166 (7)	0.0126 (7)	−0.0003 (6)	0.0046 (6)	0.0009 (5)
C5	0.0158 (7)	0.0131 (7)	0.0152 (7)	0.0019 (6)	0.0040 (6)	0.0028 (5)
C6	0.0136 (7)	0.0148 (7)	0.0125 (7)	−0.0014 (6)	0.0019 (5)	0.0030 (5)
C7	0.0142 (7)	0.0159 (7)	0.0132 (7)	0.0002 (6)	0.0033 (6)	0.0037 (5)
C8	0.0191 (8)	0.0175 (7)	0.0136 (7)	0.0022 (6)	0.0041 (6)	0.0032 (6)
C9	0.0177 (8)	0.0176 (7)	0.0169 (7)	0.0013 (6)	0.0038 (6)	0.0043 (6)
C10	0.0164 (7)	0.0154 (7)	0.0155 (7)	0.0012 (6)	0.0035 (6)	0.0042 (6)
C11	0.0153 (7)	0.0175 (7)	0.0134 (7)	−0.0011 (6)	0.0027 (6)	0.0046 (6)
C12	0.0202 (8)	0.0174 (7)	0.0194 (8)	−0.0010 (6)	0.0042 (6)	0.0031 (6)
C13	0.0249 (9)	0.0226 (8)	0.0191 (8)	−0.0037 (7)	0.0070 (7)	−0.0005 (6)
C14	0.0242 (9)	0.0322 (9)	0.0145 (7)	−0.0084 (7)	0.0028 (6)	0.0054 (6)
C15	0.0185 (8)	0.0264 (8)	0.0191 (8)	−0.0041 (7)	0.0002 (6)	0.0109 (6)
C16	0.0137 (7)	0.0184 (7)	0.0178 (7)	−0.0017 (6)	0.0016 (6)	0.0054 (6)

Geometric parameters (Å, º)

O1—C2	1.3777 (18)	C1—C2	1.383 (2)
O1—H1o	0.845 (9)	C1—C6	1.393 (2)
O2—C3	1.3615 (18)	C1—H1	0.9500
O2—H2o	0.839 (10)	C2—C3	1.392 (2)
O3—C4	1.3801 (17)	C3—C4	1.392 (2)
O3—H3o	0.851 (10)	C4—C5	1.379 (2)
O4—C7	1.2400 (17)	C5—C6	1.399 (2)
O1w—H11	0.850 (10)	C5—H5	0.9500
O1w—H12	0.855 (10)	C6—C7	1.490 (2)
O2w—H21	0.843 (10)	C8—C10	1.433 (2)
O2w—H22	0.846 (10)	C8—H8	0.9500
O3w—H31	0.854 (10)	C9—C10	1.381 (2)
O3w—H32	0.848 (10)	C9—H9	0.9500
O4w—H41	0.848 (10)	C10—C11	1.441 (2)
O4w—H42	0.839 (10)	C11—C12	1.404 (2)
O5w—H51	0.847 (10)	C11—C16	1.408 (2)
O5w—H52	0.850 (10)	C12—C13	1.380 (2)
N1—C7	1.3434 (19)	C12—H12A	0.9500
N1—N2	1.3910 (17)	C13—C14	1.402 (2)
N1—H1n	0.882 (9)	C13—H13	0.9500
N2—C8	1.288 (2)	C14—C15	1.375 (2)
N3—C9	1.354 (2)	C14—H14	0.9500
N3—C16	1.376 (2)	C15—C16	1.394 (2)
N3—H3n	0.882 (10)	C15—H15	0.9500
C2—O1—H1o	106.5 (16)	C5—C6—C7	123.54 (13)
C3—O2—H2o	115.8 (15)	O4—C7—N1	122.36 (13)
C4—O3—H3o	107.5 (14)	O4—C7—C6	121.46 (13)
H11—O1w—H12	112 (2)	N1—C7—C6	116.18 (13)
H21—O2w—H22	114 (3)	N2—C8—C10	123.34 (14)
H31—O3w—H32	109 (2)	N2—C8—H8	118.3
H41—O4w—H42	107 (2)	C10—C8—H8	118.3

H51—O5w—H52	106 (3)	N3—C9—C10	110.20 (14)
C7—N1—N2	119.24 (12)	N3—C9—H9	124.9
C7—N1—H1n	122.5 (12)	C10—C9—H9	124.9
N2—N1—H1n	118.0 (12)	C9—C10—C8	123.34 (14)
C8—N2—N1	113.26 (12)	C9—C10—C11	106.25 (13)
C9—N3—C16	109.03 (13)	C8—C10—C11	130.40 (14)
C9—N3—H3n	125.2 (15)	C12—C11—C16	119.25 (14)
C16—N3—H3n	125.7 (15)	C12—C11—C10	134.26 (14)
C2—C1—C6	120.49 (13)	C16—C11—C10	106.36 (13)
C2—C1—H1	119.8	C13—C12—C11	118.14 (15)
C6—C1—H1	119.8	C13—C12—H12A	120.9
O1—C2—C1	122.20 (13)	C11—C12—H12A	120.9
O1—C2—C3	117.48 (13)	C12—C13—C14	121.62 (15)
C1—C2—C3	120.29 (14)	C12—C13—H13	119.2
O2—C3—C4	116.52 (13)	C14—C13—H13	119.2
O2—C3—C2	124.59 (14)	C15—C14—C13	121.35 (15)
C4—C3—C2	118.89 (13)	C15—C14—H14	119.3
O3—C4—C5	123.17 (14)	C13—C14—H14	119.3
O3—C4—C3	115.42 (13)	C14—C15—C16	117.23 (15)
C5—C4—C3	121.41 (13)	C14—C15—H15	121.4
C4—C5—C6	119.40 (14)	C16—C15—H15	121.4
C4—C5—H5	120.3	N3—C16—C15	129.42 (14)
C6—C5—H5	120.3	N3—C16—C11	108.14 (13)
C1—C6—C5	119.50 (13)	C15—C16—C11	122.40 (15)
C1—C6—C7	116.96 (13)		

C7—N1—N2—C8	−179.15 (14)	N1—N2—C8—C10	178.78 (14)
C6—C1—C2—O1	−176.94 (13)	C16—N3—C9—C10	−1.24 (18)
C6—C1—C2—C3	0.9 (2)	N3—C9—C10—C8	179.52 (14)
O1—C2—C3—O2	−1.9 (2)	N3—C9—C10—C11	0.96 (18)
C1—C2—C3—O2	−179.82 (14)	N2—C8—C10—C9	172.92 (15)
O1—C2—C3—C4	177.27 (13)	N2—C8—C10—C11	−8.9 (3)
C1—C2—C3—C4	−0.7 (2)	C9—C10—C11—C12	175.33 (17)
O2—C3—C4—O3	0.3 (2)	C8—C10—C11—C12	−3.1 (3)
C2—C3—C4—O3	−178.94 (13)	C9—C10—C11—C16	−0.34 (17)
O2—C3—C4—C5	−179.82 (13)	C8—C10—C11—C16	−178.76 (16)
C2—C3—C4—C5	1.0 (2)	C16—C11—C12—C13	−0.6 (2)
O3—C4—C5—C6	178.43 (13)	C10—C11—C12—C13	−175.81 (16)
C3—C4—C5—C6	−1.5 (2)	C11—C12—C13—C14	−0.4 (2)
C2—C1—C6—C5	−1.4 (2)	C12—C13—C14—C15	0.9 (3)
C2—C1—C6—C7	178.38 (13)	C13—C14—C15—C16	−0.3 (2)
C4—C5—C6—C1	1.7 (2)	C9—N3—C16—C15	−176.86 (16)
C4—C5—C6—C7	−178.10 (13)	C9—N3—C16—C11	0.99 (17)
N2—N1—C7—O4	2.7 (2)	C14—C15—C16—N3	176.83 (16)
N2—N1—C7—C6	−176.87 (12)	C14—C15—C16—C11	−0.8 (2)
C1—C6—C7—O4	18.6 (2)	C12—C11—C16—N3	−176.83 (14)
C5—C6—C7—O4	−161.64 (14)	C10—C11—C16—N3	−0.38 (17)
C1—C6—C7—N1	−161.86 (13)	C12—C11—C16—C15	1.2 (2)

C5—C6—C7—N1	17.9 (2)	C10—C11—C16—C15	177.65 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*o*···O4^{i}	0.85 (1)	1.90 (1)	2.740 (2)	174 (2)
O2—H2*o*···O2*w*	0.84 (1)	1.94 (1)	2.697 (2)	149 (2)
O3—H3*o*···O3*w*	0.85 (1)	1.90 (1)	2.724 (2)	164 (2)
N1—H1*n*···O1*w*^{ii}	0.88 (1)	2.11 (1)	2.978 (2)	169 (2)
N3—H3*n*···O4*w*^{iii}	0.88 (1)	2.15 (1)	3.024 (2)	171 (2)
O1*w*—H11···O1	0.85 (1)	1.93 (1)	2.771 (2)	170 (3)
O1*w*—H12···O3*w*^{iv}	0.86 (1)	1.94 (1)	2.760 (2)	161 (3)
O2*w*—H21···O3^{v}	0.84 (1)	2.29 (1)	3.123 (2)	172 (2)
O2*w*—H22···O5*w*	0.85 (1)	1.94 (2)	2.753 (2)	161 (3)
O3*w*—H31···O5*w*^{vi}	0.85 (1)	1.95 (1)	2.796 (2)	172 (3)
O3*w*—H32···O3^{vii}	0.85 (1)	2.06 (1)	2.890 (2)	165 (2)
O4*w*—H41···O1*w*	0.85 (1)	1.97 (1)	2.803 (2)	169 (2)
O4*w*—H42···O4^{viii}	0.84 (1)	2.37 (2)	2.921 (2)	124 (2)
O4*w*—H42···N2^{viii}	0.84 (1)	2.39 (1)	3.211 (2)	166 (2)
O5*w*—H51···O4*w*^{ix}	0.85 (1)	1.97 (1)	2.798 (2)	167 (2)
O5*w*—H52···O2*w*^{x}	0.85 (1)	1.97 (1)	2.810 (2)	168 (3)

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