Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Hamid Khaledi, Hapipah Mohd Ali and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

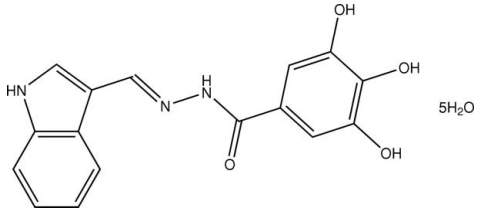
Received 22 November 2008; accepted 22 November 2008

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).

We thank the University of Malaya for funding this study (Science Fund grants 12–02-03–2031 and 12–02-03–2051).

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.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
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.

supplementary materials

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

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

H. Khaledi, H. Mohd Ali and S. W. Ng

Comment

(type here to add)

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.

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.

Figures

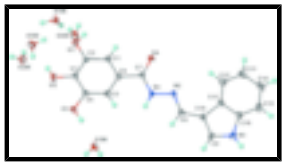


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{16}H_{13}N_3O_4.5H2O$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

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

Crystal data

$C_{16}H_{13}N_3O_4·5H_2O$	$Z = 2$
$M_r = 401.37$	$F_{000} = 424$
Triclinic, $P\bar{1}$	$D_x = 1.471$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.4379$ (2) Å	Cell parameters from 2461 reflections
$b = 9.1178$ (2) Å	$\theta = 2.3$–28.0º
$c = 14.1966$ (3) Å	$\mu = 0.12$ mm^{-1}
$\alpha = 103.814$ (1)º	$T = 100$ (2) K
$\beta = 103.716$ (1)º	Plate, pale-yellow
$\gamma = 90.613$ (2)º	0.30 × 0.25 × 0.04 mm
$V = 905.95$ (4) Å^3	

Data collection

Bruker SMART APEX diffractometer	3285 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.023$
Monochromator: graphite	$\theta_{max} = 27.5^{o}$
$T = 100(2)$ K	$\theta_{min} = 2.3^{o}$
ω scans	$h = -9 \rightarrow 9$
Absorption correction: None	$k = -11 \rightarrow 11$
7524 measured reflections	$l = -18 \rightarrow 18$
4096 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.1789P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
4096 reflections	$\Delta\rho_{max} = 0.35$ e Å^{-3}
313 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
15 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	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, °)

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)

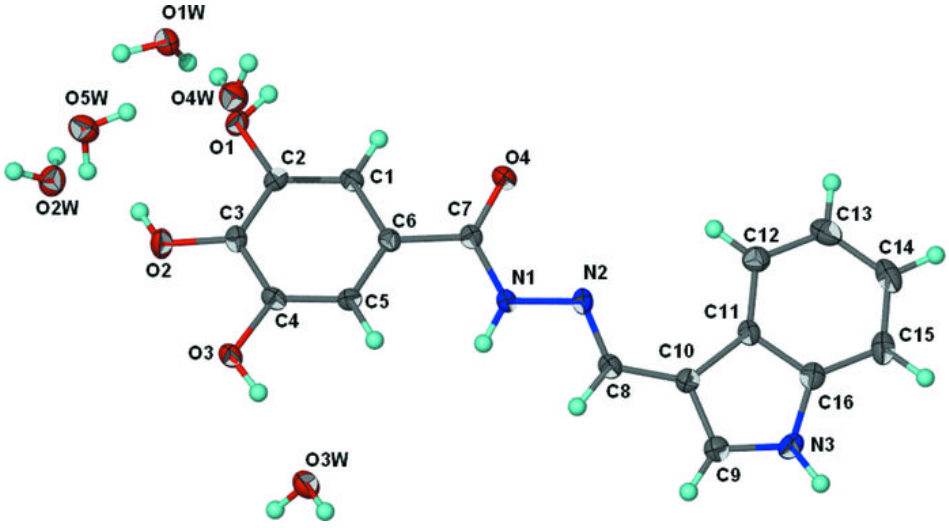
C5—C6—C7—O4	−161.64 (14)	C10—C11—C16—N3	−0.38 (17)
C1—C6—C7—N1	−161.86 (13)	C12—C11—C16—C15	1.2 (2)
C5—C6—C7—N1	17.9 (2)	C10—C11—C16—C15	177.65 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1o···O4^{i}	0.85 (1)	1.90 (1)	2.740 (2)	174 (2)
O2—H2o···O2w	0.84 (1)	1.94 (1)	2.697 (2)	149 (2)
O3—H3o···O3w	0.85 (1)	1.90 (1)	2.724 (2)	164 (2)
N1—H1n···O1w^{ii}	0.88 (1)	2.11 (1)	2.978 (2)	169 (2)
N3—H3n···O4w^{iii}	0.88 (1)	2.15 (1)	3.024 (2)	171 (2)
O1w—H11···O1	0.85 (1)	1.93 (1)	2.771 (2)	170 (3)
O1w—H12···O3w^{iv}	0.86 (1)	1.94 (1)	2.760 (2)	161 (3)
O2w—H21···O3^{v}	0.84 (1)	2.29 (1)	3.123 (2)	172 (2)
O2w—H22···O5w	0.85 (1)	1.94 (2)	2.753 (2)	161 (3)
O3w—H31···O5w^{vi}	0.85 (1)	1.95 (1)	2.796 (2)	172 (3)
O3w—H32···O3^{vii}	0.85 (1)	2.06 (1)	2.890 (2)	165 (2)
O4w—H41···O1w	0.85 (1)	1.97 (1)	2.803 (2)	169 (2)
O4w—H42···O4^{viii}	0.84 (1)	2.37 (2)	2.921 (2)	124 (2)
O4w—H42···N2^{viii}	0.84 (1)	2.39 (1)	3.211 (2)	166 (2)
O5w—H51···O4w^{ix}	0.85 (1)	1.97 (1)	2.798 (2)	167 (2)
O5w—H52···O2w^{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.

Fig. 1


O1W
O4W
O5W
O1
C2
C1
O4
O2W
C3
C6
C7
C12
C13
O2
N1
N2
C14
C5
C11
C4
C15
O3
C10
C8
C16
N3
O3W
C9