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(*E*)-4-Methoxy-*N*′-(2,3,4-trimethoxybenzylidene)-benzohydrazide monohydrate

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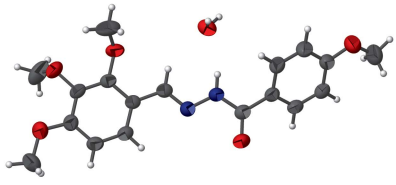
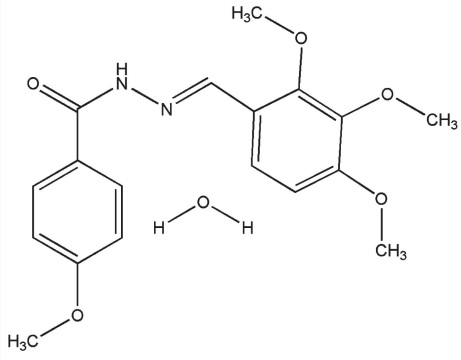
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{18}H_{20}N_2O_5\cdot H_2O$, consists of a benzohydrazide molecule which exists in an *E* conformation with respect to the C=N imine bond and a water molecule. The dihedral angle between the aromatic rings is 41.67 (9)°. The methoxy substituent of the 4-methoxyphenyl group is twisted at an angle of 6.8 (3)° out of the plane of the attached benzene ring. In the 2,4,5-trimethoxyphenyl unit, the *para*-methoxy group is coplanar with the ring [C—C—O—C = −1.5 (3)°], whereas the *ortho*- and *meta*-methoxy groups are twisted out of the plane of the ring [C—C—O—C = 75.4 (2) and −67.1 (2)°, respectively]. Two molecules are connected by two water molecules *via* O—H···O hydrogen bonds, generating an $R_2^2(8)$ ring motif. One of the water H atoms forms an additional hydrogen bond to an N atom. The water molecules act as an acceptor for an N—H···O hydrogen bond. As a result, a three-dimensional network is formed.

3D view



Chemical scheme



Structure description

Benzohydrazide derivatives possess biological activities such as antifungal (Loncle *et al.*, 2004), antimalarial (Melnyk *et al.*, 2006) and antiproliferative (Raj *et al.*, 2007). We report the synthesis and the crystal structure of the title compound (Fig. 1) whose geometric parameters are comparable with those of related structures (Fun *et al.*, 2012; Horkaew *et al.*, 2011). The dihedral angle between the planes of the C2–C7 and C10–C15 aromatic rings is 41.67 (9)°.

The benzohydrazide molecule exists in an *E* conformation with respect to the C9=N2 imine bond [1.277 (2) Å] and the N1—N2—C9—C10 torsion angle is 179.79 (14)°. The

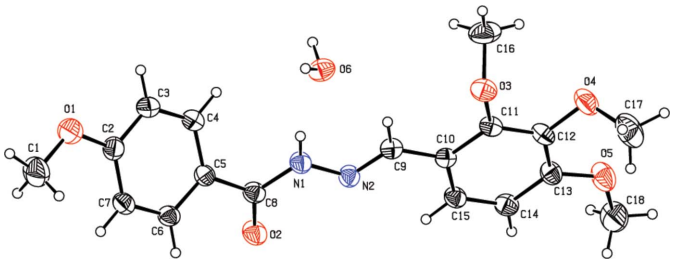


Figure 1
The molecular structure of the title compound, showing the atom labelling and 30% probability displacement ellipsoids.

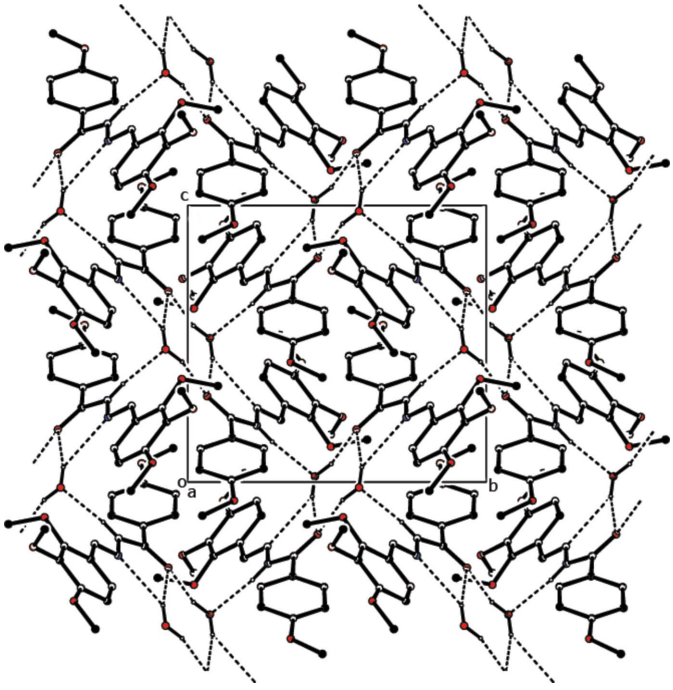


Figure 2
The crystal packing of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involving in hydrogen bonding have been omitted for clarity.

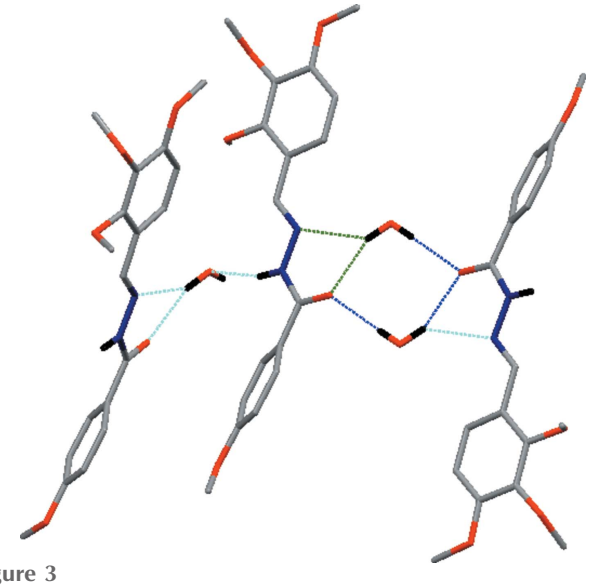


Figure 3
A partial view of the crystal packing, showing the various ring motifs.

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

*Cg*1 and *Cg*2 are the centroids of the C2–C7 and C10–C15 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O6	0.86 (1)	2.07 (1)	2.905 (2)	164 (2)
C9—H9···O6	0.93	2.45	3.258 (2)	146
O6—H6*A*···O2^{i}	0.87 (1)	1.98 (1)	2.8204 (18)	163 (2)
O6—H6*B*···O2^{ii}	0.86 (1)	2.11 (1)	2.914 (2)	156 (2)
O6—H6*B*···N2^{ii}	0.86 (1)	2.54 (2)	3.1880 (19)	133 (2)
C1—H1*C*···*Cg*2^{iii}	0.96	2.95	3.900 (3)	171
C16—H16*C*···*Cg*1^{i}	0.96	2.79	3.713 (2)	162

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{20}N_2O_5\cdot H_2O$
M_r	362.37
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, *b*, *c* (Å)	16.1090 (9), 11.2205 (5), 10.7515 (5)
β (°)	104.888 (2)
V (Å^3)	1878.11 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.30 × 0.28 × 0.24
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.962, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14944, 4685, 2334
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.145, 0.99
No. of reflections	4685
No. of parameters	249
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.21

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

methoxy substituent of 4-methoxyphenyl is twisted at an C7—C2—O1—C1 angle of 6.8 (3)°, with the attached benzene ring. The three methoxy groups of 2,4,5-trimethoxyphenyl unit have two different orientations: the *para*-methoxy group (at atom C13) is coplanar [C18—O5—C13—C12 = 178.49 (19)°] with the ring, whereas the *ortho*- and *meta*-methoxy groups (attached at atoms C11 and C12) are twisted out of the ring plane [C16—O3—C11—C10 = −108.9 (2)° and C17—O4—C12—C11 = 114.9 (2)°].

In the crystal (Fig. 2), the benzohydrazide and water molecules are linked by N—H···O hydrogen bonds and a C—H···O contact (Table 1). A pair of O—H···O (O6—H6*A*···O2^{i} and O6—H6*B*···O2^{ii}) hydrogen bonds generate

an $R_2^2(8)$ ring motif and O—H···O (O6—H6*B*···O2^{ii}) and O—H···N (O6—H6*B*···N2^{ii}) hydrogen bonds generate a bifurcated $R_1^2(6)$ ring motif (Fig. 3 and Table 1). As a result, a three-dimensional network is formed (Fig. 2), which is additionally stabilized by C—H···π interactions.

Synthesis and crystallization

4-Methoxybenzohydrazide (0.001 mmol, 0.17 g) was dissolved in ethanol (10 ml). 2,3,4-trimethoxybenzaldehyde (0.001 mmol, 0.145 g) was added slowly followed by addition of concentrated HCl (0.2 mmol). The mixture was stirred continuously for 30 min at room temperature. The precipitate formed was filtered, then washed with petroleum ether (40–60%) and dried in a vacuum desiccator, and the crystals suitable for X-ray diffraction were harvested.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The reflection 100 was omitted during refinement due to being obscured by the beam stop.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161526 [doi:10.1107/S2414314616015261]

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Crystal data

$C_{18}H_{20}N_2O_5·H_2O$
M_r = 362.37
Monoclinic, $P2_1/c$
a = 16.1090 (9) Å
b = 11.2205 (5) Å
c = 10.7515 (5) Å
β = 104.888 (2)°
V = 1878.11 (16) Å^3
Z = 4
$F(000)$ = 768
D_x = 1.282 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2417 reflections
θ = 2.1–28.3°
μ = 0.10 mm^{-1}
T = 295 K
Block, colourless
0.30 × 0.28 × 0.24 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.962, T_{max} = 0.986
14944 measured reflections
4685 independent reflections
2334 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 28.4°, θ_{min} = 2.6°
h = −21→19
k = −15→14
l = −11→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.145
S = 0.99
4685 reflections
249 parameters
3 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	1.24421 (17)	0.0490 (2)	−0.1222 (3)	0.0886 (8)

H1A	1.280361	0.069028	−0.177490	0.133*
H1B	1.193612	0.009106	−0.171245	0.133*
H1C	1.274869	−0.002702	−0.054730	0.133*
C2	1.16371 (12)	0.14659 (18)	0.00676 (19)	0.0545 (5)
C3	1.13670 (13)	0.25364 (18)	0.0479 (2)	0.0647 (6)
H3	1.158028	0.325170	0.025187	0.078*
C4	1.07928 (13)	0.25478 (17)	0.1212 (2)	0.0581 (5)
H4	1.061002	0.327246	0.146745	0.070*
C5	1.04751 (11)	0.14890 (16)	0.15839 (16)	0.0447 (4)
C6	1.07691 (12)	0.04319 (16)	0.11999 (17)	0.0471 (5)
H6	1.057605	−0.028326	0.146181	0.056*
C7	1.13406 (12)	0.04018 (17)	0.04393 (18)	0.0504 (5)
H7	1.152323	−0.032192	0.018120	0.060*
C8	0.98183 (12)	0.14453 (16)	0.23180 (17)	0.0474 (5)
C9	0.79901 (11)	0.31185 (16)	0.22430 (16)	0.0442 (4)
H9	0.803603	0.361590	0.157194	0.053*
C10	0.72665 (11)	0.32514 (15)	0.27982 (15)	0.0403 (4)
C11	0.66504 (12)	0.41359 (15)	0.23211 (16)	0.0437 (4)
C12	0.59547 (12)	0.42884 (16)	0.28314 (17)	0.0497 (5)
C13	0.58618 (12)	0.35767 (16)	0.38446 (17)	0.0506 (5)
C14	0.64630 (12)	0.26918 (16)	0.43072 (17)	0.0512 (5)
H14	0.640208	0.220152	0.497556	0.061*
C15	0.71445 (12)	0.25373 (16)	0.37852 (16)	0.0469 (5)
H15	0.753788	0.193422	0.410268	0.056*
C16	0.69663 (16)	0.6007 (2)	0.1529 (2)	0.0836 (8)
H16A	0.657851	0.639264	0.194522	0.125*
H16B	0.694892	0.640562	0.073201	0.125*
H16C	0.753916	0.604094	0.207760	0.125*
C17	0.45299 (16)	0.4792 (2)	0.1714 (3)	0.1005 (10)
H17A	0.447906	0.473042	0.080714	0.151*
H17B	0.411900	0.535857	0.186205	0.151*
H17C	0.442236	0.402774	0.204290	0.151*
C18	0.50355 (17)	0.3094 (2)	0.5323 (2)	0.0897 (8)
H18A	0.494895	0.228135	0.503843	0.135*
H18B	0.453681	0.337232	0.556795	0.135*
H18C	0.552753	0.314100	0.604811	0.135*
N2	0.85666 (10)	0.23302 (13)	0.26582 (14)	0.0473 (4)
N1	0.92169 (10)	0.23108 (14)	0.20414 (15)	0.0483 (4)
O1	1.22019 (10)	0.15475 (13)	−0.06744 (16)	0.0771 (5)
O2	0.97921 (8)	0.06501 (12)	0.31030 (13)	0.0609 (4)
O3	0.67178 (9)	0.47970 (11)	0.12780 (12)	0.0582 (4)
O4	0.53704 (9)	0.51746 (12)	0.23501 (15)	0.0699 (4)
O5	0.51735 (10)	0.38125 (13)	0.43079 (14)	0.0729 (4)
O6	0.89533 (9)	0.42585 (12)	0.02007 (13)	0.0578 (4)
H1	0.9222 (11)	0.2829 (13)	0.1455 (13)	0.051 (5)*
H6A	0.9271 (12)	0.4808 (15)	0.0652 (18)	0.076*
H6B	0.9070 (14)	0.417 (2)	−0.0528 (13)	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0936 (19)	0.0836 (18)	0.1047 (19)	0.0148 (14)	0.0550 (16)	0.0022 (15)
C2	0.0486 (11)	0.0563 (13)	0.0610 (12)	0.0044 (9)	0.0182 (10)	0.0093 (10)
C3	0.0633 (14)	0.0437 (11)	0.0948 (16)	0.0003 (10)	0.0341 (12)	0.0114 (11)
C4	0.0572 (12)	0.0415 (11)	0.0798 (14)	0.0042 (9)	0.0252 (11)	0.0023 (10)
C5	0.0427 (10)	0.0435 (10)	0.0459 (10)	0.0040 (8)	0.0076 (8)	0.0055 (8)
C6	0.0474 (11)	0.0412 (10)	0.0490 (10)	0.0014 (8)	0.0058 (9)	0.0077 (8)
C7	0.0517 (12)	0.0439 (11)	0.0533 (11)	0.0069 (9)	0.0092 (9)	0.0020 (9)
C8	0.0500 (11)	0.0440 (10)	0.0453 (10)	0.0018 (9)	0.0069 (9)	0.0025 (9)
C9	0.0482 (11)	0.0444 (10)	0.0370 (9)	−0.0022 (8)	0.0056 (8)	0.0016 (8)
C10	0.0429 (10)	0.0391 (9)	0.0359 (9)	−0.0022 (8)	0.0047 (7)	0.0006 (8)
C11	0.0525 (11)	0.0402 (10)	0.0356 (9)	0.0003 (8)	0.0066 (8)	0.0016 (8)
C12	0.0597 (13)	0.0402 (10)	0.0477 (10)	0.0121 (9)	0.0112 (9)	0.0041 (9)
C13	0.0547 (12)	0.0516 (11)	0.0477 (11)	0.0070 (9)	0.0169 (9)	−0.0020 (9)
C14	0.0599 (12)	0.0486 (11)	0.0447 (10)	0.0027 (9)	0.0129 (9)	0.0086 (9)
C15	0.0489 (11)	0.0436 (10)	0.0452 (10)	0.0045 (8)	0.0069 (8)	0.0059 (9)
C16	0.0892 (18)	0.0592 (14)	0.0907 (17)	−0.0149 (12)	0.0019 (14)	0.0268 (13)
C17	0.0813 (19)	0.099 (2)	0.103 (2)	0.0370 (15)	−0.0102 (16)	0.0022 (16)
C18	0.1019 (19)	0.0920 (18)	0.0959 (18)	0.0139 (16)	0.0632 (16)	0.0193 (15)
N2	0.0458 (9)	0.0488 (9)	0.0476 (8)	0.0028 (7)	0.0125 (7)	0.0042 (7)
N1	0.0503 (10)	0.0473 (9)	0.0489 (9)	0.0064 (7)	0.0155 (7)	0.0119 (8)
O1	0.0806 (11)	0.0649 (10)	0.1004 (12)	0.0059 (8)	0.0497 (9)	0.0103 (9)
O2	0.0664 (9)	0.0581 (8)	0.0600 (8)	0.0134 (7)	0.0195 (7)	0.0202 (7)
O3	0.0713 (9)	0.0526 (8)	0.0499 (8)	0.0039 (7)	0.0141 (6)	0.0169 (6)
O4	0.0737 (11)	0.0588 (9)	0.0795 (10)	0.0268 (8)	0.0236 (8)	0.0181 (7)
O5	0.0831 (11)	0.0767 (10)	0.0708 (9)	0.0247 (8)	0.0414 (8)	0.0134 (8)
O6	0.0684 (10)	0.0563 (9)	0.0507 (8)	−0.0118 (7)	0.0189 (7)	−0.0035 (7)

Geometric parameters (Å, º)

C1—O1	1.422 (3)	C11—C12	1.379 (3)
C1—H1A	0.9600	C12—O4	1.376 (2)
C1—H1B	0.9600	C12—C13	1.389 (3)
C1—H1C	0.9600	C13—O5	1.353 (2)
C2—O1	1.359 (2)	C13—C14	1.387 (2)
C2—C7	1.383 (3)	C14—C15	1.366 (2)
C2—C3	1.388 (3)	C14—H14	0.9300
C3—C4	1.361 (3)	C15—H15	0.9300
C3—H3	0.9300	C16—O3	1.422 (2)
C4—C5	1.392 (3)	C16—H16A	0.9600
C4—H4	0.9300	C16—H16B	0.9600
C5—C6	1.379 (2)	C16—H16C	0.9600
C5—C8	1.474 (3)	C17—O4	1.418 (3)
C6—C7	1.380 (3)	C17—H17A	0.9600
C6—H6	0.9300	C17—H17B	0.9600
C7—H7	0.9300	C17—H17C	0.9600

C8—O2	1.236 (2)	C18—O5	1.420 (3)
C8—N1	1.350 (2)	C18—H18A	0.9600
C9—N2	1.277 (2)	C18—H18B	0.9600
C9—C10	1.447 (2)	C18—H18C	0.9600
C9—H9	0.9300	N2—N1	1.376 (2)
C10—C15	1.383 (2)	N1—H1	0.859 (9)
C10—C11	1.404 (2)	O6—H6A	0.865 (9)
C11—O3	1.372 (2)	O6—H6B	0.858 (9)

O1—C1—H1A	109.5	C11—C12—C13	120.19 (16)
O1—C1—H1B	109.5	O5—C13—C14	124.80 (18)
H1A—C1—H1B	109.5	O5—C13—C12	116.09 (16)
O1—C1—H1C	109.5	C14—C13—C12	119.11 (19)
H1A—C1—H1C	109.5	C15—C14—C13	120.29 (17)
H1B—C1—H1C	109.5	C15—C14—H14	119.9
O1—C2—C7	124.14 (18)	C13—C14—H14	119.9
O1—C2—C3	116.16 (18)	C14—C15—C10	121.95 (16)
C7—C2—C3	119.7 (2)	C14—C15—H15	119.0
C4—C3—C2	120.54 (19)	C10—C15—H15	119.0
C4—C3—H3	119.7	O3—C16—H16A	109.5
C2—C3—H3	119.7	O3—C16—H16B	109.5
C3—C4—C5	120.87 (18)	H16A—C16—H16B	109.5
C3—C4—H4	119.6	O3—C16—H16C	109.5
C5—C4—H4	119.6	H16A—C16—H16C	109.5
C6—C5—C4	117.90 (18)	H16B—C16—H16C	109.5
C6—C5—C8	118.71 (16)	O4—C17—H17A	109.5
C4—C5—C8	123.33 (17)	O4—C17—H17B	109.5
C5—C6—C7	122.08 (17)	H17A—C17—H17B	109.5
C5—C6—H6	119.0	O4—C17—H17C	109.5
C7—C6—H6	119.0	H17A—C17—H17C	109.5
C6—C7—C2	118.87 (18)	H17B—C17—H17C	109.5
C6—C7—H7	120.6	O5—C18—H18A	109.5
C2—C7—H7	120.6	O5—C18—H18B	109.5
O2—C8—N1	121.41 (19)	H18A—C18—H18B	109.5
O2—C8—C5	122.99 (17)	O5—C18—H18C	109.5
N1—C8—C5	115.55 (16)	H18A—C18—H18C	109.5
N2—C9—C10	121.17 (16)	H18B—C18—H18C	109.5
N2—C9—H9	119.4	C9—N2—N1	114.68 (15)
C10—C9—H9	119.4	C8—N1—N2	119.82 (16)
C15—C10—C11	117.60 (17)	C8—N1—H1	120.5 (12)
C15—C10—C9	123.02 (16)	N2—N1—H1	119.6 (12)
C11—C10—C9	119.39 (16)	C2—O1—C1	118.76 (17)
O3—C11—C12	120.08 (16)	C11—O3—C16	116.04 (15)
O3—C11—C10	118.94 (17)	C12—O4—C17	116.03 (16)
C12—C11—C10	120.84 (16)	C13—O5—C18	118.47 (17)
O4—C12—C11	119.17 (17)	H6A—O6—H6B	111 (2)
O4—C12—C13	120.61 (18)		

O1—C2—C3—C4	179.10 (18)	C10—C11—C12—C13	1.1 (3)
C7—C2—C3—C4	−2.0 (3)	O4—C12—C13—O5	0.1 (3)
C2—C3—C4—C5	1.1 (3)	C11—C12—C13—O5	178.15 (16)
C3—C4—C5—C6	0.8 (3)	O4—C12—C13—C14	−179.95 (16)
C3—C4—C5—C8	−176.64 (17)	C11—C12—C13—C14	−1.9 (3)
C4—C5—C6—C7	−1.9 (3)	O5—C13—C14—C15	−178.97 (17)
C8—C5—C6—C7	175.68 (16)	C12—C13—C14—C15	1.1 (3)
C5—C6—C7—C2	1.0 (3)	C13—C14—C15—C10	0.6 (3)
O1—C2—C7—C6	179.75 (17)	C11—C10—C15—C14	−1.4 (2)
C3—C2—C7—C6	1.0 (3)	C9—C10—C15—C14	178.98 (16)
C6—C5—C8—O2	34.9 (2)	C10—C9—N2—N1	−179.79 (14)
C4—C5—C8—O2	−147.69 (19)	O2—C8—N1—N2	1.2 (3)
C6—C5—C8—N1	−142.51 (16)	C5—C8—N1—N2	178.68 (14)
C4—C5—C8—N1	34.9 (2)	C9—N2—N1—C8	−173.92 (15)
N2—C9—C10—C15	−0.9 (2)	C7—C2—O1—C1	6.8 (3)
N2—C9—C10—C11	179.46 (16)	C3—C2—O1—C1	−174.4 (2)
C15—C10—C11—O3	−175.04 (14)	C12—C11—O3—C16	75.4 (2)
C9—C10—C11—O3	4.6 (2)	C10—C11—O3—C16	−108.9 (2)
C15—C10—C11—C12	0.6 (2)	C11—C12—O4—C17	114.9 (2)
C9—C10—C11—C12	−179.80 (15)	C13—C12—O4—C17	−67.1 (2)
O3—C11—C12—O4	−5.3 (3)	C14—C13—O5—C18	−1.5 (3)
C10—C11—C12—O4	179.15 (15)	C12—C13—O5—C18	178.49 (19)
O3—C11—C12—C13	176.63 (16)		

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C2–C7 and C10–C15 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O6	0.86 (1)	2.07 (1)	2.905 (2)	164 (2)
C9—H9···O6	0.93	2.45	3.258 (2)	146
O6—H6*A*···O2^{i}	0.87 (1)	1.98 (1)	2.8204 (18)	163 (2)
O6—H6*B*···O2^{ii}	0.86 (1)	2.11 (1)	2.914 (2)	156 (2)
O6—H6*B*···N2^{ii}	0.86 (1)	2.54 (2)	3.1880 (19)	133 (2)
C1—H1*C*···*Cg*2^{iii}	0.96	2.95	3.900 (3)	171
C16—H16*C*···*Cg*1^{i}	0.96	2.79	3.713 (2)	162

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