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4-[(2-Phenylethyl)amino]benzoic acid

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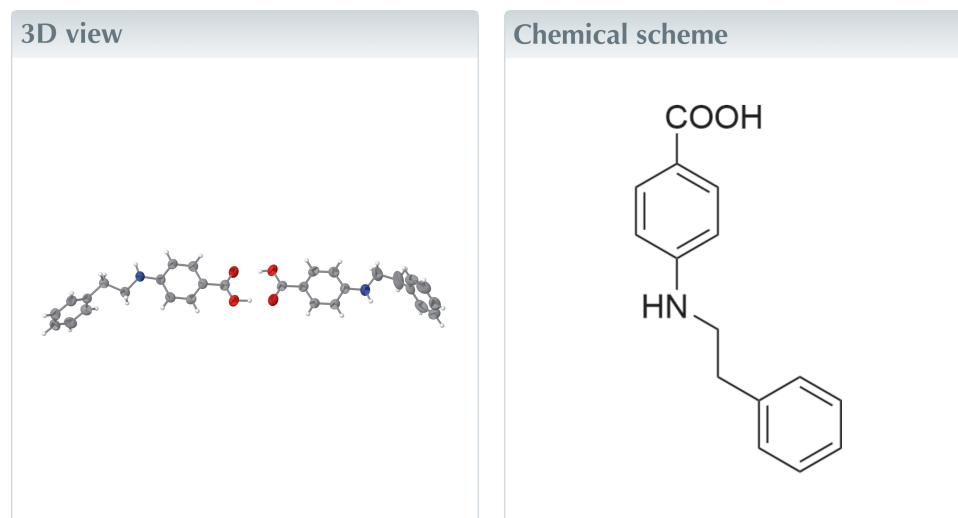
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Keywords: synthon; hydrogen bond; acid–acid dimer; crystal structure.

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

The title compound, $C_{15}H_{15}NO_2$, crystallizes with two molecules in the asymmetric unit. In the crystal, the two molecules associate to form an acid–acid dimer by pairwise $O-H\cdots O$ hydrogen bonds.



Structure description

Non-steroidal anti-inflammatory drugs (NSAIDs) constitute approximately 5–10% of all prescribed medications worldwide as antipyretic, anti-inflammatory, and analgesic agents (Sohail *et al.*, 2023). As part of our ongoing studies in this area (Liu & Long, 2023), the title compound, $C_{15}H_{15}NO_2$, was synthesized employing the Borch reductive amination reaction.

There are two molecules, *A* (containing C1) and *B* (containing C16), in the asymmetric unit (Fig. 1). Both molecules are twisted with dihedral angles between their aromatic rings of $80.98(9)^\circ$ (molecule *A*) and $83.54(11)^\circ$ (molecule *B*). The main difference between the molecules lies in the geometries of the linking ethyl-amino chains: the N1–C8–C9–C10 (molecule *A*) torsion angle of $166.11(15)^\circ$ indicates an *anti* conformation whereas the N2–C23–C24–C25 (molecule *B*) torsion angle of $-59.3(4)^\circ$ is *gauche*. In the extended structure, the molecules form *A–B* carboxylic acid dimers linked by pairs of $O-H\cdots O$ hydrogen bonds (Table 1, Fig. 2). Conversely, the NH groups do not participate in hydrogen bonds, presumably due to steric crowding.

Synthesis and crystallization

The title compound was obtained by the reaction of 4-aminobenzoic acid and 2-phenylacetaldehyde using methanol as solvent in the presence of 2-picoline borane complex (Fig. 3). The crude product was recovered by filtration and purified by silica gel column chromatography. Colourless needles were produced by recrystallization from acetonitrile solution.



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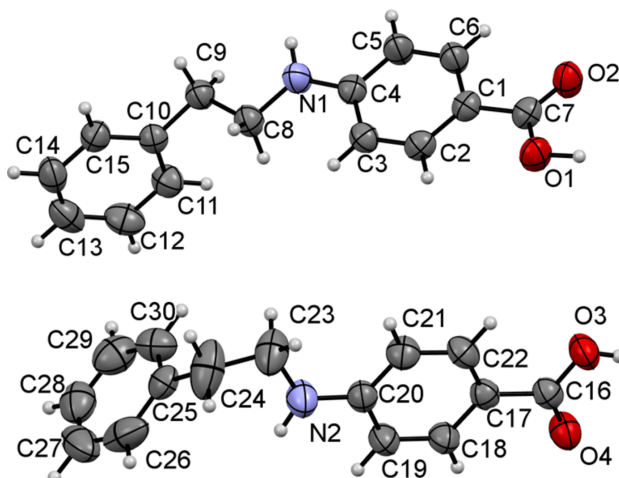


Figure 1
The molecular structures of molecules *A* and *B* in title compound with displacement ellipsoids drawn at the 50% probability level.

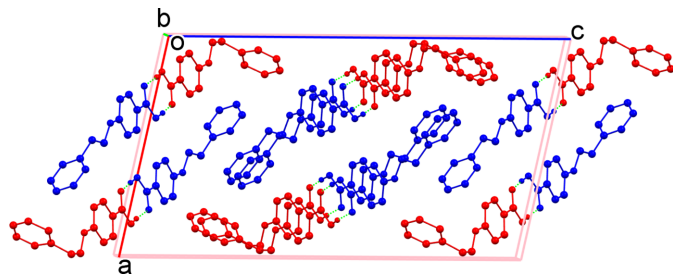


Figure 2
Packing of the molecules in the title compound: C1 molecule shown in blue, C16 molecule shown in red (for clarity, H atoms not involved in hydrogen bonding are omitted).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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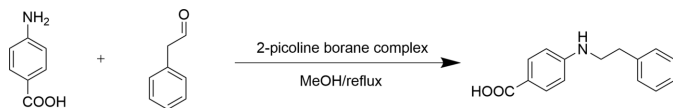


Figure 3
Synthesis scheme for the title compound.

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1···O4	1.05 (4)	1.58 (4)	2.6380 (19)	177 (3)
O3—H3A···O2	0.82	1.81	2.6246 (18)	175

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₅ H ₁₅ NO ₂
<i>M_r</i>	241.28
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	305
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.7698 (7), 6.6730 (3), 26.2392 (12)
β (°)	102.231 (5)
<i>V</i> (Å ³)	2527.4 (2)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.16 × 0.05 × 0.04
Data collection	
Diffractometer	XtaLAB Synergy R, DW system, HyPix
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2022)
<i>T</i> _{min} , <i>T</i> _{max}	0.598, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	26873, 6498, 3944
<i>R</i> _{int}	0.033
(sin θ / λ) _{max} (Å ⁻¹)	0.725
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.058, 0.175, 1.03
No. of reflections	6498
No. of parameters	330
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.52, -0.28

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

References

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full crystallographic data

IUCrData (2024). **9**, x240753 [https://doi.org/10.1107/S2414314624007533]

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Crystal data

$C_{15}H_{15}NO_2$

$M_r = 241.28$

Monoclinic, $P2_1/c$

$a = 14.7698$ (7) Å

$b = 6.6730$ (3) Å

$c = 26.2392$ (12) Å

$\beta = 102.231$ (5)°

$V = 2527.4$ (2) Å³

$Z = 8$

$F(000) = 1024$

$D_x = 1.268$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6437 reflections

$\theta = 1.9$ – 27.2 °

$\mu = 0.08$ mm⁻¹

$T = 305$ K

Needle, colourless

$0.16 \times 0.05 \times 0.04$ mm

Data collection

XtaLAB Synergy R, DW system, HyPix diffractometer

Radiation source: Rotating-anode X-ray tube, Rigaku (Mo) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)

$T_{\min} = 0.598$, $T_{\max} = 1.000$

26873 measured reflections

6498 independent reflections

3944 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 31.0$ °, $\theta_{\min} = 1.9$ °

$h = -21 \rightarrow 19$

$k = -8 \rightarrow 9$

$l = -32 \rightarrow 34$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.058$

$wR(F^2) = 0.175$

$S = 1.03$

6498 reflections

330 parameters

0 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0816P)^2 + 0.4926P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.52$ e Å⁻³

$\Delta\rho_{\min} = -0.28$ 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.

Refinement. The positions of H atoms attached to N1 and O1 were obtained from a difference Fourier map. Other H atoms were positioned geometrically with O—H = 0.82, N—H = 0.86 and C—H = 0.93 Å and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.63928 (9)	0.5549 (2)	0.49996 (5)	0.0608 (4)
H1	0.661 (2)	0.687 (5)	0.4841 (12)	0.139 (12)*
O2	0.78373 (9)	0.5311 (2)	0.54712 (6)	0.0623 (4)
N1	0.62345 (10)	−0.2690 (2)	0.62201 (6)	0.0556 (4)
H1A	0.670942	−0.343326	0.633528	0.067*
C1	0.67845 (12)	0.2741 (2)	0.55501 (6)	0.0448 (4)
C2	0.58830 (12)	0.2008 (3)	0.54624 (7)	0.0475 (4)
H2	0.540867	0.273251	0.525216	0.057*
C3	0.56779 (12)	0.0226 (3)	0.56814 (7)	0.0473 (4)
H3	0.506936	−0.022989	0.561997	0.057*
C4	0.63833 (12)	−0.0896 (3)	0.59955 (7)	0.0461 (4)
C5	0.72918 (12)	−0.0169 (3)	0.60742 (8)	0.0575 (5)
H5	0.777273	−0.090155	0.627617	0.069*
C6	0.74806 (13)	0.1609 (3)	0.58571 (8)	0.0539 (5)
H6	0.808861	0.206790	0.591675	0.065*
C7	0.70333 (13)	0.4639 (3)	0.53328 (7)	0.0485 (4)
C8	0.53414 (12)	−0.3427 (3)	0.62782 (7)	0.0523 (4)
H8A	0.496079	−0.374358	0.593891	0.063*
H8B	0.502589	−0.241065	0.643982	0.063*
C9	0.54902 (12)	−0.5296 (3)	0.66167 (7)	0.0496 (4)
H9A	0.567642	−0.638343	0.641589	0.060*
H9B	0.599654	−0.504918	0.691190	0.060*
C10	0.46542 (11)	−0.5960 (2)	0.68191 (6)	0.0439 (4)
C11	0.43655 (13)	−0.4860 (3)	0.72026 (7)	0.0554 (5)
H11	0.466372	−0.366526	0.731813	0.067*
C12	0.36428 (14)	−0.5512 (4)	0.74149 (8)	0.0678 (6)
H12	0.345739	−0.476165	0.767353	0.081*
C13	0.31917 (13)	−0.7279 (4)	0.72450 (9)	0.0671 (6)
H13	0.270503	−0.772369	0.738992	0.080*
C14	0.34607 (13)	−0.8363 (3)	0.68665 (8)	0.0629 (5)
H14	0.315378	−0.954661	0.674913	0.075*
C15	0.41898 (12)	−0.7717 (3)	0.66540 (7)	0.0525 (4)
H15	0.437040	−0.847735	0.639567	0.063*
O3	0.84499 (10)	0.8497 (2)	0.50638 (6)	0.0662 (4)
H3A	0.822533	0.751596	0.517918	0.099*
O4	0.69836 (10)	0.8856 (2)	0.46252 (6)	0.0632 (4)
N2	0.87828 (12)	1.6586 (3)	0.38333 (7)	0.0675 (5)
H2A	0.833024	1.729992	0.366770	0.081*
C16	0.78021 (12)	0.9463 (3)	0.47444 (7)	0.0496 (4)
C17	0.80772 (12)	1.1332 (3)	0.45255 (7)	0.0466 (4)
C18	0.74220 (12)	1.2459 (3)	0.41908 (7)	0.0538 (4)

H18	0.680858	1.203340	0.411462	0.065*
C19	0.76571 (13)	1.4194 (3)	0.39684 (8)	0.0588 (5)
H19	0.720120	1.493054	0.374767	0.071*
C20	0.85731 (12)	1.4864 (3)	0.40705 (7)	0.0506 (4)
C21	0.92346 (13)	1.3758 (3)	0.44124 (7)	0.0563 (5)
H21	0.984766	1.418640	0.449118	0.068*
C22	0.89844 (13)	1.2027 (3)	0.46351 (7)	0.0552 (5)
H22	0.943452	1.130779	0.486442	0.066*
C23	0.97058 (16)	1.7271 (4)	0.38434 (9)	0.0814 (7)
H23A	1.001736	1.630511	0.366397	0.098*
H23B	1.004391	1.734502	0.420262	0.098*
C24	0.9728 (2)	1.9283 (5)	0.35931 (10)	0.1036 (10)
H24A	1.037110	1.966035	0.362182	0.124*
H24B	0.945471	2.025064	0.379169	0.124*
C25	0.92401 (13)	1.9459 (3)	0.30261 (8)	0.0552 (5)
C26	0.86614 (18)	2.1100 (4)	0.28705 (13)	0.0890 (9)
H26	0.854239	2.202736	0.311259	0.107*
C27	0.82450 (17)	2.1318 (4)	0.23115 (15)	0.0942 (9)
H27	0.785947	2.239475	0.219054	0.113*
C28	0.84354 (17)	1.9928 (5)	0.19821 (11)	0.0813 (7)
H28	0.818089	2.005214	0.162771	0.098*
C29	0.89698 (17)	1.8403 (5)	0.21468 (11)	0.0843 (7)
H29	0.908093	1.745809	0.190688	0.101*
C30	0.93649 (15)	1.8160 (3)	0.26544 (9)	0.0701 (6)
H30	0.974023	1.704664	0.275262	0.084*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0613 (8)	0.0543 (8)	0.0630 (8)	0.0015 (6)	0.0047 (7)	0.0157 (6)
O2	0.0600 (8)	0.0528 (8)	0.0691 (9)	-0.0071 (6)	0.0024 (7)	0.0133 (6)
N1	0.0481 (8)	0.0523 (9)	0.0676 (10)	-0.0004 (7)	0.0151 (7)	0.0153 (7)
C1	0.0516 (9)	0.0429 (9)	0.0393 (9)	0.0004 (7)	0.0083 (7)	-0.0014 (7)
C2	0.0505 (10)	0.0479 (10)	0.0412 (9)	0.0034 (7)	0.0032 (7)	0.0007 (7)
C3	0.0458 (9)	0.0518 (10)	0.0441 (9)	-0.0039 (8)	0.0091 (7)	-0.0022 (7)
C4	0.0508 (9)	0.0451 (9)	0.0442 (9)	-0.0013 (7)	0.0138 (8)	-0.0006 (7)
C5	0.0459 (9)	0.0536 (11)	0.0690 (12)	0.0004 (8)	0.0035 (9)	0.0161 (9)
C6	0.0460 (9)	0.0509 (10)	0.0632 (12)	-0.0048 (8)	0.0080 (8)	0.0068 (8)
C7	0.0564 (10)	0.0440 (9)	0.0442 (9)	0.0007 (8)	0.0089 (8)	-0.0001 (7)
C8	0.0485 (9)	0.0545 (10)	0.0534 (10)	-0.0047 (8)	0.0099 (8)	0.0063 (8)
C9	0.0468 (9)	0.0494 (10)	0.0530 (10)	-0.0008 (8)	0.0113 (8)	0.0037 (8)
C10	0.0430 (8)	0.0460 (9)	0.0400 (8)	-0.0014 (7)	0.0030 (7)	0.0045 (7)
C11	0.0529 (10)	0.0597 (11)	0.0528 (10)	-0.0053 (9)	0.0092 (8)	-0.0099 (9)
C12	0.0603 (12)	0.0907 (16)	0.0558 (12)	0.0063 (11)	0.0201 (10)	-0.0033 (11)
C13	0.0450 (10)	0.0887 (16)	0.0674 (13)	-0.0044 (10)	0.0117 (9)	0.0236 (12)
C14	0.0538 (11)	0.0573 (12)	0.0734 (14)	-0.0133 (9)	0.0043 (10)	0.0092 (10)
C15	0.0545 (10)	0.0465 (10)	0.0542 (10)	-0.0002 (8)	0.0065 (8)	0.0004 (8)
O3	0.0646 (8)	0.0566 (8)	0.0739 (10)	0.0053 (6)	0.0068 (7)	0.0218 (7)

O4	0.0641 (8)	0.0550 (8)	0.0659 (9)	-0.0059 (6)	0.0033 (7)	0.0118 (6)
N2	0.0597 (10)	0.0657 (11)	0.0753 (12)	-0.0049 (8)	0.0104 (9)	0.0216 (9)
C16	0.0546 (10)	0.0474 (10)	0.0451 (9)	0.0041 (8)	0.0069 (8)	0.0023 (7)
C17	0.0517 (9)	0.0446 (9)	0.0431 (9)	0.0028 (7)	0.0093 (8)	0.0002 (7)
C18	0.0451 (9)	0.0550 (10)	0.0596 (11)	0.0006 (8)	0.0073 (8)	0.0095 (9)
C19	0.0509 (10)	0.0609 (11)	0.0626 (12)	0.0056 (9)	0.0076 (9)	0.0180 (9)
C20	0.0536 (10)	0.0489 (10)	0.0496 (10)	0.0004 (8)	0.0115 (8)	0.0030 (8)
C21	0.0477 (10)	0.0631 (12)	0.0549 (11)	-0.0058 (9)	0.0033 (8)	0.0017 (9)
C22	0.0539 (10)	0.0559 (11)	0.0509 (10)	0.0073 (8)	-0.0001 (8)	0.0056 (8)
C23	0.0672 (13)	0.1038 (19)	0.0657 (14)	-0.0280 (13)	-0.0031 (11)	0.0224 (13)
C24	0.126 (2)	0.114 (2)	0.0658 (15)	-0.0607 (19)	0.0075 (15)	0.0107 (15)
C25	0.0525 (10)	0.0566 (11)	0.0596 (11)	-0.0118 (9)	0.0191 (9)	0.0030 (9)
C26	0.0799 (15)	0.0647 (14)	0.139 (3)	-0.0150 (12)	0.0612 (17)	-0.0271 (15)
C27	0.0561 (13)	0.0780 (17)	0.145 (3)	0.0076 (12)	0.0123 (16)	0.0388 (18)
C28	0.0611 (13)	0.098 (2)	0.0812 (17)	-0.0161 (14)	0.0059 (12)	0.0191 (15)
C29	0.0666 (14)	0.108 (2)	0.0783 (17)	-0.0111 (14)	0.0154 (13)	-0.0114 (15)
C30	0.0577 (12)	0.0682 (13)	0.0840 (16)	0.0033 (10)	0.0139 (11)	-0.0099 (12)

Geometric parameters (Å, °)

O1—H1	1.05 (4)	O3—H3A	0.8200
O1—C7	1.295 (2)	O3—C16	1.301 (2)
O2—C7	1.249 (2)	O4—C16	1.250 (2)
N1—H1A	0.8600	N2—H2A	0.8600
N1—C4	1.372 (2)	N2—C20	1.373 (2)
N1—C8	1.446 (2)	N2—C23	1.433 (3)
C1—C2	1.391 (2)	C16—C17	1.466 (2)
C1—C6	1.387 (2)	C17—C18	1.383 (2)
C1—C7	1.467 (2)	C17—C22	1.389 (3)
C2—H2	0.9300	C18—H18	0.9300
C2—C3	1.382 (2)	C18—C19	1.374 (3)
C3—H3	0.9300	C19—H19	0.9300
C3—C4	1.401 (2)	C19—C20	1.396 (3)
C4—C5	1.400 (2)	C20—C21	1.390 (3)
C5—H5	0.9300	C21—H21	0.9300
C5—C6	1.370 (3)	C21—C22	1.380 (3)
C6—H6	0.9300	C22—H22	0.9300
C8—H8A	0.9700	C23—H23A	0.9700
C8—H8B	0.9700	C23—H23B	0.9700
C8—C9	1.520 (2)	C23—C24	1.498 (4)
C9—H9A	0.9700	C24—H24A	0.9700
C9—H9B	0.9700	C24—H24B	0.9700
C9—C10	1.510 (2)	C24—C25	1.514 (3)
C10—C11	1.384 (3)	C25—C26	1.396 (3)
C10—C15	1.381 (2)	C25—C30	1.346 (3)
C11—H11	0.9300	C26—H26	0.9300
C11—C12	1.375 (3)	C26—C27	1.473 (4)
C12—H12	0.9300	C27—H27	0.9300

C12—C13	1.381 (3)	C27—C28	1.337 (4)
C13—H13	0.9300	C28—H28	0.9300
C13—C14	1.354 (3)	C28—C29	1.304 (4)
C14—H14	0.9300	C29—H29	0.9300
C14—C15	1.382 (3)	C29—C30	1.346 (3)
C15—H15	0.9300	C30—H30	0.9300
C7—O1—H1	114.6 (18)	C16—O3—H3A	109.5
C4—N1—H1A	117.5	C20—N2—H2A	117.8
C4—N1—C8	125.08 (15)	C20—N2—C23	124.32 (18)
C8—N1—H1A	117.5	C23—N2—H2A	117.8
C2—C1—C7	123.29 (16)	O3—C16—C17	116.54 (16)
C6—C1—C2	118.06 (16)	O4—C16—O3	122.73 (17)
C6—C1—C7	118.65 (16)	O4—C16—C17	120.73 (16)
C1—C2—H2	119.3	C18—C17—C16	119.79 (16)
C3—C2—C1	121.34 (16)	C18—C17—C22	117.64 (16)
C3—C2—H2	119.3	C22—C17—C16	122.56 (16)
C2—C3—H3	119.9	C17—C18—H18	119.3
C2—C3—C4	120.23 (16)	C19—C18—C17	121.49 (17)
C4—C3—H3	119.9	C19—C18—H18	119.3
N1—C4—C3	123.51 (16)	C18—C19—H19	119.7
N1—C4—C5	118.33 (16)	C18—C19—C20	120.67 (17)
C5—C4—C3	118.14 (16)	C20—C19—H19	119.7
C4—C5—H5	119.6	N2—C20—C19	118.91 (17)
C6—C5—C4	120.78 (17)	N2—C20—C21	122.79 (17)
C6—C5—H5	119.6	C21—C20—C19	118.30 (17)
C1—C6—H6	119.3	C20—C21—H21	119.9
C5—C6—C1	121.43 (17)	C22—C21—C20	120.20 (17)
C5—C6—H6	119.3	C22—C21—H21	119.9
O1—C7—C1	117.37 (16)	C17—C22—H22	119.2
O2—C7—O1	122.76 (17)	C21—C22—C17	121.67 (17)
O2—C7—C1	119.88 (16)	C21—C22—H22	119.2
N1—C8—H8A	110.0	N2—C23—H23A	109.0
N1—C8—H8B	110.0	N2—C23—H23B	109.0
N1—C8—C9	108.58 (15)	N2—C23—C24	112.8 (2)
H8A—C8—H8B	108.4	H23A—C23—H23B	107.8
C9—C8—H8A	110.0	C24—C23—H23A	109.0
C9—C8—H8B	110.0	C24—C23—H23B	109.0
C8—C9—H9A	108.6	C23—C24—H24A	108.1
C8—C9—H9B	108.6	C23—C24—H24B	108.1
H9A—C9—H9B	107.6	C23—C24—C25	116.8 (2)
C10—C9—C8	114.73 (14)	H24A—C24—H24B	107.3
C10—C9—H9A	108.6	C25—C24—H24A	108.1
C10—C9—H9B	108.6	C25—C24—H24B	108.1
C11—C10—C9	120.06 (16)	C26—C25—C24	118.9 (2)
C15—C10—C9	121.85 (17)	C30—C25—C24	123.5 (2)
C15—C10—C11	117.99 (17)	C30—C25—C26	117.5 (2)
C10—C11—H11	119.6	C25—C26—H26	121.0

C12—C11—C10	120.79 (19)	C25—C26—C27	118.0 (2)
C12—C11—H11	119.6	C27—C26—H26	121.0
C11—C12—H12	119.9	C26—C27—H27	120.8
C11—C12—C13	120.1 (2)	C28—C27—C26	118.3 (2)
C13—C12—H12	119.9	C28—C27—H27	120.8
C12—C13—H13	120.1	C27—C28—H28	119.3
C14—C13—C12	119.75 (19)	C29—C28—C27	121.5 (3)
C14—C13—H13	120.1	C29—C28—H28	119.3
C13—C14—H14	119.9	C28—C29—H29	119.1
C13—C14—C15	120.25 (19)	C28—C29—C30	121.8 (3)
C15—C14—H14	119.9	C30—C29—H29	119.1
C10—C15—C14	121.07 (19)	C25—C30—H30	118.6
C10—C15—H15	119.5	C29—C30—C25	122.8 (2)
C14—C15—H15	119.5	C29—C30—H30	118.6
N1—C4—C5—C6	179.70 (18)	O3—C16—C17—C18	-178.77 (17)
N1—C8—C9—C10	166.11 (15)	O3—C16—C17—C22	2.1 (3)
C1—C2—C3—C4	-0.6 (3)	O4—C16—C17—C18	1.2 (3)
C2—C1—C6—C5	-0.7 (3)	O4—C16—C17—C22	-177.96 (18)
C2—C1—C7—O1	-7.6 (3)	N2—C20—C21—C22	-179.35 (18)
C2—C1—C7—O2	172.46 (17)	N2—C23—C24—C25	-59.3 (4)
C2—C3—C4—N1	-179.11 (16)	C16—C17—C18—C19	-178.47 (18)
C2—C3—C4—C5	-0.6 (3)	C16—C17—C22—C21	177.95 (17)
C3—C4—C5—C6	1.2 (3)	C17—C18—C19—C20	0.7 (3)
C4—N1—C8—C9	-171.47 (17)	C18—C17—C22—C21	-1.2 (3)
C4—C5—C6—C1	-0.5 (3)	C18—C19—C20—N2	178.84 (19)
C6—C1—C2—C3	1.2 (3)	C18—C19—C20—C21	-1.6 (3)
C6—C1—C7—O1	172.14 (16)	C19—C20—C21—C22	1.1 (3)
C6—C1—C7—O2	-7.8 (3)	C20—N2—C23—C24	-174.9 (2)
C7—C1—C2—C3	-179.02 (15)	C20—C21—C22—C17	0.3 (3)
C7—C1—C6—C5	179.53 (18)	C22—C17—C18—C19	0.7 (3)
C8—N1—C4—C3	-16.3 (3)	C23—N2—C20—C19	-170.4 (2)
C8—N1—C4—C5	165.28 (18)	C23—N2—C20—C21	10.0 (3)
C8—C9—C10—C11	-71.6 (2)	C23—C24—C25—C26	134.2 (3)
C8—C9—C10—C15	112.22 (19)	C23—C24—C25—C30	-49.0 (4)
C9—C10—C11—C12	-175.79 (17)	C24—C25—C26—C27	175.8 (2)
C9—C10—C15—C14	176.03 (17)	C24—C25—C30—C29	-175.8 (2)
C10—C11—C12—C13	-0.3 (3)	C25—C26—C27—C28	0.5 (3)
C11—C10—C15—C14	-0.3 (3)	C26—C25—C30—C29	1.1 (3)
C11—C12—C13—C14	-0.3 (3)	C26—C27—C28—C29	0.5 (4)
C12—C13—C14—C15	0.6 (3)	C27—C28—C29—C30	-0.7 (4)
C13—C14—C15—C10	-0.3 (3)	C28—C29—C30—C25	-0.1 (4)
C15—C10—C11—C12	0.6 (3)	C30—C25—C26—C27	-1.2 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1...O4	1.05 (4)	1.58 (4)	2.6380 (19)	177 (3)

O3—H3A...O2	0.82	1.81	2.6246 (18)	175
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