

# Diisopropyl 2-[(4-nitrobenzoyl)amino]propane-dioate

Cristi P. Deleon,<sup>a</sup> Anthony D. Ramirez,<sup>a</sup> Diana Gonzalez,<sup>a</sup> Arghya Ghosh,<sup>b</sup> László Kürti<sup>b</sup> and Muhammed Yousufuddin<sup>a\*</sup>

<sup>a</sup>University of North Texas at Dallas, 7400 University Hills Blvd., Dallas, TX 75241, USA, and <sup>b</sup>Rice University, 7400 University Hills Blvd., Houston, TX 77030, USA. \*Correspondence e-mail: muhammed.yousufuddin@untDallas.edu

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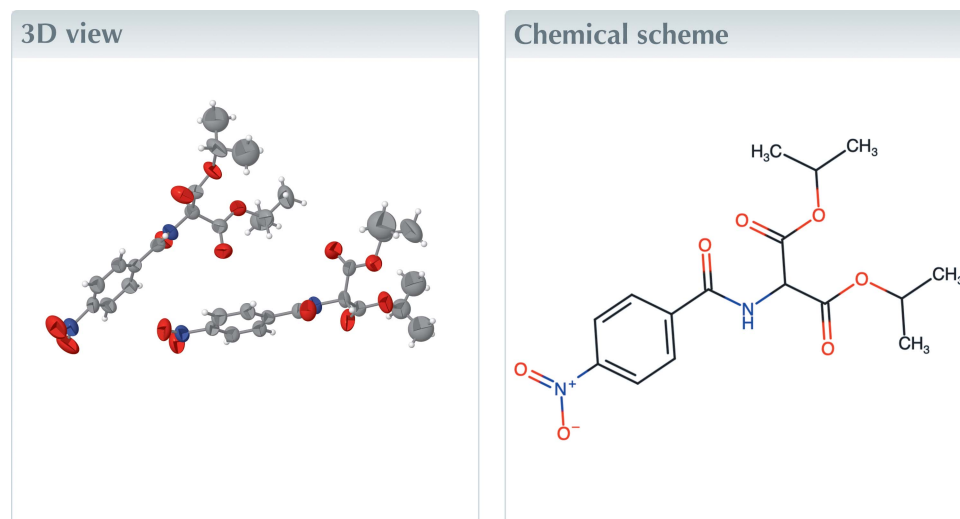
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Structural data: full structural data are available from iucrdata.iucr.org

The title compound, C<sub>16</sub>H<sub>20</sub>N<sub>2</sub>O<sub>7</sub>, crystallizes in the space group *C*2 with two molecules in the asymmetric unit. The crystal packing shows O···π interactions between the two molecules.

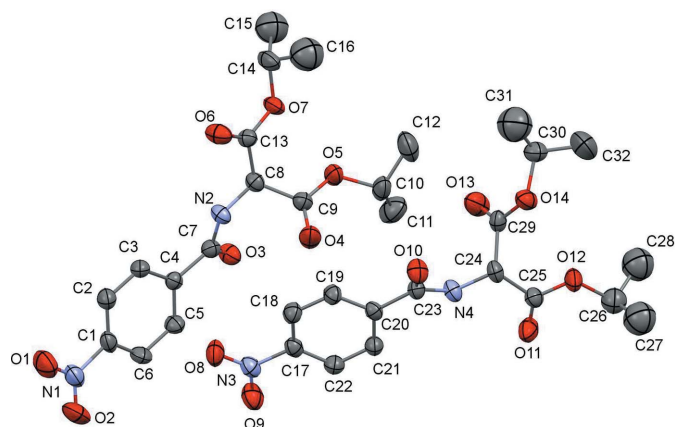


## Structure description

The title compound [alternative name: diisopropyl 2-(4-nitrobenzamido)malonate] was made in an attempt to make a compound with an N<sub>3</sub> cyclic ring. The starting material for this compound has been used previously to make symmetrical and unsymmetrical secondary amines (Kattamuri *et al.*, 2017). The title compound crystallizes in the monoclinic space group *C*2 with two molecules in the asymmetric unit (*Z* = 8). Molecule *A* contains nitro group N1–O1–O2, and molecule *B* contains nitro group N3–O8–O9 (Fig. 1). Both nitro groups are almost coplanar with their attached phenyl rings [dihedral angles = 3.7 (11)° for molecule *A* and 3.3 (8)° for molecule *B*]. An overlay of the two molecules indicates an almost complete overlap with only slight deviations in the ester groups (r.m.s. deviation = 0.268 Å; Fig. 2). The dihedral angle between the phenyl rings is 38.0 (3)°. The closest interactions in the packing are observed between the two molecules in the asymmetric unit (Fig. 3): an N3–O8···π interaction [O8···Cg1 = 3.272 (6) Å, Cg1 is the centroid of the C1–C6 ring] and a C9=O4···π interaction [O4···Cg2 = 3.552 (7) Å, Cg2 is the centroid of the C17–C22 ring].

## Synthesis and crystallization

In an oven-dried Schlenk reaction vessel, diisopropyl 2-[(tosyloxy)imino]malonate (185.7 mg, 0.5 mmol, 1.0 equiv.) was dissolved in anhydrous THF (5 ml) under Ar and cooled to 273 K on an ice bath. To the cooled solution, Et<sub>3</sub>N (1.0 mmol, 2.0 equiv.) and



**Figure 1**  
Molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. Hydrogen atoms are omitted for clarity.

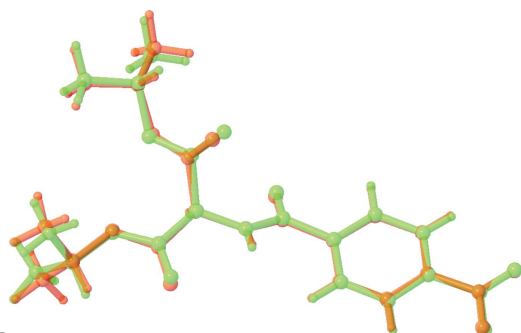
hydrazine (0.5 mmol, 1.0 equiv.) were added. The reaction mixture was allowed to stir at 273 K for 2 h. After full conversion as indicated by TLC, Et<sub>3</sub>N (1.0 mmol, 2.0 equiv.) and 4-nitrobenzoyl chloride (92.8 mg, 0.5 mmol, 1.0 equiv.) were added to the reaction mixture. After stirring the reaction mixture for 3 h at 273 K, a saturated NaHCO<sub>3</sub> solution was added and the mixture was extracted with diethyl ether. The combined organic fractions were concentrated *in vacuo*. The crude product was purified using silica gel flash column chromatography to afford the title compound (90.0 mg, 51% yield). Crystals were obtained by dissolving the compound in a minimum amount of CH<sub>2</sub>Cl<sub>2</sub> and layering with hexane at 295 K.

### Refinement

Crystal data, data collection and structure refinement are summarized in Table 1.

### Acknowledgements

The authors thank the Center for Nanostructured Materials at the University of Texas at Arlington for the use of their diffractometer. Support for this work was provided by the University of North Texas at Dallas.



**Figure 2**  
Overlay plot of the two molecules in the asymmetric unit. Molecule A is shown in green, molecule B in red.

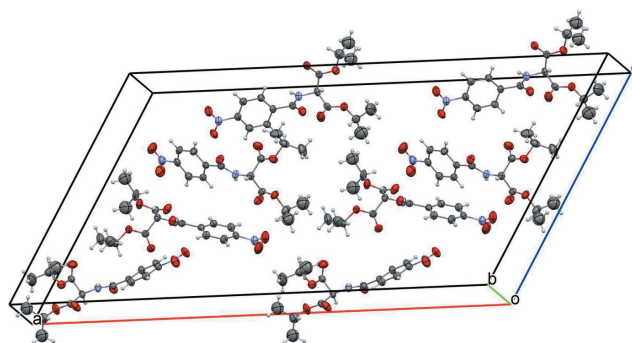
**Table 1**  
Experimental details.

<b>Crystal data</b>	
Chemical formula	C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>7</sub>
<i>M<sub>r</sub></i>	352.34
Crystal system, space group	Monoclinic, C2
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	38.408 (10), 5.1523 (13), 19.752 (5)
β (°)	115.341 (4)
<i>V</i> (Å <sup>3</sup> )	3532.7 (15)
<i>Z</i>	8
Radiation type	Mo Kα
μ (mm <sup>-1</sup> )	0.11
Crystal size (mm)	0.50 × 0.08 × 0.05
<b>Data collection</b>	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Krause <i>et al.</i> , 2015)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.534, 0.745
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	18724, 8693, 3977
<i>R<sub>int</sub></i>	0.062
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.668
<b>Refinement</b>	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.081, 0.276, 1.00
No. of reflections	8693
No. of parameters	459
No. of restraints	52
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.49, -0.34
Absolute structure	Flack <i>x</i> determined using 1214 quotients [( <i>I</i> <sup>+</sup> ) - ( <i>I</i> <sup>-</sup> )] / [( <i>I</i> <sup>+</sup> ) + ( <i>I</i> <sup>-</sup> )] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.6 (10)

Computer programs: APEX2 and SAINT (Bruker, 2016), SHELXT2014/4 (Sheldrick, 2015a), 4SHELXL2018/43 (Sheldrick, 2015b), and SHELXTL (Sheldrick, 2008).

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**Figure 3**  
Packing diagram for the title compound.

## full crystallographic data

*IUCrData* (2023). **8**, x230104 [<https://doi.org/10.1107/S2414314623001049>]

## Diisopropyl 2-[(4-nitrobenzoyl)amino]propanedioate

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## Diisopropyl 2-[(4-nitrobenzoyl)amino]propanedioate

*Crystal data*

$C_{16}H_{20}N_2O_7$

$M_r = 352.34$

Monoclinic,  $C2$

$a = 38.408$  (10) Å

$b = 5.1523$  (13) Å

$c = 19.752$  (5) Å

$\beta = 115.341$  (4)°

$V = 3532.7$  (15) Å<sup>3</sup>

$Z = 8$

$F(000) = 1488$

$D_x = 1.325$  Mg m<sup>-3</sup>

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

Cell parameters from 2123 reflections

$\theta = 2.3$ – $19.0$ °

$\mu = 0.11$  mm<sup>-1</sup>

$T = 296$  K

Needle, colourless

$0.50 \times 0.08 \times 0.05$  mm

*Data collection*

Bruker APEXII CCD

diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.534$ ,  $T_{\max} = 0.745$

18724 measured reflections

8693 independent reflections

3977 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.062$

$\theta_{\max} = 28.4$ °,  $\theta_{\min} = 2.0$ °

$h = -50 \rightarrow 50$

$k = -6 \rightarrow 6$

$l = -26 \rightarrow 26$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.081$

$wR(F^2) = 0.276$

$S = 1.00$

8693 reflections

459 parameters

52 restraints

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1417P)^2]$

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

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

$\Delta\rho_{\max} = 0.49$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.34$  e Å<sup>-3</sup>

Absolute structure: Flack  $x$  determined using

1214 quotients  $[(F^-)-(F)]/[(F^+)+(F)]$  (Parsons *et al.*, 2013)

Absolute structure parameter: 0.6 (10)

*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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.88102 (19)	0.2244 (16)	0.6329 (5)	0.118 (2)
O2	0.90133 (17)	0.5358 (18)	0.7072 (4)	0.128 (3)
O3	0.71544 (12)	0.9400 (9)	0.6084 (3)	0.0712 (13)
O4	0.67465 (15)	0.5799 (14)	0.6930 (3)	0.0944 (19)
O5	0.61676 (14)	0.7265 (11)	0.6190 (3)	0.0753 (14)
O6	0.63941 (14)	0.2095 (10)	0.4886 (3)	0.0837 (16)
O7	0.59253 (12)	0.4686 (11)	0.4841 (3)	0.0795 (15)
N1	0.87565 (19)	0.4161 (17)	0.6630 (4)	0.0811 (18)
N2	0.69438 (14)	0.5333 (10)	0.5764 (3)	0.0555 (13)
H2N2	0.700003	0.375915	0.570495	0.067*
C1	0.83549 (19)	0.4910 (16)	0.6442 (4)	0.0641 (18)
C2	0.8060 (2)	0.3469 (16)	0.5940 (4)	0.0681 (18)
H2	0.810805	0.206553	0.569638	0.082*
C3	0.76912 (18)	0.4137 (14)	0.5804 (3)	0.0577 (16)
H3	0.748686	0.313843	0.547615	0.069*
C4	0.76178 (16)	0.6251 (12)	0.6142 (3)	0.0500 (14)
C5	0.79215 (18)	0.7752 (13)	0.6635 (4)	0.0599 (16)
H5	0.787483	0.920965	0.686133	0.072*
C6	0.82960 (18)	0.7034 (15)	0.6783 (4)	0.0682 (19)
H6	0.850388	0.800012	0.711361	0.082*
C7	0.72186 (18)	0.7100 (13)	0.6000 (3)	0.0551 (15)
C8	0.65570 (17)	0.5975 (12)	0.5606 (4)	0.0555 (15)
H8	0.649966	0.764484	0.534248	0.067*
C9	0.65032 (19)	0.6329 (14)	0.6321 (4)	0.0604 (16)
C10	0.6067 (3)	0.7816 (19)	0.6811 (4)	0.086 (3)
H10	0.622571	0.675836	0.724629	0.103*
C11	0.6145 (3)	1.065 (2)	0.6998 (6)	0.122 (4)
H11A	0.641204	1.100776	0.713532	0.182*
H11B	0.608425	1.107266	0.740821	0.182*
H11C	0.598852	1.167367	0.656892	0.182*
C12	0.5657 (3)	0.712 (2)	0.6551 (7)	0.120 (4)
H12A	0.550242	0.819530	0.613445	0.181*
H12B	0.558195	0.736768	0.695147	0.181*
H12C	0.562101	0.532895	0.639884	0.181*
C13	0.62848 (17)	0.3987 (13)	0.5080 (3)	0.0539 (15)
C14	0.5632 (2)	0.3031 (18)	0.4300 (5)	0.089 (3)
H14	0.574593	0.184705	0.406273	0.107*
C15	0.5350 (4)	0.490 (3)	0.3721 (8)	0.156 (5)
H15A	0.518994	0.570858	0.392476	0.235*
H15B	0.519074	0.395818	0.327625	0.235*
H15C	0.549129	0.621206	0.359918	0.235*
C16	0.5450 (4)	0.157 (4)	0.4700 (9)	0.172 (6)
H16A	0.564320	0.061675	0.510334	0.258*
H16B	0.526439	0.038554	0.436017	0.258*
H16C	0.532346	0.275346	0.489680	0.258*

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O8	0.80326 (17)	0.2861 (12)	0.7820 (3)	0.0891 (17)
O9	0.81622 (17)	0.6196 (13)	0.8529 (4)	0.0951 (18)
O10	0.66470 (15)	-0.0673 (10)	0.8979 (3)	0.0747 (13)
O11	0.65449 (17)	0.6482 (13)	1.0333 (3)	0.0934 (18)
O12	0.60149 (14)	0.4539 (13)	1.0243 (3)	0.0924 (18)
O13	0.58449 (16)	0.4185 (15)	0.8261 (3)	0.103 (2)
O14	0.56464 (13)	0.1570 (11)	0.8898 (3)	0.0754 (14)
N3	0.79752 (15)	0.4276 (13)	0.8251 (3)	0.0664 (15)
N4	0.65984 (14)	0.3465 (11)	0.9276 (3)	0.0595 (14)
H4N4	0.668115	0.503086	0.930582	0.071*
C17	0.76625 (18)	0.3554 (13)	0.8470 (4)	0.0572 (16)
C18	0.7437 (2)	0.1486 (14)	0.8140 (4)	0.0645 (17)
H18	0.747804	0.051632	0.778358	0.077*
C19	0.71472 (18)	0.0839 (13)	0.8336 (4)	0.0585 (16)
H19	0.699443	-0.060793	0.812472	0.070*
C20	0.70813 (17)	0.2356 (12)	0.8855 (3)	0.0507 (14)
C21	0.73146 (18)	0.4425 (14)	0.9176 (4)	0.0594 (16)
H21	0.727253	0.542696	0.952543	0.071*
C22	0.76095 (19)	0.5053 (15)	0.8993 (4)	0.0639 (17)
H22	0.776969	0.645826	0.921640	0.077*
C23	0.67578 (17)	0.1561 (13)	0.9041 (3)	0.0532 (15)
C24	0.62899 (17)	0.2893 (13)	0.9479 (4)	0.0575 (16)
H24	0.632877	0.115292	0.969983	0.069*
C25	0.63007 (19)	0.4888 (14)	1.0067 (4)	0.0604 (16)
C26	0.5982 (3)	0.642 (2)	1.0786 (5)	0.101 (3)
H26	0.618275	0.775429	1.092635	0.121*
C27	0.6031 (4)	0.483 (4)	1.1412 (8)	0.166 (5)
H27A	0.583457	0.351385	1.125663	0.249*
H27B	0.601108	0.587697	1.179561	0.249*
H27C	0.627983	0.401613	1.160547	0.249*
C28	0.5600 (4)	0.757 (3)	1.0432 (9)	0.163 (5)
H28A	0.541281	0.622836	1.019716	0.245*
H28B	0.559144	0.880016	1.006063	0.245*
H28C	0.554309	0.842906	1.080354	0.245*
C29	0.5902 (2)	0.2985 (14)	0.8801 (4)	0.0601 (16)
C30	0.5250 (2)	0.1611 (18)	0.8325 (4)	0.080 (2)
H30	0.522370	0.300077	0.796814	0.096*
C31	0.5161 (5)	-0.083 (4)	0.7929 (10)	0.184 (6)
H31A	0.515314	-0.218117	0.825734	0.277*
H31B	0.535656	-0.122663	0.776323	0.277*
H31C	0.491564	-0.071294	0.750378	0.277*
C32	0.5000 (3)	0.216 (5)	0.8673 (8)	0.185 (8)
H32A	0.473706	0.210829	0.830379	0.277*
H32B	0.505665	0.386042	0.889470	0.277*
H32C	0.503806	0.089532	0.905427	0.277*

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*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.083 (4)	0.128 (6)	0.150 (6)	0.017 (4)	0.058 (4)	-0.019 (5)
O2	0.050 (3)	0.177 (8)	0.134 (6)	0.000 (4)	0.019 (4)	-0.021 (6)
O3	0.059 (3)	0.056 (3)	0.094 (3)	0.000 (2)	0.029 (2)	-0.010 (3)
O4	0.073 (3)	0.142 (6)	0.064 (3)	0.034 (4)	0.025 (3)	0.015 (3)
O5	0.063 (3)	0.101 (4)	0.063 (3)	0.023 (3)	0.028 (2)	0.000 (3)
O6	0.063 (3)	0.064 (3)	0.103 (4)	0.005 (2)	0.015 (3)	-0.014 (3)
O7	0.041 (2)	0.100 (4)	0.090 (3)	-0.005 (3)	0.021 (2)	-0.031 (3)
N1	0.058 (4)	0.105 (6)	0.087 (4)	0.008 (4)	0.038 (4)	0.009 (4)
N2	0.045 (3)	0.047 (3)	0.074 (3)	-0.002 (2)	0.024 (3)	-0.001 (2)
C1	0.054 (4)	0.084 (5)	0.065 (4)	0.007 (4)	0.036 (3)	0.011 (4)
C2	0.064 (4)	0.075 (4)	0.072 (4)	-0.001 (4)	0.036 (4)	-0.008 (4)
C3	0.051 (3)	0.067 (4)	0.054 (3)	-0.007 (3)	0.021 (3)	-0.009 (3)
C4	0.050 (3)	0.053 (3)	0.047 (3)	-0.001 (3)	0.021 (3)	0.006 (3)
C5	0.056 (4)	0.056 (4)	0.065 (4)	-0.005 (3)	0.023 (3)	-0.012 (3)
C6	0.044 (4)	0.080 (5)	0.073 (4)	-0.014 (3)	0.018 (3)	-0.011 (4)
C7	0.055 (4)	0.057 (4)	0.049 (3)	-0.003 (3)	0.019 (3)	0.000 (3)
C8	0.053 (4)	0.051 (4)	0.063 (4)	0.004 (3)	0.025 (3)	0.002 (3)
C9	0.054 (4)	0.066 (4)	0.057 (4)	0.004 (3)	0.020 (3)	0.000 (3)
C10	0.083 (6)	0.116 (7)	0.067 (5)	0.034 (5)	0.039 (4)	-0.001 (5)
C11	0.136 (9)	0.121 (9)	0.097 (7)	0.020 (7)	0.039 (7)	-0.030 (7)
C12	0.096 (7)	0.151 (10)	0.145 (9)	0.020 (7)	0.081 (7)	0.011 (8)
C13	0.050 (4)	0.053 (4)	0.053 (3)	0.002 (3)	0.017 (3)	-0.002 (3)
C14	0.047 (4)	0.104 (6)	0.107 (6)	0.010 (4)	0.023 (4)	-0.036 (5)
C15	0.154 (5)	0.156 (5)	0.153 (5)	-0.004 (3)	0.060 (3)	0.004 (3)
C16	0.171 (6)	0.172 (6)	0.171 (6)	-0.009 (3)	0.071 (3)	0.002 (3)
O8	0.101 (4)	0.101 (4)	0.094 (4)	-0.011 (3)	0.070 (3)	-0.013 (3)
O9	0.094 (4)	0.094 (4)	0.120 (5)	-0.019 (4)	0.068 (4)	-0.005 (4)
O10	0.088 (3)	0.056 (3)	0.095 (3)	-0.010 (3)	0.054 (3)	-0.003 (3)
O11	0.102 (4)	0.113 (4)	0.090 (4)	-0.045 (4)	0.064 (3)	-0.032 (3)
O12	0.076 (3)	0.124 (5)	0.098 (4)	-0.021 (3)	0.057 (3)	-0.046 (4)
O13	0.082 (4)	0.141 (6)	0.083 (4)	-0.008 (4)	0.034 (3)	0.038 (4)
O14	0.060 (3)	0.092 (4)	0.072 (3)	-0.013 (3)	0.026 (3)	0.006 (3)
N3	0.057 (3)	0.071 (4)	0.077 (4)	-0.004 (3)	0.034 (3)	0.007 (3)
N4	0.055 (3)	0.052 (3)	0.081 (4)	0.000 (2)	0.038 (3)	0.003 (3)
C17	0.051 (3)	0.064 (4)	0.059 (4)	0.003 (3)	0.026 (3)	0.012 (3)
C18	0.072 (4)	0.064 (4)	0.065 (4)	-0.001 (4)	0.036 (3)	-0.009 (3)
C19	0.058 (4)	0.056 (4)	0.066 (4)	0.000 (3)	0.031 (3)	-0.010 (3)
C20	0.046 (3)	0.050 (3)	0.057 (3)	0.005 (3)	0.023 (3)	0.006 (3)
C21	0.058 (4)	0.064 (4)	0.062 (4)	-0.004 (3)	0.031 (3)	-0.008 (3)
C22	0.059 (4)	0.069 (4)	0.064 (4)	-0.008 (3)	0.026 (3)	-0.008 (3)
C23	0.055 (4)	0.052 (4)	0.057 (4)	0.000 (3)	0.029 (3)	0.002 (3)
C24	0.055 (4)	0.062 (4)	0.071 (4)	0.004 (3)	0.041 (3)	0.006 (3)
C25	0.057 (4)	0.068 (4)	0.061 (4)	-0.008 (4)	0.029 (3)	0.002 (3)
C26	0.101 (3)	0.104 (3)	0.101 (3)	-0.0013 (14)	0.0461 (17)	-0.0033 (14)
C27	0.169 (5)	0.166 (5)	0.162 (5)	0.011 (3)	0.070 (3)	-0.003 (3)

C28	0.164 (5)	0.164 (5)	0.162 (5)	0.009 (3)	0.071 (3)	-0.002 (3)
C29	0.067 (4)	0.067 (4)	0.058 (4)	0.006 (3)	0.038 (3)	0.007 (3)
C30	0.066 (5)	0.088 (5)	0.074 (5)	-0.007 (4)	0.020 (4)	-0.009 (4)
C31	0.182 (6)	0.182 (7)	0.185 (7)	0.003 (3)	0.075 (4)	-0.005 (3)
C32	0.087 (7)	0.32 (2)	0.153 (11)	0.015 (11)	0.056 (8)	-0.026 (15)

*Geometric parameters (Å, °)*

O1—N1	1.216 (10)	O8—N3	1.210 (7)
O2—N1	1.174 (9)	O9—N3	1.207 (8)
O3—C7	1.236 (8)	O10—C23	1.215 (8)
O4—C9	1.197 (7)	O11—C25	1.186 (8)
O5—C9	1.294 (8)	O12—C25	1.297 (8)
O5—C10	1.463 (9)	O12—C26	1.491 (11)
O6—C13	1.188 (8)	O13—C29	1.170 (8)
O7—C13	1.304 (8)	O14—C29	1.299 (8)
O7—C14	1.452 (9)	O14—C30	1.459 (9)
N1—C1	1.475 (9)	N3—C17	1.488 (8)
N2—C7	1.318 (8)	N4—C23	1.340 (8)
N2—C8	1.420 (7)	N4—C24	1.434 (7)
N2—H2N2	0.8600	N4—H4N4	0.8600
C1—C6	1.354 (10)	C17—C18	1.353 (10)
C1—C2	1.363 (10)	C17—C22	1.373 (9)
C2—C3	1.368 (9)	C18—C19	1.367 (9)
C2—H2	0.9300	C18—H18	0.9300
C3—C4	1.368 (9)	C19—C20	1.395 (8)
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.391 (8)	C20—C21	1.362 (9)
C4—C7	1.501 (9)	C20—C23	1.496 (8)
C5—C6	1.389 (9)	C21—C22	1.367 (9)
C5—H5	0.9300	C21—H21	0.9300
C6—H6	0.9300	C22—H22	0.9300
C8—C13	1.514 (9)	C24—C29	1.520 (9)
C8—C9	1.525 (9)	C24—C25	1.538 (10)
C8—H8	0.9800	C24—H24	0.9800
C10—C12	1.475 (13)	C26—C27	1.430 (17)
C10—C11	1.504 (15)	C26—C28	1.454 (16)
C10—H10	0.9800	C26—H26	0.9800
C11—H11A	0.9600	C27—H27A	0.9600
C11—H11B	0.9600	C27—H27B	0.9600
C11—H11C	0.9600	C27—H27C	0.9600
C12—H12A	0.9600	C28—H28A	0.9600
C12—H12B	0.9600	C28—H28B	0.9600
C12—H12C	0.9600	C28—H28C	0.9600
C14—C16	1.465 (16)	C30—C32	1.427 (13)
C14—C15	1.534 (17)	C30—C31	1.44 (2)
C14—H14	0.9800	C30—H30	0.9800
C15—H15A	0.9600	C31—H31A	0.9600

C15—H15B	0.9600	C31—H31B	0.9600
C15—H15C	0.9600	C31—H31C	0.9600
C16—H16A	0.9600	C32—H32A	0.9600
C16—H16B	0.9600	C32—H32B	0.9600
C16—H16C	0.9600	C32—H32C	0.9600
C9—O5—C10	120.1 (5)	C25—O12—C26	116.4 (7)
C13—O7—C14	118.2 (6)	C29—O14—C30	118.8 (6)
O2—N1—O1	121.8 (8)	O9—N3—O8	124.2 (6)
O2—N1—C1	120.3 (8)	O9—N3—C17	118.0 (6)
O1—N1—C1	117.9 (8)	O8—N3—C17	117.8 (6)
C7—N2—C8	121.4 (5)	C23—N4—C24	120.1 (6)
C7—N2—H2N2	119.3	C23—N4—H4N4	120.0
C8—N2—H2N2	119.3	C24—N4—H4N4	120.0
C6—C1—C2	122.6 (6)	C18—C17—C22	122.4 (6)
C6—C1—N1	117.7 (7)	C18—C17—N3	119.1 (6)
C2—C1—N1	119.6 (7)	C22—C17—N3	118.5 (6)
C1—C2—C3	118.3 (7)	C17—C18—C19	119.1 (6)
C1—C2—H2	120.8	C17—C18—H18	120.5
C3—C2—H2	120.8	C19—C18—H18	120.5
C2—C3—C4	121.1 (6)	C18—C19—C20	119.8 (6)
C2—C3—H3	119.4	C18—C19—H19	120.1
C4—C3—H3	119.4	C20—C19—H19	120.1
C3—C4—C5	119.9 (6)	C21—C20—C19	119.3 (6)
C3—C4—C7	123.2 (6)	C21—C20—C23	123.4 (5)
C5—C4—C7	116.9 (6)	C19—C20—C23	117.3 (6)
C6—C5—C4	118.8 (6)	C20—C21—C22	121.1 (6)
C6—C5—H5	120.6	C20—C21—H21	119.4
C4—C5—H5	120.6	C22—C21—H21	119.4
C1—C6—C5	119.2 (6)	C21—C22—C17	118.2 (6)
C1—C6—H6	120.4	C21—C22—H22	120.9
C5—C6—H6	120.4	C17—C22—H22	120.9
O3—C7—N2	122.3 (6)	O10—C23—N4	122.4 (6)
O3—C7—C4	120.0 (6)	O10—C23—C20	121.8 (6)
N2—C7—C4	117.7 (6)	N4—C23—C20	115.8 (6)
N2—C8—C13	110.1 (5)	N4—C24—C29	111.4 (5)
N2—C8—C9	111.6 (5)	N4—C24—C25	108.4 (5)
C13—C8—C9	112.9 (5)	C29—C24—C25	110.1 (5)
N2—C8—H8	107.3	N4—C24—H24	109.0
C13—C8—H8	107.3	C29—C24—H24	109.0
C9—C8—H8	107.3	C25—C24—H24	109.0
O4—C9—O5	124.7 (6)	O11—C25—O12	125.2 (7)
O4—C9—C8	123.2 (6)	O11—C25—C24	123.9 (6)
O5—C9—C8	112.1 (5)	O12—C25—C24	110.9 (6)
O5—C10—C12	106.7 (7)	C27—C26—C28	112.4 (11)
O5—C10—C11	107.3 (8)	C27—C26—O12	103.2 (10)
C12—C10—C11	113.2 (9)	C28—C26—O12	107.3 (9)
O5—C10—H10	109.9	C27—C26—H26	111.2



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C12—C10—H10	109.9	C28—C26—H26	111.2
C11—C10—H10	109.9	O12—C26—H26	111.2
C10—C11—H11A	109.5	C26—C27—H27A	109.5
C10—C11—H11B	109.5	C26—C27—H27B	109.5
H11A—C11—H11B	109.5	H27A—C27—H27B	109.5
C10—C11—H11C	109.5	C26—C27—H27C	109.5
H11A—C11—H11C	109.5	H27A—C27—H27C	109.5
H11B—C11—H11C	109.5	H27B—C27—H27C	109.5
C10—C12—H12A	109.5	C26—C28—H28A	109.5
C10—C12—H12B	109.5	C26—C28—H28B	109.5
H12A—C12—H12B	109.5	H28A—C28—H28B	109.5
C10—C12—H12C	109.5	C26—C28—H28C	109.5
H12A—C12—H12C	109.5	H28A—C28—H28C	109.5
H12B—C12—H12C	109.5	H28B—C28—H28C	109.5
O6—C13—O7	125.1 (6)	O13—C29—O14	124.9 (7)
O6—C13—C8	122.7 (6)	O13—C29—C24	123.3 (7)
O7—C13—C8	112.0 (6)	O14—C29—C24	111.8 (5)
O7—C14—C16	107.7 (9)	C32—C30—C31	112.6 (13)
O7—C14—C15	104.9 (9)	C32—C30—O14	108.9 (8)
C16—C14—C15	112.2 (9)	C31—C30—O14	109.4 (9)
O7—C14—H14	110.6	C32—C30—H30	108.6
C16—C14—H14	110.6	C31—C30—H30	108.6
C15—C14—H14	110.6	O14—C30—H30	108.6
C14—C15—H15A	109.5	C30—C31—H31A	109.5
C14—C15—H15B	109.5	C30—C31—H31B	109.5
H15A—C15—H15B	109.5	H31A—C31—H31B	109.5
C14—C15—H15C	109.5	C30—C31—H31C	109.5
H15A—C15—H15C	109.5	H31A—C31—H31C	109.5
H15B—C15—H15C	109.5	H31B—C31—H31C	109.5
C14—C16—H16A	109.5	C30—C32—H32A	109.5
C14—C16—H16B	109.5	C30—C32—H32B	109.5
H16A—C16—H16B	109.5	H32A—C32—H32B	109.5
C14—C16—H16C	109.5	C30—C32—H32C	109.5
H16A—C16—H16C	109.5	H32A—C32—H32C	109.5
H16B—C16—H16C	109.5	H32B—C32—H32C	109.5

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