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## Structure Reports

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## 2,3-Dimethoxybenzaldehyde azine

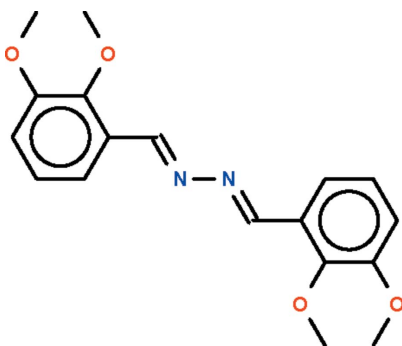
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 Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.046;  $wR$  factor = 0.125; data-to-parameter ratio = 17.2.

There are one-and-a-half independent molecules in the asymmetric unit of the title compound,  $\text{C}_{18}\text{H}_{20}\text{N}_2\text{O}_4$ . One molecule is centrosymmetric with the mid-point of the N—N bond located on a center of inversion. In the other, which lies on a general position, the benzene rings are aligned at  $21.6(1)^\circ$ . Weak intermolecular C—H $\cdots$ O hydrogen bonding is present in the crystal structure.

## Related literature

 For the structure of 2,4-dibenzaldehyde azine, see: Islam *et al.* (2009).


## Experimental

## Crystal data

 $\text{C}_{18}\text{H}_{20}\text{N}_2\text{O}_4$ 
 $M_r = 328.36$ 

 Monoclinic,  $P2_1/n$   
 $a = 8.0294(2)$  Å  
 $b = 17.9415(5)$  Å  
 $c = 17.5258(4)$  Å  
 $\beta = 96.660(2)^\circ$   
 $V = 2507.72(11)$  Å<sup>3</sup>
 $Z = 6$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.30 \times 0.25 \times 0.20$  mm

## Data collection

 Agilent SuperNova Dual diffractometer with an Atlas detector  
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)  
 $T_{\min} = 0.770$ ,  $T_{\max} = 1.000$ 

 12722 measured reflections  
 5600 independent reflections  
 4465 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.029$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.125$   
 $S = 1.03$   
 5600 reflections

 325 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.22$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9B $\cdots$ O3 <sup>i</sup>	0.98	2.45	3.288 (2)	143
C14—H14A $\cdots$ O5 <sup>ii</sup>	0.95	2.37	3.2890 (19)	161
C18—H18C $\cdots$ O6 <sup>ii</sup>	0.98	2.54	3.5229 (19)	178
C27—H27C $\cdots$ O2 <sup>iii</sup>	0.98	2.52	3.2656 (19)	133

 Symmetry codes: (i)  $x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$ ; (ii)  $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (iii)  $x - 2, y, z$ .

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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: *publCIF* (Westrip, 2010).

We thank the Higher Education Commission of Pakistan and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5148).

## References

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## supporting information

*Acta Cryst.* (2011). E67, o531 [doi:10.1107/S1600536811003217]

## 2,3-Dimethoxybenzaldehyde azine

Qamar Ali, Itrat Anis, M. Raza Shah and Seik Weng Ng

### S1. Comment

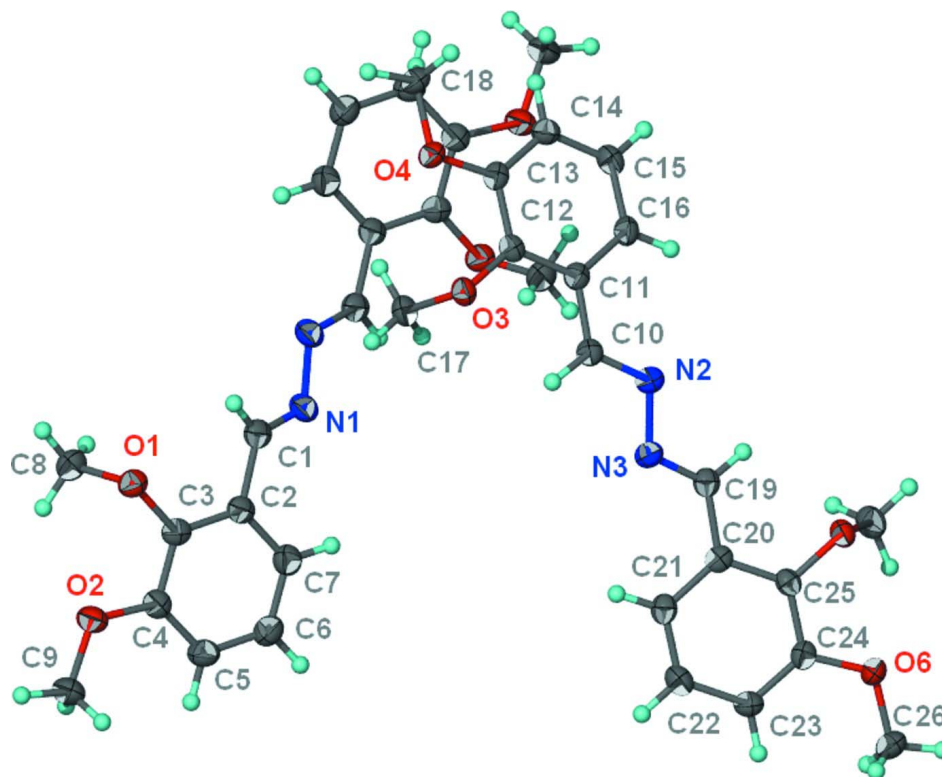
Several methoxy-substituted benzaldehyde azines have been reported, *e.g.*, 2,4-dimethoxybenzaldehyde azine (Islam *et al.*, 2009). The compounds feature a C=N–N=C linkage that allows the two aromatic systems to interact. Such interaction results in a deep yellow coloration. In the reported compound, the rings are nearly co-planar. In the 2,3-dimethoxy analog (Scheme I), the rings are co-planar in the independent molecule lying on a center-of-inversion; in the other molecule, the rings are severely twisted (Fig. 1). Intermolecular weak C—H···O hydrogen bonding is present in the crystal structure (Table 1).

### S2. Experimental

2,3-Dimethoxybenzaldehyde (1 g, 6 mmol) was dissolved in ethanol (15 ml) and to the solution was added hydrazine hydrate (0.3 ml, 6 mmol) followed by 5 drops of acetic acid. The mixture was heated for 3 h; slow evaporation of the solvent gave yellow crystals in 80% yield.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 to 0.98 Å,  $U_{\text{iso}}(\text{H})$  1.2 to 1.5  $U_{\text{eq}}(\text{C})$ ] and were included in the refinement in the riding model approximation.

**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of the two molecules of  $C_{18}H_{20}N_2O_4$  at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

### 2,3-Dimethoxybenzaldehyde azine

#### Crystal data

$C_{18}H_{20}N_2O_4$   
 $M_r = 328.36$   
 Monoclinic,  $P2_1/n$   
 Hall symbol:  $-P\ 2_1/n$   
 $a = 8.0294\ (2)\ \text{\AA}$   
 $b = 17.9415\ (5)\ \text{\AA}$   
 $c = 17.5258\ (4)\ \text{\AA}$   
 $\beta = 96.660\ (2)^\circ$   
 $V = 2507.72\ (11)\ \text{\AA}^3$   
 $Z = 6$

$F(000) = 1044$   
 $D_x = 1.305\ \text{Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$   
 Cell parameters from 5647 reflections  
 $\theta = 2.3\text{--}29.3^\circ$   
 $\mu = 0.09\ \text{mm}^{-1}$   
 $T = 100\ \text{K}$   
 Prism, yellow  
 $0.30 \times 0.25 \times 0.20\ \text{mm}$

#### Data collection

Agilent SuperNova Dual  
 diffractometer with an Atlas detector  
 Radiation source: SuperNova (Mo) X-ray  
 Source  
 Mirror monochromator  
 Detector resolution:  $10.4041\ \text{pixels mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (*CrysAlis PRO*; Agilent, 2010)

$T_{\min} = 0.770$ ,  $T_{\max} = 1.000$   
 12722 measured reflections  
 5600 independent reflections  
 4465 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.029$   
 $\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 2.3^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -18 \rightarrow 22$   
 $l = -15 \rightarrow 22$

Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.125$

$S = 1.03$

5600 reflections

325 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 1.0146P]$

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

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

$\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$

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	1.44670 (14)	0.12618 (6)	0.46827 (6)	0.0233 (3)
O2	1.51150 (15)	0.22434 (7)	0.36049 (6)	0.0274 (3)
O3	0.80577 (13)	0.08624 (6)	0.73656 (6)	0.0206 (2)
O4	0.88407 (14)	-0.04039 (6)	0.81165 (6)	0.0229 (3)
O5	-0.14383 (13)	0.28732 (6)	0.56994 (6)	0.0207 (3)
O6	-0.24191 (14)	0.39718 (7)	0.47148 (6)	0.0270 (3)
N1	0.99742 (18)	0.02682 (8)	0.47015 (7)	0.0244 (3)
N2	0.33013 (17)	0.14903 (8)	0.66135 (7)	0.0230 (3)
N3	0.32823 (17)	0.21485 (8)	0.61681 (7)	0.0219 (3)
C1	1.1291 (2)	0.06789 (9)	0.47776 (9)	0.0227 (3)
H1	1.2113	0.0607	0.5207	0.027*
C2	1.1546 (2)	0.12573 (9)	0.42122 (9)	0.0216 (3)
C3	1.3166 (2)	0.15129 (9)	0.41631 (8)	0.0210 (3)
C4	1.3473 (2)	0.20464 (9)	0.36085 (9)	0.0225 (3)
C5	1.2143 (2)	0.23323 (10)	0.31222 (9)	0.0270 (4)
H5	1.2338	0.2696	0.2749	0.032*
C6	1.0521 (2)	0.20851 (10)	0.31822 (10)	0.0284 (4)
H6	0.9613	0.2289	0.2852	0.034*
C7	1.0209 (2)	0.15493 (10)	0.37118 (9)	0.0263 (4)
H7	0.9097	0.1379	0.3738	0.032*
C8	1.5554 (2)	0.07435 (10)	0.43631 (10)	0.0290 (4)
H8A	1.6445	0.0589	0.4761	0.044*
H8B	1.6052	0.0982	0.3940	0.044*
H8C	1.4907	0.0306	0.4169	0.044*
C9	1.5503 (2)	0.27571 (11)	0.30281 (11)	0.0336 (4)
H9A	1.6713	0.2852	0.3087	0.050*
H9B	1.4902	0.3226	0.3083	0.050*
H9C	1.5161	0.2545	0.2519	0.050*
C10	0.4791 (2)	0.12549 (9)	0.68026 (8)	0.0200 (3)
H10A	0.5707	0.1537	0.6659	0.024*
C11	0.51268 (19)	0.05616 (9)	0.72347 (8)	0.0195 (3)
C12	0.67881 (19)	0.03737 (9)	0.74863 (8)	0.0186 (3)
C13	0.71782 (19)	-0.02919 (9)	0.78884 (8)	0.0194 (3)
C14	0.5896 (2)	-0.07717 (9)	0.80322 (9)	0.0218 (3)

H14A	0.6145	-0.1224	0.8303	0.026*
C15	0.4237 (2)	-0.05849 (10)	0.77768 (9)	0.0235 (4)
H15A	0.3363	-0.0916	0.7874	0.028*
C16	0.3841 (2)	0.00711 (9)	0.73868 (9)	0.0222 (3)
H16A	0.2704	0.0191	0.7222	0.027*
C17	0.9006 (2)	0.06256 (10)	0.67612 (9)	0.0262 (4)
H17A	0.9887	0.0991	0.6700	0.039*
H17B	0.8259	0.0585	0.6279	0.039*
H17C	0.9517	0.0139	0.6892	0.039*
C18	0.9285 (2)	-0.10591 (10)	0.85626 (9)	0.0253 (4)
H18A	1.0505	-0.1078	0.8691	0.038*
H18B	0.8907	-0.1503	0.8265	0.038*
H18C	0.8746	-0.1044	0.9036	0.038*
C19	0.1780 (2)	0.23233 (9)	0.59042 (8)	0.0210 (3)
H19A	0.0886	0.2030	0.6053	0.025*
C20	0.1376 (2)	0.29503 (9)	0.53866 (8)	0.0193 (3)
C21	0.2569 (2)	0.32947 (9)	0.49745 (8)	0.0216 (3)
H21A	0.3706	0.3139	0.5048	0.026*
C22	0.2081 (2)	0.38584 (10)	0.44645 (9)	0.0246 (4)
H22A	0.2887	0.4084	0.4182	0.030*
C23	0.0420 (2)	0.41041 (9)	0.43554 (9)	0.0234 (4)
H23A	0.0103	0.4496	0.4004	0.028*
C24	-0.0767 (2)	0.37737 (9)	0.47628 (9)	0.0209 (3)
C25	-0.02836 (19)	0.31907 (9)	0.52731 (8)	0.0191 (3)
C26	-0.2977 (2)	0.45460 (11)	0.41808 (11)	0.0309 (4)
H26A	-0.4175	0.4637	0.4199	0.046*
H26B	-0.2793	0.4390	0.3661	0.046*
H26C	-0.2347	0.5004	0.4315	0.046*
C27	-0.2600 (2)	0.23775 (10)	0.52664 (9)	0.0273 (4)
H27A	-0.3380	0.2173	0.5603	0.041*
H27B	-0.1981	0.1969	0.5057	0.041*
H27C	-0.3231	0.2652	0.4844	0.041*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0249 (6)	0.0233 (6)	0.0214 (5)	0.0023 (5)	0.0017 (4)	0.0007 (4)
O2	0.0256 (6)	0.0275 (7)	0.0292 (6)	-0.0034 (5)	0.0027 (5)	0.0083 (5)
O3	0.0180 (6)	0.0206 (6)	0.0235 (5)	-0.0015 (5)	0.0043 (4)	-0.0011 (4)
O4	0.0182 (6)	0.0238 (6)	0.0262 (6)	0.0018 (5)	-0.0002 (4)	0.0054 (5)
O5	0.0182 (6)	0.0237 (6)	0.0205 (5)	-0.0017 (5)	0.0041 (4)	0.0006 (4)
O6	0.0200 (6)	0.0308 (7)	0.0307 (6)	0.0066 (5)	0.0051 (5)	0.0103 (5)
N1	0.0263 (8)	0.0247 (8)	0.0235 (7)	-0.0004 (6)	0.0086 (6)	0.0015 (6)
N2	0.0227 (7)	0.0229 (7)	0.0232 (7)	0.0017 (6)	0.0017 (5)	0.0029 (5)
N3	0.0223 (7)	0.0206 (7)	0.0225 (7)	0.0019 (6)	0.0012 (5)	0.0020 (5)
C1	0.0254 (9)	0.0215 (9)	0.0222 (8)	0.0028 (7)	0.0065 (6)	-0.0016 (6)
C2	0.0251 (9)	0.0188 (8)	0.0217 (8)	0.0015 (7)	0.0068 (6)	-0.0012 (6)
C3	0.0267 (9)	0.0175 (8)	0.0189 (7)	0.0014 (7)	0.0033 (6)	-0.0028 (6)

C4	0.0237 (9)	0.0213 (9)	0.0227 (8)	-0.0008 (7)	0.0041 (6)	-0.0019 (6)
C5	0.0312 (9)	0.0266 (9)	0.0234 (8)	0.0024 (8)	0.0045 (7)	0.0048 (7)
C6	0.0265 (9)	0.0305 (10)	0.0281 (8)	0.0053 (8)	0.0020 (7)	0.0035 (7)
C7	0.0249 (9)	0.0259 (9)	0.0289 (8)	0.0013 (7)	0.0059 (7)	0.0002 (7)
C8	0.0284 (9)	0.0244 (9)	0.0348 (9)	0.0052 (8)	0.0062 (7)	0.0016 (7)
C9	0.0312 (10)	0.0310 (10)	0.0397 (10)	-0.0009 (8)	0.0086 (8)	0.0133 (8)
C10	0.0196 (8)	0.0220 (8)	0.0182 (7)	-0.0002 (7)	0.0016 (6)	-0.0004 (6)
C11	0.0203 (8)	0.0216 (8)	0.0166 (7)	0.0014 (7)	0.0027 (6)	-0.0019 (6)
C12	0.0192 (8)	0.0196 (8)	0.0174 (7)	-0.0019 (6)	0.0035 (6)	-0.0031 (6)
C13	0.0182 (8)	0.0225 (8)	0.0173 (7)	0.0012 (7)	0.0013 (6)	-0.0026 (6)
C14	0.0249 (8)	0.0205 (8)	0.0203 (7)	0.0008 (7)	0.0038 (6)	0.0018 (6)
C15	0.0212 (8)	0.0258 (9)	0.0241 (8)	-0.0043 (7)	0.0048 (6)	-0.0002 (6)
C16	0.0169 (8)	0.0266 (9)	0.0230 (8)	0.0007 (7)	0.0025 (6)	0.0002 (6)
C17	0.0226 (9)	0.0284 (9)	0.0291 (9)	0.0017 (7)	0.0089 (7)	0.0018 (7)
C18	0.0227 (9)	0.0249 (9)	0.0276 (8)	0.0043 (7)	-0.0002 (6)	0.0064 (7)
C19	0.0206 (8)	0.0221 (9)	0.0203 (7)	0.0004 (7)	0.0030 (6)	-0.0021 (6)
C20	0.0212 (8)	0.0185 (8)	0.0176 (7)	0.0008 (7)	-0.0001 (6)	-0.0027 (6)
C21	0.0184 (8)	0.0244 (9)	0.0217 (8)	-0.0003 (7)	0.0011 (6)	-0.0026 (6)
C22	0.0235 (9)	0.0268 (9)	0.0241 (8)	-0.0041 (7)	0.0058 (6)	0.0004 (7)
C23	0.0247 (9)	0.0231 (9)	0.0221 (8)	0.0011 (7)	0.0019 (6)	0.0046 (6)
C24	0.0189 (8)	0.0228 (9)	0.0211 (7)	0.0021 (7)	0.0021 (6)	-0.0016 (6)
C25	0.0194 (8)	0.0208 (8)	0.0175 (7)	-0.0024 (7)	0.0036 (6)	-0.0020 (6)
C26	0.0245 (9)	0.0291 (10)	0.0385 (10)	0.0055 (8)	0.0012 (7)	0.0116 (8)
C27	0.0224 (9)	0.0302 (10)	0.0288 (9)	-0.0065 (8)	0.0013 (7)	0.0000 (7)

*Geometric parameters (Å, °)*

O1—C3	1.3792 (19)	C10—C11	1.465 (2)
O1—C8	1.433 (2)	C10—H10A	0.9500
O2—C4	1.366 (2)	C11—C12	1.397 (2)
O2—C9	1.429 (2)	C11—C16	1.405 (2)
O3—C12	1.3794 (18)	C12—C13	1.403 (2)
O3—C17	1.4383 (19)	C13—C14	1.387 (2)
O4—C13	1.3632 (19)	C14—C15	1.396 (2)
O4—C18	1.4339 (19)	C14—H14A	0.9500
O5—C25	1.3796 (18)	C15—C16	1.380 (2)
O5—C27	1.440 (2)	C15—H15A	0.9500
O6—C24	1.3664 (19)	C16—H16A	0.9500
O6—C26	1.429 (2)	C17—H17A	0.9800
N1—C1	1.283 (2)	C17—H17B	0.9800
N1—N1 <sup>i</sup>	1.419 (3)	C17—H17C	0.9800
N2—C10	1.276 (2)	C18—H18A	0.9800
N2—N3	1.4146 (19)	C18—H18B	0.9800
N3—C19	1.280 (2)	C18—H18C	0.9800
C1—C2	1.465 (2)	C19—C20	1.458 (2)
C1—H1	0.9500	C19—H19A	0.9500
C2—C3	1.392 (2)	C20—C25	1.393 (2)
C2—C7	1.406 (2)	C20—C21	1.407 (2)

C3—C4	1.406 (2)	C21—C22	1.376 (2)
C4—C5	1.385 (2)	C21—H21A	0.9500
C5—C6	1.391 (2)	C22—C23	1.396 (2)
C5—H5	0.9500	C22—H22A	0.9500
C6—C7	1.379 (2)	C23—C24	1.388 (2)
C6—H6	0.9500	C23—H23A	0.9500
C7—H7	0.9500	C24—C25	1.401 (2)
C8—H8A	0.9800	C26—H26A	0.9800
C8—H8B	0.9800	C26—H26B	0.9800
C8—H8C	0.9800	C26—H26C	0.9800
C9—H9A	0.9800	C27—H27A	0.9800
C9—H9B	0.9800	C27—H27B	0.9800
C9—H9C	0.9800	C27—H27C	0.9800
C3—O1—C8	113.74 (12)	C13—C14—C15	119.57 (15)
C4—O2—C9	117.40 (13)	C13—C14—H14A	120.2
C12—O3—C17	112.88 (12)	C15—C14—H14A	120.2
C13—O4—C18	117.00 (12)	C16—C15—C14	121.34 (15)
C25—O5—C27	113.87 (11)	C16—C15—H15A	119.3
C24—O6—C26	117.17 (13)	C14—C15—H15A	119.3
C1—N1—N1 <sup>i</sup>	111.08 (16)	C15—C16—C11	119.75 (15)
C10—N2—N3	111.68 (13)	C15—C16—H16A	120.1
C19—N3—N2	110.69 (13)	C11—C16—H16A	120.1
N1—C1—C2	120.95 (15)	O3—C17—H17A	109.5
N1—C1—H1	119.5	O3—C17—H17B	109.5
C2—C1—H1	119.5	H17A—C17—H17B	109.5
C3—C2—C7	119.36 (15)	O3—C17—H17C	109.5
C3—C2—C1	118.68 (15)	H17A—C17—H17C	109.5
C7—C2—C1	121.96 (15)	H17B—C17—H17C	109.5
O1—C3—C2	119.57 (14)	O4—C18—H18A	109.5
O1—C3—C4	119.93 (15)	O4—C18—H18B	109.5
C2—C3—C4	120.45 (15)	H18A—C18—H18B	109.5
O2—C4—C5	125.23 (15)	O4—C18—H18C	109.5
O2—C4—C3	115.20 (14)	H18A—C18—H18C	109.5
C5—C4—C3	119.57 (16)	H18B—C18—H18C	109.5
C4—C5—C6	119.79 (16)	N3—C19—C20	123.12 (15)
C4—C5—H5	120.1	N3—C19—H19A	118.4
C6—C5—H5	120.1	C20—C19—H19A	118.4
C7—C6—C5	121.20 (16)	C25—C20—C21	119.17 (14)
C7—C6—H6	119.4	C25—C20—C19	117.91 (14)
C5—C6—H6	119.4	C21—C20—C19	122.85 (14)
C6—C7—C2	119.61 (16)	C22—C21—C20	119.77 (15)
C6—C7—H7	120.2	C22—C21—H21A	120.1
C2—C7—H7	120.2	C20—C21—H21A	120.1
O1—C8—H8A	109.5	C21—C22—C23	121.09 (15)
O1—C8—H8B	109.5	C21—C22—H22A	119.5
H8A—C8—H8B	109.5	C23—C22—H22A	119.5
O1—C8—H8C	109.5	C24—C23—C22	119.76 (15)

H8A—C8—H8C	109.5	C24—C23—H23A	120.1
H8B—C8—H8C	109.5	C22—C23—H23A	120.1
O2—C9—H9A	109.5	O6—C24—C23	125.21 (14)
O2—C9—H9B	109.5	O6—C24—C25	115.38 (14)
H9A—C9—H9B	109.5	C23—C24—C25	119.41 (15)
O2—C9—H9C	109.5	O5—C25—C20	119.13 (14)
H9A—C9—H9C	109.5	O5—C25—C24	120.00 (14)
H9B—C9—H9C	109.5	C20—C25—C24	120.79 (14)
N2—C10—C11	121.74 (15)	O6—C26—H26A	109.5
N2—C10—H10A	119.1	O6—C26—H26B	109.5
C11—C10—H10A	119.1	H26A—C26—H26B	109.5
C12—C11—C16	118.99 (15)	O6—C26—H26C	109.5
C12—C11—C10	118.67 (14)	H26A—C26—H26C	109.5
C16—C11—C10	122.32 (14)	H26B—C26—H26C	109.5
O3—C12—C11	119.60 (14)	O5—C27—H27A	109.5
O3—C12—C13	119.47 (14)	O5—C27—H27B	109.5
C11—C12—C13	120.88 (14)	H27A—C27—H27B	109.5
O4—C13—C14	125.27 (14)	O5—C27—H27C	109.5
O4—C13—C12	115.25 (14)	H27A—C27—H27C	109.5
C14—C13—C12	119.47 (14)	H27B—C27—H27C	109.5
C10—N2—N3—C19	171.89 (14)	C18—O4—C13—C12	176.95 (13)
N1 <sup>i</sup> —N1—C1—C2	177.86 (15)	O3—C12—C13—O4	-1.4 (2)
N1—C1—C2—C3	-158.74 (15)	C11—C12—C13—O4	-178.69 (13)
N1—C1—C2—C7	20.1 (2)	O3—C12—C13—C14	177.86 (13)
C8—O1—C3—C2	106.62 (16)	C11—C12—C13—C14	0.5 (2)
C8—O1—C3—C4	-75.95 (18)	O4—C13—C14—C15	178.95 (14)
C7—C2—C3—O1	176.09 (14)	C12—C13—C14—C15	-0.2 (2)
C1—C2—C3—O1	-5.0 (2)	C13—C14—C15—C16	-0.4 (2)
C7—C2—C3—C4	-1.3 (2)	C14—C15—C16—C11	0.6 (2)
C1—C2—C3—C4	177.54 (14)	C12—C11—C16—C15	-0.2 (2)
C9—O2—C4—C5	-3.4 (2)	C10—C11—C16—C15	178.05 (14)
C9—O2—C4—C3	177.07 (15)	N2—N3—C19—C20	-176.19 (13)
O1—C3—C4—O2	3.9 (2)	N3—C19—C20—C25	-165.89 (15)
C2—C3—C4—O2	-178.72 (14)	N3—C19—C20—C21	17.2 (2)
O1—C3—C4—C5	-175.72 (14)	C25—C20—C21—C22	-0.4 (2)
C2—C3—C4—C5	1.7 (2)	C19—C20—C21—C22	176.53 (15)
O2—C4—C5—C6	179.92 (15)	C20—C21—C22—C23	0.9 (2)
C3—C4—C5—C6	-0.5 (2)	C21—C22—C23—C24	-0.4 (2)
C4—C5—C6—C7	-1.0 (3)	C26—O6—C24—C23	2.5 (2)
C5—C6—C7—C2	1.3 (3)	C26—O6—C24—C25	-177.83 (14)
C3—C2—C7—C6	-0.2 (2)	C22—C23—C24—O6	178.95 (15)
C1—C2—C7—C6	-179.01 (15)	C22—C23—C24—C25	-0.7 (2)
N3—N2—C10—C11	-177.09 (13)	C27—O5—C25—C20	-107.31 (16)
N2—C10—C11—C12	-173.93 (14)	C27—O5—C25—C24	75.94 (18)
N2—C10—C11—C16	7.8 (2)	C21—C20—C25—O5	-177.46 (13)
C17—O3—C12—C11	-105.52 (16)	C19—C20—C25—O5	5.5 (2)
C17—O3—C12—C13	77.10 (17)	C21—C20—C25—C24	-0.7 (2)



C16—C11—C12—O3	-177.65 (13)	C19—C20—C25—C24	-177.79 (14)
C10—C11—C12—O3	4.0 (2)	O6—C24—C25—O5	-1.7 (2)
C16—C11—C12—C13	-0.3 (2)	C23—C24—C25—O5	177.97 (14)
C10—C11—C12—C13	-178.66 (13)	O6—C24—C25—C20	-178.42 (13)
C18—O4—C13—C14	-2.2 (2)	C23—C24—C25—C20	1.3 (2)

Symmetry code: (i)  $-x+2, -y, -z+1$ .

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C9—H9B...O3 <sup>ii</sup>	0.98	2.45	3.288 (2)	143
C14—H14A...O5 <sup>iii</sup>	0.95	2.37	3.2890 (19)	161
C18—H18C...O6 <sup>iii</sup>	0.98	2.54	3.5229 (19)	178
C27—H27C...O2 <sup>iv</sup>	0.98	2.52	3.2656 (19)	133

Symmetry codes: (ii)  $x+1/2, -y+1/2, z-1/2$ ; (iii)  $-x+1/2, y-1/2, -z+3/2$ ; (iv)  $x-2, y, z$ .