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N′-[(*E*)-4-Methoxybenzylidene]-2-(4-methylphenoxy)acetohydrazide

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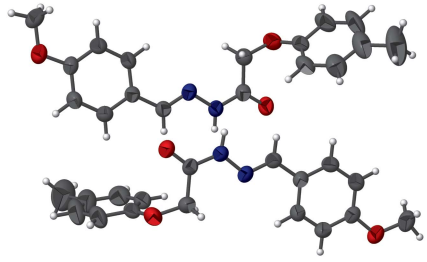
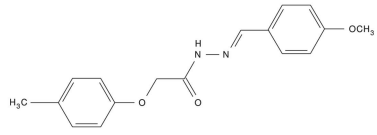
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{17}H_{18}N_2O_3$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The dihedral angle between the 4-methoxyphenyl ring and the toluene ring is 88.13 (10)° in molecule *A* and 61.47 (10)° in molecule *B*. In the crystal, molecules are linked *via* pairs of N—H···O hydrogen bonds, forming *A*–*A* and *B*–*B* inversion dimers with $R_2^2(8)$ ring motifs. The *B*–*B* dimers are linked by C—H···O hydrogen bonds, forming chains propagating along the [110] direction. The molecules are also linked by a series of C—H···π interactions, forming a three-dimensional structure.

3D view



Chemical scheme



Structure description

A number of industrial and biologically active compounds can be synthesized by using Schiff bases as the substrates *via* cycloaddition, ring closure and replacement reactions. In addition, Schiff bases are also known to have biological activities such as antifungal (Singh & Dash, 1988) antimicrobial (El-masry *et al.*, 2000, Pandeya *et al.*, 1999), antitumor and as herbicides. Schiff bases have also been employed as ligands for complexation of metal ions (Aydogan *et al.*, 2001), since many of these complexes may be useful and serve as the models for biologically important species. They have wide range of applications on the industrial scale such as dyes and pigments. In view of the importance of Schiff base hydrazones, we report herein on the synthesis and crystal structure of title compound.

The molecular structure of the two independent molecules (*A* and *B*) of the title compound is shown in Fig. 1. The dihedral angle between the 4-methoxyphenyl ring and the toluene ring is 88.13 (10)° in molecule *A* and 61.47 (10)° in molecule *B*. The methoxy

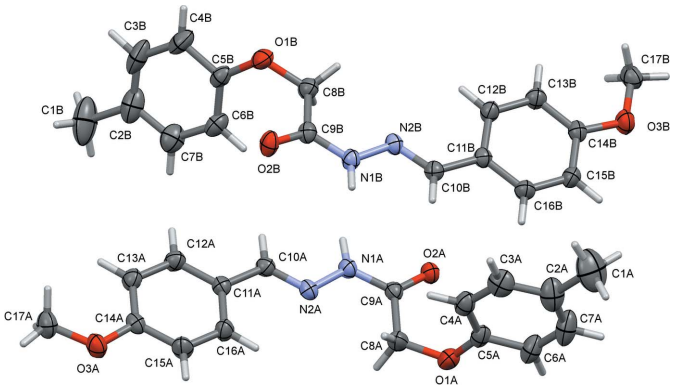


Figure 1
View of the molecular structure of the two independent molecules (*A* and *B*) of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

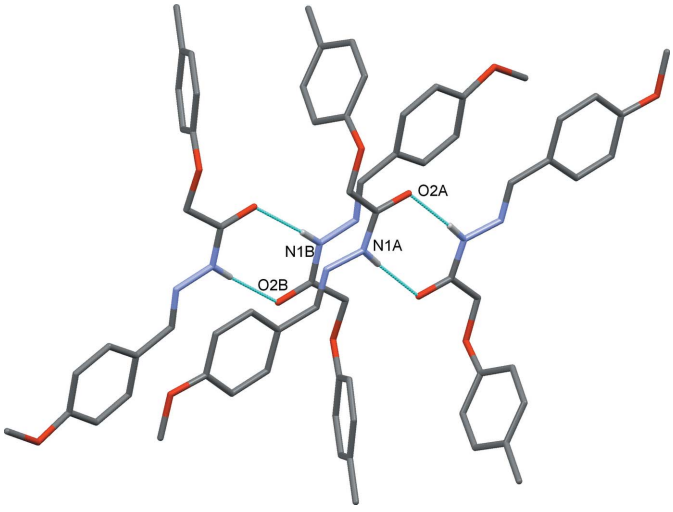


Figure 2
A view of the pairs of N—H···O hydrogen bonds forming the *A*–*A* and *B*–*B* inversion dimers with $R_2^2(8)$ ring motifs (see Table 1).

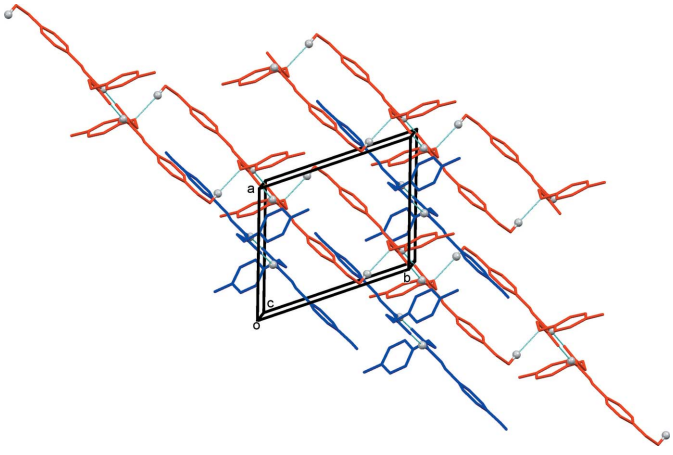


Figure 3
A view along the *c* axis of the crystal packing of the title compound (colour code: molecule *A* blue, molecule *B* red). The hydrogen bonds are shown as dashed lines (see Table 1), and only the H atoms (grey balls) involved in hydrogen bonding have been included.

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

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the C2*A*–C7*A*, C11*A*–C16*A*, C2*B*–C7*B* and C11*B*–C16*B* rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O2*A*^{i}	0.86	2.07	2.9226 (17)	173
N1*B*—H1*B*···O2*B*^{ii}	0.86	2.07	2.9207 (17)	171
C17*B*—H17*C*···O1*B*^{iii}	0.96	2.45	3.394 (2)	167
C3*A*—H3*A*···*Cg*3^{ii}	0.93	2.95	3.549 (2)	123
C6*A*—H6*A*···*Cg*3^{i}	0.93	2.98	3.698 (2)	135
C16*B*—H16*B*···*Cg*1	0.93	2.81	3.742 (2)	177
C17*B*—H17*A*···*Cg*2^{i}	0.96	2.81	3.569 (2)	136
C17*A*—H17*D*···*Cg*4^{ii}	0.96	2.93	3.619 (2)	130

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

group in both molecules lies in the plane of the phenyl ring as indicated by the torsion angles of 4.2 (3)° for C17*A*—O3*A*—C14*A*—C13*A* and −6.1 (2)° for C17*B*—O3*B*—C14*B*—C13*B*.

In the crystal, molecules are linked *via* pairs of N—H···O hydrogen bonds forming *A*–*A* and *B*–*B* inversion dimers with $R_2^2(8)$ ring motifs (Fig. 2 and Table 1). The *B*–*B* dimers are linked by C—H···O hydrogen bonds, forming chains propagating along [110]; see Table 1 and Fig. 3. The molecules are also linked by a series of C—H···π interactions (Table 1), forming a three-dimensional structure.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{18}N_2O_3$
M_r	298.33
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, *b*, *c* (Å)	9.4835 (3), 11.9112 (4), 15.5727 (4)
α, β, γ (°)	72.136 (1), 86.122 (1), 70.688 (1)
V (Å^3)	1578.95 (8)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.09
Crystal size (mm)	0.29 × 0.27 × 0.25
Data collection	
Diffractometer	Bruker APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2011)
T_{min}, T_{max}	0.984, 0.987
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21401, 5906, 3766
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.609
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.042, 0.128, 1.02
No. of reflections	5906
No. of parameters	401
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.13, −0.15

Computer programs: *APEX2* and *SAINT* (Bruker, 2011), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

Synthesis and crystallization

A mixture of 2-(4-methylphenoxy)acetohydrazide (1.8 g, 0.01 mol), anisaldehyde (1.36 g, 0.01 mol) and hydrazine hydrate (0.6 ml, 0.012 mol) in 15 ml of 2-propanol containing two drops of sulfuric acid, was refluxed for *ca* 3 h. On cooling, the solid that separated was filtered and recrystallized from DMF. On slow evaporation of the solvent colourless block-like crystals were obtained (yield 78%, m.p. 478 K).

Refinement

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

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full crystallographic data

IUCrData (2016). **1**, x161877 [https://doi.org/10.1107/S2414314616018770]

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Crystal data

$C_{17}H_{18}N_2O_3$
M_r = 298.33
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.4835 (3) Å
b = 11.9112 (4) Å
c = 15.5727 (4) Å
α = 72.136 (1)°
β = 86.122 (1)°
γ = 70.688 (1)°
V = 1578.95 (8) Å^3
Z = 4
$F(000)$ = 632
D_x = 1.255 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3766 reflections
θ = 2.0–25.7°
μ = 0.09 mm^{-1}
T = 296 K
Block, colourless
0.29 × 0.27 × 0.25 mm

Data collection

Bruker APEXII diffractometer
Radiation source: Enraf Nonius FR590
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
CCD rotation images, thick slices scans
Absorption correction: multi-scan (SADABS; Bruker, 2011)
T_{min} = 0.984, T_{max} = 0.987
21401 measured reflections
5906 independent reflections
3766 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.7°, θ_{min} = 2.0°
h = −11→11
k = −14→13
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.128
S = 1.02
5906 reflections
401 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
$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.0979P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1A	0.62766 (15)	−0.10667 (12)	0.25322 (8)	0.0693 (5)
O2A	0.48929 (12)	0.00034 (10)	0.38205 (7)	0.0523 (4)
O3A	1.42111 (13)	−0.61212 (11)	0.69317 (8)	0.0640 (4)
N1A	0.67734 (14)	−0.11448 (11)	0.48438 (8)	0.0473 (5)
N2A	0.81426 (14)	−0.20652 (11)	0.50537 (9)	0.0466 (4)
C1A	0.7133 (4)	0.3263 (3)	0.00499 (19)	0.1448 (16)
C2A	0.6947 (3)	0.2086 (2)	0.07176 (14)	0.0903 (9)
C3A	0.7806 (2)	0.1485 (2)	0.15016 (15)	0.0784 (8)
C4A	0.7635 (2)	0.04332 (18)	0.21292 (12)	0.0654 (7)
C5A	0.65672 (19)	−0.00312 (17)	0.19669 (11)	0.0567 (6)
C6A	0.5715 (2)	0.0539 (2)	0.11750 (12)	0.0763 (8)
C7A	0.5910 (3)	0.1585 (3)	0.05705 (14)	0.0952 (9)
C8A	0.6934 (2)	−0.15650 (16)	0.34117 (11)	0.0655 (7)
C9A	0.61066 (17)	−0.08207 (14)	0.40320 (10)	0.0439 (5)
C10A	0.86917 (17)	−0.23483 (14)	0.58434 (11)	0.0469 (5)
C11A	1.01379 (17)	−0.33017 (14)	0.61346 (10)	0.0445 (5)
C12A	1.07332 (18)	−0.36059 (15)	0.69929 (11)	0.0545 (6)
C13A	1.20890 (19)	−0.45358 (16)	0.72909 (11)	0.0554 (6)
C14A	1.28807 (17)	−0.51757 (14)	0.67161 (11)	0.0483 (5)
C15A	1.2317 (2)	−0.48595 (16)	0.58491 (11)	0.0617 (6)
C16A	1.09718 (19)	−0.39536 (15)	0.55635 (11)	0.0564 (6)
C17A	1.4796 (2)	−0.65423 (18)	0.78254 (13)	0.0728 (7)
O1B	0.81558 (13)	0.13675 (11)	0.72848 (8)	0.0634 (5)
O2B	0.98466 (12)	0.01561 (11)	0.61375 (7)	0.0603 (4)
O3B	0.11002 (13)	0.58182 (11)	0.21213 (8)	0.0640 (4)
N1B	0.80908 (13)	0.10968 (11)	0.50178 (8)	0.0479 (4)
N2B	0.67169 (14)	0.19796 (11)	0.47024 (9)	0.0464 (4)
C1B	0.8441 (4)	−0.2943 (3)	1.02392 (17)	0.1524 (13)
C2B	0.8360 (2)	−0.1803 (3)	0.94423 (15)	0.0907 (9)
C3B	0.8593 (2)	−0.0773 (3)	0.95466 (14)	0.0964 (12)
C4B	0.8521 (2)	0.0272 (2)	0.88290 (14)	0.0794 (9)
C5B	0.81862 (18)	0.03015 (17)	0.79686 (11)	0.0548 (6)
C6B	0.7916 (2)	−0.07031 (18)	0.78532 (12)	0.0651 (7)
C7B	0.8018 (2)	−0.1739 (2)	0.85892 (14)	0.0800 (8)
C8B	0.75049 (19)	0.15668 (16)	0.64326 (11)	0.0569 (6)

C9B	0.85908 (18)	0.08797 (14)	0.58578 (10)	0.0470 (6)
C10B	0.63556 (17)	0.21631 (14)	0.38850 (10)	0.0456 (5)
C11B	0.49714 (17)	0.31029 (14)	0.34541 (10)	0.0437 (5)
C12B	0.40738 (18)	0.39544 (15)	0.38652 (11)	0.0528 (6)
C13B	0.27787 (19)	0.48620 (16)	0.34533 (11)	0.0545 (6)
C14B	0.23462 (17)	0.49484 (14)	0.25990 (10)	0.0481 (6)
C15B	0.32298 (19)	0.41067 (15)	0.21760 (11)	0.0557 (6)
C16B	0.45144 (19)	0.31997 (15)	0.25966 (11)	0.0548 (6)
C17B	0.0093 (2)	0.66292 (16)	0.25662 (13)	0.0662 (7)
H1A	0.63450	−0.07770	0.52340	0.0570*
H3A	0.85310	0.17950	0.16150	0.0940*
H4A	0.82350	0.00450	0.26550	0.0780*
H1A1	0.75270	0.30900	−0.04970	0.2170*
H6A	0.50100	0.02170	0.10500	0.0920*
H1A2	0.78090	0.35300	0.03080	0.2170*
H7A	0.53170	0.19680	0.00420	0.1140*
H1A3	0.61790	0.39100	−0.00820	0.2170*
H8A1	0.79630	−0.15750	0.33820	0.0790*
H8A2	0.69410	−0.24200	0.36610	0.0790*
H10A	0.81580	−0.19370	0.62440	0.0560*
H12A	1.02080	−0.31730	0.73830	0.0650*
H13A	1.24610	−0.47260	0.78740	0.0670*
H15	1.28630	−0.52710	0.54520	0.0740*
H16A	1.06060	−0.37690	0.49790	0.0680*
H17D	1.49320	−0.58610	0.79770	0.1090*
H17E	1.57410	−0.71930	0.78770	0.1090*
H17F	1.41130	−0.68600	0.82310	0.1090*
H1B1	0.94640	−0.33820	1.04460	0.2280*
H1B	0.86260	0.06860	0.46760	0.0570*
H1B2	0.80420	−0.34820	1.00580	0.2280*
H1B3	0.78680	−0.26860	1.07190	0.2280*
H3B	0.88080	−0.07810	1.01230	0.1160*
H8B1	0.71670	0.24530	0.61130	0.0680*
H4B	0.86960	0.09510	0.89220	0.0950*
H8B2	0.66380	0.12890	0.65260	0.0680*
H6B	0.76640	−0.06900	0.72820	0.0780*
H7B	0.78460	−0.24190	0.84980	0.0960*
H10B	0.69940	0.16830	0.35560	0.0550*
H12B	0.43550	0.39110	0.44380	0.0630*
H13B	0.21950	0.54160	0.37490	0.0650*
H15B	0.29500	0.41560	0.16010	0.0670*
H16B	0.50900	0.26390	0.23030	0.0660*
H17A	−0.02200	0.61410	0.31100	0.0990*
H17B	−0.07640	0.71560	0.21750	0.0990*
H17C	0.05870	0.71360	0.27130	0.0990*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0851 (10)	0.0679 (8)	0.0536 (7)	−0.0146 (7)	−0.0097 (6)	−0.0253 (7)
O2A	0.0465 (7)	0.0512 (7)	0.0523 (7)	−0.0065 (6)	−0.0064 (5)	−0.0145 (5)
O3A	0.0514 (7)	0.0578 (7)	0.0666 (8)	−0.0002 (6)	−0.0040 (6)	−0.0140 (6)
N1A	0.0422 (8)	0.0463 (8)	0.0474 (8)	−0.0051 (6)	−0.0014 (6)	−0.0153 (6)
N2A	0.0428 (8)	0.0410 (7)	0.0500 (8)	−0.0084 (6)	−0.0011 (6)	−0.0104 (6)
C1A	0.130 (3)	0.140 (3)	0.119 (2)	−0.043 (2)	0.0296 (19)	0.0176 (19)
C2A	0.0645 (14)	0.1090 (18)	0.0666 (14)	−0.0113 (13)	0.0162 (12)	−0.0051 (13)
C3A	0.0530 (12)	0.0982 (16)	0.0811 (15)	−0.0190 (11)	0.0149 (11)	−0.0319 (13)
C4A	0.0507 (11)	0.0791 (13)	0.0564 (11)	−0.0025 (10)	−0.0043 (8)	−0.0255 (10)
C5A	0.0463 (10)	0.0711 (12)	0.0448 (10)	−0.0008 (9)	−0.0010 (8)	−0.0257 (9)
C6A	0.0575 (12)	0.1120 (17)	0.0502 (11)	−0.0164 (12)	−0.0063 (9)	−0.0221 (12)
C7A	0.0648 (14)	0.139 (2)	0.0517 (12)	−0.0155 (14)	−0.0048 (10)	−0.0048 (13)
C8A	0.0810 (13)	0.0513 (11)	0.0533 (11)	−0.0023 (9)	−0.0048 (9)	−0.0200 (9)
C9A	0.0453 (10)	0.0380 (9)	0.0466 (9)	−0.0136 (8)	−0.0016 (7)	−0.0096 (7)
C10A	0.0436 (9)	0.0475 (9)	0.0487 (10)	−0.0111 (8)	0.0021 (7)	−0.0173 (8)
C11A	0.0423 (9)	0.0414 (9)	0.0473 (9)	−0.0132 (7)	0.0004 (7)	−0.0103 (7)
C12A	0.0487 (10)	0.0612 (11)	0.0531 (10)	−0.0095 (9)	0.0007 (8)	−0.0257 (9)
C13A	0.0506 (10)	0.0626 (11)	0.0509 (10)	−0.0138 (9)	−0.0069 (8)	−0.0174 (9)
C14A	0.0412 (9)	0.0418 (9)	0.0557 (10)	−0.0107 (8)	0.0017 (8)	−0.0091 (8)
C15A	0.0626 (12)	0.0592 (11)	0.0496 (10)	−0.0015 (9)	0.0070 (9)	−0.0184 (9)
C16A	0.0593 (11)	0.0567 (11)	0.0417 (9)	−0.0056 (9)	−0.0011 (8)	−0.0125 (8)
C17A	0.0544 (12)	0.0709 (13)	0.0746 (13)	−0.0051 (10)	−0.0117 (10)	−0.0101 (10)
O1B	0.0652 (8)	0.0699 (8)	0.0634 (8)	−0.0194 (6)	−0.0090 (6)	−0.0324 (7)
O2B	0.0399 (7)	0.0756 (8)	0.0530 (7)	−0.0063 (6)	−0.0058 (5)	−0.0140 (6)
O3B	0.0532 (7)	0.0641 (8)	0.0594 (7)	−0.0026 (6)	−0.0110 (6)	−0.0126 (6)
N1B	0.0388 (7)	0.0516 (8)	0.0461 (8)	−0.0066 (6)	−0.0026 (6)	−0.0129 (6)
N2B	0.0392 (7)	0.0460 (8)	0.0490 (8)	−0.0110 (6)	−0.0023 (6)	−0.0098 (6)
C1B	0.123 (2)	0.207 (3)	0.0850 (18)	−0.075 (2)	−0.0123 (16)	0.041 (2)
C2B	0.0595 (13)	0.140 (2)	0.0596 (14)	−0.0362 (14)	0.0009 (10)	−0.0076 (14)
C3B	0.0687 (15)	0.168 (3)	0.0447 (12)	−0.0283 (16)	−0.0057 (10)	−0.0310 (16)
C4B	0.0650 (13)	0.1193 (18)	0.0658 (13)	−0.0235 (12)	−0.0068 (10)	−0.0499 (13)
C5B	0.0406 (9)	0.0756 (13)	0.0501 (10)	−0.0111 (8)	−0.0008 (7)	−0.0297 (10)
C6B	0.0693 (12)	0.0877 (14)	0.0474 (10)	−0.0317 (11)	0.0051 (8)	−0.0270 (10)
C7B	0.0797 (15)	0.0969 (16)	0.0651 (13)	−0.0399 (12)	0.0099 (11)	−0.0162 (12)
C8B	0.0534 (10)	0.0603 (11)	0.0568 (10)	−0.0124 (9)	−0.0070 (8)	−0.0222 (9)
C9B	0.0425 (10)	0.0494 (10)	0.0475 (10)	−0.0172 (8)	−0.0006 (7)	−0.0094 (8)
C10B	0.0434 (9)	0.0468 (9)	0.0454 (9)	−0.0142 (7)	0.0024 (7)	−0.0130 (7)
C11B	0.0434 (9)	0.0436 (9)	0.0428 (9)	−0.0151 (7)	0.0019 (7)	−0.0103 (7)
C12B	0.0495 (10)	0.0608 (11)	0.0425 (9)	−0.0100 (9)	−0.0029 (7)	−0.0156 (8)
C13B	0.0508 (10)	0.0589 (11)	0.0499 (10)	−0.0096 (9)	0.0040 (8)	−0.0204 (8)
C14B	0.0432 (9)	0.0473 (10)	0.0486 (10)	−0.0139 (8)	−0.0039 (7)	−0.0069 (8)
C15B	0.0599 (11)	0.0589 (11)	0.0455 (9)	−0.0128 (9)	−0.0093 (8)	−0.0166 (8)
C16B	0.0552 (11)	0.0542 (10)	0.0514 (10)	−0.0078 (8)	−0.0017 (8)	−0.0210 (8)
C17B	0.0514 (11)	0.0553 (11)	0.0814 (13)	−0.0036 (9)	−0.0063 (9)	−0.0190 (10)

Geometric parameters (Å, º)

O1A—C5A	1.378 (2)	C8A—H8A2	0.9700
O1A—C8A	1.410 (2)	C10A—H10A	0.9300
O2A—C9A	1.226 (2)	C12A—H12A	0.9300
O3A—C14A	1.363 (2)	C13A—H13A	0.9300
O3A—C17A	1.410 (2)	C15A—H15	0.9300
O1B—C8B	1.421 (2)	C16A—H16A	0.9300
O1B—C5B	1.378 (2)	C17A—H17F	0.9600
O2B—C9B	1.230 (2)	C17A—H17D	0.9600
O3B—C14B	1.364 (2)	C17A—H17E	0.9600
O3B—C17B	1.427 (2)	C1B—C2B	1.517 (4)
N1A—N2A	1.3751 (19)	C2B—C7B	1.362 (3)
N1A—C9A	1.340 (2)	C2B—C3B	1.374 (5)
N2A—C10A	1.270 (2)	C3B—C4B	1.380 (3)
N1A—H1A	0.8600	C4B—C5B	1.385 (3)
N1B—C9B	1.3409 (19)	C5B—C6B	1.368 (3)
N1B—N2B	1.3813 (19)	C6B—C7B	1.383 (3)
N2B—C10B	1.275 (2)	C8B—C9B	1.516 (2)
N1B—H1B	0.8600	C10B—C11B	1.454 (2)
C1A—C2A	1.524 (4)	C11B—C16B	1.391 (2)
C2A—C7A	1.371 (4)	C11B—C12B	1.385 (2)
C2A—C3A	1.371 (3)	C12B—C13B	1.375 (3)
C3A—C4A	1.383 (3)	C13B—C14B	1.382 (2)
C4A—C5A	1.373 (3)	C14B—C15B	1.384 (2)
C5A—C6A	1.376 (3)	C15B—C16B	1.372 (3)
C6A—C7A	1.372 (4)	C1B—H1B1	0.9600
C8A—C9A	1.516 (2)	C1B—H1B2	0.9600
C10A—C11A	1.454 (2)	C1B—H1B3	0.9600
C11A—C16A	1.393 (2)	C3B—H3B	0.9300
C11A—C12A	1.381 (2)	C4B—H4B	0.9300
C12A—C13A	1.385 (3)	C6B—H6B	0.9300
C13A—C14A	1.377 (2)	C7B—H7B	0.9300
C14A—C15A	1.380 (2)	C8B—H8B1	0.9700
C15A—C16A	1.364 (3)	C8B—H8B2	0.9700
C1A—H1A2	0.9600	C10B—H10B	0.9300
C1A—H1A1	0.9600	C12B—H12B	0.9300
C1A—H1A3	0.9600	C13B—H13B	0.9300
C3A—H3A	0.9300	C15B—H15B	0.9300
C4A—H4A	0.9300	C16B—H16B	0.9300
C6A—H6A	0.9300	C17B—H17A	0.9600
C7A—H7A	0.9300	C17B—H17B	0.9600
C8A—H8A1	0.9700	C17B—H17C	0.9600
C5A—O1A—C8A	117.56 (15)	H17D—C17A—H17E	110.00
C14A—O3A—C17A	118.43 (14)	O3A—C17A—H17D	109.00
C5B—O1B—C8B	118.15 (14)	O3A—C17A—H17E	109.00
C14B—O3B—C17B	117.61 (13)	O3A—C17A—H17F	109.00

N2A—N1A—C9A	120.10 (13)	H17D—C17A—H17F	109.00
N1A—N2A—C10A	116.76 (13)	H17E—C17A—H17F	109.00
N2A—N1A—H1A	120.00	C3B—C2B—C7B	116.7 (2)
C9A—N1A—H1A	120.00	C1B—C2B—C3B	121.8 (2)
N2B—N1B—C9B	120.00 (13)	C1B—C2B—C7B	121.6 (3)
N1B—N2B—C10B	115.87 (13)	C2B—C3B—C4B	122.5 (2)
C9B—N1B—H1B	120.00	C3B—C4B—C5B	119.4 (2)
N2B—N1B—H1B	120.00	O1B—C5B—C6B	124.87 (15)
C1A—C2A—C7A	121.9 (2)	O1B—C5B—C4B	116.09 (17)
C1A—C2A—C3A	121.2 (3)	C4B—C5B—C6B	119.04 (17)
C3A—C2A—C7A	116.9 (2)	C5B—C6B—C7B	119.73 (17)
C2A—C3A—C4A	122.4 (2)	C2B—C7B—C6B	122.7 (2)
C3A—C4A—C5A	119.20 (18)	O1B—C8B—C9B	112.34 (15)
O1A—C5A—C6A	115.23 (17)	N1B—C9B—C8B	115.72 (15)
C4A—C5A—C6A	119.47 (18)	O2B—C9B—C8B	122.86 (14)
O1A—C5A—C4A	125.29 (16)	O2B—C9B—N1B	121.41 (15)
C5A—C6A—C7A	119.7 (2)	N2B—C10B—C11B	121.70 (15)
C2A—C7A—C6A	122.4 (2)	C12B—C11B—C16B	117.24 (15)
O1A—C8A—C9A	112.24 (15)	C10B—C11B—C12B	121.81 (14)
N1A—C9A—C8A	115.43 (14)	C10B—C11B—C16B	120.94 (15)
O2A—C9A—N1A	121.74 (14)	C11B—C12B—C13B	122.09 (15)
O2A—C9A—C8A	122.81 (14)	C12B—C13B—C14B	119.87 (16)
N2A—C10A—C11A	121.36 (15)	O3B—C14B—C15B	116.09 (14)
C12A—C11A—C16A	117.31 (16)	O3B—C14B—C13B	124.99 (15)
C10A—C11A—C16A	121.46 (14)	C13B—C14B—C15B	118.92 (16)
C10A—C11A—C12A	121.23 (15)	C14B—C15B—C16B	120.67 (15)
C11A—C12A—C13A	122.05 (16)	C11B—C16B—C15B	121.22 (16)
C12A—C13A—C14A	119.41 (15)	C2B—C1B—H1B1	109.00
O3A—C14A—C15A	115.78 (15)	C2B—C1B—H1B2	110.00
C13A—C14A—C15A	119.13 (16)	C2B—C1B—H1B3	109.00
O3A—C14A—C13A	125.09 (15)	H1B1—C1B—H1B2	110.00
C14A—C15A—C16A	121.15 (16)	H1B1—C1B—H1B3	109.00
C11A—C16A—C15A	120.92 (15)	H1B2—C1B—H1B3	109.00
H1A1—C1A—H1A2	110.00	C2B—C3B—H3B	119.00
C2A—C1A—H1A1	109.00	C4B—C3B—H3B	119.00
C2A—C1A—H1A2	109.00	C3B—C4B—H4B	120.00
C2A—C1A—H1A3	109.00	C5B—C4B—H4B	120.00
H1A1—C1A—H1A3	109.00	C5B—C6B—H6B	120.00
H1A2—C1A—H1A3	110.00	C7B—C6B—H6B	120.00
C2A—C3A—H3A	119.00	C2B—C7B—H7B	119.00
C4A—C3A—H3A	119.00	C6B—C7B—H7B	119.00
C3A—C4A—H4A	120.00	O1B—C8B—H8B1	109.00
C5A—C4A—H4A	120.00	O1B—C8B—H8B2	109.00
C5A—C6A—H6A	120.00	C9B—C8B—H8B1	109.00
C7A—C6A—H6A	120.00	C9B—C8B—H8B2	109.00
C6A—C7A—H7A	119.00	H8B1—C8B—H8B2	108.00
C2A—C7A—H7A	119.00	N2B—C10B—H10B	119.00
C9A—C8A—H8A2	109.00	C11B—C10B—H10B	119.00

O1A—C8A—H8A1	109.00	C11B—C12B—H12B	119.00
O1A—C8A—H8A2	109.00	C13B—C12B—H12B	119.00
C9A—C8A—H8A1	109.00	C12B—C13B—H13B	120.00
H8A1—C8A—H8A2	108.00	C14B—C13B—H13B	120.00
N2A—C10A—H10A	119.00	C14B—C15B—H15B	120.00
C11A—C10A—H10A	119.00	C16B—C15B—H15B	120.00
C13A—C12A—H12A	119.00	C11B—C16B—H16B	119.00
C11A—C12A—H12A	119.00	C15B—C16B—H16B	119.00
C12A—C13A—H13A	120.00	O3B—C17B—H17A	109.00
C14A—C13A—H13A	120.00	O3B—C17B—H17B	109.00
C14A—C15A—H15	119.00	O3B—C17B—H17C	109.00
C16A—C15A—H15	119.00	H17A—C17B—H17B	110.00
C15A—C16A—H16A	120.00	H17A—C17B—H17C	109.00
C11A—C16A—H16A	120.00	H17B—C17B—H17C	109.00

C8A—O1A—C5A—C4A	11.6 (3)	C12A—C11A—C16A—C15A	0.4 (3)
C8A—O1A—C5A—C6A	−169.82 (17)	C10A—C11A—C16A—C15A	−178.99 (17)
C5A—O1A—C8A—C9A	78.4 (2)	C16A—C11A—C12A—C13A	−1.2 (3)
C17A—O3A—C14A—C13A	4.2 (3)	C11A—C12A—C13A—C14A	0.5 (3)
C17A—O3A—C14A—C15A	−175.89 (16)	C12A—C13A—C14A—C15A	1.2 (3)
C5B—O1B—C8B—C9B	−83.13 (19)	C12A—C13A—C14A—O3A	−178.86 (16)
C8B—O1B—C5B—C6B	13.8 (3)	C13A—C14A—C15A—C16A	−2.1 (3)
C8B—O1B—C5B—C4B	−166.35 (17)	O3A—C14A—C15A—C16A	177.98 (17)
C17B—O3B—C14B—C13B	−6.1 (2)	C14A—C15A—C16A—C11A	1.3 (3)
C17B—O3B—C14B—C15B	174.49 (16)	C7B—C2B—C3B—C4B	−1.4 (4)
C9A—N1A—N2A—C10A	−178.18 (15)	C1B—C2B—C3B—C4B	−179.9 (3)
N2A—N1A—C9A—C8A	2.3 (2)	C1B—C2B—C7B—C6B	179.1 (3)
N2A—N1A—C9A—O2A	−179.33 (15)	C3B—C2B—C7B—C6B	0.5 (4)
N1A—N2A—C10A—C11A	−179.54 (14)	C2B—C3B—C4B—C5B	0.7 (4)
N2B—N1B—C9B—O2B	−175.47 (15)	C3B—C4B—C5B—O1B	−179.08 (19)
C9B—N1B—N2B—C10B	177.21 (15)	C3B—C4B—C5B—C6B	0.8 (3)
N2B—N1B—C9B—C8B	5.3 (2)	C4B—C5B—C6B—C7B	−1.6 (3)
N1B—N2B—C10B—C11B	−177.30 (14)	O1B—C5B—C6B—C7B	178.25 (18)
C3A—C2A—C7A—C6A	0.6 (4)	C5B—C6B—C7B—C2B	1.0 (3)
C1A—C2A—C7A—C6A	−178.8 (3)	O1B—C8B—C9B—O2B	5.5 (2)
C7A—C2A—C3A—C4A	−1.0 (4)	O1B—C8B—C9B—N1B	−175.26 (14)
C1A—C2A—C3A—C4A	178.4 (2)	N2B—C10B—C11B—C12B	8.7 (3)
C2A—C3A—C4A—C5A	−0.1 (3)	N2B—C10B—C11B—C16B	−172.91 (16)
C3A—C4A—C5A—C6A	1.6 (3)	C10B—C11B—C12B—C13B	178.64 (17)
C3A—C4A—C5A—O1A	−179.9 (2)	C16B—C11B—C12B—C13B	0.2 (3)
C4A—C5A—C6A—C7A	−2.0 (3)	C10B—C11B—C16B—C15B	−178.20 (17)
O1A—C5A—C6A—C7A	179.4 (2)	C12B—C11B—C16B—C15B	0.3 (3)
C5A—C6A—C7A—C2A	0.9 (4)	C11B—C12B—C13B—C14B	−0.5 (3)
O1A—C8A—C9A—O2A	9.7 (2)	C12B—C13B—C14B—O3B	−179.03 (16)
O1A—C8A—C9A—N1A	−171.96 (15)	C12B—C13B—C14B—C15B	0.4 (3)
N2A—C10A—C11A—C16A	−0.8 (3)	O3B—C14B—C15B—C16B	179.53 (16)
N2A—C10A—C11A—C12A	179.88 (16)	C13B—C14B—C15B—C16B	0.0 (3)
C10A—C11A—C12A—C13A	178.13 (17)	C14B—C15B—C16B—C11B	−0.4 (3)

Hydrogen-bond geometry (Å, º)

Cg1, Cg2, Cg3 and Cg4 are the centroids of the C2*A*–C7*A*, C11*A*–C16*A*, C2*B*–C7*B* and C11*B*–C16*B* rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O2*A*^{i}	0.86	2.07	2.9226 (17)	173
N1*B*—H1*B*···O2*B*^{ii}	0.86	2.07	2.9207 (17)	171
C17*B*—H17*C*···O1*B*^{iii}	0.96	2.45	3.394 (2)	167
C3*A*—H3*A*···*Cg*3^{ii}	0.93	2.95	3.549 (2)	123
C6*A*—H6*A*···*Cg*3^{i}	0.93	2.98	3.698 (2)	135
C16*B*—H16*B*···*Cg*1	0.93	2.81	3.742 (2)	177
C17*B*—H17*A*···*Cg*2^{i}	0.96	2.81	3.569 (2)	136
C17*A*—H17*D*···*Cg*4^{ii}	0.96	2.93	3.619 (2)	130

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