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(1*R*,2*R*)-*N*,*N*′-Bis(4-nitrophenylmethylene)-cyclohexane-1,2-diamine

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.006 Å
R factor = 0.060
wR factor = 0.124
Data-to-parameter ratio = 9.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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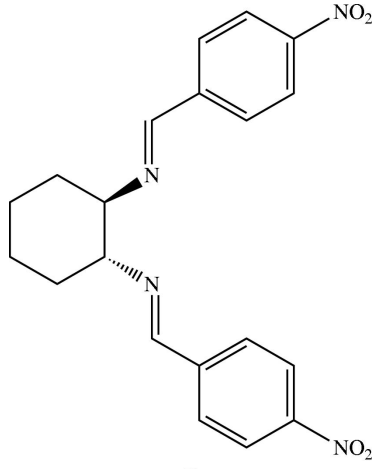
The title compound, $C_{20}H_{20}N_4O_4$, crystallizes with two molecules in the asymmetric unit. Each independent molecule exhibits approximate twofold rotation symmetry, but conformational differences between the molecules preclude any higher symmetry.

Comment

Following on from our study of the crystal structures of the diimines, *N*,*N*′-bis(4-nitrobenzylidene)ethane-1,2-diamine and -propane-1,3-diamine, obtained from 4-nitrobenzaldehyde and the appropriate α,ω-diaminoalkanes (Bomfim *et al.*, 2005), we have now studied the structure of the title compound, (I), in which the functional groups are on adjacent carbon sites in a carbocyclic ring.



(I)

In the two independent molecules of compound (I) (Fig. 1), the corresponding bond distances and interbond angles are very similar, showing no unusual values. There are clear differences between the single C—N and double C═N bonds (Table 1). The four independent chains which are pendent from the cyclohexane rings all occupy equatorial sites (Fig. 1) and all have fairly similar conformations (Table 1), such that each molecule has approximate, although not exact, twofold rotational symmetry. The biggest difference between the two independent molecules arises from the torsion angles between the nitro groups on the benzene rings, 9.8 (2) and 17.6 (2)° in molecule *A*, but only 0.8 (2) and 1.3 (2)° in molecule *B*. These differences suffice to preclude the possibility of any additional crystallographic symmetry. There is only one direction-specific interaction between the molecules (Table 2) which might be of significance. Otherwise, the structure consists of isolated pseudosymmetric molecules.

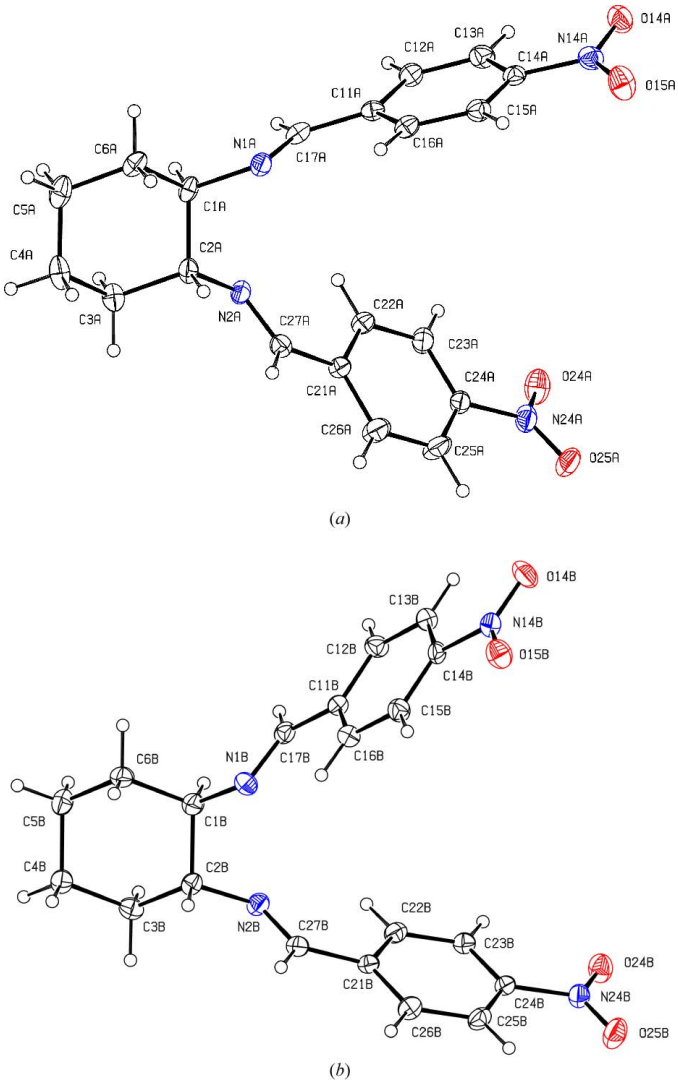


Figure 1
The two independent molecules of compound (I), showing the atom-labelling scheme for (*a*) molecule *A* and (*b*) molecule *B*. Displacement ellipsoids are drawn at the 30% probability level.

Experimental

A mixture of (1*R*,2*R*)-cyclohexane-1,2-diamine (0.228 g, 2 mmol) and 4-nitrobenzaldehyde (0.604 g, 4 mmol) in MeOH (30 ml) was heated under reflux for 30 min. The solution was then cooled to ambient temperature and the solvent was removed. The resulting solid was recrystallized from aqueous ethanol (m.p. 381–382 K). IR (KBr disk) (ν, cm^{-1}): 2924, 2853, 1644, 1602, 1521, 1347, 1140, 1107, 936, 860, 829, 747, 690, 584, 484, 444.

Crystal data

$C_{20}H_{20}N_4O_4$
M_r = 380.40
Monoclinic, *C*2
a = 52.275 (3) Å
b = 5.3605 (2) Å
c = 14.0209 (8) Å
β = 104.952 (2)°
V = 3795.9 (3) Å^3
Z = 8
D_x = 1.331 Mg m^{-3}
Mo Kα radiation
Cell parameters from 4774 reflections
θ = 3.0–27.7°
μ = 0.10 mm^{-1}
T = 120 (2) K
Needle, yellow
0.38 × 0.06 × 0.04 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.956, T_{max} = 0.996
19 060 measured reflections
4774 independent reflections
2943 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 27.7°
$h = -67 \rightarrow 67$
$k = -6 \rightarrow 6$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.124
S = 1.02
4774 reflections
505 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 2.286P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Friedel pairs merged

Table 1
Selected geometric parameters (Å, °).

C1*A*—N1*A*	1.468 (5)	C1*B*—N1*B*	1.448 (5)
C2*A*—N2*A*	1.467 (5)	C2*B*—N2*B*	1.460 (5)
N1*A*—C17*A*	1.254 (5)	N1*B*—C17*B*	1.262 (5)
N2*A*—C27*A*	1.277 (5)	N2*B*—C27*B*	1.269 (5)
C2*A*—C1*A*—N1*A*—C17*A*	108.4 (4)	C2*B*—C1*B*—N1*B*—C17*B*	136.7 (4)
C1*A*—N1*A*—C17*A*—C11*A*	−176.0 (4)	C1*B*—N1*B*—C17*B*—C11*B*	177.1 (4)
N1*A*—C17*A*—C11*A*—C12*A*	−178.8 (4)	N1*B*—C17*B*—C11*B*—C12*B*	−176.5 (4)
C13*A*—C14*A*—N14*A*—O14*A*	10.2 (6)	C13*B*—C14*B*—N14*B*—O14*B*	−2.0 (6)
C1*A*—C2*A*—N2*A*—C27*A*	137.6 (4)	C1*B*—C2*B*—N2*B*—C27*B*	122.2 (4)
C2*A*—N2*A*—C27*A*—C21*A*	−173.2 (3)	C2*B*—N2*B*—C27*B*—C21*B*	−173.6 (3)
N2*A*—C27*A*—C21*A*—C26*A*	−172.5 (4)	N2*B*—C27*B*—C21*B*—C26*B*	177.6 (4)
C23*A*—C24*A*—N24*A*—O24*A*	−15.9 (6)	C23*B*—C24*B*—N24*B*—O24*B*	−2.5 (5)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15*B*—H15*B*···O25*A*^{i}	0.95	2.48	3.392 (6)	161

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

All H atoms were located in difference maps and then treated as riding atoms with C—H distances of 0.95 (aromatic and CH—), 0.99 (CH_2) or 1.00 Å (aliphatic CH), and with U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering, Friedel pairs were merged prior to the final refinement, and the absolute configuration was set according to the known absolute configuration of the (1*R*,2*R*)-1,2-diaminocyclohexane employed in the synthesis.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* (McArdle, 2003) and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England; the authors thank the staff for all their help and advice. JLW thanks CNPq and FAPERJ for financial support.

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Hall symbol: C 2y
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$c = 14.0209$ (8) Å
$\beta = 104.952$ (2)°
$V = 3795.9$ (3) Å^3
$Z = 8$
$F(000) = 1600$
$D_x = 1.331$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4774 reflections
$\theta = 3.0$–27.7°
$\mu = 0.10$ mm^{-1}
$T = 120$ K
Needle, yellow
0.38 × 0.06 × 0.04 mm

Data collection

Bruker–Nonius 95mm CCD camera on κ goniostat diffractometer
Radiation source: Bruker–Nonius FR91 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.956$, $T_{max} = 0.996$
19060 measured reflections
4774 independent reflections
2943 reflections with $I > 2\sigma(I)$
$R_{int} = 0.086$
$\theta_{max} = 27.7°$, $\theta_{min} = 3.0°$
$h = -67\rightarrow67$
$k = -6\rightarrow6$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.124$
$S = 1.02$
4774 reflections
505 parameters
1 restraint
Primary atom site location: Patterson
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 2.286P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Absolute structure: Friedel pairs merged

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1A	0.50443 (8)	0.3481 (8)	0.8160 (3)	0.0290 (10)

C2A	0.49925 (8)	0.2985 (9)	0.7057 (3)	0.0319 (10)
C3A	0.52537 (8)	0.2552 (9)	0.6788 (3)	0.0386 (11)
C4A	0.54347 (9)	0.4825 (9)	0.7079 (4)	0.0439 (12)
C5A	0.54826 (8)	0.5380 (9)	0.8169 (4)	0.0440 (12)
C6A	0.52257 (8)	0.5728 (9)	0.8457 (3)	0.0363 (11)
N1A	0.47915 (6)	0.3949 (7)	0.8403 (2)	0.0310 (8)
C17A	0.47026 (8)	0.2321 (8)	0.8874 (3)	0.0306 (10)
C11A	0.44432 (8)	0.2550 (8)	0.9096 (3)	0.0273 (9)
C12A	0.43571 (8)	0.0703 (8)	0.9638 (3)	0.0324 (10)
C13A	0.41095 (9)	0.0825 (9)	0.9809 (3)	0.0355 (11)
C14A	0.39483 (8)	0.2809 (8)	0.9421 (3)	0.0296 (10)
C15A	0.40263 (8)	0.4671 (9)	0.8887 (3)	0.0331 (10)
C16A	0.42775 (8)	0.4562 (8)	0.8741 (3)	0.0324 (10)
N14A	0.36808 (7)	0.2899 (7)	0.9575 (3)	0.0363 (9)
O14A	0.36241 (6)	0.1425 (6)	1.0152 (2)	0.0469 (9)
O15A	0.35262 (6)	0.4470 (6)	0.9124 (3)	0.0518 (9)
N2A	0.48190 (6)	0.0800 (7)	0.6809 (3)	0.0307 (8)
C27A	0.46312 (8)	0.0903 (8)	0.6020 (3)	0.0303 (10)
C21A	0.44289 (8)	−0.1038 (8)	0.5754 (3)	0.0295 (10)
C22A	0.44032 (8)	−0.2850 (8)	0.6428 (3)	0.0328 (10)
C23A	0.41974 (8)	−0.4565 (9)	0.6204 (3)	0.0374 (11)
C24A	0.40137 (8)	−0.4370 (8)	0.5304 (3)	0.0317 (10)
C25A	0.40383 (9)	−0.2639 (10)	0.4614 (3)	0.0454 (12)
C26A	0.42484 (9)	−0.0984 (10)	0.4839 (3)	0.0458 (13)
N24A	0.37859 (7)	−0.6069 (8)	0.5089 (3)	0.0406 (10)
O24A	0.37956 (6)	−0.7927 (7)	0.5606 (3)	0.0544 (9)
O25A	0.35923 (6)	−0.5499 (7)	0.4413 (2)	0.0536 (9)
C1B	0.74978 (8)	0.4396 (9)	0.8373 (3)	0.0325 (10)
C2B	0.76180 (8)	0.4089 (8)	0.7489 (3)	0.0298 (10)
C3B	0.78859 (8)	0.2805 (9)	0.7791 (3)	0.0354 (11)
C4B	0.80765 (8)	0.4167 (9)	0.8627 (3)	0.0354 (11)
C5B	0.79599 (8)	0.4411 (9)	0.9512 (3)	0.0378 (11)
C6B	0.76935 (8)	0.5748 (9)	0.9223 (3)	0.0346 (11)
N1B	0.72597 (7)	0.5891 (7)	0.8079 (3)	0.0327 (9)
C17B	0.70609 (8)	0.5181 (8)	0.8361 (3)	0.0300 (10)
C11B	0.68122 (8)	0.6610 (8)	0.8147 (3)	0.0305 (10)
C12B	0.66043 (8)	0.5796 (9)	0.8525 (3)	0.0337 (11)
C13B	0.63698 (8)	0.7128 (9)	0.8339 (3)	0.0340 (11)
C14B	0.63492 (8)	0.9244 (8)	0.7771 (3)	0.0288 (10)
C15B	0.65521 (8)	1.0133 (9)	0.7398 (3)	0.0343 (11)
C16B	0.67853 (9)	0.8809 (9)	0.7598 (3)	0.0333 (11)
N14B	0.60994 (7)	1.0675 (8)	0.7559 (3)	0.0387 (10)
O14B	0.59175 (6)	0.9868 (7)	0.7879 (2)	0.0513 (9)
O15B	0.60827 (6)	1.2569 (7)	0.7062 (2)	0.0467 (8)
N2B	0.74318 (7)	0.2571 (7)	0.6764 (2)	0.0323 (9)
C27B	0.73370 (8)	0.3451 (8)	0.5905 (3)	0.0301 (10)
C21B	0.71275 (8)	0.2157 (8)	0.5160 (3)	0.0286 (10)
C22B	0.70190 (8)	−0.0074 (8)	0.5390 (3)	0.0310 (10)

C23B	0.68042 (8)	−0.1134 (8)	0.4735 (3)	0.0313 (10)
C24B	0.67008 (8)	0.0033 (8)	0.3847 (3)	0.0290 (10)
C25B	0.68072 (8)	0.2215 (9)	0.3581 (3)	0.0342 (11)
C26B	0.70255 (9)	0.3261 (8)	0.4248 (3)	0.0330 (11)
N24B	0.64679 (7)	−0.1063 (8)	0.3148 (3)	0.0366 (9)
O24B	0.63809 (6)	−0.3038 (6)	0.3376 (2)	0.0446 (8)
O25B	0.63765 (6)	0.0013 (7)	0.2362 (2)	0.0513 (9)
H1A	0.5131	0.1982	0.8533	0.035*
H2A	0.4901	0.4465	0.6684	0.038*
H3A1	0.5219	0.2255	0.6069	0.046*
H3A2	0.5342	0.1054	0.7137	0.046*
H4A1	0.5606	0.4502	0.6923	0.053*
H4A2	0.5352	0.6293	0.6691	0.053*
H5A1	0.5583	0.3988	0.8556	0.053*
H5A2	0.5591	0.6912	0.8331	0.053*
H6A1	0.5135	0.7242	0.8132	0.044*
H6A2	0.5264	0.5974	0.9180	0.044*
H17A	0.4807	0.0881	0.9097	0.037*
H12A	0.4470	−0.0660	0.9892	0.039*
H13A	0.4051	−0.0426	1.0184	0.043*
H15A	0.3910	0.6006	0.8623	0.040*
H16A	0.4338	0.5869	0.8395	0.039*
H27A	0.4623	0.2291	0.5592	0.036*
H22A	0.4528	−0.2920	0.7053	0.039*
H23A	0.4183	−0.5840	0.6659	0.045*
H25A	0.3913	−0.2576	0.3989	0.055*
H26A	0.4269	0.0201	0.4361	0.055*
H1B	0.7454	0.2720	0.8601	0.039*
H2B	0.7637	0.5762	0.7199	0.036*
H3B1	0.7862	0.1075	0.8000	0.042*
H3B2	0.7962	0.2723	0.7215	0.042*
H4B1	0.8114	0.5847	0.8402	0.042*
H4B2	0.8246	0.3239	0.8823	0.042*
H5B1	0.8084	0.5359	1.0042	0.045*
H5B2	0.7936	0.2732	0.9771	0.045*
H6B1	0.7720	0.7477	0.9018	0.041*
H6B2	0.7618	0.5831	0.9802	0.041*
H17B	0.7072	0.3670	0.8724	0.036*
H12B	0.6624	0.4321	0.8913	0.040*
H13B	0.6227	0.6596	0.8596	0.041*
H15B	0.6531	1.1615	0.7014	0.041*
H16B	0.6929	0.9396	0.7361	0.040*
H27B	0.7403	0.4995	0.5735	0.036*
H22B	0.7094	−0.0868	0.6004	0.037*
H23B	0.6729	−0.2641	0.4894	0.038*
H25B	0.6733	0.2976	0.2959	0.041*
H26B	0.7104	0.4735	0.4078	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.021 (2)	0.025 (2)	0.037 (3)	0.0028 (18)	−0.0001 (19)	0.0048 (19)
C2A	0.023 (2)	0.035 (3)	0.037 (3)	0.001 (2)	0.007 (2)	0.007 (2)
C3A	0.032 (3)	0.038 (3)	0.048 (3)	−0.002 (2)	0.014 (2)	−0.001 (2)
C4A	0.030 (3)	0.035 (3)	0.071 (4)	0.000 (2)	0.022 (2)	0.008 (3)
C5A	0.030 (3)	0.037 (3)	0.061 (3)	−0.007 (2)	0.003 (2)	0.012 (3)
C6A	0.032 (2)	0.035 (3)	0.036 (3)	−0.007 (2)	−0.002 (2)	0.002 (2)
N1A	0.026 (2)	0.033 (2)	0.032 (2)	−0.0022 (17)	0.0046 (16)	0.0004 (18)
C17A	0.032 (2)	0.027 (3)	0.027 (2)	0.000 (2)	−0.0031 (19)	−0.001 (2)
C11A	0.033 (2)	0.024 (2)	0.024 (2)	−0.001 (2)	0.0052 (18)	−0.0006 (19)
C12A	0.033 (2)	0.031 (3)	0.032 (2)	0.001 (2)	0.006 (2)	0.001 (2)
C13A	0.040 (3)	0.035 (3)	0.031 (3)	0.000 (2)	0.009 (2)	0.006 (2)
C14A	0.031 (2)	0.031 (3)	0.025 (2)	0.001 (2)	0.0050 (19)	−0.007 (2)
C15A	0.035 (3)	0.034 (3)	0.030 (2)	0.004 (2)	0.006 (2)	0.001 (2)
C16A	0.034 (3)	0.029 (3)	0.030 (2)	−0.001 (2)	0.0014 (19)	0.002 (2)
N14A	0.039 (2)	0.036 (2)	0.035 (2)	0.005 (2)	0.0120 (19)	−0.0043 (19)
O14A	0.041 (2)	0.059 (2)	0.044 (2)	−0.0001 (17)	0.0165 (17)	0.0113 (17)
O15A	0.045 (2)	0.044 (2)	0.071 (2)	0.0171 (19)	0.0233 (19)	0.012 (2)
N2A	0.0234 (19)	0.035 (2)	0.032 (2)	−0.0019 (17)	0.0048 (16)	0.0005 (17)
C27A	0.030 (2)	0.031 (2)	0.031 (2)	0.002 (2)	0.010 (2)	0.003 (2)
C21A	0.029 (2)	0.032 (3)	0.027 (2)	−0.001 (2)	0.0047 (19)	−0.002 (2)
C22A	0.030 (2)	0.039 (3)	0.027 (2)	0.004 (2)	0.0021 (19)	0.004 (2)
C23A	0.028 (2)	0.044 (3)	0.040 (3)	−0.002 (2)	0.008 (2)	0.003 (2)
C24A	0.025 (2)	0.037 (3)	0.033 (3)	−0.003 (2)	0.008 (2)	−0.008 (2)
C25A	0.044 (3)	0.054 (3)	0.030 (3)	−0.006 (3)	−0.007 (2)	0.005 (3)
C26A	0.047 (3)	0.051 (3)	0.033 (3)	−0.013 (3)	0.000 (2)	0.005 (3)
N24A	0.029 (2)	0.044 (3)	0.050 (3)	−0.006 (2)	0.012 (2)	−0.017 (2)
O24A	0.042 (2)	0.047 (2)	0.074 (3)	−0.0147 (18)	0.0148 (19)	0.001 (2)
O25A	0.0317 (19)	0.071 (3)	0.051 (2)	−0.0090 (19)	−0.0009 (17)	−0.020 (2)
C1B	0.031 (2)	0.038 (3)	0.029 (2)	0.003 (2)	0.0067 (19)	0.002 (2)
C2B	0.032 (2)	0.028 (2)	0.027 (2)	−0.002 (2)	0.0045 (19)	−0.001 (2)
C3B	0.034 (3)	0.037 (3)	0.038 (3)	0.004 (2)	0.014 (2)	−0.002 (2)
C4B	0.032 (2)	0.039 (3)	0.034 (2)	0.000 (2)	0.006 (2)	−0.002 (2)
C5B	0.034 (3)	0.042 (3)	0.033 (2)	0.001 (2)	0.001 (2)	0.000 (2)
C6B	0.034 (2)	0.041 (3)	0.031 (2)	0.004 (2)	0.012 (2)	−0.002 (2)
N1B	0.029 (2)	0.032 (2)	0.038 (2)	0.0027 (17)	0.0111 (17)	0.0002 (17)
C17B	0.033 (2)	0.030 (3)	0.026 (2)	−0.006 (2)	0.0046 (19)	−0.0029 (19)
C11B	0.028 (2)	0.037 (3)	0.026 (2)	−0.003 (2)	0.0073 (19)	−0.006 (2)
C12B	0.034 (3)	0.035 (3)	0.033 (3)	0.002 (2)	0.011 (2)	0.005 (2)
C13B	0.030 (2)	0.039 (3)	0.033 (3)	−0.006 (2)	0.008 (2)	−0.002 (2)
C14B	0.020 (2)	0.036 (3)	0.028 (2)	0.004 (2)	0.0014 (17)	−0.003 (2)
C15B	0.031 (2)	0.037 (3)	0.034 (3)	0.001 (2)	0.007 (2)	0.004 (2)
C16B	0.031 (2)	0.039 (3)	0.032 (2)	−0.002 (2)	0.010 (2)	0.000 (2)
N14B	0.030 (2)	0.050 (3)	0.033 (2)	−0.003 (2)	0.0036 (18)	−0.006 (2)
O14B	0.0289 (18)	0.069 (2)	0.059 (2)	0.0013 (18)	0.0175 (17)	0.006 (2)
O15B	0.0394 (19)	0.043 (2)	0.056 (2)	0.0021 (17)	0.0112 (17)	0.0052 (19)

N2B	0.036 (2)	0.032 (2)	0.028 (2)	−0.0038 (18)	0.0066 (17)	−0.0012 (18)
C27B	0.032 (3)	0.030 (3)	0.030 (2)	−0.001 (2)	0.011 (2)	−0.001 (2)
C21B	0.029 (2)	0.035 (3)	0.023 (2)	0.002 (2)	0.0087 (19)	−0.002 (2)
C22B	0.034 (2)	0.034 (3)	0.025 (2)	0.004 (2)	0.0078 (19)	0.001 (2)
C23B	0.031 (2)	0.034 (3)	0.029 (2)	0.001 (2)	0.009 (2)	−0.002 (2)
C24B	0.028 (2)	0.036 (3)	0.023 (2)	0.002 (2)	0.0063 (18)	−0.0020 (19)
C25B	0.038 (3)	0.039 (3)	0.024 (2)	0.007 (2)	0.004 (2)	0.004 (2)
C26B	0.039 (3)	0.029 (3)	0.030 (2)	0.003 (2)	0.007 (2)	0.006 (2)
N24B	0.029 (2)	0.045 (3)	0.033 (2)	0.002 (2)	0.0046 (18)	−0.005 (2)
O24B	0.042 (2)	0.041 (2)	0.047 (2)	−0.0096 (17)	0.0055 (16)	0.0015 (17)
O25B	0.050 (2)	0.058 (2)	0.0364 (19)	−0.0061 (18)	−0.0056 (16)	0.0076 (18)

Geometric parameters (Å, º)

C1A—N1A	1.468 (5)	C1B—N1B	1.448 (5)
C1A—C6A	1.523 (6)	C1B—C2B	1.537 (5)
C1A—C2A	1.524 (6)	C1B—C6B	1.537 (6)
C1A—H1A	1.00	C1B—H1B	1.00
C2A—N2A	1.467 (5)	C2B—N2B	1.460 (5)
C2A—C3A	1.524 (5)	C2B—C3B	1.519 (6)
C2A—H2A	1.00	C2B—H2B	1.00
C3A—C4A	1.532 (6)	C3B—C4B	1.516 (6)
C3A—H3A1	0.99	C3B—H3B1	0.99
C3A—H3A2	0.99	C3B—H3B2	0.99
C4A—C5A	1.514 (6)	C4B—C5B	1.522 (5)
C4A—H4A1	0.99	C4B—H4B1	0.99
C4A—H4A2	0.99	C4B—H4B2	0.99
C5A—C6A	1.510 (6)	C5B—C6B	1.525 (6)
C5A—H5A1	0.99	C5B—H5B1	0.99
C5A—H5A2	0.99	C5B—H5B2	0.99
C6A—H6A1	0.99	C6B—H6B1	0.99
C6A—H6A2	0.99	C6B—H6B2	0.99
N1A—C17A	1.254 (5)	N1B—C17B	1.262 (5)
C17A—C11A	1.473 (5)	C17B—C11B	1.472 (6)
C17A—H17A	0.95	C17B—H17B	0.95
C11A—C12A	1.391 (6)	C11B—C16B	1.395 (6)
C11A—C16A	1.393 (6)	C11B—C12B	1.396 (5)
C12A—C13A	1.378 (6)	C12B—C13B	1.384 (6)
C12A—H12A	0.95	C12B—H12B	0.95
C13A—C14A	1.379 (6)	C13B—C14B	1.374 (6)
C13A—H13A	0.95	C13B—H13B	0.95
C14A—C15A	1.371 (6)	C14B—C15B	1.383 (5)
C14A—N14A	1.470 (5)	C14B—N14B	1.477 (5)
C15A—C16A	1.382 (5)	C15B—C16B	1.375 (6)
C15A—H15A	0.95	C15B—H15B	0.95
C16A—H16A	0.95	C16B—H16B	0.95
N14A—O14A	1.220 (4)	N14B—O15B	1.222 (5)
N14A—O15A	1.224 (5)	N14B—O14B	1.230 (4)

N2A—C27A	1.277 (5)	N2B—C27B	1.269 (5)
C27A—C21A	1.462 (6)	C27B—C21B	1.477 (6)
C27A—H27A	0.95	C27B—H27B	0.95
C21A—C26A	1.382 (6)	C21B—C26B	1.384 (5)
C21A—C22A	1.386 (6)	C21B—C22B	1.396 (6)
C22A—C23A	1.388 (6)	C22B—C23B	1.376 (6)
C22A—H22A	0.95	C22B—H22B	0.95
C23A—C24A	1.379 (6)	C23B—C24B	1.374 (6)
C23A—H23A	0.95	C23B—H23B	0.95
C24A—C25A	1.369 (6)	C24B—C25B	1.387 (6)
C24A—N24A	1.468 (5)	C24B—N24B	1.474 (5)
C25A—C26A	1.383 (6)	C25B—C26B	1.393 (6)
C25A—H25A	0.95	C25B—H25B	0.95
C26A—H26A	0.95	C26B—H26B	0.95
N24A—O24A	1.225 (5)	N24B—O25B	1.226 (4)
N24A—O25A	1.234 (5)	N24B—O24B	1.227 (5)

N1A—C1A—C6A	109.6 (3)	N1B—C1B—C2B	109.3 (3)
N1A—C1A—C2A	109.3 (3)	N1B—C1B—C6B	108.1 (4)
C6A—C1A—C2A	110.5 (3)	C2B—C1B—C6B	110.3 (3)
N1A—C1A—H1A	109.1	N1B—C1B—H1B	109.7
C6A—C1A—H1A	109.1	C2B—C1B—H1B	109.7
C2A—C1A—H1A	109.1	C6B—C1B—H1B	109.7
N2A—C2A—C1A	108.4 (3)	N2B—C2B—C3B	110.0 (3)
N2A—C2A—C3A	111.0 (3)	N2B—C2B—C1B	106.5 (3)
C1A—C2A—C3A	110.0 (3)	C3B—C2B—C1B	111.3 (3)
N2A—C2A—H2A	109.1	N2B—C2B—H2B	109.7
C1A—C2A—H2A	109.1	C3B—C2B—H2B	109.7
C3A—C2A—H2A	109.1	C1B—C2B—H2B	109.7
C2A—C3A—C4A	110.1 (4)	C4B—C3B—C2B	111.8 (4)
C2A—C3A—H3A1	109.6	C4B—C3B—H3B1	109.2
C4A—C3A—H3A1	109.6	C2B—C3B—H3B1	109.2
C2A—C3A—H3A2	109.6	C4B—C3B—H3B2	109.2
C4A—C3A—H3A2	109.6	C2B—C3B—H3B2	109.2
H3A1—C3A—H3A2	108.1	H3B1—C3B—H3B2	107.9
C5A—C4A—C3A	110.8 (4)	C3B—C4B—C5B	110.5 (3)
C5A—C4A—H4A1	109.5	C3B—C4B—H4B1	109.5
C3A—C4A—H4A1	109.5	C5B—C4B—H4B1	109.5
C5A—C4A—H4A2	109.5	C3B—C4B—H4B2	109.5
C3A—C4A—H4A2	109.5	C5B—C4B—H4B2	109.5
H4A1—C4A—H4A2	108.1	H4B1—C4B—H4B2	108.1
C6A—C5A—C4A	111.6 (4)	C4B—C5B—C6B	110.7 (4)
C6A—C5A—H5A1	109.3	C4B—C5B—H5B1	109.5
C4A—C5A—H5A1	109.3	C6B—C5B—H5B1	109.5
C6A—C5A—H5A2	109.3	C4B—C5B—H5B2	109.5
C4A—C5A—H5A2	109.3	C6B—C5B—H5B2	109.5
H5A1—C5A—H5A2	108.0	H5B1—C5B—H5B2	108.1
C5A—C6A—C1A	111.3 (4)	C5B—C6B—C1B	111.4 (4)

C5A—C6A—H6A1	109.4	C5B—C6B—H6B1	109.4
C1A—C6A—H6A1	109.4	C1B—C6B—H6B1	109.4
C5A—C6A—H6A2	109.4	C5B—C6B—H6B2	109.4
C1A—C6A—H6A2	109.4	C1B—C6B—H6B2	109.4
H6A1—C6A—H6A2	108.0	H6B1—C6B—H6B2	108.0
C17A—N1A—C1A	118.8 (4)	C17B—N1B—C1B	117.5 (4)
N1A—C17A—C11A	122.7 (4)	N1B—C17B—C11B	122.3 (4)
N1A—C17A—H17A	118.7	N1B—C17B—H17B	118.8
C11A—C17A—H17A	118.7	C11B—C17B—H17B	118.8
C12A—C11A—C16A	119.2 (4)	C16B—C11B—C12B	119.8 (4)
C12A—C11A—C17A	120.1 (4)	C16B—C11B—C17B	120.7 (4)
C16A—C11A—C17A	120.7 (4)	C12B—C11B—C17B	119.6 (4)
C13A—C12A—C11A	120.8 (4)	C13B—C12B—C11B	120.4 (4)
C13A—C12A—H12A	119.6	C13B—C12B—H12B	119.8
C11A—C12A—H12A	119.6	C11B—C12B—H12B	119.8
C12A—C13A—C14A	118.3 (4)	C14B—C13B—C12B	117.9 (4)
C12A—C13A—H13A	120.8	C14B—C13B—H13B	121.0
C14A—C13A—H13A	120.8	C12B—C13B—H13B	121.0
C15A—C14A—C13A	122.6 (4)	C13B—C14B—C15B	123.4 (4)
C15A—C14A—N14A	119.0 (4)	C13B—C14B—N14B	118.6 (4)
C13A—C14A—N14A	118.4 (4)	C15B—C14B—N14B	118.0 (4)
C14A—C15A—C16A	118.6 (4)	C16B—C15B—C14B	118.1 (4)
C14A—C15A—H15A	120.7	C16B—C15B—H15B	120.9
C16A—C15A—H15A	120.7	C14B—C15B—H15B	120.9
C15A—C16A—C11A	120.5 (4)	C15B—C16B—C11B	120.4 (4)
C15A—C16A—H16A	119.8	C15B—C16B—H16B	119.8
C11A—C16A—H16A	119.8	C11B—C16B—H16B	119.8
O14A—N14A—O15A	123.1 (4)	O15B—N14B—O14B	123.5 (4)
O14A—N14A—C14A	118.6 (4)	O15B—N14B—C14B	118.4 (4)
O15A—N14A—C14A	118.2 (4)	O14B—N14B—C14B	118.1 (4)
C27A—N2A—C2A	117.4 (4)	C27B—N2B—C2B	118.7 (4)
N2A—C27A—C21A	122.3 (4)	N2B—C27B—C21B	122.2 (4)
N2A—C27A—H27A	118.8	N2B—C27B—H27B	118.9
C21A—C27A—H27A	118.8	C21B—C27B—H27B	118.9
C26A—C21A—C22A	119.0 (4)	C26B—C21B—C22B	119.8 (4)
C26A—C21A—C27A	119.9 (4)	C26B—C21B—C27B	119.4 (4)
C22A—C21A—C27A	121.0 (4)	C22B—C21B—C27B	120.7 (4)
C21A—C22A—C23A	121.1 (4)	C23B—C22B—C21B	120.7 (4)
C21A—C22A—H22A	119.5	C23B—C22B—H22B	119.7
C23A—C22A—H22A	119.5	C21B—C22B—H22B	119.7
C24A—C23A—C22A	118.2 (4)	C24B—C23B—C22B	118.6 (4)
C24A—C23A—H23A	120.9	C24B—C23B—H23B	120.7
C22A—C23A—H23A	120.9	C22B—C23B—H23B	120.7
C25A—C24A—C23A	121.9 (4)	C23B—C24B—C25B	122.5 (4)
C25A—C24A—N24A	119.6 (4)	C23B—C24B—N24B	119.1 (4)
C23A—C24A—N24A	118.5 (4)	C25B—C24B—N24B	118.5 (4)
C24A—C25A—C26A	119.1 (4)	C24B—C25B—C26B	118.3 (4)
C24A—C25A—H25A	120.4	C24B—C25B—H25B	120.8

C26A—C25A—H25A	120.4	C26B—C25B—H25B	120.8
C21A—C26A—C25A	120.7 (4)	C21B—C26B—C25B	120.1 (4)
C21A—C26A—H26A	119.7	C21B—C26B—H26B	119.9
C25A—C26A—H26A	119.7	C25B—C26B—H26B	119.9
O24A—N24A—O25A	123.9 (4)	O25B—N24B—O24B	123.7 (4)
O24A—N24A—C24A	118.4 (4)	O25B—N24B—C24B	118.3 (4)
O25A—N24A—C24A	117.7 (4)	O24B—N24B—C24B	117.9 (4)
N1A—C1A—C2A—N2A	−59.7 (4)	N1B—C1B—C2B—N2B	−67.0 (4)
C6A—C1A—C2A—N2A	179.6 (3)	C6B—C1B—C2B—N2B	174.2 (4)
N1A—C1A—C2A—C3A	178.8 (3)	N1B—C1B—C2B—C3B	173.1 (4)
C6A—C1A—C2A—C3A	58.1 (4)	C6B—C1B—C2B—C3B	54.3 (5)
N2A—C2A—C3A—C4A	−178.4 (4)	N2B—C2B—C3B—C4B	−173.5 (3)
C1A—C2A—C3A—C4A	−58.5 (5)	C1B—C2B—C3B—C4B	−55.7 (5)
C2A—C3A—C4A—C5A	57.2 (5)	C2B—C3B—C4B—C5B	56.8 (5)
C3A—C4A—C5A—C6A	−55.6 (5)	C3B—C4B—C5B—C6B	−57.0 (5)
C4A—C5A—C6A—C1A	55.3 (5)	C4B—C5B—C6B—C1B	57.0 (5)
N1A—C1A—C6A—C5A	−176.9 (3)	N1B—C1B—C6B—C5B	−174.7 (3)
C2A—C1A—C6A—C5A	−56.4 (5)	C2B—C1B—C6B—C5B	−55.3 (5)
C6A—C1A—N1A—C17A	−130.3 (4)	C2B—C1B—N1B—C17B	136.7 (4)
C2A—C1A—N1A—C17A	108.4 (4)	C6B—C1B—N1B—C17B	−103.2 (4)
C1A—N1A—C17A—C11A	−176.0 (4)	C1B—N1B—C17B—C11B	177.1 (4)
N1A—C17A—C11A—C12A	−178.8 (4)	N1B—C17B—C11B—C16B	1.4 (6)
N1A—C17A—C11A—C16A	3.4 (6)	N1B—C17B—C11B—C12B	−176.5 (4)
C16A—C11A—C12A—C13A	1.1 (6)	C16B—C11B—C12B—C13B	1.5 (6)
C17A—C11A—C12A—C13A	−176.7 (4)	C17B—C11B—C12B—C13B	179.5 (4)
C11A—C12A—C13A—C14A	0.7 (6)	C11B—C12B—C13B—C14B	0.4 (6)
C12A—C13A—C14A—C15A	−0.9 (6)	C12B—C13B—C14B—C15B	−1.5 (6)
C12A—C13A—C14A—N14A	178.0 (4)	C12B—C13B—C14B—N14B	179.5 (4)
C13A—C14A—C15A—C16A	−0.7 (6)	C13B—C14B—C15B—C16B	0.7 (6)
N14A—C14A—C15A—C16A	−179.6 (4)	N14B—C14B—C15B—C16B	179.7 (4)
C14A—C15A—C16A—C11A	2.5 (6)	C14B—C15B—C16B—C11B	1.2 (6)
C12A—C11A—C16A—C15A	−2.7 (6)	C12B—C11B—C16B—C15B	−2.3 (6)
C17A—C11A—C16A—C15A	175.0 (4)	C17B—C11B—C16B—C15B	179.8 (4)
C15A—C14A—N14A—O14A	−170.8 (4)	C13B—C14B—N14B—O15B	179.3 (4)
C13A—C14A—N14A—O14A	10.2 (6)	C15B—C14B—N14B—O15B	0.2 (6)
C15A—C14A—N14A—O15A	8.5 (6)	C13B—C14B—N14B—O14B	−2.0 (6)
C13A—C14A—N14A—O15A	−170.5 (4)	C15B—C14B—N14B—O14B	179.0 (4)
C1A—C2A—N2A—C27A	137.6 (4)	C3B—C2B—N2B—C27B	−117.1 (4)
C3A—C2A—N2A—C27A	−101.5 (4)	C1B—C2B—N2B—C27B	122.2 (4)
C2A—N2A—C27A—C21A	−173.2 (3)	C2B—N2B—C27B—C21B	−173.6 (3)
N2A—C27A—C21A—C26A	−172.5 (4)	N2B—C27B—C21B—C26B	177.6 (4)
N2A—C27A—C21A—C22A	11.9 (6)	N2B—C27B—C21B—C22B	2.1 (6)
C26A—C21A—C22A—C23A	−1.2 (6)	C26B—C21B—C22B—C23B	−2.8 (6)
C27A—C21A—C22A—C23A	174.5 (4)	C27B—C21B—C22B—C23B	172.7 (4)
C21A—C22A—C23A—C24A	−2.1 (6)	C21B—C22B—C23B—C24B	0.8 (6)
C22A—C23A—C24A—C25A	3.8 (6)	C22B—C23B—C24B—C25B	1.0 (6)
C22A—C23A—C24A—N24A	−176.0 (4)	C22B—C23B—C24B—N24B	−179.0 (3)

C23A—C24A—C25A—C26A	−2.2 (7)	C23B—C24B—C25B—C26B	−0.7 (6)
N24A—C24A—C25A—C26A	177.6 (4)	N24B—C24B—C25B—C26B	179.3 (4)
C22A—C21A—C26A—C25A	2.9 (7)	C22B—C21B—C26B—C25B	3.1 (6)
C27A—C21A—C26A—C25A	−172.9 (4)	C27B—C21B—C26B—C25B	−172.4 (4)
C24A—C25A—C26A—C21A	−1.2 (7)	C24B—C25B—C26B—C21B	−1.4 (6)
C25A—C24A—N24A—O24A	164.3 (4)	C23B—C24B—N24B—O25B	179.4 (4)
C23A—C24A—N24A—O24A	−15.9 (6)	C25B—C24B—N24B—O25B	−0.6 (5)
C25A—C24A—N24A—O25A	−17.7 (6)	C23B—C24B—N24B—O24B	−2.5 (5)
C23A—C24A—N24A—O25A	162.1 (4)	C25B—C24B—N24B—O24B	177.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15*B*—H15*B*···O25*A*^{i}	0.95	2.48	3.392 (6)	161

Symmetry code: (i) −*x*+1, *y*+2, −*z*+1.