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3,3′-({4-[(4,5-Dicyano-1*H*-imidazol-2-yl)-diazenyl]phenyl}imino)dipropionic acid

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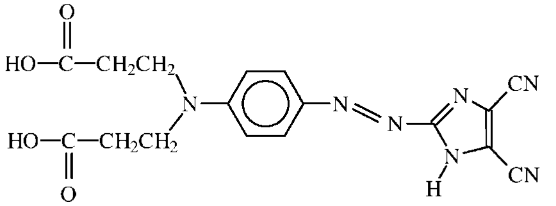
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.075; wR factor = 0.216; data-to-parameter ratio = 15.6.

The title compound, $C_{17}H_{15}N_7O_4$, is a push–pull non-linear optical chromophore containing a dialkylamino donor group and the dicyanoimidazolyl acceptor separated by a π-conjugated path. The benzene and imidazole rings are not coplanar, making a dihedral angle of 10.0 (2)°. In the crystal, molecules are linked by an extended set of hydrogen bonds and several motifs are recognized. Pairs of molecules are held together by hydrogen bonding between carboxy O—H donor groups and diazenyl N-atom acceptors, forming $R_2^2(24)$ ring patterns across inversion centres. Four-molecule $R_4^4(28)$ ring motifs are formed, again across inversion centres, through hydrogen bonding involving carboxy O—H donor groups and diazenyl and imidazole N-atom acceptors. Four-molecule $R_4^4(42)$ patterns are formed among molecules related by translation and involve carboxy O—H and imidazole N—H donor groups with carbonyl O-atom and imidazole N-atom acceptors.

Related literature

For a general survey of advanced materials based on heterocycles, see: Dalton (2002); Heeger (2010). For semiconductor, optoelectronic and piezoelectric materials containing heterocycles, see: Centore, Ricciotti *et al.* (2012); Centore, Concilio *et al.* (2012). For structural analysis of conjugation in heterocycle-based organic molecules, see: Carella, Centore, Fort *et al.* (2004); Gainsford *et al.* (2008). For structural and theoretical analysis of conjugation in metallorganic compounds containing heterocycles, see: Takjoo *et al.* (2011); Takjoo & Centore (2013). For theoretical computations on π-conjugated compounds, see: Capobianco *et al.* (2012, 2013). For the synthesis of related heterocyclic compounds, see: Carella, Centore, Sirigu *et al.* (2004); Piccialli *et al.* (2013); Centore, Fusco, Capobianco *et al.* (2013). For the local packing modes of non-linear optical chromophores see: Thallapally *et al.* (2002); Centore & Piccialli (2012); Centore, Piccialli & Tuzi (2013). For hydrogen bonding in crystal structures, see: Allen *et al.* (1999); Steiner (2002); Centore, Jazbinsek *et al.* (2012); Centore, Fusco, Jazbinsek *et al.* (2013). For the synthesis of similar diazo-chromophores, see: Centore *et al.* (2007).



Experimental

Crystal data

$C_{17}H_{15}N_7O_4$
M_r = 381.36
Triclinic, $P\bar{1}$
a = 6.895 (5) Å
b = 10.443 (3) Å
c = 13.373 (3) Å
α = 105.40 (2)°
β = 103.96 (4)°
γ = 104.84 (4)°
V = 846.5 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.26 × 0.13 × 0.07 mm

Data collection

Enraf–Nonius MACH3 diffractometer
4256 measured reflections
4082 independent reflections
1220 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
1 standard reflections every 120 min intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.216
S = 0.91
4082 reflections
262 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N5^{i}	0.80 (6)	2.12 (6)	2.896 (6)	162 (6)
O3—H3···N3^{ii}	0.88 (5)	1.89 (6)	2.750 (6)	165 (5)
N4—H4···O4^{iii}	0.81 (5)	1.98 (5)	2.740 (6)	156 (5)

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

Data collection: *MACH3/PC* Software (Nonius, 1996); cell refinement: *CELLFITW* (Centore, 2004); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2439).

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supporting information

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3,3′-({4-[(4,5-Dicyano-1*H*-imidazol-2-yl)diazenyl]phenyl}imino)dipropionic acid

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S1. Comment

Aromatic heterocycles are playing a fundamental role in modern material chemistry as building blocks of conjugated active molecules in many fields of organic electronics and optoelectronics: conjugated conducting polymers and organic solar cells (Heeger, 2010), organic field-effect transistors (Centore, Ricciotti *et al.*, 2012), nonlinear optically active and piezoelectric compounds (Dalton, 2002; Centore, Concilio *et al.*, 2012). In those fields, the chemical investigation is devoted to the synthesis of new molecules or conjugated polymers containing heterocyclic moieties and to the measurement of their spectroscopic and electronic properties relevant for device performances. However, also the structural investigation of the molecules is a relevant point for the evaluation of the structural parameters related to the conjugation (Carella, Centore, Fort *et al.*, 2004; Gainsford *et al.*, 2008; Capobianco *et al.*, 2012; Capobianco *et al.*, 2013). The rationalization of the local packing modes of chromophore units (Thallapally *et al.*, 2002; Centore & Piccialli, 2012; Centore, Piccialli & Tuzi, 2013) is another crucial point, because many properties required for optimum device performances (*e. g.* electron mobility) critically depend on the packing not less than on strictly molecular properties. In our research group we are interested in the synthesis of new heterocyclic compounds, including metal containing heterocyclic compounds (Takjoo *et al.*, 2011; Takjoo & Centore, 2013), for applications as advanced materials and bioactive compounds (Piccialli *et al.*, 2013), and in the analysis of crystal structures controlled by the formation of H bonds (Centore, Jazbinsek *et al.*, 2012; Centore, Fusco, Jazbinsek *et al.*, 2013). Following these issues, we report, in the present paper, the structural investigation of the title compound, shown in the Scheme. The title compound is a typical push-pull azo-dye, containing the dialkylamino as donor group and two cyano acceptor groups. Moreover, the cyano groups are attached to an electron poor imidazole ring. The chromophore unit has been used in the synthesis of polymers showing quadratic NLO behaviour (Carella, Centore, Sirigu *et al.*, 2004).

The molecular structure is shown in Fig. 1. The geometry around the donor N1 atom is substantially planar indicating sp^2 hybridization (the sum of valence angles at N1 is 360°) and the pattern of bond lenghts within the adjacent phenyl ring shows a certain degree of quinoidal character. All these structural features are in accordance with the expected π conjugation and push-pull character of the chromophore group.

The two aromatic rings are not coplanar, the dihedral angle between the mean planes being 10.0 (2)°; the π-conjugated part of the molecule has a slighlty curved shape, as the result of small torsions around the bonds C10—N2, N2–N3 and N3–C13.

The molecules of the title compound have several H bonding donor and acceptor groups, and the crystal packing is dominated by the formation of H bonds, Table 1. Several H bonding motifs are recognized in the crystal packing (Allen *et al.*, 1999; Steiner, 2002) and some of them are shown in Fig. 2. Couples of molecules are held by H bonding between carboxy O–H donors and azo N acceptors, forming $R^2_2(24)$ ring patterns across inversion centres. Four-molecule ring motifs $R^4_4(28)$ are formed, again across inversion centres, through H bonding involving carboxy O–H donors and azo and imidazole N acceptors. Four-molecule ring motifs $R^4_4(42)$ are formed, among molecules related by translation, through H bonding involving carboxy O–H and imidazole N–H donors and carbonyl and imidazole N acceptors.

S2. Experimental

The title compound was prepared by diazotization of 2-amino-4,5-dicyanoimidazole followed by coupling with *N,N*-(*bis*2-carboxyethylamino)aniline. The procedure of diazo-coupling is analogous to that we have already described for the synthesis of similar diazo-chromophores (Centore *et al.*, 2007). Purification was obtained by recrystallization from hot acetic acid. The final yield for the diazotization/coupling step was 91%. Mp. 230 °C (dec). Single crystals were obtained by slow evaporation from acetic acid solutions. ^{1}H-NMR (DMSO-d$_6$) δ 2.45 (tr, 4H), 3.61 (tr, 4H), 6.79 (d, 2H, J = 9 Hz), 7.69 (d, 2H, J = 9 Hz). λ_{max}(DMF) = 452 nm, ε_{max}(DMF)= 2.5 × 10 ^{4} L mol^{-1}cm^{-1}.

S3. Refinement

The H atoms of the carboxy groups and of the imidazole ring were located in difmaps and their coordinates were refined. All other H atoms were generated stereochemically and were refined by the riding model. For all H atoms U_{iso}=1.2×U_{eq} of the carrier atom was assumed.

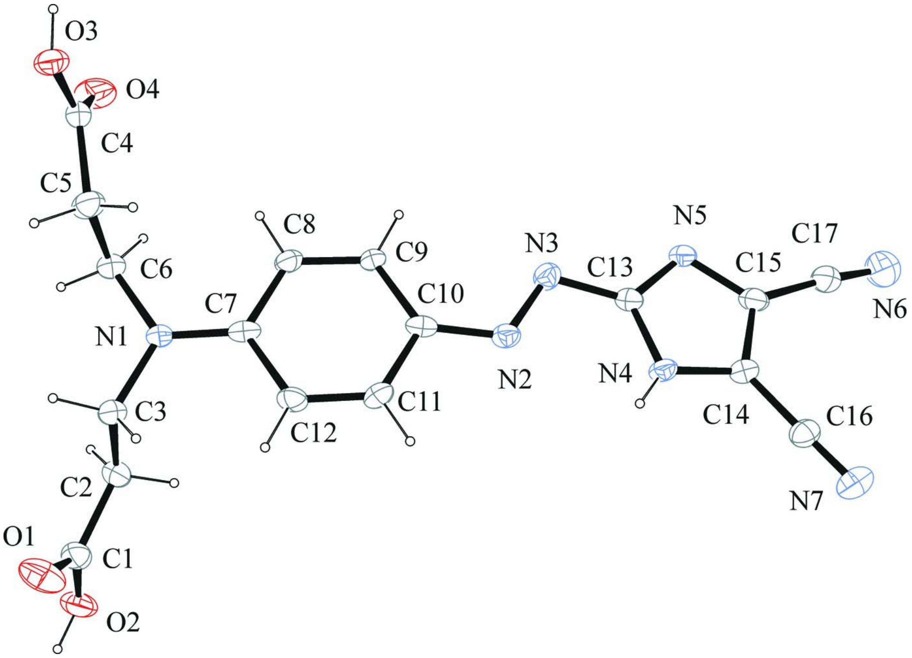

Figure 1

ORTEP view of the molecular structure of the title compound. Thermal ellipsoids are drawn at 30% probability level.

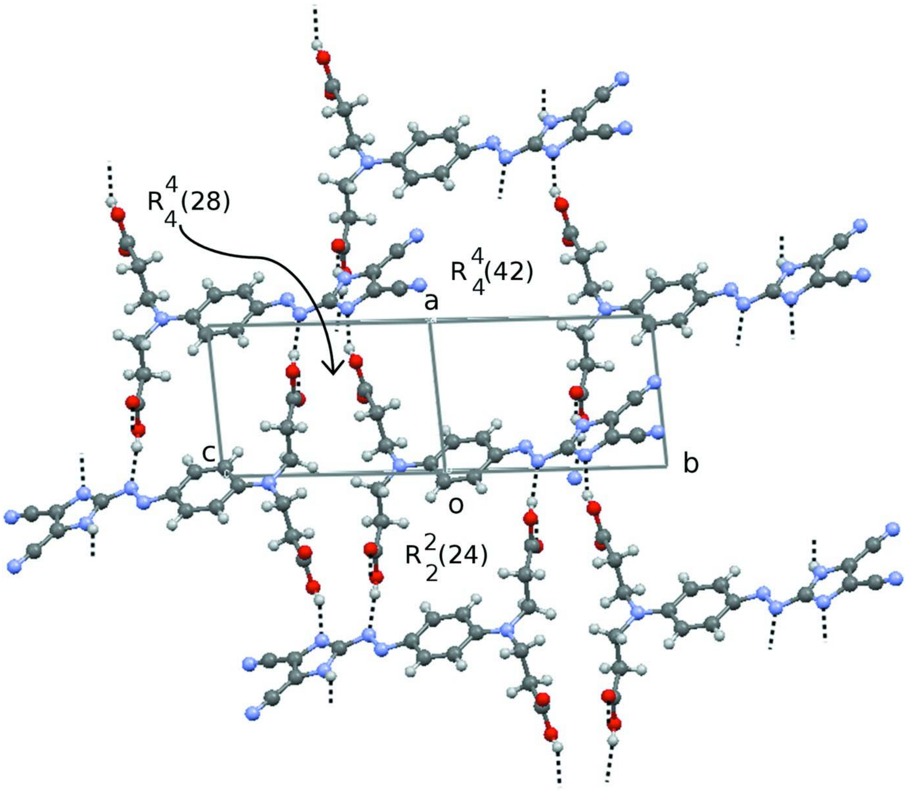

Figure 2

Packing of the title compound viewed along *b* + *c*. H bonds are represented by dashed lines.

3,3′-({4-[(4,5-Dicyano-1*H*-imidazol-2-yl)diazenyl]phenyl}imino)dipropionic acid

Crystal data

$C_{17}H_{15}N_7O_4$
$M_r = 381.36$
Triclinic, $P\overline{1}$
$a = 6.895$ (5) Å
$b = 10.443$ (3) Å
$c = 13.373$ (3) Å
$\alpha = 105.40$ (2)°
$\beta = 103.96$ (4)°
$\gamma = 104.84$ (4)°
$V = 846.5$ (7) Å^3

$Z = 2$
$F(000) = 396$
$D_x = 1.496$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 7.2$–9.8°
$\mu = 0.11$ mm^{-1}
$T = 293$ K
Plate, red
0.26 × 0.13 × 0.07 mm

Data collection

Enraf–Nonius MACH3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Nonprofiled ω scans
4256 measured reflections
4082 independent reflections
1220 reflections with $I > 2\sigma(I)$

$R_{\mathrm{int}} = 0.074$
$\theta_{\max} = 28.0°$, $\theta_{\min} = 1.7°$
$h = -9 \rightarrow 8$
$k = -13 \rightarrow 13$
$l = 0 \rightarrow 17$
1 standard reflections every 120 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.075$
$wR(F^2) = 0.216$
$S = 0.91$
4082 reflections
262 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.072P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *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.
Several crystal specimens were tested but their quality was, in general, rather poor, as witnessed by the relatively high fraction of low intensity reflections. The poorly diffracting nature of the crystals is the reason for the relatively high *R* factors.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5087 (7)	0.2972 (5)	0.6271 (4)	0.0695 (14)
O2	0.7415 (7)	0.2144 (5)	0.5641 (3)	0.0546 (13)
H2	0.828 (10)	0.252 (7)	0.625 (5)	0.065*
O3	−0.6820 (6)	−0.1393 (4)	0.2211 (3)	0.0449 (11)
H3	−0.791 (9)	−0.207 (6)	0.168 (4)	0.054*
O4	−0.4973 (6)	−0.2424 (4)	0.1314 (3)	0.0579 (13)
N1	0.0479 (6)	0.1074 (4)	0.3096 (3)	0.0347 (11)
N2	0.1576 (6)	0.3969 (4)	0.0245 (3)	0.0330 (11)
N3	0.0616 (7)	0.3422 (4)	−0.0794 (4)	0.0351 (11)
N4	0.2872 (7)	0.5635 (5)	−0.0763 (4)	0.0321 (12)
H4	0.327 (8)	0.603 (6)	−0.010 (4)	0.039*
N5	0.0928 (6)	0.3985 (4)	−0.2380 (3)	0.0350 (11)
N6	0.2377 (9)	0.5392 (6)	−0.4342 (5)	0.0736 (18)
N7	0.5606 (7)	0.8734 (5)	−0.1101 (4)	0.0530 (15)
C1	0.5542 (10)	0.2307 (6)	0.5524 (5)	0.0443 (16)
C2	0.4013 (8)	0.1581 (6)	0.4388 (4)	0.0410 (15)
H2A	0.3851	0.0586	0.4165	0.049*
H2B	0.4604	0.1965	0.3898	0.049*
C3	0.1838 (8)	0.1715 (6)	0.4252 (4)	0.0390 (14)
H3A	0.1175	0.1254	0.4685	0.047*
H3B	0.1990	0.2707	0.4522	0.047*
C4	−0.5053 (8)	−0.1506 (6)	0.2034 (4)	0.0360 (14)

C5	−0.3145 (8)	−0.0271 (6)	0.2831 (4)	0.0443 (15)
H5A	−0.3144	−0.0190	0.3570	0.053*
H5B	−0.3294	0.0582	0.2714	0.053*
C6	−0.1030 (8)	−0.0340 (6)	0.2757 (4)	0.0379 (14)
H6A	−0.0501	−0.0828	0.3226	0.045*
H6B	−0.1197	−0.0867	0.2007	0.045*
C7	0.0604 (7)	0.1772 (6)	0.2383 (4)	0.0327 (13)
C8	−0.0607 (8)	0.1135 (5)	0.1257 (4)	0.0327 (13)
H8	−0.1607	0.0232	0.1005	0.039*
C9	−0.0354 (7)	0.1804 (5)	0.0534 (4)	0.0318 (13)
H9	−0.1138	0.1331	−0.0208	0.038*
C10	0.1061 (7)	0.3192 (5)	0.0874 (4)	0.0319 (13)
C11	0.2172 (8)	0.3865 (5)	0.2009 (4)	0.0354 (14)
H11	0.3079	0.4797	0.2262	0.042*
C12	0.1978 (8)	0.3213 (5)	0.2750 (4)	0.0350 (13)
H12	0.2732	0.3700	0.3494	0.042*
C13	0.1445 (7)	0.4320 (5)	−0.1300 (4)	0.0303 (13)
C14	0.3292 (8)	0.6199 (5)	−0.1517 (4)	0.0342 (14)
C15	0.2101 (8)	0.5140 (6)	−0.2531 (4)	0.0371 (14)
C16	0.4603 (8)	0.7600 (6)	−0.1284 (4)	0.0382 (14)
C17	0.2170 (9)	0.5250 (6)	−0.3564 (5)	0.0457 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.074 (3)	0.066 (3)	0.041 (3)	0.025 (3)	−0.002 (2)	−0.005 (2)
O2	0.041 (3)	0.058 (3)	0.042 (3)	0.008 (2)	−0.007 (2)	0.010 (2)
O3	0.031 (2)	0.048 (3)	0.039 (2)	−0.0005 (19)	0.0067 (19)	0.007 (2)
O4	0.051 (3)	0.051 (3)	0.040 (2)	0.001 (2)	0.010 (2)	−0.013 (2)
N1	0.031 (2)	0.030 (3)	0.029 (3)	−0.002 (2)	0.001 (2)	0.008 (2)
N2	0.030 (2)	0.030 (3)	0.030 (3)	0.005 (2)	0.007 (2)	0.005 (2)
N3	0.037 (3)	0.030 (3)	0.034 (3)	0.007 (2)	0.012 (2)	0.009 (2)
N4	0.029 (2)	0.025 (3)	0.030 (2)	0.001 (2)	0.006 (2)	0.003 (2)
N5	0.027 (2)	0.030 (3)	0.035 (3)	0.003 (2)	−0.001 (2)	0.010 (2)
N6	0.074 (4)	0.083 (5)	0.053 (4)	0.009 (3)	0.015 (3)	0.029 (3)
N7	0.044 (3)	0.040 (3)	0.067 (4)	0.005 (3)	0.020 (3)	0.015 (3)
C1	0.052 (4)	0.030 (4)	0.037 (4)	0.005 (3)	0.002 (3)	0.010 (3)
C2	0.041 (3)	0.040 (4)	0.033 (3)	0.007 (3)	0.003 (3)	0.012 (3)
C3	0.033 (3)	0.041 (4)	0.033 (3)	0.001 (3)	0.007 (3)	0.011 (3)
C4	0.034 (3)	0.038 (4)	0.031 (3)	0.004 (3)	0.007 (3)	0.015 (3)
C5	0.039 (3)	0.040 (4)	0.039 (3)	0.000 (3)	0.011 (3)	0.005 (3)
C6	0.034 (3)	0.035 (3)	0.034 (3)	0.002 (3)	0.005 (3)	0.010 (3)
C7	0.021 (3)	0.029 (3)	0.035 (3)	0.005 (2)	0.005 (2)	0.000 (3)
C8	0.027 (3)	0.026 (3)	0.036 (3)	0.002 (2)	0.006 (2)	0.007 (3)
C9	0.029 (3)	0.024 (3)	0.030 (3)	−0.002 (2)	0.002 (2)	0.007 (2)
C10	0.022 (3)	0.032 (3)	0.032 (3)	0.009 (2)	0.002 (2)	0.002 (3)
C11	0.033 (3)	0.025 (3)	0.040 (3)	0.002 (2)	0.012 (3)	0.006 (3)
C12	0.035 (3)	0.033 (3)	0.024 (3)	0.006 (3)	0.005 (2)	0.000 (2)

C13	0.024 (3)	0.033 (3)	0.028 (3)	0.008 (2)	0.006 (2)	0.006 (2)
C14	0.029 (3)	0.031 (3)	0.036 (3)	0.005 (3)	0.008 (2)	0.008 (3)
C15	0.028 (3)	0.042 (4)	0.031 (3)	0.007 (3)	0.003 (2)	0.008 (3)
C16	0.031 (3)	0.038 (4)	0.045 (4)	0.011 (3)	0.013 (3)	0.014 (3)
C17	0.040 (3)	0.049 (4)	0.037 (4)	0.004 (3)	0.006 (3)	0.014 (3)

Geometric parameters (Å, º)

O1—C1	1.213 (7)	C2—H2B	0.9700
O2—C1	1.323 (7)	C3—H3A	0.9700
O2—H2	0.80 (6)	C3—H3B	0.9700
O3—C4	1.324 (7)	C4—C5	1.502 (7)
O3—H3	0.88 (5)	C5—C6	1.504 (7)
O4—C4	1.187 (6)	C5—H5A	0.9700
N1—C7	1.350 (7)	C5—H5B	0.9700
N1—C6	1.449 (6)	C6—H6A	0.9700
N1—C3	1.465 (6)	C6—H6B	0.9700
N2—N3	1.278 (5)	C7—C8	1.408 (7)
N2—C10	1.361 (6)	C7—C12	1.434 (7)
N3—C13	1.384 (6)	C8—C9	1.353 (7)
N4—C13	1.346 (6)	C8—H8	0.9300
N4—C14	1.347 (7)	C9—C10	1.404 (7)
N4—H4	0.81 (5)	C9—H9	0.9300
N5—C13	1.325 (6)	C10—C11	1.408 (7)
N5—C15	1.363 (6)	C11—C12	1.356 (7)
N6—C17	1.127 (7)	C11—H11	0.9300
N7—C16	1.133 (6)	C12—H12	0.9300
C1—C2	1.483 (7)	C14—C15	1.392 (7)
C2—C3	1.514 (7)	C14—C16	1.415 (8)
C2—H2A	0.9700	C15—C17	1.427 (8)

C1—O2—H2	116 (5)	N1—C6—C5	110.1 (4)
C4—O3—H3	108 (4)	N1—C6—H6A	109.6
C7—N1—C6	121.5 (4)	C5—C6—H6A	109.6
C7—N1—C3	121.7 (4)	N1—C6—H6B	109.6
C6—N1—C3	116.7 (4)	C5—C6—H6B	109.6
N3—N2—C10	118.0 (4)	H6A—C6—H6B	108.2
N2—N3—C13	109.7 (4)	N1—C7—C8	122.1 (5)
C13—N4—C14	108.1 (4)	N1—C7—C12	120.9 (5)
C13—N4—H4	124 (4)	C8—C7—C12	117.0 (5)
C14—N4—H4	127 (4)	C9—C8—C7	121.7 (5)
C13—N5—C15	105.1 (4)	C9—C8—H8	119.1
O1—C1—O2	123.8 (6)	C7—C8—H8	119.1
O1—C1—C2	122.5 (6)	C8—C9—C10	121.7 (5)
O2—C1—C2	113.7 (6)	C8—C9—H9	119.1
C1—C2—C3	114.2 (5)	C10—C9—H9	119.1
C1—C2—H2A	108.7	N2—C10—C9	128.5 (5)
C3—C2—H2A	108.7	N2—C10—C11	114.8 (4)

C1—C2—H2B	108.7	C9—C10—C11	116.6 (5)
C3—C2—H2B	108.7	C12—C11—C10	122.9 (5)
H2A—C2—H2B	107.6	C12—C11—H11	118.6
N1—C3—C2	111.0 (4)	C10—C11—H11	118.6
N1—C3—H3A	109.4	C11—C12—C7	119.8 (5)
C2—C3—H3A	109.4	C11—C12—H12	120.1
N1—C3—H3B	109.4	C7—C12—H12	120.1
C2—C3—H3B	109.4	N5—C13—N4	111.6 (5)
H3A—C3—H3B	108.0	N5—C13—N3	123.9 (4)
O4—C4—O3	125.1 (5)	N4—C13—N3	124.5 (4)
O4—C4—C5	123.8 (5)	N4—C14—C15	105.3 (5)
O3—C4—C5	111.0 (5)	N4—C14—C16	125.5 (5)
C4—C5—C6	115.5 (5)	C15—C14—C16	129.1 (5)
C4—C5—H5A	108.4	N5—C15—C14	109.8 (5)
C6—C5—H5A	108.4	N5—C15—C17	125.8 (5)
C4—C5—H5B	108.4	C14—C15—C17	124.4 (5)
C6—C5—H5B	108.4	N7—C16—C14	178.1 (6)
H5A—C5—H5B	107.5	N6—C17—C15	175.0 (6)

C10—N2—N3—C13	−175.9 (4)	C9—C10—C11—C12	2.4 (8)
O1—C1—C2—C3	−1.3 (8)	C10—C11—C12—C7	0.5 (8)
O2—C1—C2—C3	177.9 (5)	N1—C7—C12—C11	176.1 (5)
C7—N1—C3—C2	−81.8 (6)	C8—C7—C12—C11	−4.6 (7)
C6—N1—C3—C2	99.1 (5)	C15—N5—C13—N4	0.6 (6)
C1—C2—C3—N1	175.3 (5)	C15—N5—C13—N3	−179.4 (5)
O4—C4—C5—C6	−7.2 (8)	C14—N4—C13—N5	0.9 (6)
O3—C4—C5—C6	175.8 (5)	C14—N4—C13—N3	−179.2 (5)
C7—N1—C6—C5	−85.4 (6)	N2—N3—C13—N5	172.9 (5)
C3—N1—C6—C5	93.7 (6)	N2—N3—C13—N4	−7.0 (7)
C4—C5—C6—N1	150.8 (5)	C13—N4—C14—C15	−2.0 (6)
C6—N1—C7—C8	−4.7 (8)	C13—N4—C14—C16	175.5 (5)
C3—N1—C7—C8	176.2 (5)	C13—N5—C15—C14	−1.8 (6)
C6—N1—C7—C12	174.7 (5)	C13—N5—C15—C17	176.3 (6)
C3—N1—C7—C12	−4.4 (7)	N4—C14—C15—N5	2.4 (6)
N1—C7—C8—C9	−174.8 (5)	C16—C14—C15—N5	−175.0 (5)
C12—C7—C8—C9	5.8 (8)	N4—C14—C15—C17	−175.8 (5)
C7—C8—C9—C10	−2.9 (8)	C16—C14—C15—C17	6.9 (10)
N3—N2—C10—C9	3.2 (8)	N4—C14—C16—N7	−92 (19)
N3—N2—C10—C11	−179.6 (5)	C15—C14—C16—N7	85 (19)
C8—C9—C10—N2	175.9 (5)	N5—C15—C17—N6	−143 (8)
C8—C9—C10—C11	−1.3 (7)	C14—C15—C17—N6	35 (9)
N2—C10—C11—C12	−175.1 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N5^{i}	0.80 (6)	2.12 (6)	2.896 (6)	162 (6)

O3—H3···N3^{ii}	0.88 (5)	1.89 (6)	2.750 (6)	165 (5)
N4—H4···O4^{iii}	0.81 (5)	1.98 (5)	2.740 (6)	156 (5)

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