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5-Nitro-1-(prop-2-yn-1-yl)-2,3-dihydro-1*H*-1,3-benzodiazol-2-one

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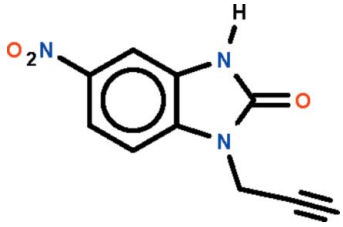
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.158; data-to-parameter ratio = 14.8.

In the two independent molecules of the title compound, $C_{10}H_7N_3O_3$, the nitro substitutent is twisted slightly with respect to the benzodiazol fused-ring system [dihedral angles = 4.9 (3) and 8.5 (1)°]. The two independent molecules are disposed about a pseudo inversion center and are held together by N—H···O hydrogen bonds. The supramolecular dimer is essentially planar [dihedral angle between the fused rings = 2.0 (1)°]. Adjacent dimers are linked by acetylene–nitro C—H···O interactions, generating a ribbon motif along (110).

Related literature

For related structures, see: Ouzidan *et al.* (2011*a*,*b*,*c*).



Experimental

Crystal data

$C_{10}H_7N_3O_3$
M_r = 217.19
Triclinic, $P\overline{1}$
a = 7.2541 (2) Å
b = 10.0362 (2) Å
c = 14.6793 (3) Å
α = 100.978 (1)°
β = 92.047 (1)°
γ = 109.043 (1)°
V = 986.20 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.27 × 0.22 × 0.13 mm

Data collection

Bruker APEX DUO diffractometer
20686 measured reflections
4506 independent reflections
2855 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.158
S = 1.05
4506 reflections
305 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4	0.96 (2)	1.81 (3)	2.766 (2)	173 (2)
N4—H4···O1	0.92 (2)	1.91 (2)	2.823 (2)	172 (2)
C4—H41···O3^{i}	0.92 (4)	2.39 (4)	3.231 (4)	153 (3)
C14—H141···O6^{ii}	0.88 (3)	2.51 (3)	3.383 (4)	169 (3)

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

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT*; 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5859).

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supplementary materials

Acta Cryst. (2012). E**68**, o1240 [doi:10.1107/S1600536812013177]

5-Nitro-1-(prop-2-yn-1-yl)-2,3-dihydro-1*H*-1,3-benzodiazol-2-one

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Comment

Benzodiazoles are of interest owing to their pharmacological properties. When the parent compound, benzodiazol-2-one, reacts with propargyl bromide, both amino groups are alkylated to give 1,3-bis(prop-2-ynyl)-benziodiazol-2-one (Ouzidan *et al.*, 2011*b*). The presence of an electron-withdrawing nitro group allows only one amino group to be alklylated, as noted from the reactions of 5-nitrobenzodiazol-2-onezol with *n*-octyl bromide and *n*-nonyl bromide (Ouzidan *et al.*, 2011*b*, 2011*c*). In the two independent molecules of $C_{10}H_7N_3O_3$ (Scheme I), the nitro substitutent is slightly bent with respect to the benzodiazol fused-ring (Fig. 2). The two are disposed about a false inversion center, and are held together by N–H···O hydrogen bonds. Adjacent dimers are linked by $C–H_{acetylene}\cdots O_{nitro}$ interactions to generate a ribbon motif (Fig. 2).

Experimental

To a mixture of 5-nitro-1*H*-benzodiazol-2(3*H*)-one (0.25 g, 1.5 mmol), potassium carbonate (0.35 g, 2.5 mmol), tetra-*n*-butylammonium bromide (0.1 g,0.2 mmol) in DMF (15 ml) was added propargyl bromide (0.14 ml, 1.6 mmol). Stirring was continued at room temperature for 6 hours. The salt was removed by filtration and the filtrate concentrated under reduced pressure. The residue was separated by chromatography on a column of silica gel with ethylacetate/hexane; yellow crystals were obtained upon evaporation of the solvent.

Refinement

All H atoms were located in a difference map. The aromatic and methylene H-atoms were placed in calculated positions (C–H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C).

The amino and acetylenic H-atoms were freely refined.

The (0 0 1) reflection was omitted owing to bad disagreement.

Computing details

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT* (Bruker, 2010); 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).

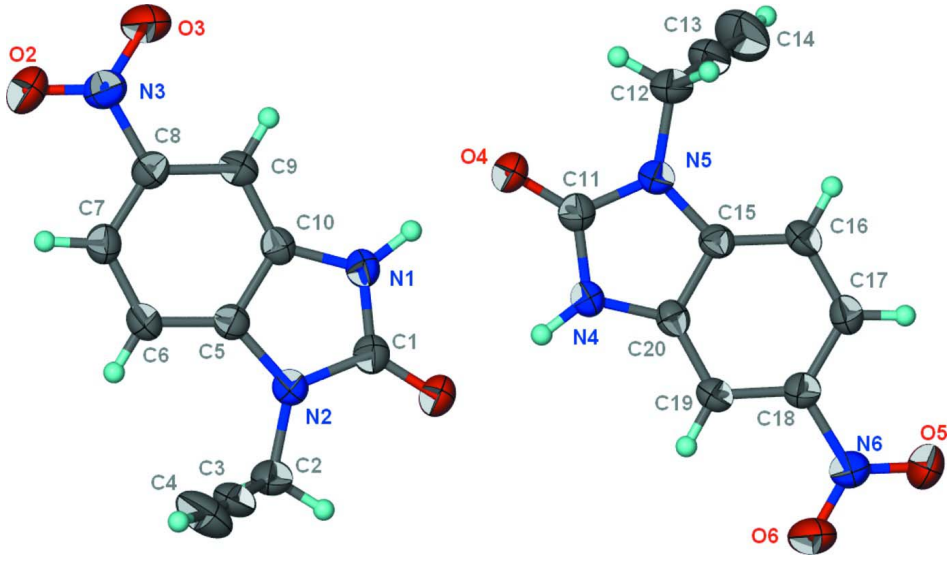

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of the two independent molecules of $C_{10}H_7N_3O_3$ molecule at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

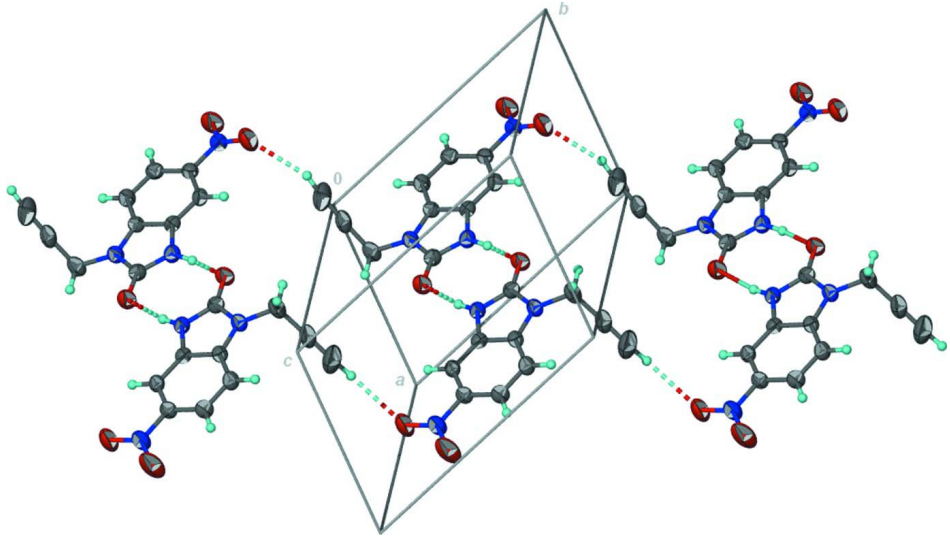

Figure 2

Anisotropic displacement ellipsoid plot (Barbour, 2001) of the hydrogen-bonded ribbon motif.

5-Nitro-1-(prop-2-yn-1-yl)-2,3-dihydro-1*H*-1,3-benzodiazol-2-one

Crystal data

$C_{10}H_7N_3O_3$
$M_r = 217.19$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.2541$ (2) Å
$b = 10.0362$ (2) Å
$c = 14.6793$ (3) Å
$\alpha = 100.978$ (1)°
$\beta = 92.047$ (1)°
$\gamma = 109.043$ (1)°
$V = 986.20$ (4) Å^3
$Z = 4$
$F(000) = 448$
$D_x = 1.463$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5674 reflections

θ = 2.2–28.0°
μ = 0.11 mm^{-1}
T = 293 K

Prism, yellow
0.27 × 0.22 × 0.13 mm

Data collection

Bruker APEX DUO diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
20686 measured reflections
4506 independent reflections

2855 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 2.2°
h = −9→9
k = −13→12
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.158
S = 1.05
4506 reflections
305 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
$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 0.2589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.4863 (2)	0.28214 (16)	0.32061 (10)	0.0583 (4)
O2	0.2729 (3)	0.70175 (19)	−0.06407 (12)	0.0780 (5)
O3	0.4106 (3)	0.84006 (18)	0.06741 (13)	0.0826 (6)
O4	0.7053 (2)	0.67457 (15)	0.41638 (10)	0.0556 (4)
O5	1.0136 (4)	0.2778 (2)	0.79280 (13)	0.1056 (8)
O6	0.8109 (3)	0.13338 (17)	0.67890 (13)	0.0826 (6)
N1	0.4993 (2)	0.47954 (18)	0.25677 (11)	0.0459 (4)
N2	0.3361 (2)	0.26206 (16)	0.17380 (10)	0.0438 (4)
N3	0.3367 (2)	0.72031 (19)	0.01736 (13)	0.0535 (4)
N4	0.7143 (2)	0.48027 (17)	0.47997 (11)	0.0416 (4)
N5	0.8738 (2)	0.70106 (16)	0.55973 (10)	0.0429 (4)
N6	0.9101 (3)	0.25456 (19)	0.72058 (13)	0.0583 (5)
C1	0.4468 (3)	0.3367 (2)	0.25799 (13)	0.0447 (4)
C2	0.2539 (3)	0.1058 (2)	0.14690 (15)	0.0555 (5)
H2A	0.3007	0.0644	0.1936	0.067*
H2B	0.2988	0.0734	0.0880	0.067*
C3	0.0406 (4)	0.0549 (2)	0.13742 (15)	0.0585 (6)
C4	−0.1296 (5)	0.0194 (3)	0.1295 (2)	0.0859 (9)
C5	0.3154 (3)	0.35855 (19)	0.12192 (12)	0.0391 (4)
C6	0.2169 (3)	0.3381 (2)	0.03563 (13)	0.0450 (4)
H6	0.1471	0.2461	0.0011	0.054*
C7	0.2259 (3)	0.4598 (2)	0.00241 (13)	0.0454 (4)
H7	0.1628	0.4505	−0.0559	0.054*

C8	0.3287 (3)	0.5950 (2)	0.05579 (13)	0.0418 (4)
C9	0.4281 (3)	0.6184 (2)	0.14315 (13)	0.0428 (4)
H9	0.4961	0.7107	0.1778	0.051*
C10	0.4197 (2)	0.49734 (19)	0.17501 (12)	0.0391 (4)
C11	0.7577 (3)	0.6231 (2)	0.47796 (13)	0.0432 (4)
C12	0.9419 (3)	0.8575 (2)	0.58554 (15)	0.0552 (5)
H12A	0.8899	0.8870	0.6430	0.066*
H12B	0.8916	0.8943	0.5372	0.066*
C13	1.1548 (4)	0.9205 (2)	0.59851 (15)	0.0621 (6)
C14	1.3251 (5)	0.9698 (3)	0.6118 (2)	0.0942 (10)
C15	0.9034 (3)	0.60770 (18)	0.61264 (12)	0.0381 (4)
C16	1.0082 (3)	0.6333 (2)	0.69790 (13)	0.0452 (4)
H16	1.0756	0.7267	0.7310	0.054*
C17	1.0092 (3)	0.5145 (2)	0.73252 (13)	0.0463 (5)
H17	1.0786	0.5271	0.7898	0.056*
C18	0.9065 (3)	0.3768 (2)	0.68142 (13)	0.0432 (4)
C19	0.7999 (3)	0.34865 (19)	0.59536 (12)	0.0404 (4)
H19	0.7318	0.2552	0.5625	0.048*
C20	0.8012 (2)	0.46764 (19)	0.56177 (12)	0.0371 (4)
H1	0.574 (3)	0.554 (3)	0.3093 (17)	0.073 (7)*
H4	0.645 (3)	0.409 (2)	0.4297 (16)	0.060 (6)*
H41	−0.263 (6)	−0.002 (4)	0.122 (3)	0.138 (14)*
H141	1.454 (5)	1.011 (3)	0.621 (2)	0.118 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0683 (9)	0.0531 (9)	0.0505 (8)	0.0149 (7)	−0.0098 (7)	0.0175 (7)
O2	0.0971 (13)	0.0713 (11)	0.0680 (11)	0.0265 (10)	−0.0142 (9)	0.0289 (9)
O3	0.1019 (14)	0.0448 (10)	0.0931 (13)	0.0164 (9)	−0.0181 (10)	0.0160 (9)
O4	0.0672 (9)	0.0501 (8)	0.0493 (8)	0.0188 (7)	−0.0090 (7)	0.0151 (7)
O5	0.169 (2)	0.0641 (12)	0.0750 (12)	0.0367 (12)	−0.0557 (13)	0.0130 (10)
O6	0.1049 (14)	0.0406 (9)	0.0919 (13)	0.0138 (9)	−0.0253 (10)	0.0156 (9)
N1	0.0484 (9)	0.0429 (9)	0.0398 (9)	0.0081 (7)	−0.0054 (7)	0.0082 (7)
N2	0.0512 (9)	0.0392 (9)	0.0398 (8)	0.0157 (7)	0.0000 (7)	0.0060 (7)
N3	0.0492 (10)	0.0468 (10)	0.0649 (12)	0.0145 (8)	0.0006 (8)	0.0172 (9)
N4	0.0445 (9)	0.0383 (9)	0.0376 (8)	0.0107 (7)	−0.0035 (7)	0.0050 (7)
N5	0.0526 (9)	0.0351 (8)	0.0396 (8)	0.0146 (7)	0.0018 (7)	0.0055 (7)
N6	0.0762 (12)	0.0428 (10)	0.0556 (11)	0.0211 (9)	−0.0062 (9)	0.0104 (8)
C1	0.0451 (10)	0.0465 (11)	0.0416 (10)	0.0147 (8)	0.0014 (8)	0.0092 (9)
C2	0.0770 (15)	0.0389 (11)	0.0518 (12)	0.0243 (10)	0.0004 (10)	0.0051 (9)
C3	0.0795 (16)	0.0329 (10)	0.0503 (12)	0.0084 (10)	−0.0016 (11)	−0.0006 (9)
C4	0.082 (2)	0.0561 (16)	0.088 (2)	−0.0025 (14)	0.0001 (16)	−0.0130 (14)
C5	0.0418 (9)	0.0385 (10)	0.0380 (9)	0.0159 (8)	0.0051 (7)	0.0064 (8)
C6	0.0519 (11)	0.0399 (10)	0.0384 (10)	0.0142 (8)	−0.0013 (8)	0.0008 (8)
C7	0.0472 (10)	0.0484 (11)	0.0404 (10)	0.0175 (9)	−0.0019 (8)	0.0081 (8)
C8	0.0400 (9)	0.0437 (10)	0.0446 (10)	0.0156 (8)	0.0057 (8)	0.0131 (8)
C9	0.0402 (10)	0.0371 (10)	0.0460 (11)	0.0087 (7)	0.0039 (8)	0.0046 (8)
C10	0.0356 (9)	0.0422 (10)	0.0363 (9)	0.0106 (7)	0.0031 (7)	0.0059 (8)
C11	0.0428 (10)	0.0440 (11)	0.0422 (10)	0.0144 (8)	0.0033 (8)	0.0089 (8)

C12	0.0725 (14)	0.0361 (11)	0.0553 (12)	0.0177 (10)	0.0026 (10)	0.0076 (9)
C13	0.0790 (17)	0.0394 (11)	0.0541 (13)	0.0046 (11)	−0.0032 (11)	0.0067 (10)
C14	0.081 (2)	0.0721 (19)	0.096 (2)	−0.0106 (16)	−0.0107 (17)	0.0092 (16)
C15	0.0429 (9)	0.0350 (9)	0.0360 (9)	0.0137 (7)	0.0070 (7)	0.0054 (7)
C16	0.0537 (11)	0.0372 (10)	0.0379 (10)	0.0119 (8)	−0.0001 (8)	−0.0008 (8)
C17	0.0558 (11)	0.0465 (11)	0.0344 (9)	0.0180 (9)	−0.0018 (8)	0.0032 (8)
C18	0.0498 (10)	0.0393 (10)	0.0415 (10)	0.0173 (8)	0.0039 (8)	0.0075 (8)
C19	0.0432 (10)	0.0337 (9)	0.0401 (10)	0.0111 (7)	0.0020 (8)	0.0021 (7)
C20	0.0365 (9)	0.0399 (10)	0.0337 (9)	0.0138 (7)	0.0040 (7)	0.0036 (7)

Geometric parameters (Å, º)

O1—C1	1.226 (2)	C4—H41	0.92 (4)
O2—N3	1.224 (2)	C5—C6	1.377 (2)
O3—N3	1.219 (2)	C5—C10	1.406 (2)
O4—C11	1.229 (2)	C6—C7	1.382 (3)
O5—N6	1.215 (2)	C6—H6	0.9300
O6—N6	1.219 (2)	C7—C8	1.380 (3)
N1—C1	1.362 (2)	C7—H7	0.9300
N1—C10	1.380 (2)	C8—C9	1.389 (3)
N1—H1	0.96 (2)	C9—C10	1.367 (3)
N2—C5	1.381 (2)	C9—H9	0.9300
N2—C1	1.385 (2)	C12—C13	1.455 (3)
N2—C2	1.452 (2)	C12—H12A	0.9700
N3—C8	1.459 (2)	C12—H12B	0.9700
N4—C11	1.370 (2)	C13—C14	1.164 (4)
N4—C20	1.383 (2)	C14—H141	0.88 (3)
N4—H4	0.92 (2)	C15—C16	1.375 (2)
N5—C11	1.379 (2)	C15—C20	1.401 (2)
N5—C15	1.387 (2)	C16—C17	1.384 (3)
N5—C12	1.452 (2)	C16—H16	0.9300
N6—C18	1.457 (2)	C17—C18	1.387 (3)
C2—C3	1.455 (3)	C17—H17	0.9300
C2—H2A	0.9700	C18—C19	1.388 (3)
C2—H2B	0.9700	C19—C20	1.373 (2)
C3—C4	1.162 (4)	C19—H19	0.9300
C1—N1—C10	110.23 (16)	C7—C8—C9	123.72 (17)
C1—N1—H1	121.9 (14)	C7—C8—N3	118.08 (17)
C10—N1—H1	127.7 (14)	C9—C8—N3	118.18 (17)
C5—N2—C1	109.67 (15)	C10—C9—C8	115.85 (17)
C5—N2—C2	126.40 (16)	C10—C9—H9	122.1
C1—N2—C2	123.92 (16)	C8—C9—H9	122.1
O3—N3—O2	122.50 (18)	C9—C10—N1	131.69 (17)
O3—N3—C8	118.46 (18)	C9—C10—C5	121.39 (16)
O2—N3—C8	119.03 (18)	N1—C10—C5	106.92 (16)
C11—N4—C20	109.80 (15)	O4—C11—N4	127.80 (18)
C11—N4—H4	120.7 (13)	O4—C11—N5	125.54 (18)
C20—N4—H4	129.3 (14)	N4—C11—N5	106.66 (16)
C11—N5—C15	109.80 (15)	N5—C12—C13	112.49 (17)

C11—N5—C12	123.13 (16)	N5—C12—H12A	109.1
C15—N5—C12	126.98 (16)	C13—C12—H12A	109.1
O5—N6—O6	122.84 (18)	N5—C12—H12B	109.1
O5—N6—C18	118.59 (18)	C13—C12—H12B	109.1
O6—N6—C18	118.57 (17)	H12A—C12—H12B	107.8
O1—C1—N1	127.84 (18)	C14—C13—C12	177.7 (3)
O1—C1—N2	125.59 (18)	C13—C14—H141	177 (2)
N1—C1—N2	106.57 (16)	C16—C15—N5	131.48 (17)
N2—C2—C3	111.72 (17)	C16—C15—C20	122.06 (16)
N2—C2—H2A	109.3	N5—C15—C20	106.46 (15)
C3—C2—H2A	109.3	C15—C16—C17	117.40 (17)
N2—C2—H2B	109.3	C15—C16—H16	121.3
C3—C2—H2B	109.3	C17—C16—H16	121.3
H2A—C2—H2B	107.9	C16—C17—C18	119.75 (17)
C4—C3—C2	177.4 (3)	C16—C17—H17	120.1
C3—C4—H41	176 (2)	C18—C17—H17	120.1
C6—C5—N2	131.73 (17)	C19—C18—C17	123.75 (17)
C6—C5—C10	121.69 (17)	C19—C18—N6	118.16 (17)
N2—C5—C10	106.58 (15)	C17—C18—N6	118.09 (17)
C5—C6—C7	117.37 (17)	C20—C19—C18	115.76 (16)
C5—C6—H6	121.3	C20—C19—H19	122.1
C7—C6—H6	121.3	C18—C19—H19	122.1
C8—C7—C6	119.97 (17)	C19—C20—N4	131.45 (16)
C8—C7—H7	120.0	C19—C20—C15	121.28 (16)
C6—C7—H7	120.0	N4—C20—C15	107.28 (15)

C10—N1—C1—O1	−177.65 (19)	C20—N4—C11—O4	−179.86 (18)
C10—N1—C1—N2	1.7 (2)	C20—N4—C11—N5	0.1 (2)
C5—N2—C1—O1	177.68 (18)	C15—N5—C11—O4	−179.94 (18)
C2—N2—C1—O1	−1.5 (3)	C12—N5—C11—O4	3.2 (3)
C5—N2—C1—N1	−1.7 (2)	C15—N5—C11—N4	0.1 (2)
C2—N2—C1—N1	179.04 (16)	C12—N5—C11—N4	−176.74 (17)
C5—N2—C2—C3	−64.0 (2)	C11—N5—C12—C13	−120.6 (2)
C1—N2—C2—C3	115.0 (2)	C15—N5—C12—C13	63.0 (3)
C1—N2—C5—C6	−178.67 (19)	C11—N5—C15—C16	179.53 (19)
C2—N2—C5—C6	0.5 (3)	C12—N5—C15—C16	−3.7 (3)
C1—N2—C5—C10	1.1 (2)	C11—N5—C15—C20	−0.27 (19)
C2—N2—C5—C10	−179.73 (17)	C12—N5—C15—C20	176.45 (17)
N2—C5—C6—C7	−179.67 (18)	N5—C15—C16—C17	−179.89 (18)
C10—C5—C6—C7	0.6 (3)	C20—C15—C16—C17	−0.1 (3)
C5—C6—C7—C8	−0.8 (3)	C15—C16—C17—C18	−0.2 (3)
C6—C7—C8—C9	0.4 (3)	C16—C17—C18—C19	0.1 (3)
C6—C7—C8—N3	179.11 (16)	C16—C17—C18—N6	−179.55 (17)
O3—N3—C8—C7	172.97 (18)	O5—N6—C18—C19	175.1 (2)
O2—N3—C8—C7	−8.4 (3)	O6—N6—C18—C19	−4.0 (3)
O3—N3—C8—C9	−8.3 (3)	O5—N6—C18—C17	−5.2 (3)
O2—N3—C8—C9	170.30 (18)	O6—N6—C18—C17	175.7 (2)
C7—C8—C9—C10	0.1 (3)	C17—C18—C19—C20	0.2 (3)
N3—C8—C9—C10	−178.55 (15)	N6—C18—C19—C20	179.91 (16)

C8—C9—C10—N1	179.90 (18)	C18—C19—C20—N4	179.50 (18)
C8—C9—C10—C5	−0.3 (2)	C18—C19—C20—C15	−0.5 (2)
C1—N1—C10—C9	178.72 (19)	C11—N4—C20—C19	179.75 (18)
C1—N1—C10—C5	−1.1 (2)	C11—N4—C20—C15	−0.23 (19)
C6—C5—C10—C9	−0.1 (3)	C16—C15—C20—C19	0.5 (3)
N2—C5—C10—C9	−179.84 (15)	N5—C15—C20—C19	−179.68 (15)
C6—C5—C10—N1	179.78 (16)	C16—C15—C20—N4	−179.52 (16)
N2—C5—C10—N1	0.01 (19)	N5—C15—C20—N4	0.30 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4	0.96 (2)	1.81 (3)	2.766 (2)	173 (2)
N4—H4···O1	0.92 (2)	1.91 (2)	2.823 (2)	172 (2)
C4—H41···O3^{i}	0.92 (4)	2.39 (4)	3.231 (4)	153 (3)
C14—H141···O6^{ii}	0.88 (3)	2.51 (3)	3.383 (4)	169 (3)

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