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N-[5-(Diphenylamino)penta-2,4-diyn-1-yl]benzamide

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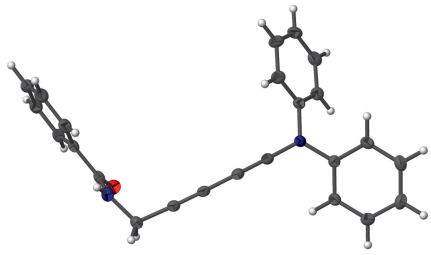
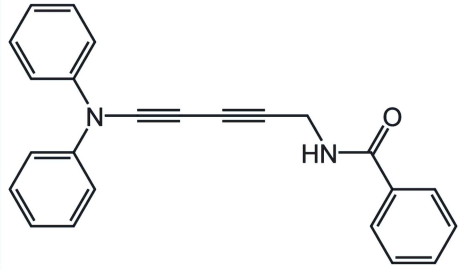
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{24}H_{18}N_2O_1$, the ynamine moiety has a near-planar structure (r.m.s. deviation = 0.0200 Å), and makes dihedral angles of 52.99 (7) and 27.91 (7)° with the phenyl rings. In the crystal, the molecules exhibit a dimeric form owing to bifurcated C—H···π interactions within a centrosymmetric dimer. Intermolecular N—H···O hydrogen bonds are also formed along the *b*-axis direction.

3D view



Chemical scheme



Structure description

The title compound is a diacetylene derivative. Solid-state polymerization is known to proceed for some diacetylene derivatives in a specific molecular arrangement. Mainly, two conditions for the molecular arrangement are required for the polymerization: (i) the molecules stack one-dimensionally with repeating intervals of 4.8–5.6 Å; (ii) the diacetylene moieties of the molecules have an inclination angle of 40–50° with the stacking axis. In order to realize such an ideal stacking structure, several kinds of intermolecular hydrogen bonds are utilized (Lauher *et al.*, 2008). In the title compound, a phenylamide group is introduced to control the molecular arrangement.

In the title compound, Fig. 1, the ynamine moiety has a near-planar structure (r.m.s. deviation = 0.0200 Å), making dihedral angles with the C1–C6 and C7–C12 phenyl rings of 52.99 (7) and 27.91 (7)°, respectively. The N2—C13 bond length is in good agreement with those reported (Tokutome *et al.*, 2012, 2013; Tabata & Okuno (2011); Tabata *et al.*, 2012). The N1/O1/C18/C19 amide group has an almost planar form (r.m.s. deviation = 0.0027 Å) and makes a dihedral angle of 17.63 (8)° with the C19–C24 phenyl ring.

In the crystal, the molecules make a dimeric form owing to bifurcated C—H···π interactions within a centrosymmetric dimer, where the H3···C14^{i} and H3···C15^{i} [symmetry code: (i) $-x+1, -y+1, -z+1$] distances are 2.81 and 2.74 Å, as shown in Fig. 2. Intermolecular N—H···O hydrogen bonds (Table 1) are also formed along the *b*-

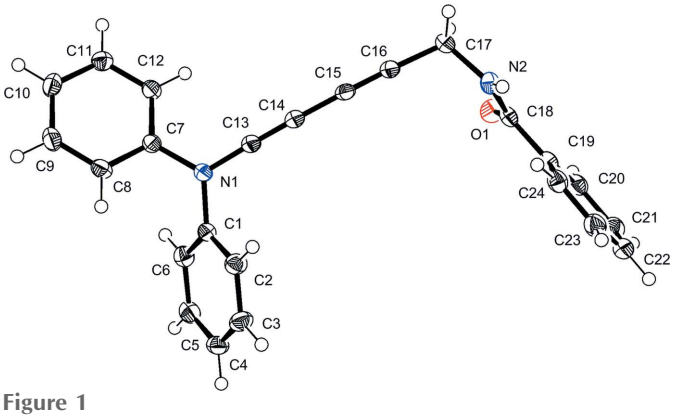


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

axis direction. Although the intermolecular N—H···O hydrogen bonds are formed as designed, the C—H···π interactions are thought to prevent a regular stack with translation.

Synthesis and crystallization

A mixture of *N*-ethynyl-*N*-phenylaniline (1.16 g, 6.0 mmol) and *N*-(prop-2-yn-1-yl)benzamide (0.80 g, 5.0 mmol) in acetone (35 ml) were reacted in the presence of Cu-TMEDA catalyst and oxygen for 12 h at 253 K. (Hay, 1962) The solution was concentrated and extracted with chloroform. The organic layer was washed with ammonium hydroxide and dried over sodium sulfate. After filtration, it was concentrated under reduced pressure. The residual solid was purified by column chromatography (SiO_2) to give 0.87 g (50%) of the title compound as a colourless solid. Single crystals of sufficient quality were obtained by slow evaporation from a dichloromethane–hexane solution.

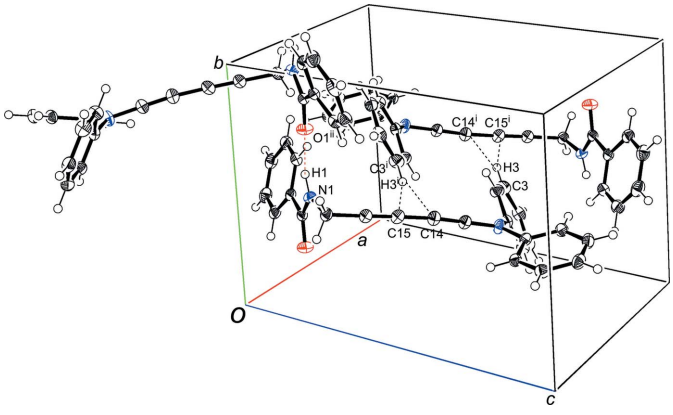


Figure 2
A view of the intermolecular interactions in the title compound. [Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.]

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···C14^{i}	0.95	2.81	3.673 (4)	152
C3—H3···C15^{i}	0.95	2.74	3.554 (4)	144
N1—H1···O1^{ii}	0.85 (3)	2.00 (3)	2.771 (3)	149 (3)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{18}N_2O$
M_r	350.42
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	93
a, b, c (Å)	12.486 (7), 9.738 (5), 16.089 (9)
β (°)	109.518 (6)
V (Å^3)	1843.8 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.10 × 0.07 × 0.04
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Numerical (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.995, 0.997
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	14614, 4155, 2929
R_{int}	0.062
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.162, 1.06
No. of reflections	4155
No. of parameters	248
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.58, −0.32

Computer programs: *CrystalClear* (Rigaku, 2008), *SHELXD2013* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *CrystalStructure* (Rigaku, 2014).

Refinement

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

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full crystallographic data

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N-[5-(Diphenylamino)penta-2,4-diyn-1-yl]benzamide

Crystal data

$C_{24}H_{18}N_2O$
M_r = 350.42
Monoclinic, $P2_1/c$
a = 12.486 (7) Å
b = 9.738 (5) Å
c = 16.089 (9) Å
β = 109.518 (6)°
V = 1843.8 (17) Å^3
Z = 4
$F(000)$ = 736.00
D_x = 1.262 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 4684 reflections
θ = 2.1–31.2°
μ = 0.08 mm^{-1}
T = 93 K
Block, colorless
0.10 × 0.07 × 0.04 mm

Data collection

Rigaku Saturn724+ diffractometer
Detector resolution: 7.111 pixels mm^{-1}
ω scans
Absorption correction: numerical (NUMABS; Rigaku, 1999)
T_{min} = 0.995, T_{max} = 0.997
14614 measured reflections
4155 independent reflections
2929 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.062
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −16→16
k = −12→12
l = −20→20

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.162
S = 1.06
4155 reflections
248 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
$w = 1/[\sigma^2(F_o^2) + (0.0816P)^2 + 0.1006P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of F^2 > 2.0 sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.02051 (13)	0.30092 (14)	0.22465 (9)	0.0308 (4)
N1	0.00394 (14)	0.51968 (17)	0.26271 (10)	0.0229 (4)
N2	0.41255 (13)	0.36679 (17)	0.68882 (10)	0.0248 (4)
C1	0.51710 (16)	0.3440 (2)	0.67100 (12)	0.0224 (4)
C2	0.55674 (17)	0.4437 (2)	0.62730 (13)	0.0276 (4)
C3	0.65474 (18)	0.4186 (2)	0.60743 (14)	0.0300 (5)
C4	0.71294 (17)	0.2951 (2)	0.63095 (13)	0.0285 (5)
C5	0.67219 (18)	0.1961 (2)	0.67443 (13)	0.0286 (5)
C6	0.57419 (17)	0.2200 (2)	0.69492 (13)	0.0256 (4)
C7	0.40326 (16)	0.34256 (19)	0.77368 (12)	0.0212 (4)
C8	0.30013 (16)	0.30123 (19)	0.78110 (12)	0.0228 (4)
C9	0.29067 (17)	0.2862 (2)	0.86391 (12)	0.0263 (4)
C10	0.38291 (19)	0.3101 (2)	0.93921 (13)	0.0287 (5)
C11	0.48588 (18)	0.3483 (2)	0.93129 (13)	0.0285 (5)
C12	0.49718 (16)	0.3653 (2)	0.84927 (13)	0.0250 (4)
C13	0.31941 (16)	0.3997 (2)	0.62021 (12)	0.0233 (4)
C14	0.23749 (16)	0.4286 (2)	0.55789 (12)	0.0249 (4)
C15	0.14353 (16)	0.4492 (2)	0.48386 (12)	0.0234 (4)
C16	0.06265 (16)	0.4636 (2)	0.41808 (12)	0.0227 (4)
C17	−0.03368 (16)	0.4829 (2)	0.33613 (12)	0.0233 (4)
C18	0.03405 (16)	0.42482 (19)	0.21431 (12)	0.0221 (4)
C19	0.08670 (16)	0.47240 (19)	0.14822 (12)	0.0215 (4)
C20	0.13380 (17)	0.6029 (2)	0.15128 (13)	0.0265 (4)
C21	0.18493 (18)	0.6402 (2)	0.09050 (13)	0.0315 (5)
C22	0.18987 (18)	0.5483 (2)	0.02646 (14)	0.0323 (5)
C23	0.14320 (18)	0.4188 (2)	0.02273 (13)	0.0302 (5)
C24	0.09132 (17)	0.3809 (2)	0.08340 (12)	0.0256 (4)
H1	0.012 (2)	0.605 (3)	0.2538 (16)	0.045 (7)*
H2	0.51728	0.52822	0.61112	0.0331*
H3	0.68247	0.48659	0.57742	0.0360*
H4	0.78019	0.27874	0.61726	0.0342*
H5	0.71144	0.11141	0.69036	0.0343*
H6	0.54645	0.15216	0.725	0.0308*
H8	0.23673	0.2835	0.72973	0.0274*
H9	0.2201	0.25907	0.86913	0.0315*
H10	0.37561	0.3005	0.99583	0.0344*
H11	0.54967	0.36294	0.98291	0.0342*
H12	0.568	0.39214	0.84442	0.0300*
H17A	−0.07853	0.39704	0.32181	0.0280*
H17B	−0.08371	0.55628	0.34498	0.0280*
H20	0.13076	0.66645	0.19525	0.0318*
H21	0.21675	0.72936	0.09278	0.0378*
H22	0.22535	0.57409	−0.01502	0.0387*
H23	0.1466	0.35561	−0.02132	0.0362*
H24	0.0589	0.292	0.08048	0.0307*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0386 (9)	0.0184 (7)	0.0381 (8)	−0.0005 (6)	0.0164 (7)	0.0003 (6)
N1	0.0270 (9)	0.0173 (8)	0.0230 (8)	0.0018 (7)	0.0065 (7)	0.0017 (7)
N2	0.0176 (8)	0.0343 (9)	0.0223 (8)	0.0021 (7)	0.0062 (7)	0.0071 (7)
C1	0.0184 (9)	0.0279 (10)	0.0200 (9)	−0.0014 (7)	0.0051 (7)	−0.0019 (8)
C2	0.0263 (10)	0.0272 (10)	0.0303 (11)	−0.0004 (8)	0.0110 (9)	0.0035 (9)
C3	0.0280 (11)	0.0343 (11)	0.0321 (11)	−0.0063 (9)	0.0157 (9)	−0.0004 (9)
C4	0.0207 (10)	0.0366 (12)	0.0290 (11)	−0.0012 (8)	0.0093 (9)	−0.0095 (9)
C5	0.0266 (11)	0.0283 (11)	0.0284 (10)	0.0041 (8)	0.0057 (9)	−0.0050 (9)
C6	0.0255 (10)	0.0238 (10)	0.0264 (10)	−0.0028 (8)	0.0071 (8)	−0.0006 (8)
C7	0.0205 (9)	0.0219 (9)	0.0213 (9)	0.0032 (7)	0.0069 (8)	0.0021 (7)
C8	0.0202 (9)	0.0236 (9)	0.0234 (9)	0.0000 (7)	0.0055 (8)	0.0022 (8)
C9	0.0239 (10)	0.0274 (11)	0.0289 (11)	−0.0012 (8)	0.0106 (9)	0.0007 (8)
C10	0.0360 (12)	0.0304 (11)	0.0206 (9)	0.0040 (9)	0.0107 (9)	0.0027 (8)
C11	0.0278 (11)	0.0310 (11)	0.0222 (10)	0.0037 (9)	0.0022 (8)	0.0006 (8)
C12	0.0183 (9)	0.0268 (10)	0.0283 (10)	−0.0010 (8)	0.0054 (8)	0.0028 (8)
C13	0.0199 (9)	0.0284 (10)	0.0233 (9)	0.0008 (8)	0.0093 (8)	0.0042 (8)
C14	0.0212 (10)	0.0326 (11)	0.0233 (9)	0.0005 (8)	0.0105 (8)	0.0034 (8)
C15	0.0206 (10)	0.0283 (10)	0.0251 (10)	0.0038 (8)	0.0126 (8)	0.0038 (8)
C16	0.0201 (9)	0.0261 (10)	0.0240 (9)	0.0013 (8)	0.0100 (8)	0.0018 (8)
C17	0.0196 (9)	0.0248 (10)	0.0241 (9)	0.0029 (8)	0.0053 (8)	0.0016 (8)
C18	0.0204 (9)	0.0188 (9)	0.0222 (9)	0.0030 (7)	0.0006 (7)	−0.0010 (8)
C19	0.0182 (9)	0.0210 (9)	0.0219 (9)	0.0034 (7)	0.0021 (7)	0.0019 (8)
C20	0.0243 (10)	0.0267 (10)	0.0246 (10)	−0.0030 (8)	0.0028 (8)	−0.0014 (8)
C21	0.0258 (11)	0.0346 (12)	0.0306 (11)	−0.0061 (9)	0.0047 (9)	0.0042 (9)
C22	0.0250 (11)	0.0428 (13)	0.0292 (11)	0.0044 (9)	0.0094 (9)	0.0093 (10)
C23	0.0283 (11)	0.0344 (11)	0.0267 (10)	0.0089 (9)	0.0076 (9)	0.0010 (9)
C24	0.0234 (10)	0.0245 (10)	0.0262 (10)	0.0058 (8)	0.0048 (8)	0.0017 (8)

Geometric parameters (Å, º)

O1—C18	1.237 (2)	C19—C24	1.388 (3)
N1—C17	1.454 (3)	C20—C21	1.383 (3)
N1—C18	1.340 (3)	C21—C22	1.382 (3)
N2—C1	1.444 (3)	C22—C23	1.382 (3)
N2—C7	1.428 (3)	C23—C24	1.390 (3)
N2—C13	1.348 (2)	N1—H1	0.85 (3)
C1—C2	1.383 (3)	C2—H2	0.950
C1—C6	1.390 (3)	C3—H3	0.950
C2—C3	1.386 (3)	C4—H4	0.950
C3—C4	1.391 (3)	C5—H5	0.950
C4—C5	1.384 (3)	C6—H6	0.950
C5—C6	1.389 (3)	C8—H8	0.950
C7—C8	1.392 (3)	C9—H9	0.950
C7—C12	1.397 (2)	C10—H10	0.950
C8—C9	1.384 (3)	C11—H11	0.950

C9—C10	1.384 (3)	C12—H12	0.950
C10—C11	1.384 (4)	C17—H17A	0.990
C11—C12	1.383 (3)	C17—H17B	0.990
C13—C14	1.202 (2)	C20—H20	0.950
C14—C15	1.379 (2)	C21—H21	0.950
C15—C16	1.202 (2)	C22—H22	0.950
C16—C17	1.470 (2)	C23—H23	0.950
C18—C19	1.498 (3)	C24—H24	0.950
C19—C20	1.395 (3)		

O1···C16	3.373 (3)	C17···H5^{x}	3.3890
O1···C17	2.762 (3)	C17···H8^{viii}	3.3058
O1···C24	2.810 (3)	C17···H20^{i}	3.2884
N1···C15	3.468 (3)	C17···H24^{iii}	3.3524
N1···C20	2.906 (3)	C18···H1^{i}	3.24 (3)
C1···C4	2.770 (3)	C18···H8^{ii}	3.1877
C1···C12	2.968 (3)	C18···H9^{ii}	3.3078
C1···C14	3.455 (3)	C19···H8^{ii}	3.1300
C2···C5	2.781 (3)	C19···H23^{ix}	3.3890
C2···C13	2.958 (3)	C20···H17A^{iii}	3.0108
C3···C6	2.772 (3)	C20···H23^{ix}	3.4498
C6···C7	3.065 (3)	C21···H12^{iv}	2.9248
C6···C12	3.269 (3)	C21···H17A^{iii}	3.3558
C6···C13	3.474 (3)	C21···H24^{ix}	3.4170
C7···C10	2.777 (3)	C22···H4^{xvi}	3.3317
C7···C14	3.498 (3)	C22···H10^{xvii}	3.4938
C8···C11	2.772 (3)	C22···H11^{iv}	3.4167
C8···C13	2.845 (3)	C22···H12^{iv}	3.0977
C9···C12	2.776 (3)	C22···H24^{ix}	3.3848
C16···C18	3.199 (3)	C23···H9^{xvii}	3.3216
C19···C22	2.780 (4)	C23···H10^{xvii}	3.2823
C20···C23	2.770 (3)	C24···H8^{ii}	2.9232
C21···C24	2.769 (3)	C24···H17B^{i}	3.3765
O1···N1^{i}	2.771 (3)	H1···O1^{iii}	2.00 (3)
O1···C8^{ii}	3.447 (3)	H1···C4^{iv}	3.46 (2)
O1···C9^{ii}	3.474 (3)	H1···C18^{iii}	3.24 (3)
O1···C17^{i}	3.268 (3)	H1···H4^{iv}	2.9546
N1···O1^{iii}	2.771 (3)	H1···H8^{viii}	3.3814
C3···C15^{iv}	3.554 (4)	H1···H9^{viii}	3.1978
C4···C20^{iv}	3.528 (3)	H1···H17A^{iii}	3.3077
C6···C12^{v}	3.578 (3)	H1···H24^{iii}	3.5752
C8···O1^{vi}	3.447 (3)	H2···C3^{iv}	3.4927
C9···O1^{vi}	3.474 (3)	H2···C7^{vii}	3.5441
C12···C6^{vii}	3.578 (3)	H2···C8^{vii}	3.5540
C14···C23^{vi}	3.564 (3)	H2···C9^{vii}	3.4025
C15···C3^{iv}	3.554 (4)	H2···C10^{vii}	3.2279
C15···C16^{viii}	3.543 (3)	H2···C11^{vii}	3.1878
C16···C15^{viii}	3.543 (3)	H2···C12^{vii}	3.3599

C16···C16^{viii}	3.557 (3)	H2···H2^{iv}	3.4989
C17···O1^{iii}	3.268 (3)	H2···H3^{iv}	3.2230
C19···C23^{ix}	3.414 (3)	H2···H6^{vii}	3.2317
C20···C4^{iv}	3.528 (3)	H2···H11^{vii}	3.5730
C22···C24^{ix}	3.432 (3)	H3···C9^{vii}	3.0499
C23···C14^{ii}	3.564 (3)	H3···C10^{vii}	3.2432
C23···C19^{ix}	3.414 (3)	H3···C13^{iv}	3.3597
C23···C24^{ix}	3.458 (3)	H3···C14^{iv}	2.8059
C24···C22^{ix}	3.432 (3)	H3···C15^{iv}	2.7413
C24···C23^{ix}	3.458 (3)	H3···C16^{iv}	3.1961
O1···H1	3.00 (3)	H3···H2^{iv}	3.2230
O1···H17A	2.4780	H3···H9^{vii}	2.9258
O1···H24	2.5220	H3···H10^{vii}	3.2692
N1···H20	2.6223	H4···O1^{xii}	3.0210
N2···H2	2.6146	H4···N1^{iv}	3.3719
N2···H6	2.6176	H4···C15^{iv}	3.4072
N2···H8	2.6222	H4···C16^{iv}	3.3491
N2···H12	2.6170	H4···C22^{xi}	3.3317
C1···H3	3.2457	H4···H1^{iv}	2.9546
C1···H5	3.2575	H4···H11^{ii}	3.2716
C1···H12	2.6877	H4···H20^{iv}	2.8948
C2···H4	3.2697	H4···H21^{xi}	3.4262
C2···H6	3.2681	H4···H22^{xi}	2.5702
C2···H12	3.4852	H5···C7^{v}	3.1294
C3···H5	3.2559	H5···C8^{v}	3.0658
C4···H2	3.2717	H5···C9^{v}	3.2831
C4···H6	3.2634	H5···C10^{v}	3.5636
C5···H3	3.2538	H5···C12^{v}	3.4389
C6···H2	3.2698	H5···C17^{xii}	3.3890
C6···H4	3.2637	H5···H8^{v}	3.4222
C6···H12	2.9540	H5···H11^{ii}	3.2830
C7···H6	2.8606	H5···H17A^{xii}	2.7660
C7···H9	3.2552	H5···H17B^{xii}	3.3385
C7···H11	3.2560	H5···H20^{iv}	3.0863
C8···H10	3.2632	H5···H22^{xi}	3.1939
C8···H12	3.2759	H6···N2^{v}	3.0712
C9···H11	3.2474	H6···C7^{v}	3.0781
C10···H8	3.2631	H6···C12^{v}	3.0155
C10···H12	3.2649	H6···C13^{v}	3.5021
C11···H9	3.2481	H6···H2^{v}	3.2317
C12···H6	3.0831	H6···H12^{v}	2.9384
C12···H8	3.2756	H6···H21^{iv}	3.5884
C12···H10	3.2641	H8···O1^{vi}	2.7971
C13···H2	2.8167	H8···C17^{viii}	3.3058
C13···H8	2.5819	H8···C18^{vi}	3.1877
C14···H2	3.4466	H8···C19^{vi}	3.1300
C14···H8	3.1079	H8···C24^{vi}	2.9232
C15···H17A	3.1485	H8···H1^{viii}	3.3814

C15···H17B	3.1456	H8···H5^{vii}	3.4222
C16···H1	2.86 (3)	H8···H17B^{viii}	2.4485
C18···H17A	2.5817	H8···H24^{vi}	2.7703
C18···H17B	3.2072	H9···O1^{vi}	2.8433
C18···H20	2.7085	H9···C14^{vi}	3.4887
C18···H24	2.6176	H9···C15^{vi}	3.1005
C19···H1	2.55 (3)	H9···C16^{vi}	3.1969
C19···H21	3.2652	H9···C18^{vi}	3.3078
C19···H23	3.2645	H9···C23^{xiii}	3.3216
C20···H1	2.59 (3)	H9···H1^{viii}	3.1978
C20···H22	3.2540	H9···H3^{v}	2.9258
C20···H24	3.2601	H9···H22^{xiii}	3.5787
C21···H23	3.2515	H9···H23^{xiii}	2.4318
C22···H20	3.2532	H10···N2^{vi}	3.3987
C22···H24	3.2569	H10···C1^{vi}	3.1174
C23···H21	3.2511	H10···C2^{vi}	3.4708
C24···H20	3.2591	H10···C6^{vi}	3.3378
C24···H22	3.2586	H10···C13^{vi}	3.0389
H1···H17A	2.7192	H10···C14^{vi}	3.1782
H1···H17B	2.2293	H10···C22^{xiii}	3.4938
H1···H20	2.0941	H10···C23^{xiii}	3.2823
H2···H3	2.3366	H10···H3^{v}	3.2692
H3···H4	2.3396	H10···H11^{xiv}	3.3934
H4···H5	2.3345	H10···H22^{xiii}	3.2294
H5···H6	2.3408	H10···H23^{xiii}	2.8308
H6···H12	2.9798	H11···C3^{vi}	3.3907
H8···H9	2.3326	H11···C4^{vi}	2.9920
H9···H10	2.3332	H11···C5^{vi}	3.0027
H10···H11	2.3320	H11···C6^{vi}	3.4181
H11···H12	2.3321	H11···C10^{xiv}	3.4217
H20···H21	2.3300	H11···C11^{xiv}	3.2281
H21···H22	2.3303	H11···C22^{iv}	3.4167
H22···H23	2.3317	H11···H2^{v}	3.5730
H23···H24	2.3375	H11···H4^{vi}	3.2716
O1···H1^{i}	2.00 (3)	H11···H5^{vi}	3.2830
O1···H4^{x}	3.0210	H11···H10^{xiv}	3.3934
O1···H8^{ii}	2.7971	H11···H11^{xiv}	3.0695
O1···H9^{ii}	2.8433	H11···H22^{iv}	2.7503
O1···H17B^{i}	2.8537	H12···C21^{iv}	2.9248
O1···H20^{i}	2.9274	H12···C22^{iv}	3.0977
N1···H4^{iv}	3.3719	H12···H6^{vii}	2.9384
N2···H6^{vii}	3.0712	H12···H21^{iv}	2.7981
N2···H10^{ii}	3.3987	H12···H22^{iv}	3.0931
C1···H10^{ii}	3.1174	H17A···C5^{x}	3.3469
C2···H10^{ii}	3.4708	H17A···C20^{i}	3.0108
C3···H2^{iv}	3.4927	H17A···C21^{i}	3.3558
C3···H11^{ii}	3.3907	H17A···H1^{i}	3.3077
C3···H20^{iv}	3.5010	H17A···H5^{x}	2.7660

C4···H1^{iv}	3.46 (2)	H17A···H20^{i}	2.3287
C4···H11^{ii}	2.9920	H17A···H21^{i}	3.0195
C4···H20^{iv}	2.8499	H17B···O1^{iii}	2.8537
C4···H22^{xi}	3.1086	H17B···C8^{viii}	3.1112
C5···H11^{ii}	3.0027	H17B···C13^{viii}	3.2031
C5···H17A^{xii}	3.3469	H17B···C14^{viii}	2.8558
C5···H20^{iv}	2.9654	H17B···C15^{viii}	3.0852
C5···H22^{xi}	3.4379	H17B···C24^{iii}	3.3765
C6···H10^{ii}	3.3378	H17B···H5^{x}	3.3385
C6···H11^{ii}	3.4181	H17B···H8^{viii}	2.4485
C6···H21^{iv}	3.5731	H17B···H24^{iii}	2.5602
C7···H2^{v}	3.5441	H20···O1^{iii}	2.9274
C7···H5^{vii}	3.1294	H20···C3^{iv}	3.5010
C7···H6^{vii}	3.0781	H20···C4^{iv}	2.8499
C8···H2^{v}	3.5540	H20···C5^{iv}	2.9654
C8···H5^{vii}	3.0658	H20···C17^{iii}	3.2884
C8···H17B^{viii}	3.1112	H20···H4^{iv}	2.8948
C9···H2^{v}	3.4025	H20···H5^{iv}	3.0863
C9···H3^{v}	3.0499	H20···H17A^{iii}	2.3287
C9···H5^{vii}	3.2831	H21···C6^{iv}	3.5731
C9···H23^{xiii}	3.0533	H21···C12^{iv}	3.5003
C10···H2^{v}	3.2279	H21···C14^{xviii}	3.4014
C10···H3^{v}	3.2432	H21···C15^{xviii}	3.5546
C10···H5^{vii}	3.5636	H21···H4^{xvi}	3.4262
C10···H11^{xiv}	3.4217	H21···H6^{iv}	3.5884
C10···H22^{xiii}	3.4622	H21···H12^{iv}	2.7981
C10···H23^{xiii}	3.2492	H21···H17A^{iii}	3.0195
C11···H2^{v}	3.1878	H22···C4^{xvi}	3.1086
C11···H11^{xiv}	3.2281	H22···C5^{xvi}	3.4379
C11···H22^{iv}	3.4844	H22···C10^{xvii}	3.4622
C12···H2^{v}	3.3599	H22···C11^{iv}	3.4844
C12···H5^{vii}	3.4389	H22···H4^{xvi}	2.5702
C12···H6^{vii}	3.0155	H22···H5^{xvi}	3.1939
C12···H21^{iv}	3.5003	H22···H9^{xvii}	3.5787
C13···H3^{iv}	3.3597	H22···H10^{xvii}	3.2294
C13···H6^{vii}	3.5021	H22···H11^{iv}	2.7503
C13···H10^{ii}	3.0389	H22···H12^{iv}	3.0931
C13···H17B^{viii}	3.2031	H22···H24^{ix}	3.5928
C13···H23^{vi}	3.5690	H23···C9^{xvii}	3.0533
C14···H3^{iv}	2.8059	H23···C10^{xvii}	3.2492
C14···H9^{ii}	3.4887	H23···C13^{ii}	3.5690
C14···H10^{ii}	3.1782	H23···C14^{ii}	3.0996
C14···H17B^{viii}	2.8558	H23···C15^{ii}	2.9697
C14···H21^{xv}	3.4014	H23···C16^{ii}	3.3206
C14···H23^{vi}	3.0996	H23···C19^{ix}	3.3890
C14···H24^{vi}	3.2035	H23···C20^{ix}	3.4498
C15···H3^{iv}	2.7413	H23···H9^{xvii}	2.4318
C15···H4^{iv}	3.4072	H23···H10^{xvii}	2.8308

C15···H9^{ii}	3.1005	H24···C14^{ii}	3.2035
C15···H17B^{viii}	3.0852	H24···C15^{ii}	3.1854
C15···H21^{xv}	3.5546	H24···C16^{i}	3.5434
C15···H23^{vi}	2.9697	H24···C17^{i}	3.3524
C15···H24^{vi}	3.1854	H24···C21^{ix}	3.4170
C16···H3^{iv}	3.1961	H24···C22^{ix}	3.3848
C16···H4^{iv}	3.3491	H24···H1^{i}	3.5752
C16···H9^{ii}	3.1969	H24···H8^{ii}	2.7703
C16···H23^{vi}	3.3206	H24···H17B^{i}	2.5602
C16···H24^{iii}	3.5434	H24···H22^{ix}	3.5928

C17—N1—C18	122.13 (17)	C18—N1—H1	120 (2)
C1—N2—C7	122.14 (14)	C1—C2—H2	120.416
C1—N2—C13	117.63 (17)	C3—C2—H2	120.421
C7—N2—C13	119.93 (18)	C2—C3—H3	119.640
N2—C1—C2	119.60 (17)	C4—C3—H3	119.651
N2—C1—C6	119.50 (19)	C3—C4—H4	120.235
C2—C1—C6	120.9 (2)	C5—C4—H4	120.231
C1—C2—C3	119.16 (19)	C4—C5—H5	119.828
C2—C3—C4	120.7 (2)	C6—C5—H5	119.814
C3—C4—C5	119.5 (2)	C1—C6—H6	120.311
C4—C5—C6	120.36 (19)	C5—C6—H6	120.311
C1—C6—C5	119.4 (2)	C7—C8—H8	120.256
N2—C7—C8	120.19 (15)	C9—C8—H8	120.261
N2—C7—C12	119.58 (19)	C8—C9—H9	119.637
C8—C7—C12	120.19 (19)	C10—C9—H9	119.637
C7—C8—C9	119.48 (16)	C9—C10—H10	120.281
C8—C9—C10	120.7 (2)	C11—C10—H10	120.288
C9—C10—C11	119.4 (2)	C10—C11—H11	119.538
C10—C11—C12	120.92 (17)	C12—C11—H11	119.542
C7—C12—C11	119.2 (2)	C7—C12—H12	120.393
N2—C13—C14	178.7 (2)	C11—C12—H12	120.383
C13—C14—C15	174.6 (2)	N1—C17—H17A	109.264
C14—C15—C16	177.9 (2)	N1—C17—H17B	109.266
C15—C16—C17	178.1 (2)	C16—C17—H17A	109.270
N1—C17—C16	111.75 (17)	C16—C17—H17B	109.274
O1—C18—N1	121.1 (2)	H17A—C17—H17B	107.935
O1—C18—C19	120.60 (19)	C19—C20—H20	119.896
N1—C18—C19	118.29 (17)	C21—C20—H20	119.889
C18—C19—C20	122.46 (18)	C20—C21—H21	119.898
C18—C19—C24	118.24 (17)	C22—C21—H21	119.896
C20—C19—C24	119.3 (2)	C21—C22—H22	119.989
C19—C20—C21	120.2 (2)	C23—C22—H22	119.981
C20—C21—C22	120.2 (2)	C22—C23—H23	119.987
C21—C22—C23	120.0 (2)	C24—C23—H23	119.985
C22—C23—C24	120.0 (2)	C19—C24—H24	119.887
C19—C24—C23	120.24 (19)	C23—C24—H24	119.871
C17—N1—H1	118 (2)		

C17—N1—C18—O1	7.2 (2)	N2—C7—C12—C11	176.76 (15)
C17—N1—C18—C19	−171.73 (13)	C8—C7—C12—C11	−1.0 (3)
C18—N1—C17—C16	84.99 (19)	C12—C7—C8—C9	1.6 (3)
C1—N2—C7—C8	−149.21 (16)	C7—C8—C9—C10	−0.8 (3)
C1—N2—C7—C12	33.1 (2)	C8—C9—C10—C11	−0.6 (3)
C7—N2—C1—C2	−132.38 (16)	C9—C10—C11—C12	1.3 (3)
C7—N2—C1—C6	50.1 (2)	C10—C11—C12—C7	−0.5 (3)
C13—N2—C1—C2	53.8 (2)	O1—C18—C19—C20	−160.81 (15)
C13—N2—C1—C6	−123.66 (17)	O1—C18—C19—C24	17.2 (2)
C13—N2—C7—C8	24.5 (3)	N1—C18—C19—C20	18.1 (2)
C13—N2—C7—C12	−153.28 (16)	N1—C18—C19—C24	−163.86 (14)
N2—C1—C2—C3	−177.48 (13)	C18—C19—C20—C21	177.75 (14)
N2—C1—C6—C5	177.35 (13)	C18—C19—C24—C23	−177.58 (13)
C2—C1—C6—C5	−0.1 (3)	C20—C19—C24—C23	0.5 (2)
C6—C1—C2—C3	−0.0 (3)	C24—C19—C20—C21	−0.3 (2)
C1—C2—C3—C4	−0.0 (3)	C19—C20—C21—C22	−0.1 (3)
C2—C3—C4—C5	0.2 (3)	C20—C21—C22—C23	0.3 (3)
C3—C4—C5—C6	−0.3 (3)	C21—C22—C23—C24	−0.0 (3)
C4—C5—C6—C1	0.3 (3)	C22—C23—C24—C19	−0.4 (3)
N2—C7—C8—C9	−176.13 (15)		

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) *x*, −*y*+1/2, *z*−1/2; (iii) −*x*, *y*+1/2, −*z*+1/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*+1, *y*−1/2, −*z*+3/2; (vi) *x*, −*y*+1/2, *z*+1/2; (vii) −*x*+1, *y*+1/2, −*z*+3/2; (viii) −*x*, −*y*+1, −*z*+1; (ix) −*x*, −*y*+1, −*z*; (x) *x*−1, −*y*+1/2, *z*−1/2; (xi) −*x*+1, *y*−1/2, −*z*+1/2; (xii) *x*+1, −*y*+1/2, *z*+1/2; (xiii) *x*, *y*, *z*+1; (xiv) −*x*+1, −*y*+1, −*z*+2; (xv) *x*, −*y*+3/2, *z*+1/2; (xvi) −*x*+1, *y*+1/2, −*z*+1/2; (xvii) *x*, *y*, *z*−1; (xviii) *x*, −*y*+3/2, *z*−1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···C14^{iv}	0.95	2.81	3.673 (4)	152
C3—H3···C15^{iv}	0.95	2.74	3.554 (4)	144
N1—H1···O1^{iii}	0.85 (3)	2.00 (3)	2.771 (3)	149 (3)

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