IUCrData

ISSN 2414-3146

5-{[1-(2,4-Dichlorophenyl)-1*H*-1,2,3-triazol-4-yl]methyl}-5*H*-dibenz[*b*,*f*]azepine

K. S. Vinay Kumar,[a] Chandra,[b] B. M. Rajesh,[c] M. Mahendra[b] and M. P. Sadashiva[a]*

[a]Department of Studies in Chemistry, Manasagangotri, University of Mysore, Mysore 570 006, India, [b]Department of Studies in Physics, Manasagangotri, University of Mysore, Mysore 570 006, India, and [c]Department of Physics, RV College of Engineering, Bengaluru 560 059, India. *Correspondence e-mail: mpsadashiva@gmail.com

Received 13 January 2016
Accepted 4 February 2016

Edited by S. Parkin, University of Kentucky, USA

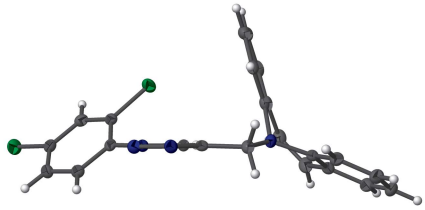
Keywords: crystal structure; azepine derivatives; medicinal importance.

CCDC reference: 1451830

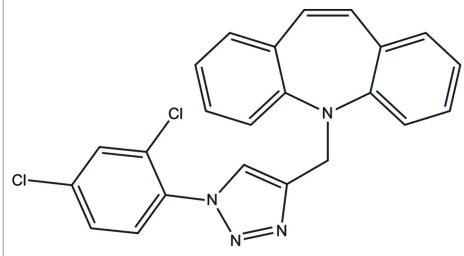
Structural data: full structural data are available from iucrdata.iucr.org

In the molecule of the title compound, $C_{23}H_{16}Cl_2N_4$, the dihedral angle between the benzene rings fused to the azepine ring is 52.00 (6)°. The plane of the triazole ring makes dihedral angles of 74.40 (5), 25.56 (8) and 44.78 (6)° with the planes of the benzene rings of the dibenzoazepine moiety and the dichlorophenyl ring, respectively. The azepine ring adopts a boat conformation. There are no classical hydrogen bonds in the crystal.

3D view



Chemical scheme



Structure description

Iminostilbene and its derivatives are found in many significant drugs such as carbamazepine, oxcarbazepine, and opipramol, which have been used to treat epilepsy (Wang *et al.*, 2015), bipolar disorder (Ghaemi *et al.*, 2003), and as an antidepressant (Moller *et al.*, 2001), respectively. Similarly, 1,2,3-triazoles also have major biological significance, with properties that include anti-tumor, anti-convulsant, anti-microbial, anti-depressant, anti-malarial and anti-inflammatory activities (Jagdish *et al.*, 2013). As a part of our ongoing research on dibenzoazepine derivatives, we present herein the crystal structure of the title compound.

In the molecular structure of the title compound (Fig. 1), the triazole ring makes dihedral angles of 74.40 (5), 25.56 (8) and 44.78 (6)° with the phenyl (C2–C7 and C10–C15) and dichlophenyl (C10–C15) rings, respectively. The dihedral angle between the phenyl rings is 52.00 (6)°. The seven-membered azepine ring adopts a boat conformation, as indicated by the puckering parameters, $Q(2)$ = 0.7122 (17), $Q(3)$ = 0.2099 (16) Å, $\varphi(2)$ = 181.58 (14), $\varphi(3)$ = 179.7 (5)° and the total puckering amplitude $Q(T)$ = 0.7424 (16) Å.

The dibenzoazepine moiety and the triazole ring are bridged by a carbon atom (C16), and this linkage is characterized by torsion angles of −158.73 (12)° (C15—N1—C16—C17) and −173.67 (13)° (N1—C16—C17—N18). The chlorine atoms are almost coplanar

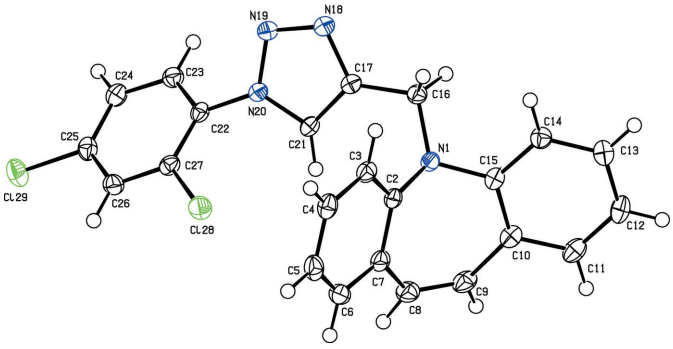


Figure 1
Perspective diagram of the title molecule, shown with 50% probability displacement ellipsoids.

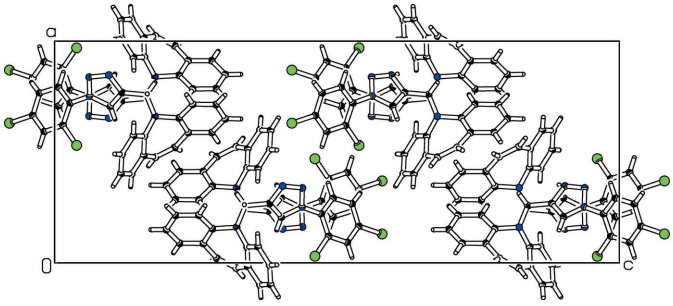


Figure 2
The packing of the molecule, viewed along the *b*-axis direction.

with the benzene ring, with atoms Cl28 and Cl29 deviating from the mean plane by −0.087 (1) and 0.029 (1) Å, respectively. There are no classical hydrogen bonds. The molecular packing exhibits layered stacking when viewed down the *b* axis, as shown in Fig. 2.

Synthesis and crystallization

5-(Prop-2-yn-1-yl)-5*H*-dibenzo[*b*,*f*]azepine (2.1 mmol) was taken in a mixture of dichloromethane and water in the ratio 1:1, cuprous iodide (0.21 mmol) was added followed by sodium ascorbate (0.21 mmol) at room temperature. After 10 minutes, 1-azido-2,4-dichlorobenzene was added (2.3 mmol) at room temperature. Then, the resulting reaction mixture was stirred for 8 h. After completion of reaction (monitored by TLC), the reaction mixture was diluted with water (50 ml). The aqueous layer was extracted with ethyl acetate (3×20 ml), the combined ethyl acetate layer was washed with brine (2×25 ml). Then, the organic layer was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure to afford crude product, which was purified by column chromatography over silica gel (60–120 mesh) using a hexane:ethyl acetate mixture in 8:2 ratio as eluent. The final compound was crystallized from ethyl acetate and hexane to obtain pale-yellow single crystals.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{16}Cl_2N_4$
M_r	419.30
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, *b*, *c* (Å)	13.2330 (11), 8.7515 (7), 33.695 (3)
V (Å^3)	3902.2 (6)
Z	8
Radiation type	Cu *Kα*
μ (mm^{-1})	3.13
Crystal size (mm)	0.29 × 0.26 × 0.23
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.464, 0.533
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20100, 3210, 3089
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.586
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.032, 0.091, 1.06
No. of reflections	3210
No. of parameters	262
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.22

Computer programs: *APEX2* (Bruker, 2009), *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

KSV gratefully acknowledges the UGC–BSR, New Delhi, for financial support. MM would like to thank the UGC, New Delhi, Government of India, for the award of a project under the head F. No. 41–920/2012(SR) dated: 25–07-2012.

References

Bruker (2009). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ghaemi, S. N., Berv, D. A., Klugman, J., Rosenquist, K. J. & Hsu, D. J. (2003). *J. Clin. Psychiatry*, **64**, 943–945.
Möller, H. J., Volz, H. P., Reimann, I. W. & Stoll, K. D. (2001). *J. Clin. Psychopharmacol.* **21**, 59–65.
Jagdish, K. S., Swastika, G. & Atul, K. (2013). *Chin. J. Nat. Med.* **11**, 456–465.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wang, P., Yin, T., Ma, H. Y., Liu, D.-Q., Sheng, Y. H., Wang, C. & Zhou, B. T. (2015). *Epilepsy Res.* **117**, 52–57.

full crystallographic data

IUCrData (2016). **1**, x160221 [https://doi.org/10.1107/S2414314616002212]

5-{[1-(2,4-Dichlorophenyl)-1*H*-1,2,3-triazol-4-yl]methyl}-5*H*-dibenz[*b*,*f*]azepine

K. S. Vinay Kumar, Chandra, B. M. Rajesh, M. Mahendra and M. P. Sadashiva

5-{[1-(2,4-Dichlorophenyl)-1*H*-1,2,3-triazol-4-yl]methyl}-5*H*-dibenz[*b*,*f*]azepine

Crystal data

$C_{23}H_{16}Cl_2N_4$
M_r = 419.30
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 13.2330 (11) Å
b = 8.7515 (7) Å
c = 33.695 (3) Å
V = 3902.2 (6) Å^3
Z = 8
F(000) = 1728
D_x = 1.427 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 3210 reflections
θ = 4.3–64.6°
μ = 3.13 mm^{-1}
T = 296 K
Block, light yellow
0.29 × 0.26 × 0.23 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 10.7 pixels mm^{-1}
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.464, T_{max} = 0.533
20100 measured reflections
3210 independent reflections
3089 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 64.6°, θ_{min} = 4.3°
h = −13→15
k = −10→8
l = −38→38

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.091
S = 1.06
3210 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 1.9833P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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}
Cl28	0.53010 (3)	0.65530 (5)	0.53902 (1)	0.0260 (1)
Cl29	0.63027 (3)	1.03517 (5)	0.42010 (1)	0.0302 (2)
N1	0.66079 (10)	0.58214 (15)	0.67786 (4)	0.0182 (4)
N18	0.84679 (10)	0.53348 (14)	0.59627 (4)	0.0193 (4)
N19	0.83790 (10)	0.59721 (15)	0.56132 (4)	0.0193 (4)
N20	0.75208 (10)	0.68295 (14)	0.56223 (4)	0.0170 (3)
C2	0.57186 (12)	0.52280 (17)	0.65898 (4)	0.0181 (4)
C3	0.57308 (12)	0.38226 (18)	0.63960 (5)	0.0205 (5)
C4	0.48933 (13)	0.32968 (19)	0.61912 (5)	0.0241 (5)
C5	0.40285 (13)	0.4183 (2)	0.61745 (5)	0.0260 (5)
C6	0.40111 (13)	0.5588 (2)	0.63632 (5)	0.0255 (5)
C7	0.48426 (12)	0.61320 (19)	0.65786 (5)	0.0212 (5)
C8	0.47687 (13)	0.7600 (2)	0.67837 (5)	0.0261 (5)
C9	0.52101 (13)	0.79772 (19)	0.71276 (5)	0.0256 (5)
C10	0.58799 (12)	0.70227 (18)	0.73680 (5)	0.0209 (5)
C11	0.58832 (13)	0.72054 (19)	0.77811 (5)	0.0254 (5)
C12	0.65044 (14)	0.6344 (2)	0.80224 (5)	0.0264 (5)
C13	0.71444 (13)	0.52698 (19)	0.78552 (5)	0.0247 (5)
C14	0.71582 (12)	0.50611 (19)	0.74478 (5)	0.0211 (5)
C15	0.65428 (12)	0.59383 (17)	0.72018 (5)	0.0184 (5)
C16	0.75821 (12)	0.53003 (17)	0.66218 (4)	0.0184 (5)
C17	0.76794 (11)	0.57852 (17)	0.61969 (4)	0.0172 (4)
C21	0.70728 (12)	0.67415 (17)	0.59844 (4)	0.0175 (4)
C22	0.72075 (12)	0.76532 (17)	0.52791 (4)	0.0177 (4)
C23	0.79272 (12)	0.84767 (18)	0.50702 (5)	0.0207 (5)
C24	0.76590 (13)	0.92902 (19)	0.47349 (5)	0.0225 (5)
C25	0.66572 (13)	0.92946 (19)	0.46149 (4)	0.0218 (5)
C26	0.59215 (13)	0.84824 (18)	0.48186 (5)	0.0214 (5)
C27	0.62067 (12)	0.76384 (18)	0.51495 (5)	0.0192 (5)
H3	0.63120	0.32260	0.64040	0.0250*
H4	0.49120	0.23510	0.60650	0.0290*
H5	0.34630	0.38380	0.60370	0.0310*
H6	0.34320	0.61870	0.63470	0.0310*
H8	0.43750	0.83480	0.66630	0.0310*
H9	0.50760	0.89520	0.72240	0.0310*
H11	0.54560	0.79250	0.78960	0.0300*
H12	0.64930	0.64840	0.82960	0.0320*
H13	0.75650	0.46880	0.80170	0.0300*
H14	0.75820	0.43280	0.73370	0.0250*

H16A	0.76260	0.41960	0.66400	0.0220*
H16B	0.81280	0.57370	0.67770	0.0220*
H21	0.64850	0.72250	0.60680	0.0210*
H23	0.85950	0.84810	0.51560	0.0250*
H24	0.81440	0.98270	0.45920	0.0270*
H26	0.52510	0.85020	0.47350	0.0260*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl28	0.0191 (2)	0.0327 (3)	0.0262 (2)	−0.0071 (2)	0.0001 (2)	0.0035 (2)
Cl29	0.0328 (3)	0.0320 (3)	0.0257 (2)	−0.0015 (2)	−0.0065 (2)	0.0086 (2)
N1	0.0192 (7)	0.0194 (7)	0.0159 (6)	0.0014 (5)	0.0018 (5)	−0.0003 (5)
N18	0.0187 (7)	0.0192 (7)	0.0200 (7)	−0.0003 (5)	0.0020 (5)	−0.0005 (5)
N19	0.0182 (7)	0.0197 (7)	0.0200 (7)	0.0015 (5)	0.0013 (5)	−0.0008 (5)
N20	0.0165 (6)	0.0174 (6)	0.0170 (6)	−0.0005 (5)	0.0015 (5)	−0.0008 (5)
C2	0.0192 (8)	0.0205 (8)	0.0146 (7)	−0.0003 (6)	0.0033 (6)	0.0041 (6)
C3	0.0226 (8)	0.0205 (8)	0.0185 (8)	0.0003 (7)	0.0033 (6)	0.0015 (6)
C4	0.0280 (9)	0.0257 (9)	0.0187 (8)	−0.0062 (7)	0.0021 (7)	0.0008 (6)
C5	0.0248 (9)	0.0343 (10)	0.0188 (8)	−0.0073 (7)	−0.0013 (7)	0.0051 (7)
C6	0.0196 (8)	0.0339 (9)	0.0229 (8)	0.0035 (7)	0.0022 (7)	0.0086 (7)
C7	0.0231 (8)	0.0233 (8)	0.0172 (8)	0.0021 (7)	0.0043 (6)	0.0052 (6)
C8	0.0276 (9)	0.0243 (9)	0.0263 (9)	0.0092 (7)	0.0039 (7)	0.0047 (7)
C9	0.0313 (9)	0.0188 (8)	0.0267 (9)	0.0068 (7)	0.0073 (7)	−0.0009 (7)
C10	0.0247 (8)	0.0164 (8)	0.0216 (8)	−0.0023 (6)	0.0036 (6)	−0.0015 (6)
C11	0.0316 (9)	0.0202 (8)	0.0244 (8)	−0.0012 (7)	0.0061 (7)	−0.0056 (7)
C12	0.0358 (10)	0.0266 (9)	0.0168 (8)	−0.0054 (7)	0.0007 (7)	−0.0037 (7)
C13	0.0290 (9)	0.0242 (9)	0.0210 (8)	−0.0015 (7)	−0.0033 (7)	0.0008 (6)
C14	0.0236 (8)	0.0185 (8)	0.0212 (8)	0.0006 (6)	0.0002 (6)	−0.0013 (6)
C15	0.0224 (8)	0.0155 (8)	0.0174 (8)	−0.0036 (6)	0.0019 (6)	−0.0010 (6)
C16	0.0195 (8)	0.0171 (8)	0.0186 (8)	0.0020 (6)	0.0008 (6)	0.0003 (6)
C17	0.0176 (8)	0.0147 (7)	0.0193 (8)	−0.0021 (6)	0.0014 (6)	−0.0029 (6)
C21	0.0196 (8)	0.0165 (7)	0.0165 (7)	−0.0013 (6)	0.0028 (6)	−0.0022 (6)
C22	0.0211 (8)	0.0164 (7)	0.0156 (7)	0.0008 (6)	0.0017 (6)	−0.0028 (6)
C23	0.0191 (8)	0.0221 (8)	0.0210 (8)	−0.0005 (6)	0.0008 (6)	−0.0017 (6)
C24	0.0244 (9)	0.0227 (8)	0.0203 (8)	−0.0021 (6)	0.0033 (7)	0.0008 (6)
C25	0.0283 (9)	0.0195 (8)	0.0177 (8)	0.0009 (7)	−0.0015 (6)	−0.0009 (6)
C26	0.0194 (8)	0.0234 (8)	0.0215 (8)	0.0002 (6)	−0.0022 (6)	−0.0038 (6)
C27	0.0191 (8)	0.0195 (8)	0.0191 (8)	−0.0016 (6)	0.0020 (6)	−0.0034 (6)

Geometric parameters (Å, º)

C2—C3	1.393 (2)	C24—C25	1.386 (2)
C2—C7	1.404 (2)	C25—C26	1.387 (2)
C3—C4	1.384 (2)	C26—C27	1.390 (2)
C4—C5	1.384 (2)	C3—H3	0.9300
C5—C6	1.384 (2)	C4—H4	0.9300
C6—C7	1.402 (2)	C5—H5	0.9300

C7—C8	1.462 (2)	C6—H6	0.9300
C8—C9	1.339 (2)	C8—H8	0.9300
C9—C10	1.463 (2)	C9—H9	0.9300
C10—C11	1.401 (2)	C11—H11	0.9300
C10—C15	1.409 (2)	C12—H12	0.9300
C11—C12	1.380 (2)	C13—H13	0.9300
C12—C13	1.385 (2)	C14—H14	0.9300
C13—C14	1.385 (2)	C16—H16A	0.9700
C14—C15	1.393 (2)	C16—H16B	0.9700
C16—C17	1.4988 (19)	C21—H21	0.9300
C17—C21	1.363 (2)	C23—H23	0.9300
C22—C23	1.386 (2)	C24—H24	0.9300
C22—C27	1.395 (2)	C26—H26	0.9300
C23—C24	1.382 (2)		

Cl28···N20	3.0494 (14)	C13···H8^{vi}	3.0800
Cl28···C21	3.0876 (16)	C14···H16B	2.6700
Cl28···C23^{i}	3.5035 (17)	C14···H16A	2.8900
Cl28···C24^{i}	3.5980 (18)	C16···H3	2.5800
Cl28···H21	2.8300	C16···H14	2.5600
Cl28···H23^{i}	2.9100	C16···H3^{v}	3.0400
Cl28···H24^{i}	3.1000	C17···H3^{v}	2.6100
Cl29···H5^{ii}	3.0500	C17···H3	2.9600
Cl29···H4^{iii}	3.0000	C21···H3^{v}	2.8700
N18···C21^{iv}	3.226 (2)	H3···C16	2.5800
N18···C22^{iv}	3.408 (2)	H3···C17	2.9600
N19···C27^{iv}	3.355 (2)	H3···H16A	2.0900
N19···C23^{iv}	3.332 (2)	H3···N18^{iv}	2.9500
N19···C22^{iv}	3.210 (2)	H3···C16^{iv}	3.0400
N20···Cl28	3.0494 (14)	H3···C17^{iv}	2.6100
N1···H21	2.7000	H3···C21^{iv}	2.8700
N18···H3^{v}	2.9500	H4···Cl29^{iii}	3.0000
N18···H21^{iv}	2.7500	H4···N18^{iv}	2.8000
N18···H4^{v}	2.8000	H5···Cl29^{i}	3.0500
N19···H23	2.7000	H5···H24^{i}	2.4600
N19···H26^{ii}	2.7800	H6···H8	2.5000
C2···C21	3.021 (2)	H8···H6	2.5000
C3···C21	3.406 (2)	H8···C12^{viii}	3.0600
C3···C17	3.170 (2)	H8···C13^{viii}	3.0800
C3···C17^{iv}	3.456 (2)	H9···H11	2.4900
C17···C3	3.170 (2)	H9···C12^{viii}	3.0700
C17···C3^{v}	3.456 (2)	H11···H9	2.4900
C21···Cl28	3.0876 (16)	H11···C2^{viii}	3.0800
C21···N18^{v}	3.226 (2)	H11···C3^{viii}	2.9600
C21···C2	3.021 (2)	H12···C4^{viii}	2.9800
C21···C3	3.406 (2)	H12···C5^{viii}	3.0400
C22···C24^{iv}	3.472 (2)	H13···C6^{ix}	2.9400
C22···N19^{v}	3.210 (2)	H13···C11^{iv}	3.0900

C22···N18^{v}	3.408 (2)	H14···C16	2.5600
C23···Cl28^{ii}	3.5035 (17)	H14···H16A	2.3500
C23···N19^{v}	3.332 (2)	H14···H16B	2.3700
C24···C22^{v}	3.472 (2)	H14···C10^{iv}	2.8700
C24···C27^{v}	3.576 (2)	H16A···C3	2.6600
C24···Cl28^{ii}	3.5980 (18)	H16A···C14	2.8900
C27···N19^{v}	3.355 (2)	H16A···H3	2.0900
C27···C24^{iv}	3.576 (2)	H16A···H14	2.3500
C2···H11^{vi}	3.0800	H16B···C14	2.6700
C2···H21	2.6800	H16B···H14	2.3700
C3···H11^{vi}	2.9600	H21···Cl28	2.8300
C3···H16A	2.6600	H21···N1	2.7000
C4···H12^{vi}	2.9800	H21···C2	2.6800
C5···H24^{i}	2.9600	H21···C7	2.9300
C5···H12^{vi}	3.0400	H21···N18^{v}	2.7500
C6···H13^{vii}	2.9400	H23···N19	2.7000
C7···H21	2.9300	H23···Cl28^{ii}	2.9100
C10···H14^{v}	2.8700	H24···Cl28^{ii}	3.1000
C11···H13^{v}	3.0900	H24···C5^{ii}	2.9600
C12···H9^{vi}	3.0700	H24···H5^{ii}	2.4600
C12···H8^{vi}	3.0600	H26···N19^{i}	2.7800

C3—C2—C7	119.65 (14)	C4—C5—H5	120.00
C2—C3—C4	121.20 (15)	C6—C5—H5	120.00
C3—C4—C5	119.75 (15)	C5—C6—H6	119.00
C4—C5—C6	119.53 (16)	C7—C6—H6	119.00
C5—C6—C7	121.77 (16)	C7—C8—H8	117.00
C2—C7—C6	118.08 (15)	C9—C8—H8	117.00
C2—C7—C8	122.53 (15)	C8—C9—H9	116.00
C6—C7—C8	119.39 (15)	C10—C9—H9	116.00
C7—C8—C9	126.62 (16)	C10—C11—H11	119.00
C8—C9—C10	127.07 (16)	C12—C11—H11	119.00
C9—C10—C11	119.14 (15)	C11—C12—H12	120.00
C9—C10—C15	122.82 (15)	C13—C12—H12	120.00
C11—C10—C15	118.03 (15)	C12—C13—H13	120.00
C10—C11—C12	121.65 (16)	C14—C13—H13	120.00
C11—C12—C13	119.69 (16)	C13—C14—H14	120.00
C12—C13—C14	120.05 (16)	C15—C14—H14	120.00
C13—C14—C15	120.63 (15)	N1—C16—H16A	110.00
C10—C15—C14	119.93 (15)	N1—C16—H16B	110.00
C16—C17—C21	128.69 (13)	C17—C16—H16A	110.00
C23—C22—C27	119.88 (14)	C17—C16—H16B	110.00
C22—C23—C24	120.43 (15)	H16A—C16—H16B	108.00
C23—C24—C25	119.06 (15)	N20—C21—H21	128.00
C24—C25—C26	121.70 (14)	C17—C21—H21	128.00
C25—C26—C27	118.60 (15)	C22—C23—H23	120.00
C22—C27—C26	120.28 (15)	C24—C23—H23	120.00
C2—C3—H3	119.00	C23—C24—H24	120.00

C4—C3—H3	119.00	C25—C24—H24	121.00
C3—C4—H4	120.00	C25—C26—H26	121.00
C5—C4—H4	120.00	C27—C26—H26	121.00
C15—N1—C2—C3	−113.85 (16)	C6—C7—C8—C9	146.28 (18)
C15—N1—C2—C7	70.45 (18)	C7—C8—C9—C10	1.6 (3)
C16—N1—C2—C3	26.1 (2)	C8—C9—C10—C11	−148.74 (18)
C16—N1—C2—C7	−149.60 (14)	C8—C9—C10—C15	32.6 (3)
C2—N1—C15—C10	−68.50 (18)	C9—C10—C11—C12	−179.55 (16)
C2—N1—C15—C14	114.92 (16)	C15—C10—C11—C12	−0.8 (2)
C16—N1—C15—C10	151.16 (14)	C9—C10—C15—N1	3.6 (2)
C16—N1—C15—C14	−25.4 (2)	C9—C10—C15—C14	−179.74 (15)
C2—N1—C16—C17	61.72 (16)	C11—C10—C15—N1	−175.10 (14)
C15—N1—C16—C17	−158.73 (12)	C11—C10—C15—C14	1.5 (2)
C17—N18—N19—N20	−0.49 (16)	C10—C11—C12—C13	0.1 (3)
N19—N18—C17—C16	−177.60 (13)	C11—C12—C13—C14	−0.1 (3)
N19—N18—C17—C21	0.09 (18)	C12—C13—C14—C15	0.9 (3)
N18—N19—N20—C21	0.74 (16)	C13—C14—C15—N1	174.92 (15)
N18—N19—N20—C22	−178.99 (12)	C13—C14—C15—C10	−1.6 (2)
N19—N20—C21—C17	−0.66 (16)	N1—C16—C17—N18	−173.67 (13)
C22—N20—C21—C17	179.03 (14)	N1—C16—C17—C21	9.1 (2)
N19—N20—C22—C23	−45.0 (2)	N18—C17—C21—N20	0.35 (16)
N19—N20—C22—C27	134.51 (15)	C16—C17—C21—N20	177.85 (14)
C21—N20—C22—C23	135.31 (16)	N20—C22—C23—C24	179.84 (14)
C21—N20—C22—C27	−45.2 (2)	C27—C22—C23—C24	0.3 (2)
N1—C2—C3—C4	−175.61 (15)	N20—C22—C27—Cl28	−2.5 (2)
C7—C2—C3—C4	0.1 (2)	N20—C22—C27—C26	178.54 (14)
N1—C2—C7—C6	174.54 (14)	C23—C22—C27—Cl28	177.04 (12)
N1—C2—C7—C8	−5.8 (2)	C23—C22—C27—C26	−1.9 (2)
C3—C2—C7—C6	−1.2 (2)	C22—C23—C24—C25	1.2 (2)
C3—C2—C7—C8	178.41 (15)	C23—C24—C25—Cl29	178.38 (13)
C2—C3—C4—C5	0.6 (3)	C23—C24—C25—C26	−1.2 (2)
C3—C4—C5—C6	0.0 (2)	Cl29—C25—C26—C27	−180.00 (13)
C4—C5—C6—C7	−1.2 (3)	C24—C25—C26—C27	−0.5 (2)
C5—C6—C7—C2	1.8 (2)	C25—C26—C27—Cl28	−177.01 (12)
C5—C6—C7—C8	−177.82 (16)	C25—C26—C27—C22	2.0 (2)
C2—C7—C8—C9	−33.4 (3)		

Symmetry codes: (i) $x-1/2, -y+3/2, -z+1$; (ii) $x+1/2, -y+3/2, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+3/2, y-1/2, z$; (v) $-x+3/2, y+1/2, z$; (vi) $-x+1, y-1/2, -z+3/2$; (vii) $x-1/2, y, -z+3/2$; (viii) $-x+1, y+1/2, -z+3/2$; (ix) $x+1/2, y, -z+3/2$.