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Bis[4-(2,4,4-trimethylpentan-2-yl)phenyl]amine

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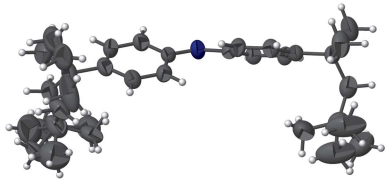
CCDC reference: 1465157

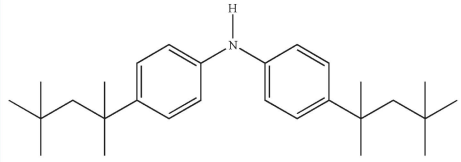
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{28}H_{43}N$, the dihedral angle between the aromatic rings is 41.15 (12)° and both side chains exhibit extensive disorder. No directional interactions beyond van der Waals contacts could be identified in the crystal.

3D view



Chemical scheme



Structure description

Alkylated diphenylamines have been investigated extensively owing to their antioxidant activity (Jensen *et al.*, 1995). Bis(4–(2,4,4–trimethylpentan–2–yl)phenyl)amine has been widely used in the synthesis of lubricating oil because of the reactive hydrogen atom bonded to the N atom (Hu *et al.*, 2006; Singh *et al.*, 2013). The title compound was synthesized by electrophilic alkylation of diphenylaminde and 2,4,4–trimethyl–1–pentene using acid clay as catalyst (Popoff *et al.*, 1960) and we now report its crystal structure (Fig. 1). The dihedral angle between the aromatic rings formed by atoms C1–C6 and C15–C20 is 41.15 (12)°. No directional interactions beyond van der Waals' contacts could be identified in the crystal (Fig. 2).

Synthesis and crystallization

The title compound was prepared according to a literature method (Popoff *et al.*, 1960). Colourless prisms were obtained by evaporation of a solution of the title compound in hexane at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Both side chains exhibit extensive disorder.

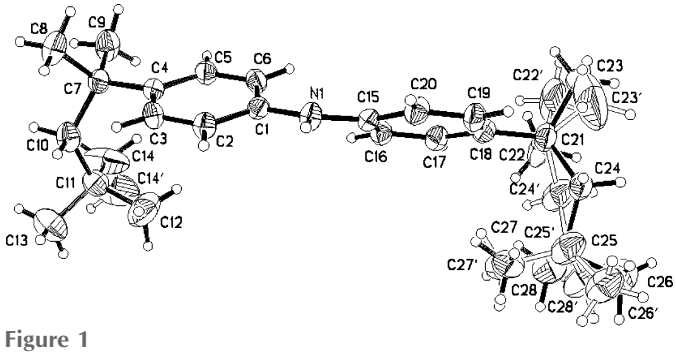


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

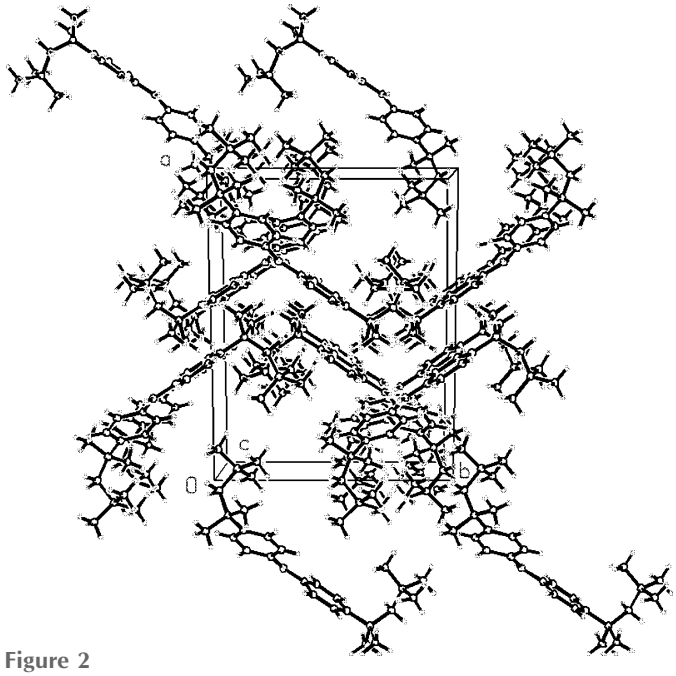


Figure 2
The crystal packing of the title compound.

Acknowledgements

The authors thank National Science Foundation of China (No. 21404114) for financial support.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{43}N$
M_r	393.63
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	17.7676 (16), 13.1380 (13), 11.4852 (11)
β (°)	108.261 (2)
V (Å^3)	2546.0 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.06
Crystal size (mm)	0.21 × 0.17 × 0.12
Data collection	
Diffractometer	Bruker SMART CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 1999)
T_{min}, T_{max}	0.639, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14525, 4735, 2969
R_{int}	0.046
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.080, 0.268, 1.07
No. of reflections	4735
No. of parameters	340
No. of restraints	75
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.67, −0.31

Computer programs: *SMART* (Bruker, 1999), *SAINT* (Bruker, 1999), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008).

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full crystallographic data

IUCrData (2016). **1**, x160424 [doi:10.1107/S2414314616004247]

Bis[4-(2,4,4-trimethylpentan-2-yl)phenyl]amine

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Crystal data

$C_{28}H_{43}N$
M_r = 393.63
Monoclinic, $P2_1/c$
a = 17.7676 (16) Å
b = 13.1380 (13) Å
c = 11.4852 (11) Å
β = 108.261 (2)°
V = 2546.0 (4) Å^3
Z = 4
$F(000)$ = 872
D_x = 1.027 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1946 reflections
θ = 4.8–40.7°
μ = 0.06 mm^{-1}
T = 293 K
Prismatic, colorless
0.21 × 0.17 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.639, T_{max} = 0.746
14525 measured reflections
4735 independent reflections
2969 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 25.5°, θ_{min} = 2.0°
h = −21→21
k = −11→15
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.268
S = 1.07
4735 reflections
340 parameters
75 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
$w = 1/[\sigma^2(F_o^2) + (0.1465P)^2 + 0.6321P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.28793 (14)	0.71370 (18)	0.1340 (2)	0.0550 (6)	
H1A	0.2884	0.7428	0.0672	0.066*	
C1	0.33224 (15)	0.6249 (2)	0.1632 (2)	0.0458 (6)	
C2	0.35062 (16)	0.5742 (2)	0.0694 (2)	0.0513 (7)	
H2A	0.3311	0.5986	−0.0105	0.062*	
C3	0.39711 (17)	0.4888 (2)	0.0930 (2)	0.0528 (7)	
H3A	0.4093	0.4575	0.0286	0.063*	
C4	0.42689 (15)	0.4470 (2)	0.2101 (2)	0.0468 (7)	
C5	0.40892 (16)	0.4997 (2)	0.3021 (2)	0.0524 (7)	
H5A	0.4286	0.4755	0.3821	0.063*	
C6	0.36305 (17)	0.5864 (2)	0.2803 (2)	0.0533 (7)	
H6A	0.3528	0.6195	0.3453	0.064*	
C7	0.47709 (17)	0.3505 (2)	0.2313 (3)	0.0559 (8)	
C8	0.5460 (2)	0.3688 (3)	0.1771 (4)	0.0851 (11)	
H8A	0.5779	0.4248	0.2187	0.128*	
H8B	0.5246	0.3841	0.0913	0.128*	
H8C	0.5782	0.3087	0.1878	0.128*	
C9	0.5169 (2)	0.3290 (3)	0.3654 (3)	0.0810 (11)	
H9A	0.4773	0.3159	0.4044	0.121*	
H9B	0.5480	0.3869	0.4032	0.121*	
H9C	0.5506	0.2706	0.3741	0.121*	
C10	0.4322 (2)	0.2591 (3)	0.1546 (3)	0.0704 (9)	
H10A	0.4700	0.2037	0.1676	0.085*	
H10B	0.4194	0.2786	0.0692	0.085*	
C11	0.3549 (2)	0.2131 (3)	0.1704 (3)	0.0706 (9)	
C12	0.2868 (3)	0.2861 (4)	0.1300 (7)	0.142 (2)	
H12A	0.2382	0.2487	0.0982	0.213*	
H12B	0.2938	0.3297	0.0671	0.213*	
H12C	0.2848	0.3265	0.1985	0.213*	
C13	0.3370 (3)	0.1250 (4)	0.0808 (4)	0.1120 (15)	
H13A	0.3575	0.1398	0.0146	0.168*	
H13B	0.2807	0.1152	0.0489	0.168*	
H13C	0.3615	0.0643	0.1220	0.168*	
C14	0.3689 (5)	0.1698 (6)	0.2948 (5)	0.144 (3)	0.797 (10)
H14A	0.4226	0.1829	0.3440	0.215*	0.797 (10)
H14B	0.3597	0.0977	0.2886	0.215*	0.797 (10)
H14C	0.3333	0.2009	0.3323	0.215*	0.797 (10)
C14′	0.304 (2)	0.148 (3)	0.261 (2)	0.146 (5)	0.203 (10)
H14D	0.3394	0.1391	0.3429	0.219*	0.203 (10)
H14E	0.2863	0.0830	0.2253	0.219*	0.203 (10)

H14F	0.2592	0.1880	0.2637	0.219*	0.203 (10)
C15	0.24268 (15)	0.7629 (2)	0.1969 (2)	0.0479 (7)	
C16	0.21175 (16)	0.7158 (2)	0.2791 (3)	0.0536 (7)	
H16A	0.2235	0.6478	0.2993	0.064*	
C17	0.16335 (17)	0.7687 (2)	0.3318 (3)	0.0569 (8)	
H17A	0.1434	0.7350	0.3870	0.068*	
C18	0.14367 (16)	0.8692 (2)	0.3055 (3)	0.0581 (8)	
C19	0.17542 (18)	0.9152 (2)	0.2240 (3)	0.0651 (8)	
H19A	0.1635	0.9831	0.2037	0.078*	
C20	0.22417 (17)	0.8643 (2)	0.1714 (3)	0.0609 (8)	
H20A	0.2450	0.8987	0.1178	0.073*	
C21	0.08906 (19)	0.9284 (3)	0.3625 (3)	0.0727 (10)	
C22	0.0681 (4)	0.8611 (6)	0.4614 (5)	0.122 (3)	0.779 (6)
H22A	0.1143	0.8533	0.5317	0.183*	0.779 (6)
H22B	0.0502	0.7953	0.4272	0.183*	0.779 (6)
H22C	0.0269	0.8935	0.4855	0.183*	0.779 (6)
C23	0.1356 (4)	1.0216 (6)	0.4278 (8)	0.125 (3)	0.779 (6)
H23A	0.1482	1.0646	0.3690	0.187*	0.779 (6)
H23B	0.1836	0.9997	0.4881	0.187*	0.779 (6)
H23C	0.1039	1.0590	0.4673	0.187*	0.779 (6)
C24	0.0145 (3)	0.9664 (4)	0.2669 (4)	0.0736 (14)	0.779 (6)
H24A	0.0318	1.0085	0.2108	0.088*	0.779 (6)
H24B	−0.0113	1.0117	0.3093	0.088*	0.779 (6)
C25	−0.0511 (6)	0.8954 (9)	0.1864 (9)	0.0969 (17)	0.779 (6)
C26	−0.1080 (6)	0.9765 (8)	0.1194 (10)	0.159 (3)	0.779 (6)
H26A	−0.1536	0.9451	0.0625	0.238*	0.779 (6)
H26B	−0.0825	1.0195	0.0756	0.238*	0.779 (6)
H26C	−0.1242	1.0165	0.1772	0.238*	0.779 (6)
C27	−0.0214 (6)	0.8335 (7)	0.1007 (7)	0.110 (3)	0.779 (6)
H27A	−0.0631	0.7903	0.0525	0.165*	0.779 (6)
H27B	0.0224	0.7924	0.1471	0.165*	0.779 (6)
H27C	−0.0044	0.8780	0.0476	0.165*	0.779 (6)
C28	−0.0974 (6)	0.8275 (8)	0.2440 (10)	0.158 (3)	0.779 (6)
H28A	−0.1347	0.7884	0.1814	0.236*	0.779 (6)
H28B	−0.1252	0.8682	0.2866	0.236*	0.779 (6)
H28C	−0.0617	0.7823	0.3009	0.236*	0.779 (6)
C22′	0.1271 (14)	0.943 (2)	0.4881 (18)	0.105 (7)	0.221 (6)
H22D	0.1635	0.9992	0.4995	0.158*	0.221 (6)
H22E	0.1555	0.8827	0.5228	0.158*	0.221 (6)
H22F	0.0883	0.9582	0.5280	0.158*	0.221 (6)
C23′	0.0859 (14)	1.0473 (14)	0.325 (2)	0.100 (7)	0.221 (6)
H23D	0.0614	1.0855	0.3748	0.150*	0.221 (6)
H23E	0.0557	1.0551	0.2404	0.150*	0.221 (6)
H23F	0.1388	1.0720	0.3386	0.150*	0.221 (6)
C24′	0.0065 (7)	0.8881 (15)	0.3270 (13)	0.074 (4)	0.221 (6)
H24C	−0.0198	0.9201	0.3798	0.088*	0.221 (6)
H24D	0.0098	0.8159	0.3457	0.088*	0.221 (6)
C25′	−0.0504 (14)	0.901 (3)	0.1871 (19)	0.073 (4)	0.221 (6)

C26′	−0.0986 (13)	0.961 (2)	0.0669 (16)	0.081 (5)	0.221 (6)
H26D	−0.1308	0.9137	0.0084	0.122*	0.221 (6)
H26E	−0.0623	0.9939	0.0324	0.122*	0.221 (6)
H26F	−0.1319	1.0108	0.0871	0.122*	0.221 (6)
C27′	−0.0232 (17)	0.804 (2)	0.136 (2)	0.077 (5)	0.221 (6)
H27D	−0.0503	0.7984	0.0498	0.116*	0.221 (6)
H27E	−0.0355	0.7451	0.1772	0.116*	0.221 (6)
H27F	0.0329	0.8065	0.1502	0.116*	0.221 (6)
C28′	−0.1175 (10)	0.8818 (18)	0.242 (2)	0.079 (4)	0.221 (6)
H28D	−0.1677	0.8893	0.1790	0.118*	0.221 (6)
H28E	−0.1139	0.9299	0.3062	0.118*	0.221 (6)
H28F	−0.1129	0.8140	0.2744	0.118*	0.221 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0585 (14)	0.0524 (14)	0.0599 (14)	0.0138 (11)	0.0269 (12)	0.0090 (11)
C1	0.0435 (14)	0.0441 (14)	0.0515 (15)	0.0001 (12)	0.0171 (12)	−0.0014 (12)
C2	0.0581 (17)	0.0544 (16)	0.0452 (15)	0.0056 (13)	0.0216 (13)	0.0056 (13)
C3	0.0643 (18)	0.0514 (16)	0.0485 (16)	0.0060 (14)	0.0261 (13)	−0.0022 (13)
C4	0.0454 (14)	0.0461 (15)	0.0492 (15)	0.0022 (12)	0.0152 (12)	−0.0017 (12)
C5	0.0541 (16)	0.0578 (17)	0.0421 (14)	0.0082 (13)	0.0103 (12)	−0.0016 (13)
C6	0.0591 (17)	0.0538 (16)	0.0458 (15)	0.0070 (14)	0.0149 (13)	−0.0099 (13)
C7	0.0544 (17)	0.0501 (16)	0.0604 (18)	0.0084 (13)	0.0141 (14)	0.0005 (14)
C8	0.077 (2)	0.091 (3)	0.096 (3)	0.027 (2)	0.040 (2)	0.008 (2)
C9	0.091 (3)	0.083 (2)	0.063 (2)	0.037 (2)	0.0160 (18)	0.0093 (18)
C10	0.085 (2)	0.063 (2)	0.068 (2)	0.0137 (18)	0.0291 (17)	0.0046 (16)
C11	0.082 (2)	0.063 (2)	0.068 (2)	−0.0060 (17)	0.0243 (17)	−0.0004 (16)
C12	0.074 (3)	0.091 (3)	0.266 (8)	−0.008 (3)	0.061 (4)	−0.019 (4)
C13	0.143 (4)	0.089 (3)	0.102 (3)	−0.015 (3)	0.036 (3)	−0.011 (3)
C14	0.177 (7)	0.186 (7)	0.075 (4)	−0.105 (6)	0.051 (4)	0.001 (4)
C14′	0.177 (11)	0.185 (10)	0.082 (8)	−0.099 (10)	0.052 (8)	−0.010 (8)
C15	0.0404 (14)	0.0460 (15)	0.0553 (16)	0.0033 (12)	0.0120 (12)	−0.0025 (12)
C16	0.0554 (17)	0.0458 (15)	0.0608 (17)	0.0045 (13)	0.0202 (14)	0.0003 (13)
C17	0.0546 (16)	0.0621 (18)	0.0564 (17)	0.0069 (14)	0.0208 (14)	0.0024 (14)
C18	0.0466 (16)	0.067 (2)	0.0577 (17)	0.0097 (14)	0.0116 (13)	−0.0084 (15)
C19	0.0601 (18)	0.0482 (17)	0.086 (2)	0.0135 (14)	0.0207 (17)	0.0009 (16)
C20	0.0551 (17)	0.0533 (17)	0.078 (2)	0.0048 (14)	0.0265 (15)	0.0083 (15)
C21	0.064 (2)	0.083 (2)	0.068 (2)	0.0249 (18)	0.0157 (16)	−0.0131 (18)
C22	0.135 (5)	0.175 (7)	0.079 (4)	0.092 (5)	0.067 (4)	0.042 (4)
C23	0.082 (4)	0.139 (6)	0.136 (6)	0.021 (4)	0.008 (4)	−0.082 (5)
C24	0.066 (2)	0.081 (3)	0.076 (3)	0.017 (2)	0.025 (2)	−0.006 (2)
C25	0.077 (3)	0.113 (3)	0.096 (3)	0.008 (3)	0.022 (3)	−0.016 (3)
C26	0.120 (5)	0.159 (6)	0.166 (7)	0.040 (5)	0.000 (5)	−0.018 (6)
C27	0.094 (4)	0.136 (6)	0.088 (5)	0.000 (5)	0.010 (4)	−0.036 (4)
C28	0.153 (6)	0.176 (7)	0.146 (6)	−0.015 (6)	0.050 (5)	0.001 (6)
C22′	0.097 (10)	0.119 (11)	0.110 (10)	0.020 (9)	0.049 (8)	−0.033 (8)
C23′	0.108 (10)	0.086 (9)	0.113 (10)	0.013 (8)	0.047 (8)	−0.021 (8)

C24′	0.051 (6)	0.111 (9)	0.065 (6)	0.008 (6)	0.025 (5)	0.001 (6)
C25′	0.045 (5)	0.112 (8)	0.065 (6)	0.005 (5)	0.024 (5)	0.002 (6)
C26′	0.059 (7)	0.121 (10)	0.059 (7)	0.007 (7)	0.013 (6)	0.010 (7)
C27′	0.048 (7)	0.112 (10)	0.068 (9)	−0.011 (7)	0.012 (7)	−0.004 (8)
C28′	0.045 (6)	0.113 (10)	0.085 (8)	0.009 (7)	0.031 (6)	0.015 (8)

Geometric parameters (Å, º)

N1—C1	1.389 (3)	C19—H19A	0.9300
N1—C15	1.396 (3)	C20—H20A	0.9300
N1—H1A	0.8600	C21—C22′	1.40 (2)
C1—C6	1.378 (4)	C21—C24′	1.491 (12)
C1—C2	1.390 (4)	C21—C24	1.516 (5)
C2—C3	1.369 (4)	C21—C23	1.536 (7)
C2—H2A	0.9300	C21—C22	1.574 (7)
C3—C4	1.395 (4)	C21—C23′	1.615 (19)
C3—H3A	0.9300	C22—H22A	0.9600
C4—C5	1.382 (4)	C22—H22B	0.9600
C4—C7	1.525 (4)	C22—H22C	0.9600
C5—C6	1.378 (4)	C23—H23A	0.9600
C5—H5A	0.9300	C23—H23B	0.9600
C6—H6A	0.9300	C23—H23C	0.9600
C7—C9	1.507 (4)	C24—C25	1.553 (13)
C7—C10	1.554 (4)	C24—H24A	0.9700
C7—C8	1.557 (4)	C24—H24B	0.9700
C8—H8A	0.9600	C25—C27	1.495 (10)
C8—H8B	0.9600	C25—C28	1.500 (11)
C8—H8C	0.9600	C25—C26	1.503 (10)
C9—H9A	0.9600	C26—H26A	0.9600
C9—H9B	0.9600	C26—H26B	0.9600
C9—H9C	0.9600	C26—H26C	0.9600
C10—C11	1.562 (5)	C27—H27A	0.9600
C10—H10A	0.9700	C27—H27B	0.9600
C10—H10B	0.9700	C27—H27C	0.9600
C11—C14	1.484 (6)	C28—H28A	0.9600
C11—C12	1.498 (6)	C28—H28B	0.9600
C11—C13	1.515 (5)	C28—H28C	0.9600
C11—C14′	1.79 (2)	C22′—H22D	0.9600
C12—H12A	0.9600	C22′—H22E	0.9600
C12—H12B	0.9600	C22′—H22F	0.9600
C12—H12C	0.9600	C23′—H23D	0.9600
C13—H13A	0.9600	C23′—H23E	0.9600
C13—H13B	0.9600	C23′—H23F	0.9600
C13—H13C	0.9600	C24′—C25′	1.617 (19)
C14—H14A	0.9600	C24′—H24C	0.9700
C14—H14B	0.9600	C24′—H24D	0.9700
C14—H14C	0.9600	C25′—C28′	1.534 (19)
C14′—H14D	0.9600	C25′—C27′	1.55 (2)

C14′—H14E	0.9600	C25′—C26′	1.583 (18)
C14′—H14F	0.9600	C26′—H26D	0.9600
C15—C16	1.379 (4)	C26′—H26E	0.9600
C15—C20	1.381 (4)	C26′—H26F	0.9600
C16—C17	1.384 (4)	C27′—H27D	0.9600
C16—H16A	0.9300	C27′—H27E	0.9600
C17—C18	1.375 (4)	C27′—H27F	0.9600
C17—H17A	0.9300	C28′—H28D	0.9600
C18—C19	1.376 (4)	C28′—H28E	0.9600
C18—C21	1.540 (4)	C28′—H28F	0.9600
C19—C20	1.375 (4)		

C1—N1—C15	129.7 (2)	C22′—C21—C24	136.8 (9)
C1—N1—H1A	115.2	C24′—C21—C24	50.0 (7)
C15—N1—H1A	115.2	C22′—C21—C23	51.2 (11)
C6—C1—N1	124.4 (2)	C24′—C21—C23	138.5 (7)
C6—C1—C2	117.6 (2)	C24—C21—C23	107.8 (4)
N1—C1—C2	117.9 (2)	C22′—C21—C18	110.0 (9)
C3—C2—C1	120.8 (3)	C24′—C21—C18	113.7 (7)
C3—C2—H2A	119.6	C24—C21—C18	112.5 (3)
C1—C2—H2A	119.6	C23—C21—C18	107.3 (3)
C2—C3—C4	122.5 (2)	C22′—C21—C22	58.8 (11)
C2—C3—H3A	118.7	C24′—C21—C22	64.1 (7)
C4—C3—H3A	118.7	C24—C21—C22	110.9 (4)
C5—C4—C3	115.6 (2)	C23—C21—C22	108.0 (5)
C5—C4—C7	123.9 (2)	C18—C21—C22	110.2 (3)
C3—C4—C7	120.5 (2)	C22′—C21—C23′	95.9 (11)
C6—C5—C4	122.7 (3)	C24′—C21—C23′	108.8 (11)
C6—C5—H5A	118.7	C24—C21—C23′	62.6 (9)
C4—C5—H5A	118.7	C23—C21—C23′	47.7 (8)
C5—C6—C1	120.8 (2)	C18—C21—C23′	110.5 (7)
C5—C6—H6A	119.6	C22—C21—C23′	137.5 (7)
C1—C6—H6A	119.6	C21—C22—H22A	109.5
C9—C7—C4	112.5 (2)	C21—C22—H22B	109.5
C9—C7—C10	115.3 (3)	C21—C22—H22C	109.5
C4—C7—C10	112.4 (2)	C21—C23—H23A	109.5
C9—C7—C8	105.2 (3)	C21—C23—H23B	109.5
C4—C7—C8	107.6 (2)	H23A—C23—H23B	109.5
C10—C7—C8	102.8 (3)	C21—C23—H23C	109.5
C7—C8—H8A	109.5	H23A—C23—H23C	109.5
C7—C8—H8B	109.5	H23B—C23—H23C	109.5
H8A—C8—H8B	109.5	C21—C24—C25	123.8 (5)
C7—C8—H8C	109.5	C21—C24—H24A	106.4
H8A—C8—H8C	109.5	C25—C24—H24A	106.4
H8B—C8—H8C	109.5	C21—C24—H24B	106.4
C7—C9—H9A	109.5	C25—C24—H24B	106.4
C7—C9—H9B	109.5	H24A—C24—H24B	106.5
H9A—C9—H9B	109.5	C27—C25—C28	108.8 (9)

C7—C9—H9C	109.5	C27—C25—C26	111.6 (8)
H9A—C9—H9C	109.5	C28—C25—C26	105.9 (9)
H9B—C9—H9C	109.5	C27—C25—C24	111.4 (8)
C7—C10—C11	123.2 (3)	C28—C25—C24	120.5 (8)
C7—C10—H10A	106.5	C26—C25—C24	97.9 (8)
C11—C10—H10A	106.5	C25—C26—H26A	109.5
C7—C10—H10B	106.5	C25—C26—H26B	109.5
C11—C10—H10B	106.5	H26A—C26—H26B	109.5
H10A—C10—H10B	106.5	C25—C26—H26C	109.5
C14—C11—C12	114.8 (5)	H26A—C26—H26C	109.5
C14—C11—C13	107.3 (4)	H26B—C26—H26C	109.5
C12—C11—C13	107.5 (4)	C25—C27—H27A	109.5
C14—C11—C10	111.8 (4)	C25—C27—H27B	109.5
C12—C11—C10	111.7 (3)	H27A—C27—H27B	109.5
C13—C11—C10	102.8 (3)	C25—C27—H27C	109.5
C14—C11—C14′	38.9 (10)	H27A—C27—H27C	109.5
C12—C11—C14′	88.8 (13)	H27B—C27—H27C	109.5
C13—C11—C14′	89.7 (10)	C25—C28—H28A	109.5
C10—C11—C14′	150.7 (11)	C25—C28—H28B	109.5
C11—C12—H12A	109.5	H28A—C28—H28B	109.5
C11—C12—H12B	109.5	C25—C28—H28C	109.5
H12A—C12—H12B	109.5	H28A—C28—H28C	109.5
C11—C12—H12C	109.5	H28B—C28—H28C	109.5
H12A—C12—H12C	109.5	C21—C22′—H22D	109.5
H12B—C12—H12C	109.5	C21—C22′—H22E	109.5
C11—C13—H13A	109.5	H22D—C22′—H22E	109.5
C11—C13—H13B	109.5	C21—C22′—H22F	109.5
H13A—C13—H13B	109.5	H22D—C22′—H22F	109.5
C11—C13—H13C	109.5	H22E—C22′—H22F	109.5
H13A—C13—H13C	109.5	C21—C23′—H23D	109.5
H13B—C13—H13C	109.5	C21—C23′—H23E	109.5
C11—C14—H14A	109.5	C21—C23′—H23F	109.5
C11—C14—H14B	109.5	C21—C24′—C25′	119.2 (14)
H14A—C14—H14B	109.5	C21—C24′—H24C	107.5
C11—C14—H14C	109.5	C25′—C24′—H24C	107.5
H14A—C14—H14C	109.5	C21—C24′—H24D	107.5
H14B—C14—H14C	109.5	C25′—C24′—H24D	107.5
C11—C14′—H14D	109.5	H24C—C24′—H24D	107.0
C11—C14′—H14E	109.5	C28′—C25′—C27′	113 (2)
H14D—C14′—H14E	109.5	C28′—C25′—C26′	99.3 (17)
C11—C14′—H14F	109.5	C27′—C25′—C26′	103.2 (19)
H14D—C14′—H14F	109.5	C28′—C25′—C24′	84.2 (13)
H14E—C14′—H14F	109.5	C27′—C25′—C24′	96.5 (17)
C16—C15—C20	117.3 (3)	C26′—C25′—C24′	157 (3)
C16—C15—N1	124.3 (2)	C25′—C26′—H26D	109.5
C20—C15—N1	118.3 (3)	C25′—C26′—H26E	109.5
C15—C16—C17	120.6 (3)	H26D—C26′—H26E	109.5
C15—C16—H16A	119.7	C25′—C26′—H26F	109.5

C17—C16—H16A	119.7	H26D—C26′—H26F	109.5
C18—C17—C16	122.5 (3)	H26E—C26′—H26F	109.5
C18—C17—H17A	118.8	C25′—C27′—H27D	109.5
C16—C17—H17A	118.8	C25′—C27′—H27E	109.5
C17—C18—C19	116.2 (3)	H27D—C27′—H27E	109.5
C17—C18—C21	122.9 (3)	C25′—C27′—H27F	109.5
C19—C18—C21	121.0 (3)	H27D—C27′—H27F	109.5
C20—C19—C18	122.3 (3)	H27E—C27′—H27F	109.5
C20—C19—H19A	118.9	C25′—C28′—H28D	109.5
C18—C19—H19A	118.9	C25′—C28′—H28E	109.5
C19—C20—C15	121.2 (3)	H28D—C28′—H28E	109.5
C19—C20—H20A	119.4	C25′—C28′—H28F	109.5
C15—C20—H20A	119.4	H28D—C28′—H28F	109.5
C22′—C21—C24′	116.5 (12)	H28E—C28′—H28F	109.5

C15—N1—C1—C6	−24.3 (4)	C18—C19—C20—C15	1.1 (5)
C15—N1—C1—C2	159.5 (3)	C16—C15—C20—C19	−1.4 (4)
C6—C1—C2—C3	0.5 (4)	N1—C15—C20—C19	175.6 (3)
N1—C1—C2—C3	177.0 (2)	C17—C18—C21—C22′	68.8 (14)
C1—C2—C3—C4	1.4 (4)	C19—C18—C21—C22′	−111.5 (13)
C2—C3—C4—C5	−2.4 (4)	C17—C18—C21—C24′	−63.9 (8)
C2—C3—C4—C7	178.8 (3)	C19—C18—C21—C24′	115.8 (8)
C3—C4—C5—C6	1.5 (4)	C17—C18—C21—C24	−118.6 (4)
C7—C4—C5—C6	−179.7 (3)	C19—C18—C21—C24	61.1 (4)
C4—C5—C6—C1	0.3 (4)	C17—C18—C21—C23	123.0 (5)
N1—C1—C6—C5	−177.6 (3)	C19—C18—C21—C23	−57.3 (5)
C2—C1—C6—C5	−1.4 (4)	C17—C18—C21—C22	5.7 (5)
C5—C4—C7—C9	−10.1 (4)	C19—C18—C21—C22	−174.6 (4)
C3—C4—C7—C9	168.6 (3)	C17—C18—C21—C23′	173.5 (10)
C5—C4—C7—C10	122.0 (3)	C19—C18—C21—C23′	−6.8 (10)
C3—C4—C7—C10	−59.2 (4)	C22′—C21—C24—C25	−124.4 (19)
C5—C4—C7—C8	−125.5 (3)	C24′—C21—C24—C25	−36.8 (10)
C3—C4—C7—C8	53.2 (4)	C23—C21—C24—C25	−176.1 (6)
C9—C7—C10—C11	68.5 (4)	C18—C21—C24—C25	65.9 (7)
C4—C7—C10—C11	−62.2 (4)	C22—C21—C24—C25	−58.1 (7)
C8—C7—C10—C11	−177.7 (3)	C23′—C21—C24—C25	168.1 (10)
C7—C10—C11—C14	−62.9 (5)	C21—C24—C25—C27	−66.0 (9)
C7—C10—C11—C12	67.3 (5)	C21—C24—C25—C28	63.2 (10)
C7—C10—C11—C13	−177.7 (3)	C21—C24—C25—C26	177.0 (6)
C7—C10—C11—C14′	−64 (2)	C22′—C21—C24′—C25′	161.2 (18)
C1—N1—C15—C16	−22.9 (5)	C24—C21—C24′—C25′	31.0 (15)
C1—N1—C15—C20	160.4 (3)	C23—C21—C24′—C25′	100.7 (17)
C20—C15—C16—C17	0.8 (4)	C18—C21—C24′—C25′	−69.3 (19)
N1—C15—C16—C17	−175.9 (3)	C22—C21—C24′—C25′	−171.2 (19)
C15—C16—C17—C18	0.1 (4)	C23′—C21—C24′—C25′	54.2 (19)
C16—C17—C18—C19	−0.5 (4)	C21—C24′—C25′—C28′	−161.1 (16)
C16—C17—C18—C21	179.3 (3)	C21—C24′—C25′—C27′	86 (2)
C17—C18—C19—C20	−0.1 (5)	C21—C24′—C25′—C26′	−61 (5)

C21—C18—C19—C20	−179.8 (3)