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N-(2,6-Dimethylphenyl)-2,2,2-trimethylacetamide

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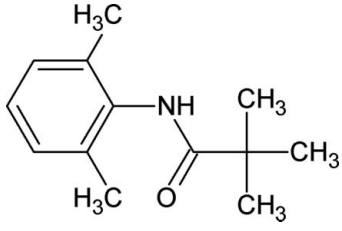
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.054; wR factor = 0.119; data-to-parameter ratio = 17.7.

The title compound, $C_{13}H_{19}NO$, crystallizes with four molecules in the asymmetric unit. Its molecular conformation is similar to those of *N*-(2,6-dimethylphenyl)acetamide, 2,2,2-trimethyl-*N*-(2-methylphenyl)acetamide, *N*-(3,5-dimethylphenyl)-2,2,2-trimethylacetamide, 2,2,2-trichloro-*N*-(2,6-dimethylphenyl)acetamide and other closely related acetanilides, with somewhat slightly different bond parameters. The molecules are linked through N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2004, 2007); Gowda, Foro & Fuess (2007*a*, 2007*b*); Gowda, Kožíšek, Tokarčík & Fuess (2007*a*, 2007*b*).



Experimental

Crystal data

$C_{13}H_{19}NO$
M_r = 205.29
Triclinic, $P\overline{1}$
a = 10.799 (1) Å
b = 15.330 (1) Å
c = 16.173 (1) Å
α = 70.004 (8)°
β = 89.800 (7)°
γ = 81.487 (7)°
V = 2485.1 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 100 (2) K
0.36 × 0.16 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.976, T_{max} = 0.989
26845 measured reflections
10127 independent reflections
4638 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.119
S = 0.97
10127 reflections
571 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···O4^{i}	0.849 (18)	2.009 (19)	2.802 (2)	155.1 (19)
N2—H2*A*···O1^{ii}	0.874 (18)	2.006 (19)	2.876 (2)	173.4 (19)
N3—H3*A*···O2	0.850 (18)	2.042 (19)	2.879 (2)	168.4 (19)
N4—H4*A*···O3	0.874 (19)	2.07 (2)	2.937 (2)	174.2 (18)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2405).

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supplementary materials

Acta Cryst. (2007). E**63**, o3324 [**doi:10.1107/S1600536807030395**]

N-(2,6-Dimethylphenyl)-2,2,2-trimethylacetamide

B. T. Gowda, I. Svoboda and H. Fuess

Comment

In the present work, the structure of *N*-(2,6-dimethylphenyl)-2,2,2- trimethylacetamide has been determined, as part of our study of the effect of ring and side chain substitutions on the solid state structures of chemically and biologically significant compounds such as acetanilides (Gowda, Foro, & Fuess, 2007*a*; Gowda, Foro, & Fuess, 2007*b*; Gowda *et al.*, 2007; Gowda, Kožíšek, Tokarčík & Fuess, 2007*a*, 2007*b*). The title compound crystallizes with four molecules in the asymmetric unit (Figs. 1 & 2). The structure of resembles those of *N*-(2,6-dimethylphenyl)-acetamide (Gowda, Foro, & Fuess, 2007*a*, *b*), *N*-(2-methylphenyl)- 2,2,2-trimethylacetamide (Gowda, Kožíšek, Tokarčík & Fuess, 2007*b*), *N*-(3,5-dimethylphenyl)-2,2,2-trimethylacetamide (Gowda, Kožíšek, Tokarčík & Fuess, 2007*a*), *N*-(2,6-dimethylphenyl)-2,2,2-trichloroacetamide (Gowda, Foro, & Fuess, 2007*a*) and other closely related acetanilides (Gowda *et al.*, 2007), with somewhat slightly different bond parameters. The molecules are linked into chains through N—H···O hydrogen bonds (Table 1).

Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2004). The purity of the compound was checked by determining its melting point. The compound was further characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2004). Single crystals of the title compound were obtained from a slow evaporation of an ethanolic solution.

Refinement

H atoms bonded to C were refined using a riding model with C—H ranging from 0.95 to 0.98Å and U_{iso}(H) = 1.2 U_{eq}(C). The methyl groups were allowed to rotate but not to tip. H atoms bonded to N were located in difference map and their positions were refined with U_{iso}(H) = 1.2 U_{eq}(N).

Figures

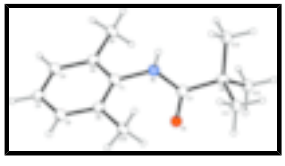
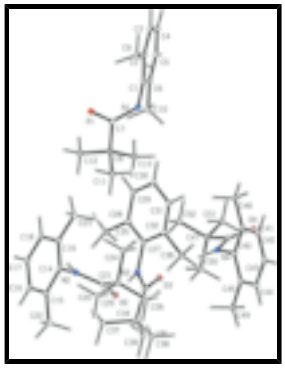


Fig. 1 & 2. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.



N-(2,6-Dimethylphenyl)-2,2,2-trimethylacetamide

Crystal data

$C_{13}H_{19}NO$	$Z = 8$
$M_r = 205.29$	$F_{000} = 896$
Triclinic, $P\overline{1}$	$D_x = 1.097$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.799$ (1) Å	Cell parameters from 4489 reflections
$b = 15.330$ (1) Å	$\theta = 2.2$–21.9º
$c = 16.173$ (1) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 70.004$ (8)º	$T = 100$ (2) K
$\beta = 89.800$ (7)º	Prism, colourless
$\gamma = 81.487$ (7)º	0.36 × 0.16 × 0.16 mm
$V = 2485.1$ (3) Å^3	

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	10127 independent reflections
Radiation source: Enhance (Mo) X-ray Source	4638 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.056$
Detector resolution: 8.4012 pixels mm^{-1}	$\theta_{max} = 26.4$º
$T = 100(2)$ K	$\theta_{min} = 2.4$º
Rotation method data acquisition using ω and φ scans	$h = -12 \rightarrow 13$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)	$k = -19 \rightarrow 19$
$T_{min} = 0.976$, $T_{max} = 0.989$	$l = -20 \rightarrow 19$
26845 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$

$wR(F^2) = 0.119$

$S = 0.97$

10127 reflections

571 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.21$ e Å^{-3}

$\Delta\rho_{min} = -0.21$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0018 (4)

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0649 (2)	0.14871 (14)	0.78936 (14)	0.0315 (6)
C2	0.0007 (2)	0.12608 (15)	0.86686 (16)	0.0389 (6)
C3	0.0677 (3)	0.11314 (16)	0.94468 (15)	0.0488 (7)
H3	0.0267	0.0973	0.9987	0.059*
C4	0.1927 (3)	0.12295 (16)	0.94443 (18)	0.0518 (8)
H4	0.2368	0.1151	0.9979	0.062*
C5	0.2535 (3)	0.14408 (15)	0.86678 (18)	0.0465 (7)
H5	0.3399	0.1497	0.8674	0.056*
C6	0.1912 (2)	0.15735 (14)	0.78768 (15)	0.0332 (6)
C7	−0.00024 (19)	0.10499 (15)	0.66636 (13)	0.0256 (5)
C8	−0.07001 (19)	0.13618 (14)	0.57685 (13)	0.0249 (5)
C9	−0.1353 (2)	0.11504 (17)	0.86599 (15)	0.0536 (7)
H9A	−0.1451	0.0640	0.8442	0.064*
H9B	−0.1846	0.1738	0.8273	0.064*
H9C	−0.1648	0.1001	0.9259	0.064*
C10	0.2571 (2)	0.17881 (15)	0.70316 (15)	0.0462 (7)
H10A	0.2171	0.2394	0.6614	0.055*
H10B	0.2521	0.1294	0.6782	0.055*
H10C	0.3453	0.1816	0.7145	0.055*
C11	0.0291 (2)	0.15985 (15)	0.50841 (13)	0.0400 (6)
H11A	0.0941	0.1048	0.5189	0.048*
H11B	0.0672	0.2123	0.5132	0.048*

H11C	−0.0102	0.1777	0.4493	0.048*
C12	−0.1291 (2)	0.05423 (14)	0.57049 (14)	0.0369 (6)
H12A	−0.1917	0.0389	0.6151	0.044*
H12B	−0.0639	−0.0006	0.5805	0.044*
H12C	−0.1697	0.0717	0.5118	0.044*
C13	−0.1715 (2)	0.22187 (15)	0.56060 (15)	0.0435 (7)
H13A	−0.1327	0.2756	0.5610	0.052*
H13B	−0.2316	0.2081	0.6071	0.052*
H13C	−0.2151	0.2368	0.5033	0.052*
C14	0.61128 (18)	0.06586 (13)	0.22279 (14)	0.0250 (5)
C15	0.5538 (2)	0.05535 (14)	0.15060 (14)	0.0281 (6)
C16	0.4501 (2)	0.00871 (14)	0.16555 (15)	0.0355 (6)
H16	0.4090	0.0007	0.1174	0.043*
C17	0.4061 (2)	−0.02609 (15)	0.24876 (16)	0.0403 (6)
H17	0.3360	−0.0585	0.2577	0.048*
C18	0.4640 (2)	−0.01373 (15)	0.31906 (15)	0.0355 (6)
H18	0.4330	−0.0376	0.3762	0.043*
C19	0.5669 (2)	0.03308 (14)	0.30732 (14)	0.0291 (6)
C20	0.7244 (2)	0.20128 (15)	0.17613 (13)	0.0230 (5)
C21	0.85034 (19)	0.23408 (13)	0.18171 (13)	0.0231 (5)
C22	0.6029 (2)	0.09186 (14)	0.06028 (13)	0.0375 (6)
H22A	0.6910	0.0641	0.0617	0.045*
H22B	0.5961	0.1604	0.0413	0.045*
H22C	0.5537	0.0750	0.0189	0.045*
C23	0.6297 (2)	0.04825 (15)	0.38334 (13)	0.0362 (6)
H23A	0.6244	0.1158	0.3717	0.043*
H23B	0.7179	0.0191	0.3902	0.043*
H23C	0.5875	0.0197	0.4375	0.043*
C24	0.88453 (19)	0.21409 (14)	0.27880 (13)	0.0327 (6)
H24A	0.8987	0.1461	0.3103	0.039*
H24B	0.8158	0.2436	0.3047	0.039*
H24C	0.9610	0.2398	0.2837	0.039*
C25	0.9524 (2)	0.18120 (15)	0.14211 (14)	0.0402 (6)
H25A	0.9301	0.1950	0.0797	0.048*
H25B	0.9590	0.1135	0.1738	0.048*
H25C	1.0329	0.2014	0.1476	0.048*
C26	0.83978 (19)	0.33891 (13)	0.13096 (13)	0.0308 (6)
H26A	0.7719	0.3730	0.1536	0.037*
H26B	0.8217	0.3511	0.0683	0.037*
H26C	0.9190	0.3601	0.1383	0.037*
C27	0.41393 (18)	0.29916 (14)	0.30430 (13)	0.0228 (5)
C28	0.34897 (19)	0.23532 (14)	0.36472 (14)	0.0273 (5)
C29	0.3737 (2)	0.21754 (15)	0.45409 (14)	0.0356 (6)
H29	0.3305	0.1747	0.4967	0.043*
C30	0.4598 (2)	0.26134 (16)	0.48133 (15)	0.0400 (6)
H30	0.4764	0.2478	0.5425	0.048*
C31	0.5220 (2)	0.32462 (15)	0.42045 (15)	0.0343 (6)
H31	0.5808	0.3547	0.4400	0.041*
C32	0.49984 (19)	0.34489 (14)	0.33076 (14)	0.0267 (5)

C33	0.2896 (2)	0.36453 (14)	0.16344 (14)	0.0245 (5)
C34	0.28635 (18)	0.37096 (13)	0.06697 (13)	0.0220 (5)
C35	0.25744 (19)	0.18665 (14)	0.33497 (14)	0.0371 (6)
H35A	0.2944	0.1625	0.2901	0.045*
H35B	0.1808	0.2312	0.3099	0.045*
H35C	0.2370	0.1343	0.3853	0.045*
C36	0.5656 (2)	0.41565 (15)	0.26390 (14)	0.0391 (6)
H36A	0.5053	0.4723	0.2338	0.047*
H36B	0.6017	0.3886	0.2207	0.047*
H36C	0.6326	0.4321	0.2938	0.047*
C37	0.3138 (2)	0.27300 (14)	0.06025 (13)	0.0352 (6)
H37A	0.2541	0.2342	0.0944	0.042*
H37B	0.3993	0.2439	0.0837	0.042*
H37C	0.3056	0.2781	−0.0016	0.042*
C38	0.38569 (19)	0.42933 (14)	0.01940 (13)	0.0353 (6)
H38A	0.4688	0.3985	0.0470	0.042*
H38B	0.3679	0.4922	0.0235	0.042*
H38C	0.3839	0.4345	−0.0427	0.042*
C39	0.15722 (18)	0.41861 (14)	0.02437 (13)	0.0313 (6)
H39A	0.1372	0.4800	0.0316	0.038*
H39B	0.0945	0.3793	0.0526	0.038*
H39C	0.1567	0.4272	−0.0385	0.038*
C40	0.2864 (2)	0.58984 (14)	0.27000 (15)	0.0304 (6)
C41	0.3581 (2)	0.58250 (14)	0.34470 (14)	0.0304 (6)
C42	0.4648 (2)	0.62495 (15)	0.33164 (16)	0.0408 (6)
H42	0.5150	0.6212	0.3813	0.049*
C43	0.4999 (2)	0.67262 (16)	0.24805 (18)	0.0510 (7)
H43	0.5735	0.7011	0.2405	0.061*
C44	0.4275 (2)	0.67875 (15)	0.17535 (16)	0.0443 (7)
H44	0.4526	0.7109	0.1179	0.053*
C45	0.3193 (2)	0.63888 (14)	0.18489 (15)	0.0360 (6)
C46	0.0722 (2)	0.57113 (15)	0.31516 (14)	0.0288 (6)
C47	−0.0358 (2)	0.51674 (14)	0.31754 (14)	0.0291 (6)
C48	0.3221 (2)	0.52920 (15)	0.43530 (13)	0.0363 (6)
H48A	0.3061	0.4671	0.4377	0.044*
H48B	0.2461	0.5638	0.4495	0.044*
H48C	0.3904	0.5218	0.4780	0.044*
C49	0.2376 (2)	0.64833 (16)	0.10600 (14)	0.0472 (7)
H49A	0.1558	0.6849	0.1077	0.057*
H49B	0.2262	0.5858	0.1070	0.057*
H49C	0.2778	0.6804	0.0520	0.057*
C50	−0.0809 (2)	0.53427 (16)	0.22283 (14)	0.0463 (7)
H50A	−0.0118	0.5129	0.1915	0.056*
H50B	−0.1095	0.6016	0.1929	0.056*
H50C	−0.1503	0.4995	0.2234	0.056*
C51	−0.1421 (2)	0.55081 (18)	0.36546 (17)	0.0558 (8)
H51A	−0.1702	0.6181	0.3350	0.067*
H51B	−0.1132	0.5401	0.4260	0.067*
H51C	−0.2120	0.5163	0.3664	0.067*

C52	0.0073 (2)	0.41170 (14)	0.36543 (15)	0.0461 (7)
H52A	0.0357	0.4011	0.4261	0.055*
H52B	0.0766	0.3893	0.3348	0.055*
H52C	−0.0626	0.3774	0.3661	0.055*
N1	−0.00496 (17)	0.16643 (12)	0.70878 (12)	0.0296 (5)
H1A	−0.0395 (18)	0.2230 (13)	0.6835 (13)	0.036*
N2	0.72269 (16)	0.10847 (12)	0.21176 (11)	0.0252 (5)
H2A	0.7912 (18)	0.0703 (13)	0.2367 (12)	0.030*
N3	0.39556 (17)	0.31548 (12)	0.21201 (12)	0.0257 (5)
H3A	0.4578 (18)	0.2954 (14)	0.1876 (12)	0.031*
N4	0.17862 (18)	0.54433 (12)	0.28008 (11)	0.0294 (5)
H4A	0.1836 (18)	0.4990 (13)	0.2583 (12)	0.035*
O1	0.06421 (13)	0.02588 (9)	0.69633 (9)	0.0342 (4)
O2	0.62806 (13)	0.25735 (9)	0.14412 (9)	0.0283 (4)
O3	0.20194 (13)	0.40129 (9)	0.19555 (9)	0.0301 (4)
O4	0.06294 (14)	0.63754 (10)	0.34287 (9)	0.0392 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0514 (18)	0.0205 (13)	0.0228 (15)	0.0053 (12)	−0.0123 (13)	−0.0119 (11)
C2	0.0454 (18)	0.0364 (15)	0.0342 (17)	0.0095 (12)	−0.0102 (14)	−0.0175 (13)
C3	0.078 (2)	0.0408 (16)	0.0255 (16)	0.0170 (15)	−0.0076 (15)	−0.0195 (12)
C4	0.079 (2)	0.0352 (16)	0.043 (2)	0.0090 (15)	−0.0288 (17)	−0.0223 (14)
C5	0.0647 (19)	0.0283 (15)	0.0482 (18)	−0.0031 (13)	−0.0219 (16)	−0.0168 (13)
C6	0.0444 (17)	0.0227 (13)	0.0339 (16)	−0.0035 (12)	−0.0091 (13)	−0.0122 (11)
C7	0.0280 (14)	0.0232 (13)	0.0262 (14)	−0.0066 (11)	0.0020 (11)	−0.0084 (11)
C8	0.0314 (14)	0.0220 (12)	0.0216 (13)	0.0026 (11)	−0.0053 (11)	−0.0106 (10)
C9	0.062 (2)	0.0597 (18)	0.0350 (16)	0.0135 (15)	0.0100 (14)	−0.0200 (14)
C10	0.0508 (18)	0.0342 (15)	0.0525 (18)	−0.0076 (13)	−0.0069 (14)	−0.0132 (13)
C11	0.0494 (17)	0.0419 (15)	0.0237 (14)	−0.0095 (13)	−0.0054 (12)	−0.0039 (12)
C12	0.0374 (15)	0.0359 (14)	0.0425 (16)	−0.0074 (12)	−0.0073 (12)	−0.0191 (12)
C13	0.0476 (17)	0.0404 (15)	0.0435 (16)	0.0067 (13)	−0.0192 (13)	−0.0209 (13)
C14	0.0197 (13)	0.0203 (12)	0.0331 (15)	−0.0048 (10)	−0.0043 (11)	−0.0063 (11)
C15	0.0315 (15)	0.0217 (13)	0.0296 (15)	−0.0014 (11)	−0.0043 (12)	−0.0082 (11)
C16	0.0384 (16)	0.0349 (14)	0.0373 (16)	−0.0091 (12)	−0.0060 (13)	−0.0163 (12)
C17	0.0304 (15)	0.0436 (16)	0.0504 (18)	−0.0145 (12)	0.0026 (14)	−0.0170 (14)
C18	0.0282 (15)	0.0390 (15)	0.0375 (16)	−0.0121 (12)	0.0058 (12)	−0.0084 (12)
C19	0.0329 (14)	0.0252 (13)	0.0257 (15)	−0.0027 (11)	−0.0020 (12)	−0.0052 (11)
C20	0.0262 (14)	0.0277 (14)	0.0149 (12)	−0.0015 (12)	0.0056 (10)	−0.0085 (10)
C21	0.0247 (13)	0.0233 (13)	0.0202 (13)	−0.0025 (10)	0.0024 (10)	−0.0067 (10)
C22	0.0471 (16)	0.0323 (14)	0.0326 (15)	−0.0068 (12)	−0.0051 (12)	−0.0101 (12)
C23	0.0414 (16)	0.0390 (15)	0.0267 (14)	−0.0062 (12)	0.0037 (12)	−0.0096 (11)
C24	0.0286 (14)	0.0353 (14)	0.0340 (15)	−0.0123 (11)	−0.0043 (11)	−0.0088 (11)
C25	0.0346 (15)	0.0358 (15)	0.0482 (16)	−0.0059 (12)	0.0105 (12)	−0.0120 (13)
C26	0.0323 (14)	0.0317 (14)	0.0286 (14)	−0.0072 (11)	0.0039 (11)	−0.0098 (11)
C27	0.0182 (13)	0.0242 (13)	0.0261 (14)	0.0011 (10)	−0.0037 (10)	−0.0106 (11)
C28	0.0263 (14)	0.0236 (13)	0.0311 (15)	−0.0007 (11)	0.0013 (11)	−0.0098 (11)

C29	0.0419 (16)	0.0327 (14)	0.0258 (15)	−0.0003 (12)	0.0025 (12)	−0.0044 (11)
C30	0.0465 (17)	0.0403 (16)	0.0299 (15)	0.0052 (13)	−0.0080 (13)	−0.0127 (13)
C31	0.0271 (14)	0.0373 (15)	0.0421 (17)	0.0040 (12)	−0.0093 (12)	−0.0217 (13)
C32	0.0238 (13)	0.0267 (13)	0.0278 (15)	0.0019 (11)	−0.0004 (11)	−0.0094 (11)
C33	0.0257 (14)	0.0201 (13)	0.0282 (14)	−0.0123 (11)	−0.0004 (12)	−0.0054 (11)
C34	0.0176 (12)	0.0236 (12)	0.0256 (13)	−0.0068 (10)	0.0009 (10)	−0.0081 (10)
C35	0.0363 (15)	0.0369 (14)	0.0399 (15)	−0.0122 (12)	0.0093 (12)	−0.0128 (12)
C36	0.0339 (15)	0.0419 (15)	0.0473 (16)	−0.0090 (12)	0.0046 (12)	−0.0216 (13)
C37	0.0373 (15)	0.0407 (15)	0.0313 (14)	−0.0097 (12)	0.0005 (11)	−0.0157 (12)
C38	0.0350 (15)	0.0401 (15)	0.0283 (14)	−0.0085 (12)	0.0015 (11)	−0.0078 (12)
C39	0.0270 (14)	0.0388 (14)	0.0255 (13)	−0.0096 (11)	−0.0016 (11)	−0.0059 (11)
C40	0.0340 (15)	0.0224 (13)	0.0356 (15)	−0.0063 (11)	−0.0086 (12)	−0.0103 (11)
C41	0.0387 (15)	0.0230 (13)	0.0311 (15)	−0.0025 (11)	−0.0069 (12)	−0.0124 (11)
C42	0.0468 (17)	0.0347 (15)	0.0417 (17)	−0.0097 (13)	−0.0146 (13)	−0.0126 (13)
C43	0.0547 (19)	0.0370 (16)	0.060 (2)	−0.0247 (14)	−0.0106 (16)	−0.0077 (15)
C44	0.0533 (18)	0.0355 (15)	0.0426 (17)	−0.0220 (14)	0.0007 (14)	−0.0052 (13)
C45	0.0524 (18)	0.0242 (13)	0.0283 (15)	−0.0074 (12)	−0.0103 (13)	−0.0043 (11)
C46	0.0392 (16)	0.0222 (13)	0.0219 (14)	0.0010 (12)	−0.0115 (12)	−0.0058 (11)
C47	0.0327 (14)	0.0291 (14)	0.0305 (14)	0.0013 (11)	−0.0011 (11)	−0.0192 (11)
C48	0.0391 (16)	0.0378 (15)	0.0303 (15)	0.0062 (12)	−0.0107 (12)	−0.0145 (12)
C49	0.0671 (19)	0.0420 (16)	0.0297 (15)	−0.0181 (14)	−0.0052 (14)	−0.0047 (12)
C50	0.0391 (16)	0.0617 (18)	0.0450 (17)	−0.0166 (13)	−0.0035 (13)	−0.0236 (14)
C51	0.0468 (18)	0.0698 (19)	0.071 (2)	−0.0114 (15)	0.0131 (15)	−0.0492 (16)
C52	0.0481 (17)	0.0353 (15)	0.0566 (17)	−0.0143 (13)	0.0114 (13)	−0.0150 (13)
N1	0.0423 (13)	0.0185 (10)	0.0262 (12)	0.0040 (9)	−0.0077 (10)	−0.0090 (9)
N2	0.0234 (12)	0.0206 (11)	0.0264 (11)	0.0008 (9)	−0.0025 (9)	−0.0033 (9)
N3	0.0206 (12)	0.0320 (11)	0.0245 (12)	−0.0006 (9)	0.0012 (9)	−0.0115 (9)
N4	0.0345 (13)	0.0258 (12)	0.0321 (12)	−0.0047 (10)	−0.0021 (10)	−0.0153 (9)
O1	0.0420 (10)	0.0205 (9)	0.0370 (10)	0.0055 (8)	−0.0149 (8)	−0.0103 (7)
O2	0.0247 (9)	0.0235 (9)	0.0324 (9)	0.0020 (7)	−0.0028 (7)	−0.0066 (7)
O3	0.0275 (10)	0.0328 (9)	0.0323 (9)	0.0011 (7)	0.0019 (7)	−0.0163 (8)
O4	0.0534 (11)	0.0255 (9)	0.0407 (10)	0.0008 (8)	−0.0124 (8)	−0.0165 (8)

Geometric parameters (Å, °)

C1—C6	1.389 (3)	C27—N3	1.436 (2)
C1—C2	1.393 (3)	C28—C29	1.395 (3)
C1—N1	1.430 (3)	C28—C35	1.494 (3)
C2—C3	1.393 (3)	C29—C30	1.379 (3)
C2—C9	1.504 (3)	C29—H29	0.9500
C3—C4	1.381 (3)	C30—C31	1.377 (3)
C3—H3	0.9500	C30—H30	0.9500
C4—C5	1.375 (3)	C31—C32	1.389 (3)
C4—H4	0.9500	C31—H31	0.9500
C5—C6	1.385 (3)	C32—C36	1.507 (3)
C5—H5	0.9500	C33—O3	1.234 (2)
C6—C10	1.496 (3)	C33—N3	1.356 (2)
C7—O1	1.241 (2)	C33—C34	1.529 (3)
C7—N1	1.337 (2)	C34—C39	1.521 (2)

C7—C8	1.523 (3)	C34—C37	1.528 (3)
C8—C12	1.524 (3)	C34—C38	1.533 (3)
C8—C13	1.528 (3)	C35—H35A	0.9800
C8—C11	1.528 (3)	C35—H35B	0.9800
C9—H9A	0.9800	C35—H35C	0.9800
C9—H9B	0.9800	C36—H36A	0.9800
C9—H9C	0.9800	C36—H36B	0.9800
C10—H10A	0.9800	C36—H36C	0.9800
C10—H10B	0.9800	C37—H37A	0.9800
C10—H10C	0.9800	C37—H37B	0.9800
C11—H11A	0.9800	C37—H37C	0.9800
C11—H11B	0.9800	C38—H38A	0.9800
C11—H11C	0.9800	C38—H38B	0.9800
C12—H12A	0.9800	C38—H38C	0.9800
C12—H12B	0.9800	C39—H39A	0.9800
C12—H12C	0.9800	C39—H39B	0.9800
C13—H13A	0.9800	C39—H39C	0.9800
C13—H13B	0.9800	C40—C45	1.398 (3)
C13—H13C	0.9800	C40—C41	1.400 (3)
C14—C15	1.392 (3)	C40—N4	1.425 (3)
C14—C19	1.396 (3)	C41—C42	1.387 (3)
C14—N2	1.434 (2)	C41—C48	1.496 (3)
C15—C16	1.392 (3)	C42—C43	1.381 (3)
C15—C22	1.501 (3)	C42—H42	0.9500
C16—C17	1.379 (3)	C43—C44	1.383 (3)
C16—H16	0.9500	C43—H43	0.9500
C17—C18	1.381 (3)	C44—C45	1.382 (3)
C17—H17	0.9500	C44—H44	0.9500
C18—C19	1.388 (3)	C45—C49	1.506 (3)
C18—H18	0.9500	C46—O4	1.236 (2)
C19—C23	1.508 (3)	C46—N4	1.352 (3)
C20—O2	1.234 (2)	C46—C47	1.524 (3)
C20—N2	1.343 (2)	C47—C51	1.512 (3)
C20—C21	1.532 (3)	C47—C52	1.529 (3)
C21—C26	1.521 (3)	C47—C50	1.530 (3)
C21—C24	1.529 (3)	C48—H48A	0.9800
C21—C25	1.538 (3)	C48—H48B	0.9800
C22—H22A	0.9800	C48—H48C	0.9800
C22—H22B	0.9800	C49—H49A	0.9800
C22—H22C	0.9800	C49—H49B	0.9800
C23—H23A	0.9800	C49—H49C	0.9800
C23—H23B	0.9800	C50—H50A	0.9800
C23—H23C	0.9800	C50—H50B	0.9800
C24—H24A	0.9800	C50—H50C	0.9800
C24—H24B	0.9800	C51—H51A	0.9800
C24—H24C	0.9800	C51—H51B	0.9800
C25—H25A	0.9800	C51—H51C	0.9800
C25—H25B	0.9800	C52—H52A	0.9800
C25—H25C	0.9800	C52—H52B	0.9800

C26—H26A	0.9800	C52—H52C	0.9800
C26—H26B	0.9800	N1—H1A	0.849 (18)
C26—H26C	0.9800	N2—H2A	0.874 (18)
C27—C32	1.391 (3)	N3—H3A	0.850 (18)
C27—C28	1.396 (3)	N4—H4A	0.874 (19)
C6—C1—C2	122.6 (2)	C30—C29—C28	120.9 (2)
C6—C1—N1	119.8 (2)	C30—C29—H29	119.6
C2—C1—N1	117.6 (2)	C28—C29—H29	119.6
C3—C2—C1	117.4 (2)	C31—C30—C29	120.4 (2)
C3—C2—C9	121.7 (2)	C31—C30—H30	119.8
C1—C2—C9	120.9 (2)	C29—C30—H30	119.8
C4—C3—C2	121.0 (2)	C30—C31—C32	120.7 (2)
C4—C3—H3	119.5	C30—C31—H31	119.7
C2—C3—H3	119.5	C32—C31—H31	119.7
C5—C4—C3	120.0 (2)	C31—C32—C27	118.25 (19)
C5—C4—H4	120.0	C31—C32—C36	120.9 (2)
C3—C4—H4	120.0	C27—C32—C36	120.89 (19)
C4—C5—C6	121.3 (3)	O3—C33—N3	121.8 (2)
C4—C5—H5	119.3	O3—C33—C34	122.56 (19)
C6—C5—H5	119.3	N3—C33—C34	115.67 (19)
C5—C6—C1	117.7 (2)	C39—C34—C37	109.27 (16)
C5—C6—C10	121.6 (2)	C39—C34—C33	109.26 (17)
C1—C6—C10	120.7 (2)	C37—C34—C33	110.52 (16)
O1—C7—N1	121.44 (19)	C39—C34—C38	109.61 (16)
O1—C7—C8	120.05 (19)	C37—C34—C38	109.46 (17)
N1—C7—C8	118.41 (18)	C33—C34—C38	108.72 (16)
C7—C8—C12	108.39 (16)	C28—C35—H35A	109.5
C7—C8—C13	113.36 (17)	C28—C35—H35B	109.5
C12—C8—C13	109.50 (17)	H35A—C35—H35B	109.5
C7—C8—C11	105.99 (16)	C28—C35—H35C	109.5
C12—C8—C11	109.93 (17)	H35A—C35—H35C	109.5
C13—C8—C11	109.58 (17)	H35B—C35—H35C	109.5
C2—C9—H9A	109.5	C32—C36—H36A	109.5
C2—C9—H9B	109.5	C32—C36—H36B	109.5
H9A—C9—H9B	109.5	H36A—C36—H36B	109.5
C2—C9—H9C	109.5	C32—C36—H36C	109.5
H9A—C9—H9C	109.5	H36A—C36—H36C	109.5
H9B—C9—H9C	109.5	H36B—C36—H36C	109.5
C6—C10—H10A	109.5	C34—C37—H37A	109.5
C6—C10—H10B	109.5	C34—C37—H37B	109.5
H10A—C10—H10B	109.5	H37A—C37—H37B	109.5
C6—C10—H10C	109.5	C34—C37—H37C	109.5
H10A—C10—H10C	109.5	H37A—C37—H37C	109.5
H10B—C10—H10C	109.5	H37B—C37—H37C	109.5
C8—C11—H11A	109.5	C34—C38—H38A	109.5
C8—C11—H11B	109.5	C34—C38—H38B	109.5
H11A—C11—H11B	109.5	H38A—C38—H38B	109.5
C8—C11—H11C	109.5	C34—C38—H38C	109.5
H11A—C11—H11C	109.5	H38A—C38—H38C	109.5

H11B—C11—H11C	109.5	H38B—C38—H38C	109.5
C8—C12—H12A	109.5	C34—C39—H39A	109.5
C8—C12—H12B	109.5	C34—C39—H39B	109.5
H12A—C12—H12B	109.5	H39A—C39—H39B	109.5
C8—C12—H12C	109.5	C34—C39—H39C	109.5
H12A—C12—H12C	109.5	H39A—C39—H39C	109.5
H12B—C12—H12C	109.5	H39B—C39—H39C	109.5
C8—C13—H13A	109.5	C45—C40—C41	121.8 (2)
C8—C13—H13B	109.5	C45—C40—N4	118.55 (19)
H13A—C13—H13B	109.5	C41—C40—N4	119.6 (2)
C8—C13—H13C	109.5	C42—C41—C40	117.6 (2)
H13A—C13—H13C	109.5	C42—C41—C48	121.2 (2)
H13B—C13—H13C	109.5	C40—C41—C48	121.1 (2)
C15—C14—C19	122.19 (19)	C43—C42—C41	121.5 (2)
C15—C14—N2	119.67 (19)	C43—C42—H42	119.3
C19—C14—N2	118.10 (18)	C41—C42—H42	119.3
C14—C15—C16	117.5 (2)	C42—C43—C44	119.8 (2)
C14—C15—C22	121.12 (19)	C42—C43—H43	120.1
C16—C15—C22	121.32 (19)	C44—C43—H43	120.1
C17—C16—C15	121.4 (2)	C45—C44—C43	121.0 (2)
C17—C16—H16	119.3	C45—C44—H44	119.5
C15—C16—H16	119.3	C43—C44—H44	119.5
C16—C17—C18	119.9 (2)	C44—C45—C40	118.3 (2)
C16—C17—H17	120.0	C44—C45—C49	121.2 (2)
C18—C17—H17	120.0	C40—C45—C49	120.5 (2)
C17—C18—C19	120.8 (2)	O4—C46—N4	121.2 (2)
C17—C18—H18	119.6	O4—C46—C47	121.9 (2)
C19—C18—H18	119.6	N4—C46—C47	116.89 (19)
C18—C19—C14	118.12 (19)	C51—C47—C46	109.46 (18)
C18—C19—C23	121.3 (2)	C51—C47—C52	109.10 (19)
C14—C19—C23	120.57 (19)	C46—C47—C52	110.20 (17)
O2—C20—N2	121.52 (19)	C51—C47—C50	109.40 (18)
O2—C20—C21	121.90 (19)	C46—C47—C50	108.64 (18)
N2—C20—C21	116.51 (18)	C52—C47—C50	110.02 (18)
C26—C21—C24	109.68 (16)	C41—C48—H48A	109.5
C26—C21—C20	110.05 (16)	C41—C48—H48B	109.5
C24—C21—C20	108.00 (16)	H48A—C48—H48B	109.5
C26—C21—C25	108.80 (17)	C41—C48—H48C	109.5
C24—C21—C25	110.08 (17)	H48A—C48—H48C	109.5
C20—C21—C25	110.21 (17)	H48B—C48—H48C	109.5
C15—C22—H22A	109.5	C45—C49—H49A	109.5
C15—C22—H22B	109.5	C45—C49—H49B	109.5
H22A—C22—H22B	109.5	H49A—C49—H49B	109.5
C15—C22—H22C	109.5	C45—C49—H49C	109.5
H22A—C22—H22C	109.5	H49A—C49—H49C	109.5
H22B—C22—H22C	109.5	H49B—C49—H49C	109.5
C19—C23—H23A	109.5	C47—C50—H50A	109.5
C19—C23—H23B	109.5	C47—C50—H50B	109.5
H23A—C23—H23B	109.5	H50A—C50—H50B	109.5

C19—C23—H23C	109.5	C47—C50—H50C	109.5
H23A—C23—H23C	109.5	H50A—C50—H50C	109.5
H23B—C23—H23C	109.5	H50B—C50—H50C	109.5
C21—C24—H24A	109.5	C47—C51—H51A	109.5
C21—C24—H24B	109.5	C47—C51—H51B	109.5
H24A—C24—H24B	109.5	H51A—C51—H51B	109.5
C21—C24—H24C	109.5	C47—C51—H51C	109.5
H24A—C24—H24C	109.5	H51A—C51—H51C	109.5
H24B—C24—H24C	109.5	H51B—C51—H51C	109.5
C21—C25—H25A	109.5	C47—C52—H52A	109.5
C21—C25—H25B	109.5	C47—C52—H52B	109.5
H25A—C25—H25B	109.5	H52A—C52—H52B	109.5
C21—C25—H25C	109.5	C47—C52—H52C	109.5
H25A—C25—H25C	109.5	H52A—C52—H52C	109.5
H25B—C25—H25C	109.5	H52B—C52—H52C	109.5
C21—C26—H26A	109.5	C7—N1—C1	123.82 (17)
C21—C26—H26B	109.5	C7—N1—H1A	119.9 (14)
H26A—C26—H26B	109.5	C1—N1—H1A	115.2 (14)
C21—C26—H26C	109.5	C20—N2—C14	124.50 (17)
H26A—C26—H26C	109.5	C20—N2—H2A	120.0 (13)
H26B—C26—H26C	109.5	C14—N2—H2A	115.0 (13)
C32—C27—C28	122.12 (19)	C33—N3—C27	123.64 (18)
C32—C27—N3	118.72 (18)	C33—N3—H3A	120.4 (13)
C28—C27—N3	119.11 (18)	C27—N3—H3A	115.9 (13)
C29—C28—C27	117.66 (19)	C46—N4—C40	123.98 (19)
C29—C28—C35	121.04 (19)	C46—N4—H4A	120.9 (13)
C27—C28—C35	121.30 (19)	C40—N4—H4A	115.0 (13)
C6—C1—C2—C3	0.8 (3)	C30—C31—C32—C27	−0.4 (3)
N1—C1—C2—C3	−177.10 (18)	C30—C31—C32—C36	178.65 (19)
C6—C1—C2—C9	−178.5 (2)	C28—C27—C32—C31	0.9 (3)
N1—C1—C2—C9	3.6 (3)	N3—C27—C32—C31	−176.47 (18)
C1—C2—C3—C4	0.3 (3)	C28—C27—C32—C36	−178.13 (19)
C9—C2—C3—C4	179.6 (2)	N3—C27—C32—C36	4.5 (3)
C2—C3—C4—C5	−1.2 (3)	O3—C33—C34—C39	−6.0 (3)
C3—C4—C5—C6	1.0 (3)	N3—C33—C34—C39	173.96 (16)
C4—C5—C6—C1	0.1 (3)	O3—C33—C34—C37	−126.2 (2)
C4—C5—C6—C10	−179.0 (2)	N3—C33—C34—C37	53.7 (2)
C2—C1—C6—C5	−1.0 (3)	O3—C33—C34—C38	113.6 (2)
N1—C1—C6—C5	176.85 (18)	N3—C33—C34—C38	−66.5 (2)
C2—C1—C6—C10	178.06 (19)	C45—C40—C41—C42	−0.7 (3)
N1—C1—C6—C10	−4.1 (3)	N4—C40—C41—C42	177.63 (19)
O1—C7—C8—C12	42.4 (3)	C45—C40—C41—C48	−179.59 (19)
N1—C7—C8—C12	−141.14 (19)	N4—C40—C41—C48	−1.2 (3)
O1—C7—C8—C13	164.20 (19)	C40—C41—C42—C43	−0.2 (3)
N1—C7—C8—C13	−19.4 (3)	C48—C41—C42—C43	178.7 (2)
O1—C7—C8—C11	−75.6 (2)	C41—C42—C43—C44	0.1 (4)
N1—C7—C8—C11	100.9 (2)	C42—C43—C44—C45	0.9 (4)
C19—C14—C15—C16	−1.2 (3)	C43—C44—C45—C40	−1.7 (3)
N2—C14—C15—C16	176.35 (18)	C43—C44—C45—C49	177.8 (2)

C19—C14—C15—C22	179.56 (18)	C41—C40—C45—C44	1.7 (3)
N2—C14—C15—C22	−2.8 (3)	N4—C40—C45—C44	−176.7 (2)
C14—C15—C16—C17	−0.2 (3)	C41—C40—C45—C49	−177.86 (19)
C22—C15—C16—C17	179.03 (19)	N4—C40—C45—C49	3.8 (3)
C15—C16—C17—C18	0.9 (3)	O4—C46—C47—C51	−5.6 (3)
C16—C17—C18—C19	−0.3 (3)	N4—C46—C47—C51	175.32 (19)
C17—C18—C19—C14	−1.0 (3)	O4—C46—C47—C52	−125.6 (2)
C17—C18—C19—C23	179.1 (2)	N4—C46—C47—C52	55.3 (2)
C15—C14—C19—C18	1.8 (3)	O4—C46—C47—C50	113.8 (2)
N2—C14—C19—C18	−175.80 (18)	N4—C46—C47—C50	−65.3 (2)
C15—C14—C19—C23	−178.28 (19)	O1—C7—N1—C1	2.0 (3)
N2—C14—C19—C23	4.1 (3)	C8—C7—N1—C1	−174.4 (2)
O2—C20—C21—C26	−8.6 (3)	C6—C1—N1—C7	78.7 (3)
N2—C20—C21—C26	174.51 (17)	C2—C1—N1—C7	−103.3 (2)
O2—C20—C21—C24	111.1 (2)	O2—C20—N2—C14	−5.1 (3)
N2—C20—C21—C24	−65.8 (2)	C21—C20—N2—C14	171.82 (18)
O2—C20—C21—C25	−128.60 (19)	C15—C14—N2—C20	77.5 (3)
N2—C20—C21—C25	54.5 (2)	C19—C14—N2—C20	−104.8 (2)
C32—C27—C28—C29	−0.6 (3)	O3—C33—N3—C27	2.2 (3)
N3—C27—C28—C29	176.84 (18)	C34—C33—N3—C27	−177.77 (17)
C32—C27—C28—C35	−179.76 (19)	C32—C27—N3—C33	−109.8 (2)
N3—C27—C28—C35	−2.3 (3)	C28—C27—N3—C33	72.7 (3)
C27—C28—C29—C30	−0.3 (3)	O4—C46—N4—C40	−1.4 (3)
C35—C28—C29—C30	178.85 (19)	C47—C46—N4—C40	177.65 (18)
C28—C29—C30—C31	0.9 (3)	C45—C40—N4—C46	−112.3 (2)
C29—C30—C31—C32	−0.5 (3)	C41—C40—N4—C46	69.3 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O4^{i}	0.849 (18)	2.009 (19)	2.802 (2)	155.1 (19)
N2—H2A···O1^{ii}	0.874 (18)	2.006 (19)	2.876 (2)	173.4 (19)
N3—H3A···O2	0.850 (18)	2.042 (19)	2.879 (2)	168.4 (19)
N4—H4A···O3	0.874 (19)	2.07 (2)	2.937 (2)	174.2 (18)

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

Fig. 1

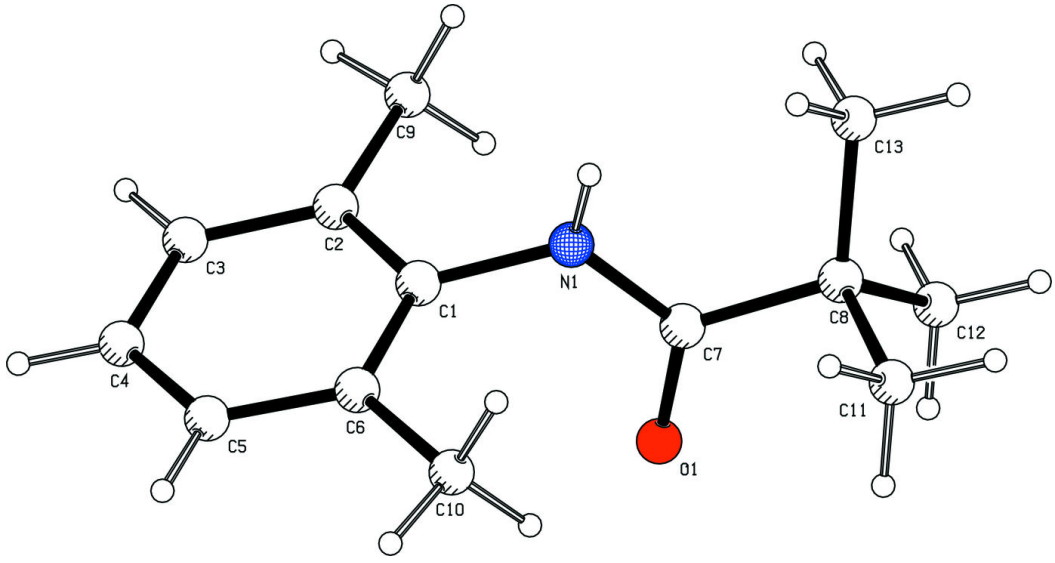
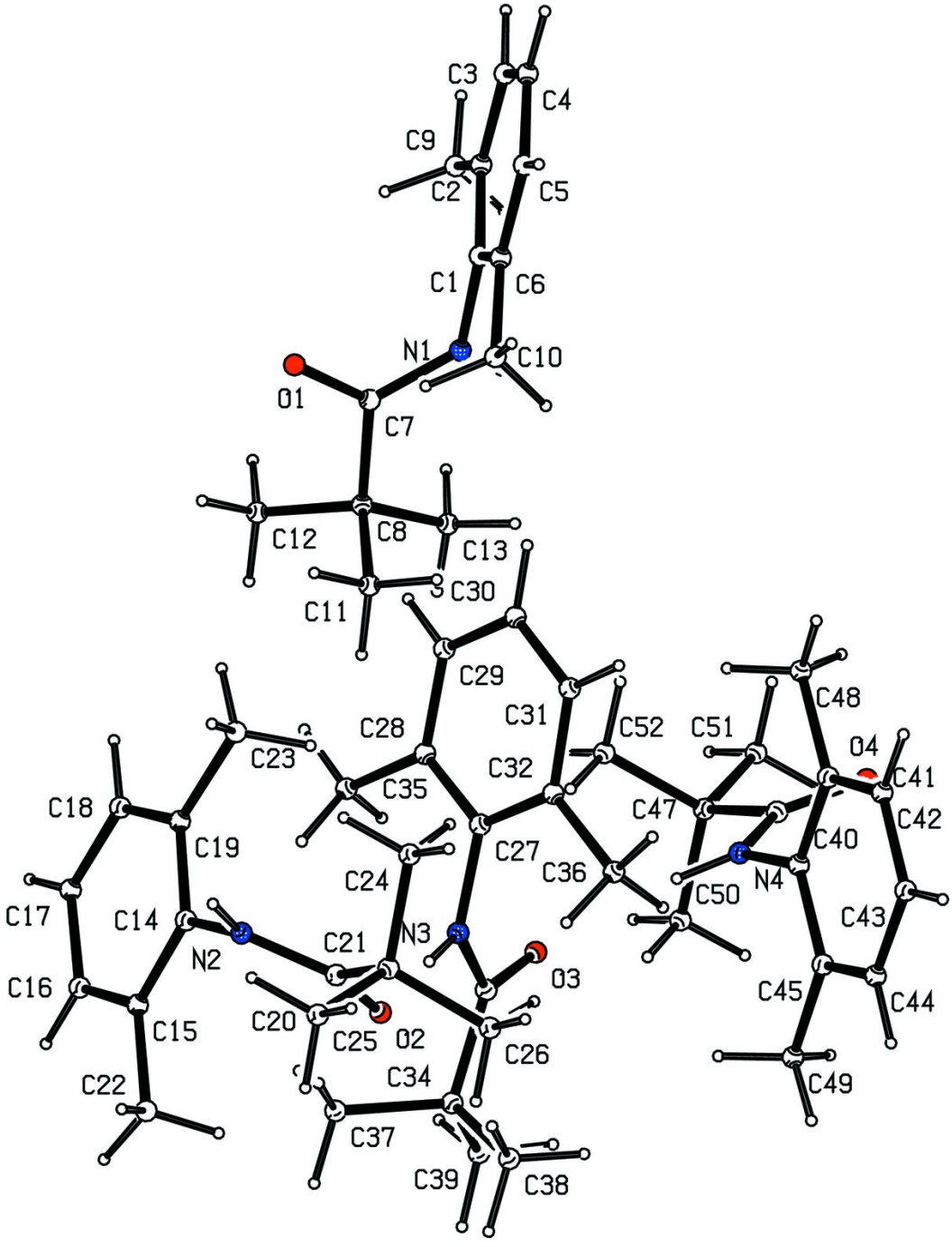


Fig. 2


C3
C4
C9
C2
C5
C1
C6
N1
C10
O1
C7
C12
C8
C13
C11
C30
C29
C31
C52
C51
C48
C28
C23
C32
O4
C41
C35
C47
C42
C18
C19
C27
C40
C24
C36
N4
C50
C17
C14
N2
C21
N3
C43
C16
O3
C45
C44
C20
C25
O2
C15
C26
C22
C34
C49
C37
C39
C38