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Bis(4,6-di-*tert*-butyl-2-{*N*-[4-(diethylamino)phenyl]-carboximidoyl}phenolato)cobalt(II)

C.Vidya Rani,[a] L. Mitu,[b] G. Chakkaravarthi[c]* and G. Rajagopal[d]*

[a]Department of Chemistry, Vaigai College of Engineering, Madurai 625122, Tamil Nadu, India, [b]Department of Chemistry, University of Pitesti, Pitesti 11040, Romania, [c]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India, and [d]PG & Research Department of Chemistry, Chikkanna Government Arts College, Tiruppur 641 602, Tamil Nadu, India. *Correspondence e-mail: chakkaravarthi_2005@yahoo.com, rajagopal18@yahoo.com

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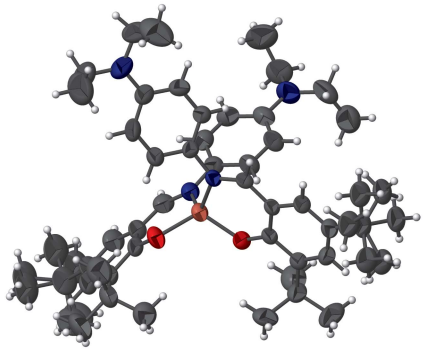
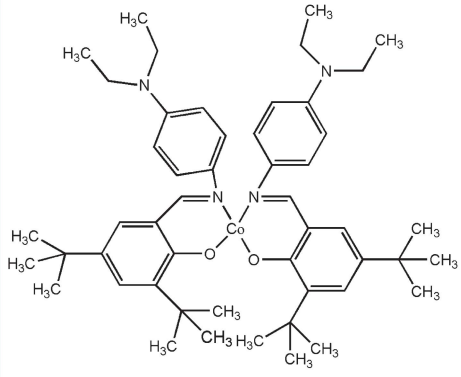
Structural data: full structural data are available from iucrdata.iucr.org

In the title complex, $[Co(C_{25}H_{35}N_2O)_2]$, the cobalt(II) atom has a distorted tetrahedral geometry provided by pairs of O and N atoms. The dihedral angles between the benzene rings of the same ligand are 52.39 (9) and 34.96 (9)°. The molecular structure is stabilized by weak intramolecular C—H···O hydrogen bonds. The crystal packing is stabilized mainly by van der Waals forces. The structure contains a solvent-accessible void of 276 Å^3 which was treated using the SQUEEZE routine from *PLATON* [Spek (2015). *Acta Cryst.* C**71**, 9–18]. The methyl C atoms of the *tert*-butyl groups are rotationally disordered, with site occupancies of 0.802 (3) and 0.548 (9) for the major components and 0.198 (3) and 0.452 (9) for the minor components.

3D view



Chemical scheme



Structure description

In our continuing work on the development of new N- and O-chelating ligands able to play a key role in the coordination of metals at the active sites of numerous metallobimolecules (Nair *et al.*, 2006), we herein report on the synthesis and the crystal structure of the title compound (Fig. 1). The cobalt(II) atom is coordinated in a distorted tetrahedral geometry by two O and two N atoms. The Co—O and Co—N bond lengths [Co1—O1 = 1.8844 (18), Co1—O2 = 1.8867 (17), Co1—N1 = 20 1.978 (2) and Co1—N2 = 1.971 (2) Å] are similar to those reported in related structures (Adam *et al.*, 1997; Chen *et al.*, 2014, 2015). Within the same ligand, the dihedral angles formed by the benzene rings are 52.39 (9) and 34.96 (9)°. The molecular structure is stabilized by weak C—H···O hydrogen bonds (Table 1). The crystal packing is mainly stabilized by van der Waals forces.

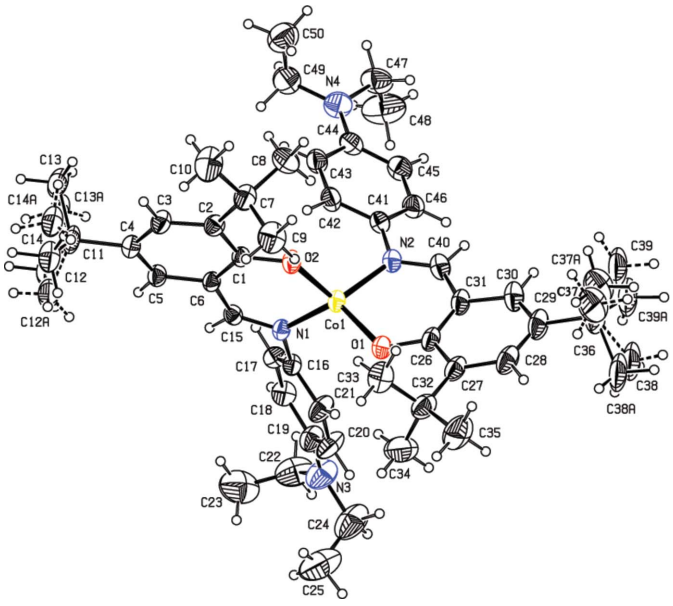


Figure 1
The molecular structure of the title compound, with the atom labelling and 30% probability displacement ellipsoids.

Synthesis and crystallization

To a solution of the Schiff base (1 mmol) in 10 ml methanol was added a solution of $Co(AcO)_2{\cdot}H_2O$ (0.5 mmol) in 10 ml ethanol. The resulting mixture was refluxed for 4–6 h and then cooled to room temperature. The precipitate obtained was filtered, washed in ice-cold ethanol and dried *in vacuo*. X-ray quality crystals were grown by layering a $CHCl_3$ solution (3 ml) of the compound with CH_3CN (5 ml).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The methyl C atoms of the *tert*-butyl groups are rotationally disordered, with site occupancies of 0.802 (3) and 0.548 (9) for the major components (C12, C13, C14 and C37*A*, C38*A*, C39*A*), and 0.198 (3) and 0.452 (9) for the minor components (C12*A*, C13*A*, C14*A* and C37, C38, C39). The C—C bond lengths involving the disordered atoms were restrained to 1.50 (1) Å. SIMU, SADI and DELU restraints were also applied. The structure contains a solvent-accessible void which was treated using the SQUEEZE routine from *PLATON* (Spek, 2015).

Acknowledgements

The authors acknowledge the SAIF, IIT, Madras, for the data collection.

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8*C*···O2	0.96	2.31	2.936 (4)	123
C9—H9*C*···O2	0.96	2.35	2.987 (4)	123
C33—H33*A*···O1	0.96	2.34	2.980 (4)	123
C34—H34*A*···O1	0.96	2.31	2.955 (4)	124

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_{25}H_{35}N_2O)_2]$
M_r	818.03
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	295
a, b, c (Å)	11.9460 (1), 13.2180 (2), 17.4340 (2)
α, β, γ (°)	109.348 (1), 96.350 (1), 98.881 (2)
V (Å^3)	2527.33 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.38
Crystal size (mm)	0.28 × 0.24 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.851, 0.928
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38553, 8091, 5894
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.579
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.146, 1.12
No. of reflections	8091
No. of parameters	592
No. of restraints	105
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, −0.36

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

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full crystallographic data

IUCrData (2017). **2**, x170784 [https://doi.org/10.1107/S2414314617007842]

Bis(4,6-di-*tert*-butyl-2-{*N*-[4-(diethylamino)phenyl]carboximidoyl}-phenolato)cobalt(II)

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Bis(4,6-di-*tert*-butyl-2-{*N*-[4-(diethylamino)phenyl]carboximidoyl}phenolato)cobalt(II)

Crystal data

$[Co(C_{25}H_{35}N_2O)_2]$
M_r = 818.03
Triclinic, $P\overline{1}$
a = 11.9460 (1) Å
b = 13.2180 (2) Å
c = 17.4340 (2) Å
α = 109.348 (1)°
β = 96.350 (1)°
γ = 98.881 (2)°
V = 2527.33 (6) Å^3
Z = 2
$F(000)$ = 882
D_x = 1.075 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8860 reflections
θ = 2.2–22.1°
μ = 0.38 mm^{-1}
T = 295 K
Block, colourless
0.28 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.851, T_{max} = 0.928
38553 measured reflections
8091 independent reflections
5894 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 24.3°, θ_{min} = 2.0°
h = −13→13
k = −15→15
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.146
S = 1.12
8091 reflections
592 parameters
105 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0808P)^2 + 0.0839P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 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. All H atoms were positioned geometrically and refined as riding, with C–H = 0.93–0.97 Å, and U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C) for methyl H atoms. A rotating model was used for the methyl groups.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.7275 (2)	−0.1630 (2)	0.29792 (15)	0.0416 (6)	
C2	0.6716 (2)	−0.2748 (2)	0.25854 (16)	0.0491 (7)	
C3	0.6434 (2)	−0.3331 (2)	0.30879 (18)	0.0555 (7)	
H3	0.606782	−0.406170	0.283027	0.067*	
C4	0.6648 (2)	−0.2921 (2)	0.39406 (18)	0.0521 (7)	
C5	0.7202 (2)	−0.1854 (2)	0.43080 (17)	0.0487 (7)	
H5	0.737078	−0.155396	0.488124	0.058*	
C6	0.7527 (2)	−0.1189 (2)	0.38531 (15)	0.0409 (6)	
C7	0.6438 (3)	−0.3258 (2)	0.16368 (18)	0.0656 (8)	
C8	0.7551 (3)	−0.3166 (3)	0.1273 (2)	0.0901 (11)	
H8A	0.737375	−0.351694	0.068397	0.135*	
H8B	0.807989	−0.351562	0.149775	0.135*	
H8C	0.789287	−0.240734	0.141175	0.135*	
C9	0.5597 (3)	−0.2679 (3)	0.1303 (2)	0.0868 (11)	
H9A	0.489036	−0.277717	0.150877	0.130*	
H9B	0.544591	−0.298377	0.071107	0.130*	
H9C	0.592624	−0.191108	0.148060	0.130*	
C10	0.5880 (4)	−0.4482 (3)	0.1350 (2)	0.1087 (15)	
H10A	0.516180	−0.456372	0.154379	0.163*	
H10B	0.638470	−0.485652	0.157071	0.163*	
H10C	0.574698	−0.479019	0.075846	0.163*	
C11	0.6289 (3)	−0.3656 (2)	0.44291 (19)	0.0719 (7)	
C12	0.5005 (4)	−0.4117 (4)	0.4184 (3)	0.0872 (9)	0.802 (3)
H12A	0.478052	−0.457883	0.448839	0.131*	0.802 (3)
H12B	0.482410	−0.453715	0.360374	0.131*	0.802 (3)
H12C	0.459748	−0.352622	0.430557	0.131*	0.802 (3)
C13	0.6935 (4)	−0.4590 (3)	0.4250 (3)	0.0826 (9)	0.802 (3)
H13A	0.774718	−0.429758	0.440593	0.124*	0.802 (3)
H13B	0.675674	−0.502009	0.367135	0.124*	0.802 (3)
H13C	0.670812	−0.504372	0.456029	0.124*	0.802 (3)
C14	0.6576 (4)	−0.3049 (3)	0.5350 (2)	0.0847 (9)	0.802 (3)
H14A	0.630550	−0.352960	0.562969	0.127*	0.802 (3)
H14B	0.621043	−0.242977	0.549303	0.127*	0.802 (3)
H14C	0.739409	−0.280172	0.551407	0.127*	0.802 (3)
C12A	0.5553 (16)	−0.3073 (13)	0.5019 (11)	0.0844 (11)	0.198 (3)
H12D	0.478014	−0.321298	0.473154	0.127*	0.198 (3)
H12E	0.586233	−0.229893	0.522812	0.127*	0.198 (3)
H12F	0.555289	−0.333744	0.546920	0.127*	0.198 (3)
C13A	0.7398 (10)	−0.3798 (15)	0.4855 (11)	0.0827 (11)	0.198 (3)
H13D	0.798941	−0.316360	0.496154	0.124*	0.198 (3)
H13E	0.762664	−0.443509	0.450615	0.124*	0.198 (3)
H13F	0.728153	−0.388602	0.536722	0.124*	0.198 (3)
C14A	0.5353 (15)	−0.4650 (12)	0.3886 (10)	0.0848 (13)	0.198 (3)
H14D	0.570244	−0.518950	0.353217	0.127*	0.198 (3)
H14E	0.481806	−0.442259	0.355656	0.127*	0.198 (3)

H14F	0.495380	−0.495857	0.423132	0.127*	0.198 (3)
C15	0.8064 (2)	−0.0076 (2)	0.43271 (15)	0.0423 (6)	
H15	0.820529	0.010026	0.489624	0.051*	
C16	0.8867 (2)	0.1774 (2)	0.46795 (16)	0.0456 (6)	
C17	0.9717 (2)	0.1937 (2)	0.53267 (17)	0.0516 (7)	
H17	1.002326	0.134701	0.536498	0.062*	
C18	1.0128 (2)	0.2958 (2)	0.59233 (18)	0.0614 (8)	
H18	1.070537	0.303851	0.635609	0.074*	
C19	0.9708 (3)	0.3870 (2)	0.5898 (2)	0.0684 (9)	
C20	0.8859 (3)	0.3693 (2)	0.5225 (2)	0.0848 (11)	
H20	0.855582	0.428129	0.517882	0.102*	
C21	0.8457 (3)	0.2674 (2)	0.46256 (19)	0.0710 (9)	
H21	0.790197	0.259023	0.417872	0.085*	
C22	1.0854 (4)	0.5023 (3)	0.7256 (3)	0.1123 (13)	
H22A	1.120568	0.579168	0.753573	0.135*	
H22B	1.146705	0.462398	0.712887	0.135*	
C23	1.0226 (5)	0.4633 (5)	0.7818 (3)	0.146 (2)	
H23A	0.956104	0.495667	0.789326	0.220*	
H23B	1.071830	0.483679	0.834146	0.220*	
H23C	0.998710	0.384988	0.758492	0.220*	
C24	0.9676 (6)	0.5846 (3)	0.6445 (3)	0.1307 (19)	
H24A	0.952787	0.579007	0.587256	0.157*	
H24B	1.025936	0.650219	0.674167	0.157*	
C25	0.8610 (6)	0.5962 (4)	0.6791 (4)	0.163 (3)	
H25A	0.803323	0.530839	0.651209	0.244*	
H25B	0.833988	0.657701	0.671764	0.244*	
H25C	0.876278	0.607672	0.736938	0.244*	
C26	0.7745 (3)	0.1623 (2)	0.18080 (17)	0.0545 (7)	
C27	0.6898 (3)	0.1961 (2)	0.13590 (18)	0.0626 (8)	
C28	0.7208 (4)	0.2304 (3)	0.0733 (2)	0.0753 (10)	
H28	0.665658	0.253495	0.044726	0.090*	
C29	0.8283 (3)	0.2333 (3)	0.0495 (2)	0.0760 (10)	
C30	0.9069 (3)	0.1995 (3)	0.09240 (19)	0.0744 (9)	
H30	0.979803	0.200811	0.078298	0.089*	
C31	0.8839 (3)	0.1624 (2)	0.15762 (17)	0.0588 (8)	
C32	0.5673 (3)	0.1897 (3)	0.1547 (2)	0.0740 (9)	
C33	0.5136 (3)	0.0718 (3)	0.1415 (2)	0.0919 (11)	
H33A	0.558636	0.046452	0.177659	0.138*	
H33B	0.511434	0.026557	0.085202	0.138*	
H33C	0.436699	0.068086	0.153190	0.138*	
C34	0.5693 (4)	0.2634 (3)	0.2430 (3)	0.1117 (14)	
H34A	0.614150	0.239439	0.280318	0.168*	
H34B	0.492138	0.259608	0.254116	0.168*	
H34C	0.602880	0.337488	0.250353	0.168*	
C35	0.4890 (4)	0.2265 (4)	0.0968 (3)	0.1154 (15)	
H35A	0.413323	0.221969	0.110867	0.173*	
H35B	0.484527	0.179699	0.040664	0.173*	
H35C	0.520294	0.300729	0.103026	0.173*	

C36	0.8494 (4)	0.2657 (3)	−0.0253 (2)	0.1072 (11)	
C37	0.7516 (10)	0.191 (2)	−0.0954 (14)	0.124 (2)	0.452 (9)
H37A	0.759247	0.206911	−0.144653	0.185*	0.452 (9)
H37B	0.678862	0.203175	−0.079981	0.185*	0.452 (9)
H37C	0.755826	0.115710	−0.105485	0.185*	0.452 (9)
C38	0.8413 (13)	0.3803 (8)	−0.0184 (10)	0.1228 (16)	0.452 (9)
H38A	0.836302	0.385919	−0.072099	0.184*	0.452 (9)
H38B	0.908460	0.430343	0.017311	0.184*	0.452 (9)
H38C	0.773976	0.397965	0.004055	0.184*	0.452 (9)
C39	0.9580 (8)	0.2355 (12)	−0.0555 (7)	0.1231 (16)	0.452 (9)
H39A	0.969990	0.260469	−0.100365	0.185*	0.452 (9)
H39B	0.950375	0.157432	−0.074110	0.185*	0.452 (9)
H39C	1.022413	0.269504	−0.011278	0.185*	0.452 (9)
C37A	0.7884 (10)	0.1753 (17)	−0.1055 (12)	0.126 (2)	0.548 (9)
H37D	0.790728	0.202322	−0.150234	0.190*	0.548 (9)
H37E	0.709729	0.152283	−0.101369	0.190*	0.548 (9)
H37F	0.826119	0.114247	−0.115670	0.190*	0.548 (9)
C38A	0.7892 (11)	0.3676 (8)	−0.0172 (8)	0.1213 (18)	0.548 (9)
H38D	0.801540	0.393020	−0.061710	0.182*	0.548 (9)
H38E	0.821645	0.425441	0.034500	0.182*	0.548 (9)
H38F	0.708090	0.345483	−0.019407	0.182*	0.548 (9)
C39A	0.9775 (8)	0.3155 (10)	−0.0167 (7)	0.1234 (15)	0.548 (9)
H39D	1.021770	0.259587	−0.021934	0.185*	0.548 (9)
H39E	1.003185	0.372552	0.036315	0.185*	0.548 (9)
H39F	0.987462	0.345512	−0.059312	0.185*	0.548 (9)
C40	0.9729 (3)	0.1215 (2)	0.19182 (17)	0.0596 (8)	
H40	1.042064	0.129469	0.172599	0.072*	
C41	1.0694 (2)	0.0376 (2)	0.27158 (16)	0.0504 (7)	
C42	1.0537 (2)	−0.0517 (2)	0.29725 (18)	0.0581 (7)	
H42	0.979620	−0.083946	0.299053	0.070*	
C43	1.1444 (2)	−0.0933 (3)	0.31992 (18)	0.0614 (8)	
H43	1.130510	−0.153533	0.336436	0.074*	
C44	1.2574 (2)	−0.0476 (3)	0.31887 (17)	0.0596 (8)	
C45	1.2722 (3)	0.0442 (2)	0.29534 (19)	0.0651 (8)	
H45	1.346297	0.078122	0.294935	0.078*	
C46	1.1813 (2)	0.0855 (2)	0.27293 (18)	0.0605 (8)	
H46	1.194956	0.147235	0.258252	0.073*	
C47	1.4628 (3)	−0.0539 (3)	0.3249 (3)	0.0932 (12)	
H47A	1.454860	−0.037022	0.274778	0.112*	
H47B	1.504118	−0.113325	0.316198	0.112*	
C48	1.5312 (3)	0.0439 (4)	0.3937 (3)	0.139 (2)	
H48A	1.487210	0.100432	0.406766	0.209*	
H48B	1.600936	0.069923	0.377348	0.209*	
H48C	1.549728	0.024581	0.441314	0.209*	
C49	1.3332 (3)	−0.1838 (3)	0.3668 (2)	0.0879 (10)	
H49A	1.272892	−0.178574	0.400026	0.105*	
H49B	1.403659	−0.181647	0.401392	0.105*	
C50	1.3027 (4)	−0.2902 (3)	0.2973 (3)	0.1095 (13)	

H50A	1.233502	−0.292744	0.262377	0.164*
H50B	1.290666	−0.348637	0.318528	0.164*
H50C	1.364097	−0.298037	0.266006	0.164*
N1	0.83819 (17)	0.07252 (16)	0.40685 (12)	0.0425 (5)
N2	0.96972 (19)	0.07446 (18)	0.24633 (13)	0.0509 (6)
N3	1.0126 (3)	0.4891 (2)	0.64881 (19)	0.0967 (10)
N4	1.3492 (2)	−0.0897 (2)	0.34047 (19)	0.0805 (8)
O1	0.74859 (17)	0.13208 (15)	0.24188 (12)	0.0600 (5)
O2	0.75399 (15)	−0.10400 (14)	0.25273 (11)	0.0515 (5)
CO1	0.82532 (3)	0.04522 (3)	0.28727 (2)	0.04779 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0400 (14)	0.0473 (15)	0.0432 (15)	0.0107 (12)	0.0066 (12)	0.0226 (13)
C2	0.0516 (16)	0.0493 (16)	0.0465 (16)	0.0101 (13)	0.0042 (13)	0.0185 (14)
C3	0.0653 (18)	0.0441 (16)	0.0550 (19)	0.0027 (13)	0.0051 (14)	0.0203 (14)
C4	0.0565 (17)	0.0516 (17)	0.0545 (18)	0.0089 (13)	0.0108 (14)	0.0274 (15)
C5	0.0573 (17)	0.0499 (16)	0.0425 (15)	0.0098 (13)	0.0081 (13)	0.0218 (13)
C6	0.0424 (14)	0.0446 (15)	0.0404 (15)	0.0102 (11)	0.0058 (11)	0.0211 (13)
C7	0.089 (2)	0.0531 (18)	0.0467 (18)	0.0040 (16)	0.0022 (16)	0.0155 (15)
C8	0.118 (3)	0.091 (3)	0.062 (2)	0.030 (2)	0.034 (2)	0.019 (2)
C9	0.092 (3)	0.101 (3)	0.056 (2)	0.008 (2)	−0.0154 (18)	0.027 (2)
C10	0.168 (4)	0.069 (2)	0.055 (2)	−0.019 (2)	−0.003 (2)	0.0048 (19)
C11	0.0978 (17)	0.0614 (16)	0.0729 (15)	0.0074 (12)	0.0216 (14)	0.0469 (14)
C12	0.0994 (17)	0.083 (2)	0.0907 (19)	0.0038 (14)	0.0222 (16)	0.0503 (17)
C13	0.110 (2)	0.0690 (17)	0.0847 (19)	0.0148 (14)	0.0173 (17)	0.0495 (15)
C14	0.114 (2)	0.0785 (19)	0.0745 (15)	0.0078 (16)	0.0229 (15)	0.0478 (14)
C12A	0.105 (2)	0.080 (2)	0.081 (2)	0.0084 (17)	0.0287 (17)	0.0464 (19)
C13A	0.110 (2)	0.074 (2)	0.080 (2)	0.0142 (17)	0.0164 (17)	0.0509 (18)
C14A	0.103 (2)	0.074 (2)	0.087 (2)	0.0041 (17)	0.0185 (19)	0.0468 (19)
C15	0.0431 (14)	0.0513 (16)	0.0349 (14)	0.0113 (12)	0.0057 (11)	0.0178 (13)
C16	0.0507 (16)	0.0426 (15)	0.0435 (15)	0.0036 (12)	0.0074 (13)	0.0179 (13)
C17	0.0483 (16)	0.0502 (17)	0.0545 (18)	0.0098 (13)	0.0043 (14)	0.0179 (15)
C18	0.0570 (18)	0.065 (2)	0.0527 (18)	0.0050 (15)	−0.0037 (14)	0.0162 (16)
C19	0.086 (2)	0.0522 (19)	0.059 (2)	0.0042 (16)	0.0000 (18)	0.0173 (16)
C20	0.131 (3)	0.0429 (18)	0.074 (2)	0.0189 (19)	−0.011 (2)	0.0210 (18)
C21	0.097 (2)	0.0518 (19)	0.0578 (19)	0.0114 (17)	−0.0149 (17)	0.0221 (16)
C22	0.118 (3)	0.082 (3)	0.094 (2)	0.016 (2)	−0.0260 (19)	−0.009 (2)
C23	0.174 (5)	0.185 (5)	0.077 (3)	0.078 (4)	0.004 (3)	0.030 (3)
C24	0.204 (6)	0.058 (3)	0.098 (4)	0.003 (3)	−0.020 (4)	0.012 (2)
C25	0.217 (7)	0.110 (4)	0.158 (6)	0.076 (4)	−0.004 (5)	0.035 (4)
C26	0.081 (2)	0.0424 (15)	0.0418 (16)	0.0072 (14)	0.0040 (15)	0.0211 (13)
C27	0.093 (2)	0.0466 (17)	0.0488 (17)	0.0129 (15)	−0.0014 (16)	0.0223 (15)
C28	0.111 (3)	0.061 (2)	0.056 (2)	0.0119 (19)	−0.006 (2)	0.0320 (17)
C29	0.108 (3)	0.073 (2)	0.0515 (19)	0.005 (2)	0.0001 (19)	0.0381 (18)
C30	0.088 (2)	0.084 (2)	0.060 (2)	0.0049 (19)	0.0132 (18)	0.0426 (19)
C31	0.075 (2)	0.0591 (18)	0.0475 (17)	0.0064 (15)	0.0057 (15)	0.0300 (15)

C32	0.090 (3)	0.068 (2)	0.075 (2)	0.0286 (18)	0.0062 (19)	0.0353 (19)
C33	0.091 (3)	0.093 (3)	0.099 (3)	0.010 (2)	0.011 (2)	0.048 (2)
C34	0.133 (4)	0.106 (3)	0.103 (3)	0.059 (3)	0.025 (3)	0.029 (3)
C35	0.112 (3)	0.127 (4)	0.133 (4)	0.040 (3)	−0.003 (3)	0.081 (3)
C36	0.162 (3)	0.114 (2)	0.0623 (18)	0.015 (2)	0.019 (2)	0.0590 (18)
C37	0.178 (4)	0.143 (5)	0.050 (5)	0.035 (6)	0.019 (6)	0.035 (3)
C38	0.172 (4)	0.124 (3)	0.109 (3)	0.014 (3)	0.042 (3)	0.090 (3)
C39	0.170 (3)	0.132 (3)	0.104 (4)	0.017 (3)	0.046 (3)	0.089 (3)
C37A	0.184 (5)	0.145 (5)	0.054 (4)	0.038 (6)	0.025 (6)	0.037 (2)
C38A	0.171 (4)	0.122 (3)	0.109 (3)	0.014 (3)	0.041 (4)	0.091 (3)
C39A	0.170 (3)	0.129 (3)	0.107 (3)	0.015 (3)	0.043 (3)	0.089 (3)
C40	0.0631 (19)	0.0670 (19)	0.0467 (17)	0.0008 (15)	0.0099 (14)	0.0230 (16)
C41	0.0524 (17)	0.0573 (17)	0.0428 (15)	0.0101 (14)	0.0112 (13)	0.0192 (14)
C42	0.0491 (17)	0.076 (2)	0.0617 (19)	0.0145 (15)	0.0160 (14)	0.0374 (17)
C43	0.0580 (19)	0.078 (2)	0.0628 (19)	0.0206 (16)	0.0171 (15)	0.0385 (17)
C44	0.0548 (19)	0.078 (2)	0.0507 (18)	0.0221 (16)	0.0126 (14)	0.0236 (16)
C45	0.0477 (17)	0.071 (2)	0.072 (2)	0.0048 (15)	0.0116 (15)	0.0218 (18)
C46	0.0601 (19)	0.0571 (18)	0.064 (2)	0.0071 (15)	0.0168 (15)	0.0215 (16)
C47	0.0572 (18)	0.106 (3)	0.118 (3)	0.030 (2)	0.022 (2)	0.033 (3)
C48	0.072 (3)	0.125 (4)	0.185 (5)	0.026 (3)	−0.010 (3)	0.016 (4)
C49	0.076 (2)	0.120 (3)	0.088 (2)	0.043 (2)	0.014 (2)	0.0536 (19)
C50	0.109 (3)	0.103 (3)	0.127 (3)	0.033 (3)	0.019 (3)	0.050 (2)
N1	0.0425 (12)	0.0460 (12)	0.0436 (12)	0.0081 (10)	0.0058 (10)	0.0227 (11)
N2	0.0563 (14)	0.0540 (14)	0.0453 (13)	0.0077 (11)	0.0082 (11)	0.0232 (12)
N3	0.127 (3)	0.0534 (17)	0.0806 (19)	0.0029 (17)	−0.0119 (16)	0.0025 (16)
N4	0.0546 (14)	0.095 (2)	0.098 (2)	0.0249 (14)	0.0105 (14)	0.0391 (18)
O1	0.0760 (13)	0.0679 (13)	0.0530 (12)	0.0266 (10)	0.0176 (10)	0.0362 (10)
O2	0.0610 (11)	0.0532 (11)	0.0426 (10)	0.0054 (9)	0.0069 (9)	0.0236 (9)
CO1	0.0559 (3)	0.0516 (3)	0.0434 (2)	0.01044 (17)	0.00958 (17)	0.02650 (19)

Geometric parameters (Å, º)

C1—O2	1.309 (3)	C26—C27	1.426 (4)
C1—C6	1.417 (3)	C27—C28	1.379 (4)
C1—C2	1.422 (3)	C27—C32	1.530 (5)
C2—C3	1.381 (4)	C28—C29	1.391 (5)
C2—C7	1.540 (4)	C28—H28	0.9300
C3—C4	1.381 (4)	C29—C30	1.355 (4)
C3—H3	0.9300	C29—C36	1.535 (5)
C4—C5	1.362 (4)	C30—C31	1.417 (4)
C4—C11	1.534 (4)	C30—H30	0.9300
C5—C6	1.406 (3)	C31—C40	1.424 (4)
C5—H5	0.9300	C32—C34	1.520 (5)
C6—C15	1.430 (3)	C32—C33	1.522 (4)
C7—C9	1.529 (4)	C32—C35	1.545 (5)
C7—C10	1.540 (4)	C33—H33A	0.9600
C7—C8	1.540 (5)	C33—H33B	0.9600
C8—H8A	0.9600	C33—H33C	0.9600

C8—H8B	0.9600	C34—H34A	0.9600
C8—H8C	0.9600	C34—H34B	0.9600
C9—H9A	0.9600	C34—H34C	0.9600
C9—H9B	0.9600	C35—H35A	0.9600
C9—H9C	0.9600	C35—H35B	0.9600
C10—H10A	0.9600	C35—H35C	0.9600
C10—H10B	0.9600	C36—C38	1.498 (7)
C10—H10C	0.9600	C36—C39	1.514 (6)
C11—C14	1.510 (4)	C36—C37A	1.522 (12)
C11—C13A	1.515 (8)	C36—C37	1.538 (8)
C11—C12	1.517 (4)	C36—C39A	1.540 (10)
C11—C12A	1.518 (8)	C36—C38A	1.595 (11)
C11—C13	1.521 (4)	C37—H37A	0.9600
C11—C14A	1.536 (8)	C37—H37B	0.9600
C12—H12A	0.9600	C37—H37C	0.9600
C12—H12B	0.9600	C38—H38A	0.9600
C12—H12C	0.9600	C38—H38B	0.9600
C13—H13A	0.9600	C38—H38C	0.9600
C13—H13B	0.9600	C39—H39A	0.9600
C13—H13C	0.9600	C39—H39B	0.9600
C14—H14A	0.9600	C39—H39C	0.9600
C14—H14B	0.9600	C37A—H37D	0.9600
C14—H14C	0.9600	C37A—H37E	0.9600
C12A—H12D	0.9600	C37A—H37F	0.9600
C12A—H12E	0.9600	C38A—H38D	0.9600
C12A—H12F	0.9600	C38A—H38E	0.9600
C13A—H13D	0.9600	C38A—H38F	0.9600
C13A—H13E	0.9600	C39A—H39D	0.9600
C13A—H13F	0.9600	C39A—H39E	0.9600
C14A—H14D	0.9600	C39A—H39F	0.9600
C14A—H14E	0.9600	C40—N2	1.297 (3)
C14A—H14F	0.9600	C40—H40	0.9300
C15—N1	1.303 (3)	C41—C46	1.383 (4)
C15—H15	0.9300	C41—C42	1.388 (4)
C16—C17	1.367 (4)	C41—N2	1.434 (3)
C16—C21	1.381 (4)	C42—C43	1.366 (4)
C16—N1	1.425 (3)	C42—H42	0.9300
C17—C18	1.377 (4)	C43—C44	1.396 (4)
C17—H17	0.9300	C43—H43	0.9300
C18—C19	1.387 (4)	C44—N4	1.374 (4)
C18—H18	0.9300	C44—C45	1.397 (4)
C19—N3	1.374 (4)	C45—C46	1.364 (4)
C19—C20	1.394 (4)	C45—H45	0.9300
C20—C21	1.375 (4)	C46—H46	0.9300
C20—H20	0.9300	C47—N4	1.452 (4)
C21—H21	0.9300	C47—C48	1.485 (5)
C22—N3	1.457 (5)	C47—H47A	0.9700
C22—C23	1.472 (7)	C47—H47B	0.9700

C22—H22A	0.9700	C48—H48A	0.9600
C22—H22B	0.9700	C48—H48B	0.9600
C23—H23A	0.9600	C48—H48C	0.9600
C23—H23B	0.9600	C49—N4	1.456 (4)
C23—H23C	0.9600	C49—C50	1.480 (5)
C24—N3	1.467 (5)	C49—H49A	0.9700
C24—C25	1.476 (7)	C49—H49B	0.9700
C24—H24A	0.9700	C50—H50A	0.9600
C24—H24B	0.9700	C50—H50B	0.9600
C25—H25A	0.9600	C50—H50C	0.9600
C25—H25B	0.9600	N1—CO1	1.978 (2)
C25—H25C	0.9600	N2—CO1	1.971 (2)
C26—O1	1.306 (3)	O1—CO1	1.8844 (18)
C26—C31	1.409 (4)	O2—CO1	1.8867 (17)

O2—C1—C6	122.0 (2)	C30—C29—C36	123.9 (4)
O2—C1—C2	119.3 (2)	C28—C29—C36	119.9 (3)
C6—C1—C2	118.6 (2)	C29—C30—C31	123.4 (3)
C3—C2—C1	117.2 (2)	C29—C30—H30	118.3
C3—C2—C7	122.7 (2)	C31—C30—H30	118.3
C1—C2—C7	120.1 (2)	C26—C31—C30	118.9 (3)
C2—C3—C4	125.6 (3)	C26—C31—C40	124.8 (2)
C2—C3—H3	117.2	C30—C31—C40	116.3 (3)
C4—C3—H3	117.2	C34—C32—C33	110.3 (3)
C5—C4—C3	116.5 (2)	C34—C32—C27	109.9 (3)
C5—C4—C11	123.0 (3)	C33—C32—C27	109.7 (3)
C3—C4—C11	120.5 (3)	C34—C32—C35	108.0 (3)
C4—C5—C6	122.5 (2)	C33—C32—C35	106.8 (3)
C4—C5—H5	118.8	C27—C32—C35	112.0 (3)
C6—C5—H5	118.8	C32—C33—H33A	109.5
C5—C6—C1	119.6 (2)	C32—C33—H33B	109.5
C5—C6—C15	115.9 (2)	H33A—C33—H33B	109.5
C1—C6—C15	124.4 (2)	C32—C33—H33C	109.5
C9—C7—C2	109.8 (2)	H33A—C33—H33C	109.5
C9—C7—C10	108.2 (3)	H33B—C33—H33C	109.5
C2—C7—C10	110.9 (2)	C32—C34—H34A	109.5
C9—C7—C8	110.2 (3)	C32—C34—H34B	109.5
C2—C7—C8	110.1 (3)	H34A—C34—H34B	109.5
C10—C7—C8	107.6 (3)	C32—C34—H34C	109.5
C7—C8—H8A	109.5	H34A—C34—H34C	109.5
C7—C8—H8B	109.5	H34B—C34—H34C	109.5
H8A—C8—H8B	109.5	C32—C35—H35A	109.5
C7—C8—H8C	109.5	C32—C35—H35B	109.5
H8A—C8—H8C	109.5	H35A—C35—H35B	109.5
H8B—C8—H8C	109.5	C32—C35—H35C	109.5
C7—C9—H9A	109.5	H35A—C35—H35C	109.5
C7—C9—H9B	109.5	H35B—C35—H35C	109.5
H9A—C9—H9B	109.5	C38—C36—C39	111.9 (7)

C7—C9—H9C	109.5	C38—C36—C29	116.8 (6)
H9A—C9—H9C	109.5	C39—C36—C29	112.2 (5)
H9B—C9—H9C	109.5	C37A—C36—C29	111.0 (12)
C7—C10—H10A	109.5	C38—C36—C37	105.6 (14)
C7—C10—H10B	109.5	C39—C36—C37	104.3 (6)
H10A—C10—H10B	109.5	C29—C36—C37	104.8 (14)
C7—C10—H10C	109.5	C37A—C36—C39A	119.1 (8)
H10A—C10—H10C	109.5	C29—C36—C39A	110.5 (4)
H10B—C10—H10C	109.5	C37A—C36—C38A	106.4 (10)
C14—C11—C12	109.2 (3)	C29—C36—C38A	105.7 (5)
C13A—C11—C12A	113.9 (11)	C39A—C36—C38A	102.9 (6)
C14—C11—C13	106.2 (3)	C36—C37—H37A	109.5
C12—C11—C13	109.5 (3)	C36—C37—H37B	109.5
C14—C11—C4	112.3 (3)	H37A—C37—H37B	109.5
C13A—C11—C4	105.9 (6)	C36—C37—H37C	109.5
C12—C11—C4	109.5 (3)	H37A—C37—H37C	109.5
C12A—C11—C4	106.7 (7)	H37B—C37—H37C	109.5
C13—C11—C4	110.0 (3)	C36—C38—H38A	109.5
C13A—C11—C14A	121.2 (10)	C36—C38—H38B	109.5
C12A—C11—C14A	98.0 (11)	H38A—C38—H38B	109.5
C4—C11—C14A	110.4 (7)	C36—C38—H38C	109.5
C11—C12—H12A	109.5	H38A—C38—H38C	109.5
C11—C12—H12B	109.5	H38B—C38—H38C	109.5
H12A—C12—H12B	109.5	C36—C39—H39A	109.5
C11—C12—H12C	109.5	C36—C39—H39B	109.5
H12A—C12—H12C	109.5	H39A—C39—H39B	109.5
H12B—C12—H12C	109.5	C36—C39—H39C	109.5
C11—C13—H13A	109.5	H39A—C39—H39C	109.5
C11—C13—H13B	109.5	H39B—C39—H39C	109.5
H13A—C13—H13B	109.5	C36—C37A—H37D	109.5
C11—C13—H13C	109.5	C36—C37A—H37E	109.5
H13A—C13—H13C	109.5	H37D—C37A—H37E	109.5
H13B—C13—H13C	109.5	C36—C37A—H37F	109.5
C11—C14—H14A	109.5	H37D—C37A—H37F	109.5
C11—C14—H14B	109.5	H37E—C37A—H37F	109.5
H14A—C14—H14B	109.5	C36—C38A—H38D	109.5
C11—C14—H14C	109.5	C36—C38A—H38E	109.5
H14A—C14—H14C	109.5	H38D—C38A—H38E	109.5
H14B—C14—H14C	109.5	C36—C38A—H38F	109.5
C11—C12A—H12D	109.5	H38D—C38A—H38F	109.5
C11—C12A—H12E	109.5	H38E—C38A—H38F	109.5
H12D—C12A—H12E	109.5	C36—C39A—H39D	109.5
C11—C12A—H12F	109.5	C36—C39A—H39E	109.5
H12D—C12A—H12F	109.5	H39D—C39A—H39E	109.5
H12E—C12A—H12F	109.5	C36—C39A—H39F	109.5
C11—C13A—H13D	109.5	H39D—C39A—H39F	109.5
C11—C13A—H13E	109.5	H39E—C39A—H39F	109.5
H13D—C13A—H13E	109.5	N2—C40—C31	128.3 (3)

C11—C13A—H13F	109.5	N2—C40—H40	115.8
H13D—C13A—H13F	109.5	C31—C40—H40	115.8
H13E—C13A—H13F	109.5	C46—C41—C42	117.2 (3)
C11—C14A—H14D	109.5	C46—C41—N2	124.4 (2)
C11—C14A—H14E	109.5	C42—C41—N2	118.4 (2)
H14D—C14A—H14E	109.5	C43—C42—C41	121.7 (3)
C11—C14A—H14F	109.5	C43—C42—H42	119.2
H14D—C14A—H14F	109.5	C41—C42—H42	119.2
H14E—C14A—H14F	109.5	C42—C43—C44	121.5 (3)
N1—C15—C6	128.7 (2)	C42—C43—H43	119.2
N1—C15—H15	115.7	C44—C43—H43	119.2
C6—C15—H15	115.7	N4—C44—C43	122.1 (3)
C17—C16—C21	117.9 (3)	N4—C44—C45	121.7 (3)
C17—C16—N1	123.2 (2)	C43—C44—C45	116.2 (3)
C21—C16—N1	118.9 (2)	C46—C45—C44	121.9 (3)
C16—C17—C18	121.3 (3)	C46—C45—H45	119.0
C16—C17—H17	119.3	C44—C45—H45	119.0
C18—C17—H17	119.3	C45—C46—C41	121.4 (3)
C17—C18—C19	122.0 (3)	C45—C46—H46	119.3
C17—C18—H18	119.0	C41—C46—H46	119.3
C19—C18—H18	119.0	N4—C47—C48	112.9 (3)
N3—C19—C18	122.1 (3)	N4—C47—H47A	109.0
N3—C19—C20	122.0 (3)	C48—C47—H47A	109.0
C18—C19—C20	115.9 (3)	N4—C47—H47B	109.0
C21—C20—C19	122.0 (3)	C48—C47—H47B	109.0
C21—C20—H20	119.0	H47A—C47—H47B	107.8
C19—C20—H20	119.0	C47—C48—H48A	109.5
C20—C21—C16	120.8 (3)	C47—C48—H48B	109.5
C20—C21—H21	119.6	H48A—C48—H48B	109.5
C16—C21—H21	119.6	C47—C48—H48C	109.5
N3—C22—C23	113.3 (4)	H48A—C48—H48C	109.5
N3—C22—H22A	108.9	H48B—C48—H48C	109.5
C23—C22—H22A	108.9	N4—C49—C50	113.5 (3)
N3—C22—H22B	108.9	N4—C49—H49A	108.9
C23—C22—H22B	108.9	C50—C49—H49A	108.9
H22A—C22—H22B	107.7	N4—C49—H49B	108.9
C22—C23—H23A	109.5	C50—C49—H49B	108.9
C22—C23—H23B	109.5	H49A—C49—H49B	107.7
H23A—C23—H23B	109.5	C49—C50—H50A	109.5
C22—C23—H23C	109.5	C49—C50—H50B	109.5
H23A—C23—H23C	109.5	H50A—C50—H50B	109.5
H23B—C23—H23C	109.5	C49—C50—H50C	109.5
N3—C24—C25	113.7 (4)	H50A—C50—H50C	109.5
N3—C24—H24A	108.8	H50B—C50—H50C	109.5
C25—C24—H24A	108.8	C15—N1—C16	117.2 (2)
N3—C24—H24B	108.8	C15—N1—CO1	120.36 (17)
C25—C24—H24B	108.8	C16—N1—CO1	122.34 (15)
H24A—C24—H24B	107.7	C40—N2—C41	119.3 (2)

C24—C25—H25A	109.5	C40—N2—CO1	119.7 (2)
C24—C25—H25B	109.5	C41—N2—CO1	120.85 (16)
H25A—C25—H25B	109.5	C19—N3—C22	120.7 (3)
C24—C25—H25C	109.5	C19—N3—C24	121.2 (3)
H25A—C25—H25C	109.5	C22—N3—C24	117.1 (3)
H25B—C25—H25C	109.5	C44—N4—C47	121.0 (3)
O1—C26—C31	122.1 (3)	C44—N4—C49	121.4 (3)
O1—C26—C27	119.2 (3)	C47—N4—C49	116.9 (3)
C31—C26—C27	118.8 (3)	C26—O1—CO1	126.01 (19)
C28—C27—C26	117.8 (3)	C1—O2—CO1	128.76 (16)
C28—C27—C32	121.4 (3)	O1—CO1—O2	116.00 (8)
C26—C27—C32	120.7 (3)	O1—CO1—N2	95.76 (8)
C27—C28—C29	125.1 (3)	O2—CO1—N2	114.94 (8)
C27—C28—H28	117.5	O1—CO1—N1	119.33 (8)
C29—C28—H28	117.5	O2—CO1—N1	95.57 (8)
C30—C29—C28	116.1 (3)	N2—CO1—N1	116.77 (9)

O2—C1—C2—C3	−178.8 (2)	C26—C27—C32—C33	−59.5 (4)
C6—C1—C2—C3	1.1 (4)	C28—C27—C32—C35	−0.5 (4)
O2—C1—C2—C7	0.7 (4)	C26—C27—C32—C35	−178.0 (3)
C6—C1—C2—C7	−179.4 (2)	C30—C29—C36—C38	−120.1 (8)
C1—C2—C3—C4	0.0 (4)	C28—C29—C36—C38	64.3 (9)
C7—C2—C3—C4	−179.4 (3)	C30—C29—C36—C39	10.9 (8)
C2—C3—C4—C5	−1.1 (4)	C28—C29—C36—C39	−164.7 (7)
C2—C3—C4—C11	179.9 (3)	C30—C29—C36—C37A	103.3 (7)
C3—C4—C5—C6	1.0 (4)	C28—C29—C36—C37A	−72.3 (8)
C11—C4—C5—C6	180.0 (3)	C30—C29—C36—C37	123.5 (8)
C4—C5—C6—C1	0.2 (4)	C28—C29—C36—C37	−52.2 (9)
C4—C5—C6—C15	177.8 (2)	C30—C29—C36—C39A	−31.2 (7)
O2—C1—C6—C5	178.7 (2)	C28—C29—C36—C39A	153.2 (6)
C2—C1—C6—C5	−1.2 (3)	C30—C29—C36—C38A	−141.8 (6)
O2—C1—C6—C15	1.2 (4)	C28—C29—C36—C38A	42.6 (6)
C2—C1—C6—C15	−178.7 (2)	C26—C31—C40—N2	2.7 (5)
C3—C2—C7—C9	116.6 (3)	C30—C31—C40—N2	−173.5 (3)
C1—C2—C7—C9	−62.8 (3)	C46—C41—C42—C43	−2.5 (4)
C3—C2—C7—C10	−2.9 (4)	N2—C41—C42—C43	178.1 (3)
C1—C2—C7—C10	177.7 (3)	C41—C42—C43—C44	0.4 (5)
C3—C2—C7—C8	−121.9 (3)	C42—C43—C44—N4	−179.1 (3)
C1—C2—C7—C8	58.7 (3)	C42—C43—C44—C45	1.5 (4)
C5—C4—C11—C14	2.3 (4)	N4—C44—C45—C46	179.2 (3)
C3—C4—C11—C14	−178.8 (3)	C43—C44—C45—C46	−1.4 (4)
C5—C4—C11—C13A	−66.3 (9)	C44—C45—C46—C41	−0.7 (5)
C3—C4—C11—C13A	112.7 (8)	C42—C41—C46—C45	2.6 (4)
C5—C4—C11—C12	123.7 (3)	N2—C41—C46—C45	−178.0 (3)
C3—C4—C11—C12	−57.3 (4)	C6—C15—N1—C16	177.9 (2)
C5—C4—C11—C12A	55.4 (9)	C6—C15—N1—CO1	−4.9 (3)
C3—C4—C11—C12A	−125.6 (9)	C17—C16—N1—C15	48.4 (3)
C5—C4—C11—C13	−115.8 (3)	C21—C16—N1—C15	−130.9 (3)

C3—C4—C11—C13	63.1 (4)	C17—C16—N1—CO1	−128.7 (2)
C5—C4—C11—C14A	160.8 (10)	C21—C16—N1—CO1	52.0 (3)
C3—C4—C11—C14A	−20.2 (10)	C31—C40—N2—C41	179.0 (3)
C5—C6—C15—N1	−175.3 (2)	C31—C40—N2—CO1	3.4 (4)
C1—C6—C15—N1	2.2 (4)	C46—C41—N2—C40	29.8 (4)
C21—C16—C17—C18	2.1 (4)	C42—C41—N2—C40	−150.9 (3)
N1—C16—C17—C18	−177.2 (2)	C46—C41—N2—CO1	−154.7 (2)
C16—C17—C18—C19	−0.2 (5)	C42—C41—N2—CO1	24.7 (3)
C17—C18—C19—N3	−179.3 (3)	C18—C19—N3—C22	−13.0 (6)
C17—C18—C19—C20	−1.1 (5)	C20—C19—N3—C22	168.9 (4)
N3—C19—C20—C21	178.7 (4)	C18—C19—N3—C24	179.4 (4)
C18—C19—C20—C21	0.5 (5)	C20—C19—N3—C24	1.3 (6)
C19—C20—C21—C16	1.4 (6)	C23—C22—N3—C19	−71.5 (5)
C17—C16—C21—C20	−2.7 (5)	C23—C22—N3—C24	96.5 (5)
N1—C16—C21—C20	176.7 (3)	C25—C24—N3—C19	83.3 (5)
O1—C26—C27—C28	178.2 (3)	C25—C24—N3—C22	−84.7 (5)
C31—C26—C27—C28	−1.9 (4)	C43—C44—N4—C47	168.8 (3)
O1—C26—C27—C32	−4.3 (4)	C45—C44—N4—C47	−11.8 (5)
C31—C26—C27—C32	175.7 (3)	C43—C44—N4—C49	−0.8 (5)
C26—C27—C28—C29	1.0 (5)	C45—C44—N4—C49	178.5 (3)
C32—C27—C28—C29	−176.5 (3)	C48—C47—N4—C44	88.3 (4)
C27—C28—C29—C30	−0.2 (5)	C48—C47—N4—C49	−101.6 (4)
C27—C28—C29—C36	175.8 (3)	C50—C49—N4—C44	83.7 (4)
C28—C29—C30—C31	0.4 (5)	C50—C49—N4—C47	−86.4 (4)
C36—C29—C30—C31	−175.4 (3)	C31—C26—O1—CO1	−20.2 (4)
O1—C26—C31—C30	−178.0 (3)	C27—C26—O1—CO1	159.71 (19)
C27—C26—C31—C30	2.1 (4)	C6—C1—O2—CO1	−1.0 (3)
O1—C26—C31—C40	5.9 (4)	C2—C1—O2—CO1	178.88 (16)
C27—C26—C31—C40	−174.0 (3)	C26—O1—CO1—O2	−100.4 (2)
C29—C30—C31—C26	−1.4 (5)	C26—O1—CO1—N2	21.0 (2)
C29—C30—C31—C40	175.1 (3)	C26—O1—CO1—N1	146.1 (2)
C28—C27—C32—C34	−120.6 (3)	C1—O2—CO1—O1	−127.7 (2)
C26—C27—C32—C34	62.0 (4)	C1—O2—CO1—N2	121.8 (2)
C28—C27—C32—C33	117.9 (3)	C1—O2—CO1—N1	−1.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*C*···O2	0.96	2.31	2.936 (4)	123
C9—H9*C*···O2	0.96	2.35	2.987 (4)	123
C33—H33*A*···O1	0.96	2.34	2.980 (4)	123
C34—H34*A*···O1	0.96	2.31	2.955 (4)	124