Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cyclo{[(6-Amino-6-deoxy-2,3:4,5-di-*O*-isopropylidene-D-galactonic acid)-(D-Phe)]$_2$}

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.048
wR factor = 0.089
Data-to-parameter ratio = 8.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 3 April 2006
Accepted 5 April 2006

Determination of the crystal structure of the title compound [systematic name: 9,25-dibenzyl-4,4,15,15,20,20,31,31-octamethyl-3,5,14,16,19,21,30,32-octaoxa-8,11,24,27-tetraazapentacyclo[27.3.0.0^{2,6}.0^{13,17}.0^{18,22}]dotriacontane-7,10,23,26-tetrone], $C_{42}H_{56}N_4O_{12}$, a cyclic tetramer, established the relative stereochemistry of its ten stereogenic C atoms; an interesting saddle-like conformation is adopted. There are two molecules in the asymmetric unit. With the exception of the phenyl and isopropylidene groups, the molecules are related by a non-crystallographic twofold rotation axis. There are varying degrees of disorder in the isopropylidene groups.

Comment

Carbohydrates which contain amine and acid groups are commonly referred to as sugar amino acids (SAAs) (Chakraborty *et al.*, 2004; Gruner *et al.*, 2002; Smith & Fleet, 1999). They have been the focus of much interest as dipeptide isosteres and library scaffolds, and their linear oligomers as foldamers (Jensen & Brask, 2005, Trabocchi *et al.*, 2005). SAAs and α-amino acids have been combined in cyclic peptides (Stockle *et al.*, 2002; van Well *et al.*, 2000) to create mimics of biologically active cyclic peptides (van Well, Over-

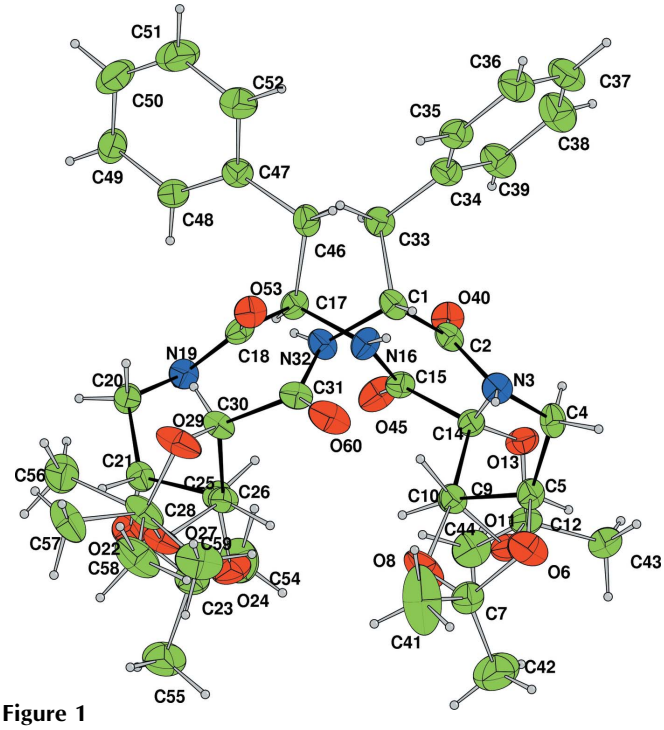
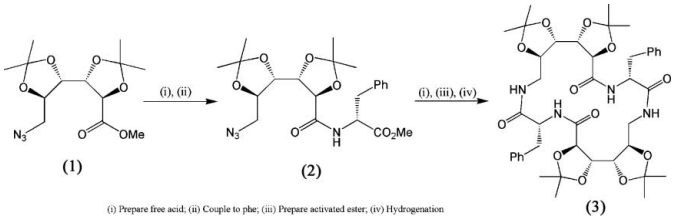


Figure 1
The title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. The bonds in the 20-membered ring are black.

kleeft *et al.*, 2003; Gruner *et al.*, 2001). Several cyclic homo-oligomers have now been prepared using oxetane, furanose and pyranose SAAs (Johnson *et al.*, 2006; van Well, Marinelli *et al.*, 2003; Chakraborty *et al.*, 2003); a cyclic hexamer of pyranose SAAs was found to form inclusion complexes akin to those of cyclodextrins (Locardi *et al.*, 2001). A new family of cyclic SAA oligomers, based on acyclic SAAs, has been established (Mayes, Stetz *et al.*, 2004; Mayes, Simon *et al.*, 2004; Mayes, Cowley *et al.*, 2004) and a cyclic dimer of galactose stereochemistry found to interact with probe compounds (Edwards *et al.*, 2005). This family has now been expanded to include heterooligomers which incorporate phenylalanine (Phe).

The X-ray crystal structure confirms the structural integrity of the title compound, (3), and the absolute stereochemistry is determined by the use of D-galactonolactone as the starting material for the synthesis of (1). The saddle-like conformation adopted by (3) is of particular interest (Fig. 1).



The material crystallizes in *P*1, with two molecules in the asymmetric unit (Fig. 2). The ring atoms in both molecules adopt the same conformation, the only differences being in the phenyl groups, which adopt different conformations in each molecule. The methyl groups on the isopropylidene rings show elongated displacement ellipsoids, and as such are probably disordered. Only two of the eight groups, one on each ring, are actually disordered enough to be modelled as such. The remaining groups were best modelled by large ADP. One of the isopropylidene rings also shows a disordered O atom, suggesting that it is the O atom on the ring, rather than the C atom with the methyl groups attached, that is flipping. Indeed, the dimethyl C atom has a small, well shaped displacement ellipsoid, suggesting that it does not move to any great degree, and the ring flips about it.

When the phenyl groups, the hydrogen and the isopropylidene methyl groups are removed, it is found that the skeletons of the two rings map on to each other, related by a pseudo-twofold rotation axis (r.m.s. deviation in atomic position = 0.137 Å; r.m.s. deviation in bond length = 0.012 Å; r.m.s. deviation in torsion angles = 5.78°).

The structure consists of ribbons of hydrogen-bonded molecules, with alternating inter- and intramolecular hydrogen bonds, parallel to the *a* axis (Table 1, and Figs. 3 and 4).

Experimental

Compound (3) was prepared by hydrogenation of the pentafluorophenyl ester of the linear SAA-Phe dimer (2) with palladized carbon in dioxane; no cyclic dimer was observed. The linear dimer (2) was prepared by coupling of the free acid of SAA (1) (Long *et al.*, 1999) with the methyl ester of D-phenylalanine using standard peptide coupling reagents (*O*-benzotriazol-1-yl-*N*,*N*,*N*′,*N*′-tetramethyluronium tetrafluoroborate and triethylamine). The sample for X-ray analysis was crystallized from methanol.

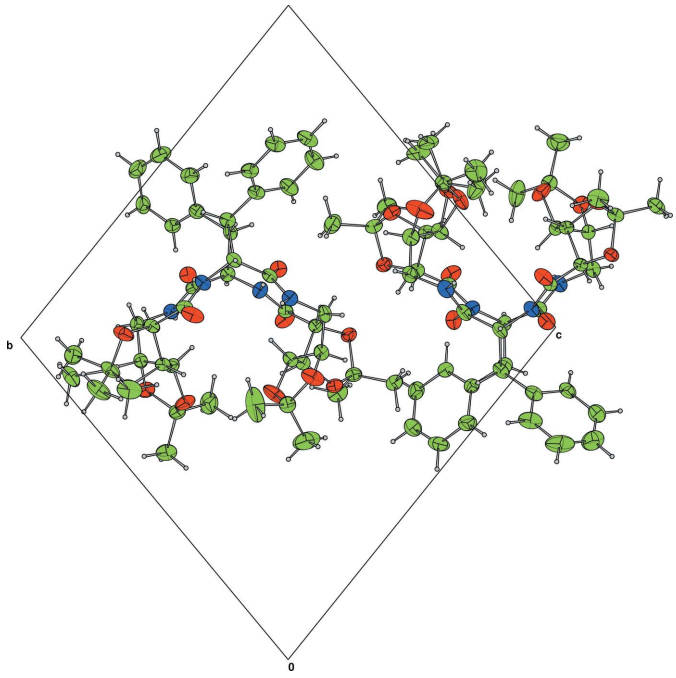


Figure 2
The asymmetric unit, viewed parallel to *a*, with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

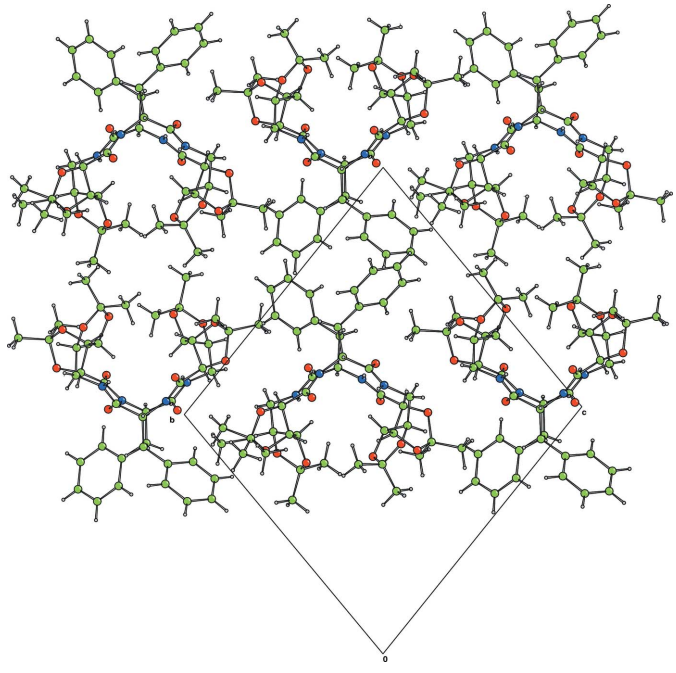


Figure 3
Packing diagram, viewed along the *a* axis, showing the hydrogen-bonded ribbons end on.

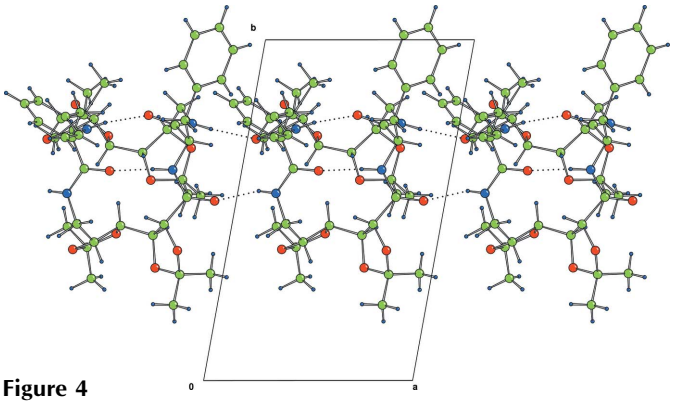


Figure 4
Packing diagram, viewed along the *c* axis, showing the hydrogen-bonded ribbons parallel to the *a* axis. Hydrogen bonds are drawn as dotted lines.

Crystal data

$C_{42}H_{56}N_4O_{12}$
M_r = 808.93
Triclinic, *P*1
a = 9.1755 (1) Å
b = 15.4193 (2) Å
c = 15.5475 (2) Å
α = 77.2624 (5)°
β = 82.0270 (5)°
γ = 78.2560 (7)°
V = 2090.45 (4) Å^3
Z = 2
D_x = 1.285 Mg m^{-3}
Mo *K*α radiation
μ = 0.09 mm^{-1}
T = 150 K
Needle, colourless
0.60 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*DENZO*/*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.621, T_{max} = 0.981
17594 measured reflections
9415 independent reflections
9411 reflections with $I > -3\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.089
S = 1.00
9411 reflections
1090 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.04P)^2 + 0.37P]$, where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N119—H1···O161	0.89	1.89	2.776 (2)	174
N16—H2···O40	0.88	1.95	2.813 (2)	170
N116—H3···O141^{i}	0.86	2.08	2.883 (2)	155
N132—H4···O156^{ii}	0.85	2.09	2.916 (2)	163
N19—H5···O60^{ii}	0.85	2.15	2.966 (2)	160
N3—H7···O45^{i}	0.85	2.08	2.897 (2)	159
N32—H8···O53	0.85	1.92	2.753 (2)	167
N102—H9···O148	0.85	1.96	2.798 (2)	167

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

In the absence of significant anomalous scattering, Friedel pairs were merged. To model the disorder, those atoms with unusually elongated displacement ellipsoids were split, and each atom given an occupancy of 0.5. Coordinates, U^{ij} values and site occupancies of these atoms were then refined. No geometric restraints were applied. The isopropylidene ring containing C56–C59 showed significant deviation from equal occupancies, ending up at 0.581 (4):0.419 (4). The isopropylidene ring containing C144–C157 showed no deviation from equal occupancies, with the occupancies converging to 0.500 (3):0.500 (3). The H atoms were all located in a difference map, but those attached to C atoms were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.98 Å, N—H in the range 0.86–0.89 Å and O—H = 0.82 Å) and displacement parameters [U_{iso}(H) in the range 1.2–1.5 times U_{eq} of the parent atom], after which they were refined with riding constraints.

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO*/*SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

Financial support from the EPSRC (AAE and SJH) is gratefully acknowledged.

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supporting information

Acta Cryst. (2006). E**62**, o1851–o1853 [https://doi.org/10.1107/S1600536806012487]

cyclo{[(6-Amino-6-deoxy-2,3:4,5-di-*O*-isopropylidene-D-galactonic acid)-(D-Phe)]$_2$}

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9,25-Dibenzyl-4,4,15,15,20,20,31,31-octamethyl-3,5,14,16,19,21,30,32- octaoxa-8,11,24,27-tetraazapentacyclo[27.3.0.0^{2,6}.0^{13,17}.0^{18,22}]dotriacontane- 7,10,23,26-tetrone

Crystal data

$C_{42}H_{56}N_4O_{12}$
M_r = 808.93
Triclinic, $P\overline{1}$
a = 9.1755 (1) Å
b = 15.4193 (2) Å
c = 15.5475 (2) Å
α = 77.2624 (5)°
β = 82.0270 (5)°
γ = 78.2560 (7)°
V = 2090.45 (4) Å^3
Z = 2
$F(000)$ = 864
D_x = 1.285 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8903 reflections
θ = 5–27°
μ = 0.09 mm^{-1}
T = 150 K
Plate, colourless
0.60 × 0.20 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Graphite monochromator
ω scans
Absorption correction: multi-scan (DENZO/SCALEPACK; Otwinowski & Minor, 1997)
T_{min} = 0.621, T_{max} = 0.981
17594 measured reflections
9415 independent reflections
9411 reflections with $I > -3\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.5°, θ_{min} = 5.1°
h = −11→11
k = −19→19
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.089
S = 1.00
9411 reflections
1090 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.04P)^2 + 0.37P]$, where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.1602 (2)	0.71407 (18)	0.51070 (16)	0.0262	
C2	0.2449 (2)	0.62211 (18)	0.55200 (16)	0.0258	
N3	0.1838 (2)	0.54939 (15)	0.55504 (14)	0.0288	
C4	0.2577 (3)	0.45965 (18)	0.59511 (17)	0.0307	
C5	0.3559 (3)	0.40664 (18)	0.53017 (17)	0.0287	
O6	0.2602 (2)	0.38501 (17)	0.47648 (14)	0.0466	
C7	0.3260 (3)	0.39140 (19)	0.38814 (18)	0.0335	
O8	0.4540 (2)	0.43120 (18)	0.38066 (13)	0.0509	
C9	0.4679 (3)	0.45482 (19)	0.46271 (16)	0.0281	
C10	0.6315 (3)	0.42641 (17)	0.48008 (17)	0.0273	
O11	0.67032 (18)	0.33075 (12)	0.50355 (12)	0.0303	
C12	0.7937 (3)	0.31125 (19)	0.55580 (18)	0.0309	
O13	0.7620 (2)	0.38134 (12)	0.60731 (12)	0.0337	
C14	0.6749 (3)	0.45836 (17)	0.56006 (16)	0.0256	
C15	0.7611 (3)	0.53791 (17)	0.52759 (16)	0.0257	
N16	0.6693 (2)	0.61835 (14)	0.51277 (15)	0.0287	
C17	0.7232 (3)	0.70397 (17)	0.47718 (17)	0.0257	
C18	0.6423 (3)	0.74983 (17)	0.39455 (17)	0.0266	
N19	0.7226 (2)	0.75454 (15)	0.31638 (14)	0.0280	
C20	0.6547 (3)	0.80035 (18)	0.23479 (17)	0.0299	
C21	0.6079 (3)	0.73727 (18)	0.18491 (17)	0.0278	
O22	0.73851 (19)	0.68299 (13)	0.15021 (13)	0.0361	
C23	0.7245 (3)	0.5896 (2)	0.17420 (19)	0.0359	
O24	0.5734 (2)	0.58864 (13)	0.20294 (15)	0.0427	
C25	0.5102 (3)	0.66950 (17)	0.23612 (17)	0.0278	
C26	0.3464 (3)	0.68978 (18)	0.21992 (17)	0.0277	
O27	0.33149 (19)	0.71847 (13)	0.12721 (12)	0.0329	
C28	0.1969 (3)	0.7806 (2)	0.11569 (18)	0.0398	
O29	0.1471 (2)	0.81080 (15)	0.19512 (13)	0.0474	
C30	0.2486 (3)	0.76843 (18)	0.25930 (16)	0.0282	
C31	0.1598 (2)	0.73525 (18)	0.34743 (17)	0.0276	
N32	0.2239 (2)	0.73839 (15)	0.41860 (13)	0.0281	
C33	0.1771 (3)	0.78708 (19)	0.55960 (17)	0.0304	
C34	0.1098 (3)	0.77502 (19)	0.65504 (17)	0.0310	
C35	−0.0334 (3)	0.82065 (19)	0.67619 (19)	0.0343	
C36	−0.0963 (3)	0.8128 (2)	0.76376 (19)	0.0415	
C37	−0.0152 (3)	0.7599 (2)	0.8311 (2)	0.0457	
C38	0.1263 (3)	0.7138 (2)	0.8109 (2)	0.0482	
C39	0.1893 (3)	0.7211 (2)	0.72352 (18)	0.0391	
O40	0.36836 (18)	0.61550 (13)	0.57846 (12)	0.0314	
C41	0.2153 (4)	0.4520 (4)	0.3287 (3)	0.0858	
C42	0.3741 (6)	0.2998 (3)	0.3679 (4)	0.0916	
C43	0.7901 (3)	0.2217 (2)	0.6183 (2)	0.0415	
C44	0.9399 (3)	0.3142 (2)	0.4985 (2)	0.0428	
O45	0.89684 (19)	0.52718 (13)	0.51393 (15)	0.0386	

C46	0.6856 (3)	0.76367 (18)	0.54684 (17)	0.0306	
C47	0.7132 (3)	0.85939 (18)	0.51639 (17)	0.0300	
C48	0.8247 (3)	0.88328 (19)	0.45017 (17)	0.0315	
C49	0.8535 (4)	0.9711 (2)	0.4280 (2)	0.0412	
C50	0.7693 (4)	1.0361 (2)	0.4722 (2)	0.0549	
C51	0.6581 (4)	1.0144 (2)	0.5367 (2)	0.0555	
C52	0.6289 (3)	0.9268 (2)	0.5588 (2)	0.0413	
O53	0.50621 (18)	0.77882 (12)	0.40329 (12)	0.0310	
C54	0.8256 (4)	0.5421 (2)	0.2462 (2)	0.0551	
C55	0.7630 (5)	0.5481 (3)	0.0924 (2)	0.0613	
C56	0.2695 (8)	0.8740 (5)	0.0700 (5)	0.0473	0.4187
C57	0.1954 (6)	0.8451 (4)	0.0331 (3)	0.0494	0.5813
C58	0.0911 (8)	0.7720 (8)	0.0633 (6)	0.0547	0.4187
C59	0.0779 (6)	0.7142 (5)	0.1204 (5)	0.0536	0.5813
O60	0.04183 (19)	0.70884 (16)	0.35092 (13)	0.0420	
C101	1.0124 (2)	0.10326 (17)	0.91125 (17)	0.0265	
N102	0.9168 (2)	0.18806 (14)	0.87479 (14)	0.0268	
C103	0.9547 (3)	0.26958 (18)	0.86707 (17)	0.0281	
C104	0.8363 (3)	0.35031 (18)	0.83034 (17)	0.0288	
O105	0.9059 (2)	0.42168 (13)	0.77952 (13)	0.0353	
C106	0.8625 (3)	0.49951 (19)	0.81951 (19)	0.0341	
O107	0.7271 (2)	0.48608 (13)	0.87359 (13)	0.0358	
C108	0.7391 (3)	0.39131 (17)	0.90704 (17)	0.0287	
C109	0.5858 (3)	0.3661 (2)	0.93319 (17)	0.0335	
O110	0.5329 (13)	0.4113 (5)	1.0096 (7)	0.0352	0.4999
O111	0.5254 (12)	0.3760 (5)	1.0195 (8)	0.0405	0.5001
C112	0.3777 (3)	0.4341 (2)	1.01408 (18)	0.0349	
O113	0.3364 (2)	0.4376 (2)	0.92944 (16)	0.0646	
C114	0.4632 (3)	0.4128 (2)	0.87110 (19)	0.0346	
C115	0.4192 (3)	0.35751 (19)	0.81228 (18)	0.0340	
N116	0.3927 (2)	0.26731 (16)	0.85571 (15)	0.0326	
C117	0.5019 (3)	0.19650 (19)	0.85376 (16)	0.0289	
C118	0.4674 (3)	0.10127 (19)	0.89230 (16)	0.0278	
N119	0.5115 (2)	0.07369 (15)	0.98252 (13)	0.0271	
C120	0.4147 (2)	0.07579 (16)	1.05509 (16)	0.0228	
C121	0.4919 (2)	0.04838 (17)	1.14107 (15)	0.0242	
O122	0.4019 (2)	0.00516 (13)	1.21258 (11)	0.0317	
C123	0.3687 (3)	0.05793 (19)	1.28157 (17)	0.0301	
O124	0.48327 (17)	0.11051 (13)	1.26527 (11)	0.0296	
C125	0.5194 (3)	0.13188 (17)	1.17195 (16)	0.0262	
C126	0.6781 (3)	0.15074 (17)	1.15177 (17)	0.0264	
O127	0.6740 (2)	0.23383 (13)	1.17970 (15)	0.0417	
C128	0.8143 (3)	0.23237 (18)	1.20760 (18)	0.0314	
O129	0.87966 (19)	0.13960 (13)	1.23320 (13)	0.0340	
C130	0.7977 (2)	0.08318 (17)	1.20512 (16)	0.0249	
C131	0.9065 (3)	0.01718 (18)	1.15686 (17)	0.0293	
N132	0.9784 (2)	0.05931 (15)	1.07287 (14)	0.0289	
C133	0.9294 (2)	0.05959 (17)	0.99621 (17)	0.0268	

C134	1.0479 (3)	0.03790 (19)	0.84773 (18)	0.0323	
C135	1.1189 (3)	0.06999 (18)	0.75547 (17)	0.0286	
C136	1.1159 (4)	0.0210 (2)	0.6911 (2)	0.0447	
C137	1.1836 (5)	0.0436 (3)	0.6064 (2)	0.0593	
C138	1.2539 (4)	0.1180 (2)	0.5838 (2)	0.0527	
C139	1.2575 (3)	0.1679 (2)	0.6461 (2)	0.0405	
C140	1.1907 (3)	0.14407 (18)	0.73208 (18)	0.0299	
O141	1.07266 (19)	0.28003 (13)	0.88842 (14)	0.0385	
C142	0.9834 (3)	0.5056 (2)	0.8739 (2)	0.0424	
C143	0.8277 (4)	0.5815 (2)	0.7472 (2)	0.0498	
C144	0.3882 (12)	0.5275 (7)	1.0146 (7)	0.0604	0.5001
C145	0.3314 (10)	0.5252 (7)	1.0470 (6)	0.0487	0.4999
C146	0.2763 (15)	0.3907 (10)	1.0917 (9)	0.0639	0.5001
C147	0.2963 (15)	0.3632 (8)	1.0670 (9)	0.0582	0.4999
O148	0.63080 (18)	0.20509 (13)	0.82270 (13)	0.0350	
C149	0.5583 (3)	0.0377 (2)	0.83273 (17)	0.0325	
C150	0.5412 (3)	−0.0596 (2)	0.85827 (17)	0.0329	
C151	0.4569 (3)	−0.0944 (3)	0.8107 (2)	0.0493	
C152	0.4525 (4)	−0.1863 (3)	0.8291 (3)	0.0708	
C153	0.5298 (5)	−0.2437 (3)	0.8948 (3)	0.0701	
C154	0.6130 (4)	−0.2102 (2)	0.9435 (2)	0.0559	
C155	0.6186 (3)	−0.1195 (2)	0.92491 (18)	0.0407	
O156	0.27963 (18)	0.09948 (14)	1.05416 (12)	0.0348	
C157	0.2166 (3)	0.1165 (2)	1.2744 (2)	0.0451	
C158	0.3852 (4)	−0.0053 (2)	1.36983 (18)	0.0454	
C159	0.7884 (5)	0.2776 (3)	1.2867 (3)	0.0631	
C160	0.9138 (4)	0.2775 (2)	1.1327 (3)	0.0599	
O161	0.81821 (18)	0.02636 (13)	0.99201 (12)	0.0333	
H11	0.0546	0.7106	0.5126	0.0304*	
H41	0.3240	0.4653	0.6370	0.0364*	
H42	0.1831	0.4241	0.6254	0.0359*	
H51	0.4078	0.3499	0.5622	0.0351*	
H91	0.4388	0.5209	0.4561	0.0347*	
H101	0.6943	0.4487	0.4266	0.0334*	
H141	0.5838	0.4770	0.5980	0.0317*	
H171	0.8306	0.6914	0.4612	0.0295*	
H201	0.7282	0.8320	0.1954	0.0357*	
H202	0.5662	0.8445	0.2490	0.0359*	
H211	0.5571	0.7728	0.1325	0.0313*	
H251	0.5165	0.6597	0.2999	0.0311*	
H261	0.3045	0.6343	0.2429	0.0327*	
H301	0.3100	0.8100	0.2697	0.0323*	
H331	0.2852	0.7868	0.5578	0.0360*	
H332	0.1258	0.8455	0.5270	0.0364*	
H351	−0.0854	0.8581	0.6298	0.0442*	
H361	−0.1956	0.8438	0.7772	0.0515*	
H371	−0.0544	0.7544	0.8898	0.0574*	
H381	0.1811	0.6784	0.8577	0.0598*	

H391	0.2867	0.6901	0.7100	0.0478*
H411	0.2644	0.4696	0.2695	0.1193*
H412	0.1759	0.5043	0.3534	0.1202*
H413	0.1357	0.4204	0.3271	0.1201*
H421	0.4165	0.3057	0.3065	0.1395*
H422	0.4485	0.2689	0.4067	0.1402*
H423	0.2882	0.2689	0.3800	0.1398*
H431	0.8665	0.2101	0.6585	0.0619*
H432	0.6933	0.2242	0.6518	0.0616*
H433	0.8096	0.1742	0.5838	0.0616*
H441	1.0218	0.3024	0.5329	0.0634*
H442	0.9351	0.3715	0.4596	0.0640*
H443	0.9560	0.2670	0.4643	0.0632*
H461	0.7418	0.7341	0.5971	0.0373*
H462	0.5793	0.7664	0.5675	0.0360*
H481	0.8809	0.8403	0.4189	0.0395*
H491	0.9293	0.9853	0.3836	0.0511*
H501	0.7869	1.0959	0.4583	0.0694*
H511	0.6011	1.0586	0.5665	0.0671*
H521	0.5512	0.9120	0.6030	0.0501*
H541	0.8136	0.4794	0.2641	0.0766*
H542	0.9296	0.5434	0.2241	0.0770*
H543	0.7966	0.5727	0.2961	0.0771*
H551	0.7413	0.4869	0.1047	0.0887*
H552	0.8701	0.5474	0.0722	0.0892*
H553	0.7018	0.5843	0.0457	0.0883*
H1011	1.1034	0.1179	0.9241	0.0308*
H1041	0.7723	0.3329	0.7929	0.0345*
H1081	0.7956	0.3750	0.9578	0.0339*
H1141	0.4930	0.4672	0.8317	0.0406*
H1151	0.3261	0.3909	0.7904	0.0408*
H1152	0.4971	0.3531	0.7634	0.0398*
H1181	0.3586	0.1030	0.8956	0.0313*
H1211	0.5878	0.0069	1.1323	0.0275*
H1251	0.4493	0.1845	1.1463	0.0311*
H1261	0.7061	0.1558	1.0879	0.0306*
H1301	0.7446	0.0482	1.2580	0.0295*
H1311	0.9859	−0.0123	1.1951	0.0332*
H1312	0.8542	−0.0263	1.1454	0.0338*
H1341	1.1150	−0.0129	0.8738	0.0391*
H1342	0.9531	0.0222	0.8416	0.0384*
H1361	1.0663	−0.0289	0.7041	0.0559*
H1371	1.1815	0.0084	0.5646	0.0740*
H1381	1.2989	0.1343	0.5259	0.0613*
H1391	1.3059	0.2198	0.6298	0.0475*
H1401	1.1940	0.1802	0.7742	0.0359*
H1421	0.9494	0.5580	0.9020	0.0659*
H1422	1.0006	0.4504	0.9183	0.0649*

H1423	1.0763	0.5141	0.8376	0.0658*	
H1431	0.7968	0.6346	0.7734	0.0749*	
H1432	0.9132	0.5876	0.7068	0.0748*	
H1433	0.7493	0.5749	0.7170	0.0746*	
H1491	0.6633	0.0418	0.8325	0.0385*	
H1492	0.5289	0.0625	0.7719	0.0383*	
H1511	0.4021	−0.0557	0.7661	0.0629*	
H1521	0.3962	−0.2077	0.7963	0.0941*	
H1531	0.5253	−0.3048	0.9060	0.0843*	
H1541	0.6674	−0.2506	0.9904	0.0639*	
H1551	0.6782	−0.0979	0.9579	0.0481*	
H1571	0.1966	0.1517	1.3202	0.0675*	
H1572	0.1436	0.0780	1.2824	0.0682*	
H1573	0.2154	0.1546	1.2164	0.0678*	
H1581	0.3663	0.0274	1.4170	0.0669*	
H1582	0.4851	−0.0402	1.3725	0.0666*	
H1583	0.3136	−0.0468	1.3817	0.0666*	
H1591	0.8886	0.2752	1.3046	0.0978*	
H1592	0.7285	0.2443	1.3326	0.0975*	
H1593	0.7364	0.3398	1.2702	0.0976*	
H1601	1.0081	0.2761	1.1526	0.0838*	
H1602	0.8707	0.3400	1.1129	0.0838*	
H1603	0.9311	0.2476	1.0811	0.0844*	
H1	0.6084	0.0563	0.9894	0.0312*	
H2	0.5729	0.6205	0.5264	0.0345*	
H3	0.3051	0.2604	0.8804	0.0388*	
H4	1.0576	0.0793	1.0738	0.0335*	
H5	0.8167	0.7367	0.3141	0.0322*	
H7	0.1004	0.5558	0.5338	0.0356*	
H8	0.3057	0.7582	0.4083	0.0344*	
H9	0.8344	0.1853	0.8571	0.0319*	
H561	0.3453	0.8803	0.1076	0.0554*	0.4187
H562	0.1878	0.9283	0.0660	0.0554*	0.4187
H563	0.3185	0.8690	0.0092	0.0554*	0.4187
H571	0.2689	0.8855	0.0310	0.0548*	0.5813
H572	0.0929	0.8822	0.0280	0.0548*	0.5813
H573	0.2232	0.8122	−0.0172	0.0548*	0.5813
H581	0.0481	0.7165	0.0906	0.0703*	0.4187
H582	0.0093	0.8262	0.0594	0.0703*	0.4187
H583	0.1400	0.7670	0.0026	0.0703*	0.4187
H591	0.0800	0.6699	0.1780	0.0665*	0.5813
H592	−0.0249	0.7510	0.1156	0.0665*	0.5813
H593	0.1054	0.6809	0.0704	0.0665*	0.5813
H1471	0.3300	0.3065	1.0430	0.0676*	0.4999
H1472	0.3178	0.3513	1.1302	0.0676*	0.4999
H1473	0.1863	0.3838	1.0632	0.0676*	0.4999
H1461	0.2755	0.3274	1.0862	0.0720*	0.5001
H1462	0.3151	0.3899	1.1489	0.0720*	0.5001

H1463	0.1722	0.4263	1.0904	0.0720*	0.5001
H1451	0.3891	0.5707	1.0093	0.0591*	0.4999
H1452	0.3534	0.5154	1.1100	0.0591*	0.4999
H1453	0.2219	0.5479	1.0429	0.0591*	0.4999
H1441	0.4560	0.5508	0.9622	0.0751*	0.5001
H1442	0.4294	0.5295	1.0703	0.0751*	0.5001
H1443	0.2865	0.5660	1.0118	0.0751*	0.5001
H1091	0.5905	0.2992	0.9500	0.0410*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0169 (10)	0.0375 (14)	0.0243 (12)	−0.0067 (9)	0.0009 (9)	−0.0064 (11)
C2	0.0187 (10)	0.0362 (15)	0.0234 (12)	−0.0074 (9)	0.0008 (9)	−0.0076 (11)
N3	0.0209 (9)	0.0360 (13)	0.0313 (11)	−0.0082 (9)	−0.0035 (8)	−0.0071 (10)
C4	0.0271 (12)	0.0357 (15)	0.0284 (13)	−0.0125 (10)	−0.0002 (10)	0.0004 (11)
C5	0.0249 (11)	0.0342 (15)	0.0296 (13)	−0.0129 (10)	−0.0022 (10)	−0.0048 (11)
O6	0.0349 (10)	0.0762 (16)	0.0428 (12)	−0.0335 (10)	0.0054 (9)	−0.0254 (11)
C7	0.0301 (13)	0.0373 (16)	0.0375 (15)	−0.0132 (11)	−0.0072 (11)	−0.0077 (12)
O8	0.0426 (11)	0.0959 (18)	0.0295 (10)	−0.0405 (11)	0.0025 (8)	−0.0229 (11)
C9	0.0264 (12)	0.0376 (15)	0.0241 (12)	−0.0149 (10)	−0.0010 (9)	−0.0063 (11)
C10	0.0248 (11)	0.0306 (15)	0.0291 (13)	−0.0109 (10)	−0.0011 (9)	−0.0068 (11)
O11	0.0279 (9)	0.0305 (10)	0.0367 (10)	−0.0081 (7)	−0.0034 (7)	−0.0125 (8)
C12	0.0297 (12)	0.0315 (15)	0.0345 (14)	−0.0062 (10)	−0.0053 (10)	−0.0110 (12)
O13	0.0426 (10)	0.0266 (10)	0.0348 (10)	−0.0043 (8)	−0.0128 (8)	−0.0083 (8)
C14	0.0260 (11)	0.0274 (14)	0.0256 (12)	−0.0092 (10)	−0.0028 (9)	−0.0056 (10)
C15	0.0239 (11)	0.0285 (14)	0.0282 (13)	−0.0079 (10)	−0.0056 (9)	−0.0083 (10)
N16	0.0184 (9)	0.0289 (12)	0.0390 (13)	−0.0083 (8)	−0.0019 (8)	−0.0044 (10)
C17	0.0193 (10)	0.0275 (13)	0.0318 (13)	−0.0085 (9)	−0.0012 (9)	−0.0057 (11)
C18	0.0242 (11)	0.0246 (13)	0.0346 (14)	−0.0106 (10)	−0.0014 (10)	−0.0084 (11)
N19	0.0220 (9)	0.0310 (12)	0.0306 (11)	−0.0044 (8)	−0.0011 (8)	−0.0065 (9)
C20	0.0319 (13)	0.0268 (14)	0.0299 (14)	−0.0068 (10)	−0.0008 (10)	−0.0031 (11)
C21	0.0242 (11)	0.0297 (14)	0.0259 (13)	0.0002 (10)	−0.0004 (9)	−0.0039 (11)
O22	0.0251 (8)	0.0380 (12)	0.0431 (11)	0.0007 (7)	0.0037 (8)	−0.0134 (9)
C23	0.0346 (13)	0.0321 (15)	0.0371 (15)	0.0056 (11)	−0.0010 (11)	−0.0108 (12)
O24	0.0371 (10)	0.0301 (11)	0.0606 (14)	0.0013 (8)	0.0043 (9)	−0.0203 (10)
C25	0.0272 (12)	0.0230 (13)	0.0310 (13)	−0.0008 (10)	−0.0014 (10)	−0.0051 (11)
C26	0.0286 (12)	0.0282 (14)	0.0278 (13)	−0.0048 (10)	−0.0007 (10)	−0.0100 (11)
O27	0.0297 (9)	0.0439 (11)	0.0260 (9)	0.0013 (8)	−0.0019 (7)	−0.0166 (8)
C28	0.0280 (13)	0.061 (2)	0.0259 (14)	0.0056 (12)	0.0001 (10)	−0.0142 (13)
O29	0.0451 (11)	0.0609 (14)	0.0309 (10)	0.0221 (10)	−0.0126 (8)	−0.0215 (10)
C30	0.0245 (11)	0.0363 (15)	0.0230 (12)	−0.0002 (10)	−0.0033 (9)	−0.0088 (11)
C31	0.0184 (11)	0.0345 (15)	0.0315 (14)	−0.0015 (9)	−0.0017 (9)	−0.0131 (11)
N32	0.0209 (9)	0.0398 (13)	0.0252 (11)	−0.0100 (8)	−0.0002 (8)	−0.0069 (10)
C33	0.0262 (12)	0.0366 (15)	0.0304 (13)	−0.0092 (10)	−0.0005 (10)	−0.0090 (12)
C34	0.0290 (12)	0.0392 (15)	0.0302 (13)	−0.0140 (11)	−0.0001 (10)	−0.0128 (12)
C35	0.0309 (13)	0.0384 (16)	0.0377 (15)	−0.0116 (11)	0.0001 (11)	−0.0136 (13)
C36	0.0351 (14)	0.0544 (19)	0.0403 (16)	−0.0167 (13)	0.0065 (12)	−0.0189 (15)

C37	0.0490 (17)	0.067 (2)	0.0306 (15)	−0.0268 (16)	0.0043 (13)	−0.0190 (15)
C38	0.0458 (17)	0.068 (2)	0.0350 (16)	−0.0184 (15)	−0.0111 (13)	−0.0082 (15)
C39	0.0336 (14)	0.0558 (19)	0.0320 (14)	−0.0123 (13)	−0.0061 (11)	−0.0111 (13)
O40	0.0207 (8)	0.0376 (11)	0.0377 (10)	−0.0074 (7)	−0.0054 (7)	−0.0080 (8)
C41	0.0428 (19)	0.116 (4)	0.081 (3)	−0.024 (2)	−0.0212 (19)	0.037 (3)
C42	0.119 (4)	0.061 (3)	0.098 (3)	−0.038 (3)	0.053 (3)	−0.043 (3)
C43	0.0515 (17)	0.0300 (16)	0.0426 (17)	−0.0067 (12)	−0.0001 (13)	−0.0100 (13)
C44	0.0240 (12)	0.0462 (19)	0.0583 (19)	−0.0052 (12)	−0.0009 (12)	−0.0137 (15)
O45	0.0201 (8)	0.0353 (11)	0.0639 (13)	−0.0084 (7)	−0.0060 (8)	−0.0130 (10)
C46	0.0298 (12)	0.0343 (15)	0.0277 (13)	−0.0108 (11)	−0.0012 (10)	−0.0025 (11)
C47	0.0290 (12)	0.0338 (15)	0.0298 (13)	−0.0072 (10)	−0.0072 (10)	−0.0078 (11)
C48	0.0344 (13)	0.0330 (15)	0.0309 (14)	−0.0103 (11)	−0.0062 (11)	−0.0088 (11)
C49	0.0573 (18)	0.0366 (17)	0.0340 (15)	−0.0210 (14)	−0.0134 (13)	0.0013 (13)
C50	0.085 (2)	0.0296 (17)	0.057 (2)	−0.0166 (16)	−0.0249 (19)	−0.0065 (15)
C51	0.071 (2)	0.0372 (19)	0.061 (2)	0.0014 (16)	−0.0120 (18)	−0.0206 (16)
C52	0.0416 (15)	0.0414 (18)	0.0415 (17)	−0.0014 (13)	−0.0046 (12)	−0.0148 (14)
O53	0.0208 (8)	0.0361 (10)	0.0374 (10)	−0.0066 (7)	−0.0030 (7)	−0.0087 (8)
C54	0.0492 (18)	0.052 (2)	0.054 (2)	0.0068 (15)	−0.0125 (15)	0.0011 (16)
C55	0.078 (2)	0.048 (2)	0.053 (2)	0.0056 (18)	0.0029 (18)	−0.0214 (17)
C56	0.043 (4)	0.042 (4)	0.049 (4)	−0.002 (3)	0.006 (3)	−0.005 (4)
C57	0.043 (3)	0.068 (4)	0.028 (3)	0.002 (3)	−0.002 (2)	−0.001 (3)
C58	0.036 (4)	0.098 (7)	0.037 (4)	−0.017 (4)	−0.006 (3)	−0.022 (5)
C59	0.028 (3)	0.077 (5)	0.064 (4)	−0.012 (3)	0.000 (3)	−0.032 (4)
O60	0.0217 (9)	0.0726 (15)	0.0403 (11)	−0.0154 (9)	0.0027 (8)	−0.0265 (11)
C101	0.0176 (10)	0.0281 (14)	0.0329 (14)	−0.0047 (9)	−0.0024 (9)	−0.0038 (11)
N102	0.0176 (9)	0.0294 (12)	0.0340 (11)	−0.0028 (8)	−0.0042 (8)	−0.0077 (9)
C103	0.0205 (11)	0.0315 (15)	0.0336 (14)	−0.0050 (10)	0.0023 (10)	−0.0122 (11)
C104	0.0232 (11)	0.0297 (14)	0.0339 (14)	−0.0046 (10)	−0.0010 (10)	−0.0082 (11)
O105	0.0412 (10)	0.0293 (10)	0.0364 (10)	−0.0105 (8)	0.0044 (8)	−0.0098 (8)
C106	0.0359 (14)	0.0284 (15)	0.0407 (15)	−0.0052 (11)	−0.0035 (11)	−0.0133 (12)
O107	0.0320 (9)	0.0295 (11)	0.0454 (11)	0.0001 (7)	−0.0042 (8)	−0.0115 (9)
C108	0.0251 (12)	0.0289 (14)	0.0324 (13)	0.0017 (10)	−0.0067 (10)	−0.0103 (11)
C109	0.0245 (12)	0.0460 (17)	0.0280 (13)	0.0016 (11)	−0.0047 (10)	−0.0090 (12)
O110	0.034 (3)	0.044 (5)	0.029 (4)	0.000 (4)	0.000 (2)	−0.017 (4)
O111	0.026 (2)	0.061 (6)	0.024 (3)	0.004 (4)	−0.0019 (18)	0.002 (4)
C112	0.0298 (13)	0.0374 (16)	0.0355 (15)	−0.0001 (11)	0.0004 (11)	−0.0107 (12)
O113	0.0260 (10)	0.115 (2)	0.0546 (14)	0.0188 (11)	−0.0112 (9)	−0.0444 (15)
C114	0.0226 (12)	0.0417 (16)	0.0379 (15)	0.0020 (11)	−0.0079 (10)	−0.0082 (12)
C115	0.0297 (13)	0.0388 (16)	0.0312 (14)	0.0015 (11)	−0.0099 (10)	−0.0047 (12)
N116	0.0197 (9)	0.0454 (14)	0.0320 (12)	−0.0060 (9)	−0.0039 (8)	−0.0053 (10)
C117	0.0198 (11)	0.0434 (16)	0.0232 (12)	−0.0060 (10)	−0.0049 (9)	−0.0042 (11)
C118	0.0197 (10)	0.0434 (16)	0.0205 (12)	−0.0068 (10)	−0.0042 (9)	−0.0044 (11)
N119	0.0171 (9)	0.0394 (13)	0.0248 (10)	−0.0063 (8)	−0.0031 (8)	−0.0048 (9)
C120	0.0205 (11)	0.0254 (13)	0.0246 (12)	−0.0078 (9)	−0.0008 (9)	−0.0070 (10)
C121	0.0228 (11)	0.0273 (13)	0.0235 (12)	−0.0053 (9)	−0.0012 (9)	−0.0071 (10)
O122	0.0411 (10)	0.0330 (10)	0.0240 (9)	−0.0153 (8)	0.0027 (7)	−0.0079 (8)
C123	0.0270 (12)	0.0383 (15)	0.0277 (13)	−0.0080 (11)	−0.0005 (10)	−0.0113 (11)
O124	0.0221 (8)	0.0426 (11)	0.0288 (9)	−0.0061 (7)	−0.0009 (7)	−0.0177 (8)

C125	0.0232 (11)	0.0281 (14)	0.0290 (13)	−0.0019 (9)	−0.0068 (9)	−0.0092 (10)
C126	0.0243 (11)	0.0253 (13)	0.0311 (13)	−0.0052 (9)	−0.0081 (10)	−0.0048 (10)
O127	0.0382 (10)	0.0250 (10)	0.0680 (14)	−0.0050 (8)	−0.0249 (9)	−0.0108 (9)
C128	0.0269 (12)	0.0328 (15)	0.0375 (14)	−0.0087 (10)	−0.0089 (10)	−0.0067 (12)
O129	0.0289 (9)	0.0320 (11)	0.0446 (11)	−0.0078 (7)	−0.0160 (8)	−0.0049 (9)
C130	0.0207 (10)	0.0270 (13)	0.0273 (12)	−0.0058 (9)	−0.0034 (9)	−0.0038 (10)
C131	0.0225 (11)	0.0326 (15)	0.0305 (13)	−0.0043 (10)	−0.0021 (10)	−0.0023 (11)
N132	0.0177 (9)	0.0392 (13)	0.0296 (11)	−0.0076 (8)	−0.0011 (8)	−0.0051 (10)
C133	0.0149 (10)	0.0317 (14)	0.0335 (13)	−0.0027 (9)	−0.0007 (9)	−0.0081 (11)
C134	0.0294 (12)	0.0308 (15)	0.0342 (14)	−0.0045 (10)	0.0028 (10)	−0.0054 (11)
C135	0.0244 (11)	0.0288 (14)	0.0312 (14)	−0.0004 (10)	−0.0017 (10)	−0.0076 (11)
C136	0.0563 (18)	0.0398 (17)	0.0431 (17)	−0.0185 (14)	0.0031 (14)	−0.0147 (14)
C137	0.088 (3)	0.058 (2)	0.0393 (18)	−0.0235 (19)	0.0081 (17)	−0.0258 (17)
C138	0.069 (2)	0.049 (2)	0.0354 (17)	−0.0126 (16)	0.0139 (15)	−0.0080 (15)
C139	0.0408 (15)	0.0345 (16)	0.0433 (17)	−0.0111 (12)	0.0060 (12)	−0.0034 (13)
C140	0.0251 (11)	0.0299 (14)	0.0351 (14)	−0.0045 (10)	−0.0027 (10)	−0.0080 (11)
O141	0.0222 (8)	0.0362 (11)	0.0616 (13)	−0.0045 (7)	−0.0091 (8)	−0.0171 (10)
C142	0.0375 (15)	0.0427 (18)	0.0525 (18)	−0.0111 (12)	−0.0077 (13)	−0.0155 (14)
C143	0.0601 (19)	0.0342 (17)	0.055 (2)	−0.0091 (14)	−0.0131 (15)	−0.0037 (15)
C144	0.066 (7)	0.052 (5)	0.071 (7)	−0.008 (5)	−0.001 (5)	−0.036 (5)
C145	0.051 (5)	0.040 (4)	0.056 (6)	0.001 (4)	0.006 (4)	−0.026 (4)
C146	0.046 (5)	0.073 (10)	0.065 (7)	−0.003 (5)	0.007 (4)	−0.013 (5)
C147	0.047 (5)	0.037 (6)	0.082 (10)	−0.014 (4)	0.011 (5)	0.001 (5)
O148	0.0224 (8)	0.0419 (11)	0.0380 (11)	−0.0088 (7)	−0.0011 (7)	−0.0002 (9)
C149	0.0295 (12)	0.0456 (17)	0.0235 (13)	−0.0108 (11)	0.0001 (10)	−0.0071 (12)
C150	0.0259 (12)	0.0471 (17)	0.0281 (13)	−0.0129 (11)	0.0062 (10)	−0.0120 (12)
C151	0.0338 (14)	0.069 (2)	0.056 (2)	−0.0166 (14)	0.0005 (13)	−0.0314 (17)
C152	0.059 (2)	0.087 (3)	0.088 (3)	−0.040 (2)	0.018 (2)	−0.054 (3)
C153	0.082 (3)	0.052 (2)	0.075 (3)	−0.031 (2)	0.035 (2)	−0.020 (2)
C154	0.075 (2)	0.048 (2)	0.0371 (17)	−0.0131 (17)	0.0220 (16)	−0.0071 (15)
C155	0.0486 (16)	0.0467 (19)	0.0263 (14)	−0.0124 (13)	0.0074 (12)	−0.0095 (13)
O156	0.0176 (8)	0.0575 (13)	0.0308 (10)	−0.0075 (8)	−0.0017 (7)	−0.0117 (9)
C157	0.0217 (12)	0.061 (2)	0.0536 (19)	−0.0039 (12)	0.0015 (12)	−0.0188 (16)
C158	0.0547 (18)	0.053 (2)	0.0264 (15)	−0.0054 (15)	−0.0007 (13)	−0.0100 (14)
C159	0.076 (2)	0.063 (2)	0.057 (2)	0.0010 (19)	−0.0230 (19)	−0.0269 (19)
C160	0.0434 (17)	0.048 (2)	0.075 (3)	−0.0137 (15)	−0.0019 (16)	0.0166 (18)
O161	0.0220 (8)	0.0443 (12)	0.0355 (10)	−0.0115 (8)	−0.0005 (7)	−0.0081 (8)

Geometric parameters (Å, º)

C1—C2	1.522 (4)	C101—C134	1.521 (4)
C1—N32	1.467 (3)	C101—H1011	0.966
C1—C33	1.533 (4)	N102—C103	1.347 (3)
C1—H11	0.978	N102—H9	0.853
C2—N3	1.341 (3)	C103—C104	1.538 (4)
C2—O40	1.235 (3)	C103—O141	1.225 (3)
N3—C4	1.455 (4)	C104—O105	1.416 (3)
N3—H7	0.854	C104—C108	1.557 (3)

C4—C5	1.520 (4)	C104—H1041	0.991
C4—H41	0.978	O105—C106	1.432 (3)
C4—H42	0.970	C106—O107	1.425 (3)
C5—O6	1.423 (3)	C106—C142	1.514 (4)
C5—C9	1.542 (3)	C106—C143	1.508 (4)
C5—H51	0.972	O107—C108	1.426 (3)
O6—C7	1.413 (3)	C108—C109	1.514 (4)
C7—O8	1.412 (3)	C108—H1081	0.963
C7—C41	1.502 (5)	C109—O110	1.484 (11)
C7—C42	1.481 (5)	C109—C114	1.543 (3)
O8—C9	1.430 (3)	C109—H1091	1.000
C9—C10	1.520 (3)	C109—O111	1.407 (12)
C9—H91	0.985	C109—C114	1.543 (3)
C10—O11	1.421 (3)	C109—H1091	1.000
C10—C14	1.561 (3)	O110—C112	1.391 (12)
C10—H101	0.982	O111—C112	1.467 (11)
O11—C12	1.428 (3)	C112—O113	1.406 (4)
C12—O13	1.443 (3)	C112—C145	1.559 (9)
C12—C43	1.507 (4)	C112—C147	1.481 (13)
C12—C44	1.507 (4)	C112—O113	1.406 (4)
O13—C14	1.407 (3)	C112—C144	1.466 (11)
C14—C15	1.548 (3)	C112—C146	1.534 (15)
C14—H141	0.984	O113—C114	1.415 (3)
C15—N16	1.343 (3)	C114—C115	1.520 (4)
C15—O45	1.218 (3)	C114—H1141	0.988
N16—C17	1.470 (3)	C115—N116	1.459 (4)
N16—H2	0.876	C115—H1151	0.967
C17—C18	1.533 (4)	C115—H1152	0.973
C17—C46	1.532 (4)	N116—C117	1.326 (3)
C17—H171	0.973	N116—H3	0.858
C18—N19	1.326 (3)	C117—C118	1.537 (4)
C18—O53	1.237 (3)	C117—O148	1.236 (3)
N19—C20	1.463 (3)	C118—N119	1.461 (3)
N19—H5	0.850	C118—C149	1.539 (4)
C20—C21	1.525 (4)	C118—H1181	0.988
C20—H201	0.978	N119—C120	1.338 (3)
C20—H202	0.981	N119—H1	0.889
C21—O22	1.428 (3)	C120—C121	1.536 (3)
C21—C25	1.532 (4)	C120—O156	1.220 (3)
C21—H211	0.993	C121—O122	1.416 (3)
O22—C23	1.433 (4)	C121—C125	1.546 (3)
C23—O24	1.398 (3)	C121—H1211	0.989
C23—C54	1.516 (4)	O122—C123	1.449 (3)
C23—C55	1.516 (4)	C123—O124	1.417 (3)
O24—C25	1.436 (3)	C123—C157	1.504 (4)
C25—C26	1.516 (3)	C123—C158	1.505 (4)
C25—H251	0.978	O124—C125	1.423 (3)
C26—O27	1.429 (3)	C125—C126	1.520 (3)

C26—C30	1.544 (3)	C125—H1251	0.973
C26—H261	0.984	C126—O127	1.433 (3)
O27—C28	1.407 (3)	C126—C130	1.544 (3)
C28—O29	1.400 (3)	C126—H1261	0.981
C28—C56	1.682 (8)	O127—C128	1.408 (3)
C28—C58	1.393 (7)	C128—O129	1.425 (3)
C28—O29	1.400 (3)	C128—C159	1.512 (4)
C28—C57	1.440 (6)	C128—C160	1.511 (4)
C28—C59	1.628 (7)	O129—C130	1.428 (3)
O29—C30	1.419 (3)	C130—C131	1.520 (3)
C30—C31	1.534 (4)	C130—H1301	1.002
C30—H301	0.987	C131—N132	1.457 (3)
C31—N32	1.337 (3)	C131—H1311	0.978
C31—O60	1.222 (3)	C131—H1312	0.959
N32—H8	0.850	N132—C133	1.330 (3)
C33—C34	1.513 (4)	N132—H4	0.848
C33—H331	0.987	C133—O161	1.247 (3)
C33—H332	0.991	C134—C135	1.512 (4)
C34—C35	1.391 (4)	C134—H1341	0.944
C34—C39	1.391 (4)	C134—H1342	0.971
C35—C36	1.393 (4)	C135—C136	1.387 (4)
C35—H351	0.939	C135—C140	1.388 (4)
C36—C37	1.381 (5)	C136—C137	1.379 (5)
C36—H361	0.958	C136—H1361	0.943
C37—C38	1.378 (5)	C137—C138	1.383 (5)
C37—H371	0.926	C137—H1371	0.938
C38—C39	1.391 (4)	C138—C139	1.371 (5)
C38—H381	0.945	C138—H1381	0.940
C39—H391	0.943	C139—C140	1.395 (4)
C41—H411	0.974	C139—H1391	0.962
C41—H412	0.953	C140—H1401	0.955
C41—H413	0.963	C142—H1421	0.976
C42—H421	0.971	C142—H1422	0.971
C42—H422	0.955	C142—H1423	0.971
C42—H423	0.977	C143—H1431	0.968
C43—H431	0.967	C143—H1432	0.942
C43—H432	0.964	C143—H1433	0.944
C43—H433	0.974	C144—H1441	1.000
C44—H441	0.947	C144—H1442	1.000
C44—H442	0.951	C144—H1443	1.000
C44—H443	0.968	C145—H1451	1.000
C46—C47	1.509 (4)	C145—H1452	1.000
C46—H461	0.972	C145—H1453	1.000
C46—H462	0.979	C146—H1461	1.000
C47—C48	1.392 (4)	C146—H1462	1.000
C47—C52	1.395 (4)	C146—H1463	1.000
C48—C49	1.392 (4)	C147—H1471	1.000
C48—H481	0.936	C147—H1472	1.000

C49—C50	1.384 (5)	C147—H1473	1.000
C49—H491	0.933	C149—C150	1.499 (4)
C50—C51	1.365 (5)	C149—H1491	0.978
C50—H501	0.941	C149—H1492	0.991
C51—C52	1.390 (5)	C150—C151	1.392 (4)
C51—H511	0.938	C150—C155	1.395 (4)
C52—H521	0.946	C151—C152	1.390 (6)
C54—H541	0.969	C151—H1511	0.939
C54—H542	0.971	C152—C153	1.370 (7)
C54—H543	0.974	C152—H1521	0.924
C55—H551	0.976	C153—C154	1.385 (6)
C55—H552	0.988	C153—H1531	0.929
C55—H553	0.980	C154—C155	1.373 (5)
C56—H561	1.000	C154—H1541	0.971
C56—H562	1.000	C155—H1551	0.949
C56—H563	1.000	C157—H1571	0.964
C57—H571	1.000	C157—H1572	0.960
C57—H572	1.000	C157—H1573	0.963
C57—H573	1.000	C158—H1581	0.957
C58—H581	1.000	C158—H1582	0.964
C58—H582	1.000	C158—H1583	0.980
C58—H583	1.000	C159—H1591	0.988
C59—H591	1.000	C159—H1592	0.959
C59—H592	1.000	C159—H1593	0.976
C59—H593	1.000	C160—H1601	0.953
C101—N102	1.464 (3)	C160—H1602	0.963
C101—C133	1.522 (4)	C160—H1603	0.989

C2—C1—N32	108.49 (19)	C133—C101—H1011	110.1
C2—C1—C33	111.0 (2)	C134—C101—H1011	110.3
N32—C1—C33	107.9 (2)	C101—N102—C103	122.88 (19)
C2—C1—H11	109.2	C101—N102—H9	118.1
N32—C1—H11	110.1	C103—N102—H9	119.0
C33—C1—H11	110.1	N102—C103—C104	114.7 (2)
C1—C2—N3	117.8 (2)	N102—C103—O141	123.6 (2)
C1—C2—O40	120.3 (2)	C104—C103—O141	121.7 (2)
N3—C2—O40	121.9 (2)	C103—C104—O105	110.39 (19)
C2—N3—C4	120.5 (2)	C103—C104—C108	110.7 (2)
C2—N3—H7	119.8	O105—C104—C108	104.5 (2)
C4—N3—H7	119.7	C103—C104—H1041	111.3
N3—C4—C5	114.7 (2)	O105—C104—H1041	109.1
N3—C4—H41	109.0	C108—C104—H1041	110.6
C5—C4—H41	105.9	C104—O105—C106	109.7 (2)
N3—C4—H42	109.5	O105—C106—O107	104.8 (2)
C5—C4—H42	107.3	O105—C106—C142	110.1 (2)
H41—C4—H42	110.3	O107—C106—C142	111.6 (2)
C4—C5—O6	107.59 (19)	O105—C106—C143	108.2 (2)
C4—C5—C9	117.8 (2)	O107—C106—C143	108.3 (2)

O6—C5—C9	103.94 (19)	C142—C106—C143	113.4 (3)
C4—C5—H51	109.9	C106—O107—C108	107.07 (18)
O6—C5—H51	107.2	C104—C108—O107	102.5 (2)
C9—C5—H51	109.8	C104—C108—C109	116.6 (2)
C5—O6—C7	110.53 (18)	O107—C108—C109	110.7 (2)
O6—C7—O8	107.7 (2)	C104—C108—H1081	108.0
O6—C7—C41	108.0 (3)	O107—C108—H1081	108.8
O8—C7—C41	109.2 (3)	C109—C108—H1081	109.8
O6—C7—C42	109.7 (3)	C108—C109—O110	101.2 (4)
O8—C7—C42	108.4 (3)	C108—C109—C114	117.1 (2)
C41—C7—C42	113.6 (4)	O110—C109—C114	100.3 (5)
C7—O8—C9	110.21 (19)	C108—C109—H1091	112.3
C5—C9—O8	104.50 (19)	O110—C109—H1091	112.3
C5—C9—C10	116.2 (2)	C114—C109—H1091	112.3
O8—C9—C10	107.3 (2)	C108—C109—O111	114.1 (5)
C5—C9—H91	110.6	C108—C109—C114	117.1 (2)
O8—C9—H91	108.3	O111—C109—C114	107.0 (5)
C10—C9—H91	109.6	C108—C109—H1091	112.3
C9—C10—O11	110.69 (19)	O111—C109—H1091	90.9
C9—C10—C14	115.4 (2)	C114—C109—H1091	112.3
O11—C10—C14	102.98 (19)	C109—O110—C112	108.2 (7)
C9—C10—H101	109.3	C109—O111—C112	108.3 (7)
O11—C10—H101	109.5	O110—C112—O113	107.2 (5)
C14—C10—H101	108.8	O110—C112—C145	107.5 (5)
C10—O11—C12	106.91 (18)	O113—C112—C145	114.2 (4)
O11—C12—O13	103.94 (19)	O110—C112—C147	115.3 (6)
O11—C12—C43	108.6 (2)	O113—C112—C147	100.0 (6)
O13—C12—C43	108.4 (2)	C145—C112—C147	112.6 (6)
O11—C12—C44	111.5 (2)	O111—C112—O113	106.3 (5)
O13—C12—C44	111.1 (2)	O111—C112—C144	110.4 (6)
C43—C12—C44	112.9 (2)	O113—C112—C144	104.5 (5)
C12—O13—C14	108.87 (18)	O111—C112—C146	105.7 (7)
C10—C14—O13	104.86 (19)	O113—C112—C146	115.1 (6)
C10—C14—C15	110.9 (2)	C144—C112—C146	114.5 (6)
O13—C14—C15	112.45 (18)	C112—O113—C114	110.92 (19)
C10—C14—H141	109.5	C109—C114—O113	104.0 (2)
O13—C14—H141	109.2	C109—C114—C115	117.8 (2)
C15—C14—H141	109.8	O113—C114—C115	108.0 (2)
C14—C15—N16	112.46 (19)	C109—C114—H1141	109.9
C14—C15—O45	122.9 (2)	O113—C114—H1141	110.1
N16—C15—O45	124.6 (2)	C115—C114—H1141	106.9
C15—N16—C17	123.05 (19)	C114—C115—N116	115.9 (2)
C15—N16—H2	118.8	C114—C115—H1151	106.3
C17—N16—H2	118.1	N116—C115—H1151	106.8
N16—C17—C18	106.95 (18)	C114—C115—H1152	107.9
N16—C17—C46	109.4 (2)	N116—C115—H1152	109.6
C18—C17—C46	110.3 (2)	H1151—C115—H1152	110.2
N16—C17—H171	109.3	C115—N116—C117	120.0 (2)

C18—C17—H171	110.1	C115—N116—H3	119.4
C46—C17—H171	110.7	C117—N116—H3	120.6
C17—C18—N19	117.7 (2)	N116—C117—C118	119.0 (2)
C17—C18—O53	119.2 (2)	N116—C117—O148	121.8 (3)
N19—C18—O53	123.1 (2)	C118—C117—O148	119.2 (2)
C18—N19—C20	120.9 (2)	C117—C118—N119	108.31 (19)
C18—N19—H5	119.5	C117—C118—C149	107.6 (2)
C20—N19—H5	119.2	N119—C118—C149	111.0 (2)
N19—C20—C21	114.3 (2)	C117—C118—H1181	109.5
N19—C20—H201	107.9	N119—C118—H1181	107.8
C21—C20—H201	107.7	C149—C118—H1181	112.6
N19—C20—H202	109.2	C118—N119—C120	123.69 (19)
C21—C20—H202	108.4	C118—N119—H1	118.0
H201—C20—H202	109.3	C120—N119—H1	118.3
C20—C21—O22	109.19 (19)	N119—C120—C121	112.85 (18)
C20—C21—C25	118.4 (2)	N119—C120—O156	124.3 (2)
O22—C21—C25	104.69 (19)	C121—C120—O156	122.8 (2)
C20—C21—H211	110.2	C120—C121—O122	112.00 (18)
O22—C21—H211	105.5	C120—C121—C125	111.5 (2)
C25—C21—H211	108.0	O122—C121—C125	104.66 (18)
C21—O22—C23	109.85 (19)	C120—C121—H1211	109.9
O22—C23—O24	105.9 (2)	O122—C121—H1211	108.7
O22—C23—C54	109.2 (2)	C125—C121—H1211	110.0
O24—C23—C54	112.3 (3)	C121—O122—C123	109.31 (18)
O22—C23—C55	109.0 (3)	O122—C123—O124	104.24 (18)
O24—C23—C55	108.2 (3)	O122—C123—C157	110.0 (2)
C54—C23—C55	112.0 (3)	O124—C123—C157	111.5 (2)
C23—O24—C25	108.9 (2)	O122—C123—C158	108.7 (2)
C21—C25—O24	103.24 (19)	O124—C123—C158	108.3 (2)
C21—C25—C26	117.2 (2)	C157—C123—C158	113.7 (2)
O24—C25—C26	105.8 (2)	C123—O124—C125	107.54 (17)
C21—C25—H251	111.1	C121—C125—O124	102.89 (19)
O24—C25—H251	111.0	C121—C125—C126	115.61 (19)
C26—C25—H251	108.3	O124—C125—C126	109.67 (18)
C25—C26—O27	110.1 (2)	C121—C125—H1251	108.5
C25—C26—C30	116.0 (2)	O124—C125—H1251	109.8
O27—C26—C30	102.98 (19)	C126—C125—H1251	110.1
C25—C26—H261	108.3	C125—C126—O127	105.67 (19)
O27—C26—H261	109.7	C125—C126—C130	116.2 (2)
C30—C26—H261	109.5	O127—C126—C130	103.73 (18)
C26—O27—C28	108.62 (18)	C125—C126—H1261	108.2
O27—C28—O29	108.5 (2)	O127—C126—H1261	112.0
O27—C28—C56	98.5 (3)	C130—C126—H1261	110.9
O29—C28—C56	92.6 (3)	C126—O127—C128	108.58 (19)
O27—C28—C58	122.7 (5)	O127—C128—O129	106.44 (19)
O29—C28—C58	118.7 (4)	O127—C128—C159	108.1 (2)
C56—C28—C58	109.4 (6)	O129—C128—C159	109.9 (2)
O27—C28—O29	108.5 (2)	O127—C128—C160	110.7 (2)

O27—C28—C57	115.0 (3)	O129—C128—C160	109.3 (2)
O29—C28—C57	119.5 (4)	C159—C128—C160	112.2 (3)
O27—C28—C59	101.8 (3)	C128—O129—C130	110.60 (17)
O29—C28—C59	99.0 (3)	C126—C130—O129	103.85 (19)
C57—C28—C59	110.3 (4)	C126—C130—C131	117.4 (2)
C28—O29—C30	109.76 (19)	O129—C130—C131	108.84 (18)
C26—C30—O29	104.14 (19)	C126—C130—H1301	107.8
C26—C30—C31	112.3 (2)	O129—C130—H1301	109.7
O29—C30—C31	109.00 (19)	C131—C130—H1301	108.9
C26—C30—H301	111.2	C130—C131—N132	114.2 (2)
O29—C30—H301	112.3	C130—C131—H1311	107.5
C31—C30—H301	107.9	N132—C131—H1311	107.1
C30—C31—N32	113.6 (2)	C130—C131—H1312	109.1
C30—C31—O60	122.3 (2)	N132—C131—H1312	108.1
N32—C31—O60	124.1 (2)	H1311—C131—H1312	110.8
C1—N32—C31	124.94 (19)	C131—N132—C133	121.2 (2)
C1—N32—H8	119.0	C131—N132—H4	118.0
C31—N32—H8	116.0	C133—N132—H4	120.5
C1—C33—C34	115.0 (2)	C101—C133—N132	118.1 (2)
C1—C33—H331	107.3	C101—C133—O161	119.5 (2)
C34—C33—H331	108.9	N132—C133—O161	122.4 (2)
C1—C33—H332	106.9	C101—C134—C135	118.2 (2)
C34—C33—H332	107.9	C101—C134—H1341	107.3
H331—C33—H332	110.8	C135—C134—H1341	106.4
C33—C34—C35	119.9 (2)	C101—C134—H1342	106.0
C33—C34—C39	121.6 (2)	C135—C134—H1342	107.4
C35—C34—C39	118.5 (2)	H1341—C134—H1342	111.7
C34—C35—C36	121.0 (3)	C134—C135—C136	118.1 (2)
C34—C35—H351	118.0	C134—C135—C140	123.8 (2)
C36—C35—H351	121.0	C136—C135—C140	118.1 (2)
C35—C36—C37	119.8 (3)	C135—C136—C137	121.6 (3)
C35—C36—H361	120.1	C135—C136—H1361	120.6
C37—C36—H361	120.1	C137—C136—H1361	117.8
C36—C37—C38	119.7 (3)	C136—C137—C138	119.7 (3)
C36—C37—H371	121.2	C136—C137—H1371	119.6
C38—C37—H371	119.1	C138—C137—H1371	120.7
C37—C38—C39	120.7 (3)	C137—C138—C139	119.8 (3)
C37—C38—H381	118.9	C137—C138—H1381	120.1
C39—C38—H381	120.5	C139—C138—H1381	120.1
C34—C39—C38	120.3 (3)	C138—C139—C140	120.3 (3)
C34—C39—H391	119.2	C138—C139—H1391	119.3
C38—C39—H391	120.5	C140—C139—H1391	120.4
C7—C41—H411	110.1	C139—C140—C135	120.5 (2)
C7—C41—H412	107.7	C139—C140—H1401	118.7
H411—C41—H412	109.8	C135—C140—H1401	120.8
C7—C41—H413	108.6	C106—C142—H1421	108.3
H411—C41—H413	110.9	C106—C142—H1422	108.6
H412—C41—H413	109.5	H1421—C142—H1422	110.7

C7—C42—H421	108.4	C106—C142—H1423	112.0
C7—C42—H422	106.3	H1421—C142—H1423	107.7
H421—C42—H422	110.4	H1422—C142—H1423	109.5
C7—C42—H423	109.0	C106—C143—H1431	109.1
H421—C42—H423	112.5	C106—C143—H1432	109.6
H422—C42—H423	110.0	H1431—C143—H1432	110.0
C12—C43—H431	110.0	C106—C143—H1433	109.5
C12—C43—H432	108.5	H1431—C143—H1433	109.2
H431—C43—H432	109.2	H1432—C143—H1433	109.3
C12—C43—H433	108.8	C112—C144—H1441	109.6
H431—C43—H433	109.0	C112—C144—H1442	109.4
H432—C43—H433	111.4	H1441—C144—H1442	109.5
C12—C44—H441	111.7	C112—C144—H1443	109.4
C12—C44—H442	109.3	H1441—C144—H1443	109.5
H441—C44—H442	110.7	H1442—C144—H1443	109.5
C12—C44—H443	108.5	C112—C145—H1451	109.6
H441—C44—H443	106.9	C112—C145—H1452	109.3
H442—C44—H443	109.7	H1451—C145—H1452	109.5
C17—C46—C47	116.2 (2)	C112—C145—H1453	109.5
C17—C46—H461	108.3	H1451—C145—H1453	109.5
C47—C46—H461	109.3	H1452—C145—H1453	109.5
C17—C46—H462	107.5	C112—C146—H1461	109.2
C47—C46—H462	107.9	C112—C146—H1462	109.6
H461—C46—H462	107.4	H1461—C146—H1462	109.5
C46—C47—C48	122.9 (2)	C112—C146—H1463	109.6
C46—C47—C52	119.2 (2)	H1461—C146—H1463	109.5
C48—C47—C52	117.8 (3)	H1462—C146—H1463	109.5
C47—C48—C49	121.2 (3)	C112—C147—H1471	109.2
C47—C48—H481	120.1	C112—C147—H1472	109.6
C49—C48—H481	118.7	H1471—C147—H1472	109.5
C48—C49—C50	119.5 (3)	C112—C147—H1473	109.6
C48—C49—H491	119.6	H1471—C147—H1473	109.5
C50—C49—H491	121.0	H1472—C147—H1473	109.5
C49—C50—C51	120.3 (3)	C118—C149—C150	116.7 (2)
C49—C50—H501	120.9	C118—C149—H1491	106.4
C51—C50—H501	118.8	C150—C149—H1491	109.3
C50—C51—C52	120.3 (3)	C118—C149—H1492	107.0
C50—C51—H511	120.2	C150—C149—H1492	109.1
C52—C51—H511	119.5	H1491—C149—H1492	108.0
C47—C52—C51	120.8 (3)	C149—C150—C151	120.4 (3)
C47—C52—H521	118.9	C149—C150—C155	121.5 (2)
C51—C52—H521	120.3	C151—C150—C155	117.9 (3)
C23—C54—H541	109.4	C150—C151—C152	120.3 (4)
C23—C54—H542	110.4	C150—C151—H1511	120.0
H541—C54—H542	108.1	C152—C151—H1511	119.6
C23—C54—H543	107.9	C151—C152—C153	120.6 (4)
H541—C54—H543	110.3	C151—C152—H1521	118.7
H542—C54—H543	110.9	C153—C152—H1521	120.8

C23—C55—H551	111.0	C152—C153—C154	119.9 (4)
C23—C55—H552	108.8	C152—C153—H1531	119.1
H551—C55—H552	110.3	C154—C153—H1531	120.9
C23—C55—H553	109.2	C153—C154—C155	119.6 (4)
H551—C55—H553	107.7	C153—C154—H1541	120.1
H552—C55—H553	109.9	C155—C154—H1541	120.3
C28—C56—H561	109.4	C150—C155—C154	121.7 (3)
C28—C56—H562	109.4	C150—C155—H1551	119.8
H561—C56—H562	109.5	C154—C155—H1551	118.5
C28—C56—H563	109.5	C123—C157—H1571	109.0
H561—C56—H563	109.5	C123—C157—H1572	108.4
H562—C56—H563	109.5	H1571—C157—H1572	109.7
C28—C57—H571	109.6	C123—C157—H1573	108.4
C28—C57—H572	109.5	H1571—C157—H1573	111.3
H571—C57—H572	109.5	H1572—C157—H1573	109.9
C28—C57—H573	109.4	C123—C158—H1581	111.0
H571—C57—H573	109.5	C123—C158—H1582	111.2
H572—C57—H573	109.5	H1581—C158—H1582	107.4
C28—C58—H581	109.3	C123—C158—H1583	111.2
C28—C58—H582	109.6	H1581—C158—H1583	106.9
H581—C58—H582	109.5	H1582—C158—H1583	108.9
C28—C58—H583	109.5	C128—C159—H1591	105.9
H581—C58—H583	109.5	C128—C159—H1592	108.1
H582—C58—H583	109.5	H1591—C159—H1592	111.5
C28—C59—H591	109.5	C128—C159—H1593	109.8
C28—C59—H592	109.5	H1591—C159—H1593	111.4
H591—C59—H592	109.5	H1592—C159—H1593	109.9
C28—C59—H593	109.5	C128—C160—H1601	109.7
H591—C59—H593	109.5	C128—C160—H1602	110.9
H592—C59—H593	109.5	H1601—C160—H1602	107.4
N102—C101—C133	107.78 (19)	C128—C160—H1603	112.1
N102—C101—C134	112.2 (2)	H1601—C160—H1603	108.6
C133—C101—C134	108.8 (2)	H1602—C160—H1603	108.0
N102—C101—H1011	107.7		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N119—H1···O161	0.89	1.89	2.776 (2)	174
N16—H2···O40	0.88	1.95	2.813 (2)	170
N116—H3···O141^{i}	0.86	2.08	2.883 (2)	155
N132—H4···O156^{ii}	0.85	2.09	2.916 (2)	163
N19—H5···O60^{ii}	0.85	2.15	2.966 (2)	160
N3—H7···O45^{i}	0.85	2.08	2.897 (2)	159
N32—H8···O53	0.85	1.92	2.753 (2)	167
N102—H9···O148	0.85	1.96	2.798 (2)	167

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