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Supplementary Material

Synthesis and Characterization of a New Group of Exo-Coordinating O_2N_2-Donor Macrocycles

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Table 1. **Crystal data and structure refinement for 1.**

Identification code	1	
Empirical formula	C52 H56 N4 O6	
Formula weight	833.01	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 10.8743(8) Å	α= 102.085(6)°
	b = 12.6588(9) Å	β= 97.529(6)°
	c = 17.2802(11) Å	γ= 110.683(7)°
Volume	2120.8(3) $Å^3$	
Z	2	
Density (calculated)	1.304 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	888	
Crystal size	0.12 x 0.09 x 0.02 mm^3	
Theta range for data collection	3.36 to 26.00°.	
Index ranges	-13<=h<=13, -15<=k<=15, -16<=l<=21	
Reflections collected	8257	
Independent reflections	8257 [R(int) = 0.0000]	
Completeness to theta = 26.00°	98.9 %	
Max. and min. transmission	0.9983 and 0.9898	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8257 / 0 / 562	
Goodness-of-fit on F^2	1.120	
Final R indices [I>2sigma(I)]	R1 = 0.1065, wR2 = 0.2868	
R indices (all data)	R1 = 0.1464, wR2 = 0.3257	
Extinction coefficient	0.008(3)	
Largest diff. peak and hole	1.183 and -0.887 e.$Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for ?.

O(14)-C(15)	1.376(5)
O(14)-C(13)	1.435(5)
O(45)-C(46)	1.371(5)
O(45)-C(44)	1.438(6)
O(11)-C(10)	1.368(5)
O(11)-C(12)	1.433(6)
O(42)-C(41)	1.371(5)
O(42)-C(43)	1.432(5)
O(31)-C(26)	1.353(5)
O(31)-H(1)	0.8144
O(62)-C(61)	1.360(5)
O(62)-H(2)	0.9508
N(32)-C(33)	1.454(5)
N(32)-C(53)	1.472(6)
N(32)-C(52)	1.483(5)
N(1)-C(21)	1.455(5)
N(1)-C(22)	1.467(5)
N(1)-C(2)	1.468(5)
N(34)-C(55)	1.464(5)
N(34)-C(35)	1.484(5)
N(34)-C(33)	1.491(5)
N(3)-C(24)	1.478(5)
N(3)-C(2)	1.487(5)
N(3)-C(4)	1.498(5)
C(51)-C(50)	1.374(6)
C(51)-C(46)	1.400(7)
C(51)-C(52)	1.521(6)
C(10)-C(5)	1.395(6)
C(10)-C(9)	1.400(6)
C(59)-C(58)	1.372(6)
C(59)-C(60)	1.390(7)
C(59)-H(59A)	0.9300
C(58)-C(57)	1.388(6)
C(58)-H(58A)	0.9300

C(55)-C(54)	1.506(6)
C(55)-H(55A)	0.9700
C(55)-H(55B)	0.9700
C(57)-C(56)	1.395(6)
C(57)-H(57A)	0.9300
C(37)-C(38)	1.378(6)
C(37)-C(36)	1.382(6)
C(37)-H(37A)	0.9300
C(7)-C(6)	1.374(6)
C(7)-C(8)	1.387(7)
C(7)-H(7A)	0.9300
C(9)-C(8)	1.384(7)
C(9)-H(9A)	0.9300
C(23)-C(22)	1.513(6)
C(23)-C(24)	1.516(6)
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(20)-C(15)	1.391(7)
C(20)-C(19)	1.392(6)
C(20)-C(21)	1.523(6)
C(15)-C(16)	1.393(6)
C(5)-C(6)	1.388(6)
C(5)-C(4)	1.507(6)
C(60)-C(61)	1.396(6)
C(60)-H(60A)	0.9300
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(54)-C(53)	1.525(6)
C(54)-H(54A)	0.9700
C(54)-H(54B)	0.9700
C(41)-C(40)	1.397(6)
C(41)-C(36)	1.400(6)
C(6)-H(6A)	0.9300
C(29)-C(28)	1.369(7)
C(29)-C(30)	1.384(6)
C(29)-H(29A)	0.9300

C(28)-C(27)	1.382(6)
C(28)-H(28A)	0.9300
C(36)-C(35)	1.502(6)
C(25)-C(30)	1.394(6)
C(25)-C(26)	1.411(6)
C(25)-C(2)	1.541(5)
C(26)-C(27)	1.398(6)
C(61)-C(56)	1.404(6)
C(43)-C(44)	1.502(6)
C(43)-H(43A)	0.9700
C(43)-H(43B)	0.9700
C(39)-C(38)	1.374(7)
C(39)-C(40)	1.387(7)
C(39)-H(39A)	0.9300
C(47)-C(48)	1.393(7)
C(47)-C(46)	1.397(6)
C(47)-H(47A)	0.9300
C(33)-C(56)	1.533(6)
C(33)-H(33A)	0.9800
C(27)-H(27A)	0.9300
C(16)-C(17)	1.390(7)
C(16)-H(16A)	0.9300
C(53)-H(53A)	0.9700
C(53)-H(53B)	0.9700
C(17)-C(18)	1.400(8)
C(17)-H(17A)	0.9300
C(48)-C(49)	1.383(8)
C(48)-H(48A)	0.9300
C(49)-C(50)	1.375(7)
C(49)-H(49A)	0.9300
C(38)-H(38A)	0.9300
C(50)-H(50A)	0.9300
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
C(8)-H(8A)	0.9300
C(44)-H(44A)	0.9700

C(44)-H(44B)	0.9700
C(52)-H(52A)	0.9700
C(52)-H(52B)	0.9700
C(40)-H(40A)	0.9300
C(30)-H(30A)	0.9300
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(19)-C(18)	1.382(7)
C(19)-H(19A)	0.9300
C(18)-H(18A)	0.9300
C(2)-H(2A)	0.9800
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(12)-C(13)	1.493(6)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700

C(15)-O(14)-C(13)	117.7(4)
C(46)-O(45)-C(44)	117.8(3)
C(10)-O(11)-C(12)	118.0(3)
C(41)-O(42)-C(43)	117.5(3)
C(26)-O(31)-H(1)	109.1
C(61)-O(62)-H(2)	104.1
C(33)-N(32)-C(53)	114.7(3)
C(33)-N(32)-C(52)	116.4(3)
C(53)-N(32)-C(52)	114.1(3)
C(21)-N(1)-C(22)	114.1(3)
C(21)-N(1)-C(2)	116.6(3)
C(22)-N(1)-C(2)	114.2(3)
C(55)-N(34)-C(35)	112.8(3)
C(55)-N(34)-C(33)	109.6(3)
C(35)-N(34)-C(33)	111.8(3)

C(24)-N(3)-C(2)	110.0(3)
C(24)-N(3)-C(4)	112.6(3)
C(2)-N(3)-C(4)	111.7(3)
C(50)-C(51)-C(46)	118.5(4)
C(50)-C(51)-C(52)	121.3(4)
C(46)-C(51)-C(52)	120.0(4)
O(11)-C(10)-C(5)	115.7(4)
O(11)-C(10)-C(9)	122.9(4)
C(5)-C(10)-C(9)	121.4(4)
C(58)-C(59)-C(60)	120.8(4)
C(58)-C(59)-H(59A)	119.6
C(60)-C(59)-H(59A)	119.6
C(59)-C(58)-C(57)	118.9(4)
C(59)-C(58)-H(58A)	120.5
C(57)-C(58)-H(58A)	120.5
N(34)-C(55)-C(54)	113.8(4)
N(34)-C(55)-H(55A)	108.8
C(54)-C(55)-H(55A)	108.8
N(34)-C(55)-H(55B)	108.8
C(54)-C(55)-H(55B)	108.8
H(55A)-C(55)-H(55B)	107.7
C(58)-C(57)-C(56)	122.5(4)
C(58)-C(57)-H(57A)	118.7
C(56)-C(57)-H(57A)	118.7
C(38)-C(37)-C(36)	123.1(5)
C(38)-C(37)-H(37A)	118.4
C(36)-C(37)-H(37A)	118.4
C(6)-C(7)-C(8)	118.4(5)
C(6)-C(7)-H(7A)	120.8
C(8)-C(7)-H(7A)	120.8
C(8)-C(9)-C(10)	118.5(4)
C(8)-C(9)-H(9A)	120.8
C(10)-C(9)-H(9A)	120.8
C(22)-C(23)-C(24)	109.4(3)
C(22)-C(23)-H(23A)	109.8
C(24)-C(23)-H(23A)	109.8

C(22)-C(23)-H(23B)	109.8
C(24)-C(23)-H(23B)	109.8
H(23A)-C(23)-H(23B)	108.2
C(15)-C(20)-C(19)	118.5(4)
C(15)-C(20)-C(21)	120.9(4)
C(19)-C(20)-C(21)	120.4(4)
O(14)-C(15)-C(20)	115.1(4)
O(14)-C(15)-C(16)	124.0(4)
C(20)-C(15)-C(16)	120.9(4)
C(6)-C(5)-C(10)	117.4(4)
C(6)-C(5)-C(4)	120.3(4)
C(10)-C(5)-C(4)	122.2(4)
C(59)-C(60)-C(61)	119.5(4)
C(59)-C(60)-H(60A)	120.2
C(61)-C(60)-H(60A)	120.2
N(3)-C(24)-C(23)	111.6(4)
N(3)-C(24)-H(24A)	109.3
C(23)-C(24)-H(24A)	109.3
N(3)-C(24)-H(24B)	109.3
C(23)-C(24)-H(24B)	109.3
H(24A)-C(24)-H(24B)	108.0
C(55)-C(54)-C(53)	109.1(3)
C(55)-C(54)-H(54A)	109.9
C(53)-C(54)-H(54A)	109.9
C(55)-C(54)-H(54B)	109.9
C(53)-C(54)-H(54B)	109.9
H(54A)-C(54)-H(54B)	108.3
O(42)-C(41)-C(40)	122.8(4)
O(42)-C(41)-C(36)	116.1(4)
C(40)-C(41)-C(36)	121.1(4)
C(7)-C(6)-C(5)	122.8(5)
C(7)-C(6)-H(6A)	118.6
C(5)-C(6)-H(6A)	118.6
C(28)-C(29)-C(30)	119.9(4)
C(28)-C(29)-H(29A)	120.1
C(30)-C(29)-H(29A)	120.1

C(29)-C(28)-C(27)	120.5(4)
C(29)-C(28)-H(28A)	119.8
C(27)-C(28)-H(28A)	119.8
C(37)-C(36)-C(41)	116.7(4)
C(37)-C(36)-C(35)	120.4(4)
C(41)-C(36)-C(35)	122.8(4)
C(30)-C(25)-C(26)	117.3(4)
C(30)-C(25)-C(2)	122.6(4)
C(26)-C(25)-C(2)	119.5(3)
O(31)-C(26)-C(27)	117.3(4)
O(31)-C(26)-C(25)	122.2(4)
C(27)-C(26)-C(25)	120.4(4)
O(62)-C(61)-C(60)	117.4(4)
O(62)-C(61)-C(56)	121.6(4)
C(60)-C(61)-C(56)	121.0(4)
O(42)-C(43)-C(44)	106.4(4)
O(42)-C(43)-H(43A)	110.4
C(44)-C(43)-H(43A)	110.4
O(42)-C(43)-H(43B)	110.4
C(44)-C(43)-H(43B)	110.4
H(43A)-C(43)-H(43B)	108.6
C(38)-C(39)-C(40)	120.2(5)
C(38)-C(39)-H(39A)	119.9
C(40)-C(39)-H(39A)	119.9
C(48)-C(47)-C(46)	118.0(5)
C(48)-C(47)-H(47A)	121.0
C(46)-C(47)-H(47A)	121.0
N(32)-C(33)-N(34)	110.2(3)
N(32)-C(33)-C(56)	118.7(3)
N(34)-C(33)-C(56)	109.2(3)
N(32)-C(33)-H(33A)	106.0
N(34)-C(33)-H(33A)	105.9
C(56)-C(33)-H(33A)	105.9
C(28)-C(27)-C(26)	119.9(4)
C(28)-C(27)-H(27A)	120.0
C(26)-C(27)-H(27A)	120.0

C(17)-C(16)-C(15)	119.6(5)
C(17)-C(16)-H(16A)	120.2
C(15)-C(16)-H(16A)	120.2
N(32)-C(53)-C(54)	109.3(4)
N(32)-C(53)-H(53A)	109.8
C(54)-C(53)-H(53A)	109.8
N(32)-C(53)-H(53B)	109.8
C(54)-C(53)-H(53B)	109.8
H(53A)-C(53)-H(53B)	108.3
C(16)-C(17)-C(18)	120.2(4)
C(16)-C(17)-H(17A)	119.9
C(18)-C(17)-H(17A)	119.9
C(49)-C(48)-C(47)	121.4(4)
C(49)-C(48)-H(48A)	119.3
C(47)-C(48)-H(48A)	119.3
C(50)-C(49)-C(48)	119.1(5)
C(50)-C(49)-H(49A)	120.4
C(48)-C(49)-H(49A)	120.4
C(39)-C(38)-C(37)	119.2(5)
C(39)-C(38)-H(38A)	120.4
C(37)-C(38)-H(38A)	120.4
C(51)-C(50)-C(49)	121.8(5)
C(51)-C(50)-H(50A)	119.1
C(49)-C(50)-H(50A)	119.1
N(34)-C(35)-C(36)	111.0(3)
N(34)-C(35)-H(35A)	109.4
C(36)-C(35)-H(35A)	109.4
N(34)-C(35)-H(35B)	109.4
C(36)-C(35)-H(35B)	109.4
H(35A)-C(35)-H(35B)	108.0
O(45)-C(46)-C(47)	123.6(5)
O(45)-C(46)-C(51)	115.3(4)
C(47)-C(46)-C(51)	121.1(4)
C(9)-C(8)-C(7)	121.5(4)
C(9)-C(8)-H(8A)	119.3
C(7)-C(8)-H(8A)	119.3

O(45)-C(44)-C(43)	106.9(3)
O(45)-C(44)-H(44A)	110.3
C(43)-C(44)-H(44A)	110.3
O(45)-C(44)-H(44B)	110.3
C(43)-C(44)-H(44B)	110.3
H(44A)-C(44)-H(44B)	108.6
N(32)-C(52)-C(51)	112.4(3)
N(32)-C(52)-H(52A)	109.1
C(51)-C(52)-H(52A)	109.1
N(32)-C(52)-H(52B)	109.1
C(51)-C(52)-H(52B)	109.1
H(52A)-C(52)-H(52B)	107.9
C(39)-C(40)-C(41)	119.6(5)
C(39)-C(40)-H(40A)	120.2
C(41)-C(40)-H(40A)	120.2
C(29)-C(30)-C(25)	121.9(4)
C(29)-C(30)-H(30A)	119.1
C(25)-C(30)-H(30A)	119.1
N(1)-C(22)-C(23)	109.7(3)
N(1)-C(22)-H(22A)	109.7
C(23)-C(22)-H(22A)	109.7
N(1)-C(22)-H(22B)	109.7
C(23)-C(22)-H(22B)	109.7
H(22A)-C(22)-H(22B)	108.2
N(1)-C(21)-C(20)	113.6(3)
N(1)-C(21)-H(21A)	108.9
C(20)-C(21)-H(21A)	108.9
N(1)-C(21)-H(21B)	108.9
C(20)-C(21)-H(21B)	108.9
H(21A)-C(21)-H(21B)	107.7
C(18)-C(19)-C(20)	121.6(5)
C(18)-C(19)-H(19A)	119.2
C(20)-C(19)-H(19A)	119.2
C(57)-C(56)-C(61)	117.0(4)
C(57)-C(56)-C(33)	122.5(4)
C(61)-C(56)-C(33)	120.0(4)

C(19)-C(18)-C(17)	119.1(4)
C(19)-C(18)-H(18A)	120.4
C(17)-C(18)-H(18A)	120.4
N(1)-C(2)-N(3)	110.3(3)
N(1)-C(2)-C(25)	118.9(3)
N(3)-C(2)-C(25)	109.2(3)
N(1)-C(2)-H(2A)	105.8
N(3)-C(2)-H(2A)	105.8
C(25)-C(2)-H(2A)	105.8
N(3)-C(4)-C(5)	110.2(3)
N(3)-C(4)-H(4A)	109.6
C(5)-C(4)-H(4A)	109.6
N(3)-C(4)-H(4B)	109.6
C(5)-C(4)-H(4B)	109.6
H(4A)-C(4)-H(4B)	108.1
O(11)-C(12)-C(13)	106.0(3)
O(11)-C(12)-H(12A)	110.5
C(13)-C(12)-H(12A)	110.5
O(11)-C(12)-H(12B)	110.5
C(13)-C(12)-H(12B)	110.5
H(12A)-C(12)-H(12B)	108.7
O(14)-C(13)-C(12)	107.4(4)
O(14)-C(13)-H(13A)	110.2
C(12)-C(13)-H(13A)	110.2
O(14)-C(13)-H(13B)	110.2
C(12)-C(13)-H(13B)	110.2
H(13A)-C(13)-H(13B)	108.5

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for ?.

C(12)-O(11)-C(10)-C(5)	153.4(4)
C(12)-O(11)-C(10)-C(9)	-28.8(6)
C(60)-C(59)-C(58)-C(57)	5.3(8)
C(35)-N(34)-C(55)-C(54)	68.2(4)
C(33)-N(34)-C(55)-C(54)	-57.0(4)
C(59)-C(58)-C(57)-C(56)	-1.7(7)
O(11)-C(10)-C(9)-C(8)	-175.1(4)
C(5)-C(10)-C(9)-C(8)	2.5(6)
C(13)-O(14)-C(15)-C(20)	170.0(4)
C(13)-O(14)-C(15)-C(16)	-11.1(6)
C(19)-C(20)-C(15)-O(14)	178.8(4)
C(21)-C(20)-C(15)-O(14)	2.8(6)
C(19)-C(20)-C(15)-C(16)	-0.1(6)
C(21)-C(20)-C(15)-C(16)	-176.1(4)
O(11)-C(10)-C(5)-C(6)	175.2(4)
C(9)-C(10)-C(5)-C(6)	-2.6(6)
O(11)-C(10)-C(5)-C(4)	-8.3(6)
C(9)-C(10)-C(5)-C(4)	173.9(4)
C(58)-C(59)-C(60)-C(61)	-4.2(7)
C(2)-N(3)-C(24)-C(23)	58.1(4)
C(4)-N(3)-C(24)-C(23)	-67.3(4)
C(22)-C(23)-C(24)-N(3)	-57.3(5)
N(34)-C(55)-C(54)-C(53)	55.6(5)
C(43)-O(42)-C(41)-C(40)	29.6(6)
C(43)-O(42)-C(41)-C(36)	-153.5(4)
C(8)-C(7)-C(6)-C(5)	1.3(7)
C(10)-C(5)-C(6)-C(7)	0.7(6)
C(4)-C(5)-C(6)-C(7)	-175.9(4)
C(30)-C(29)-C(28)-C(27)	-2.2(7)
C(38)-C(37)-C(36)-C(41)	-0.4(7)
C(38)-C(37)-C(36)-C(35)	176.0(4)
O(42)-C(41)-C(36)-C(37)	-175.7(4)
C(40)-C(41)-C(36)-C(37)	1.3(6)
O(42)-C(41)-C(36)-C(35)	8.1(6)

C(40)-C(41)-C(36)-C(35)	-174.9(4)
C(30)-C(25)-C(26)-O(31)	178.1(4)
C(2)-C(25)-C(26)-O(31)	-10.4(6)
C(30)-C(25)-C(26)-C(27)	-3.3(6)
C(2)-C(25)-C(26)-C(27)	168.2(4)
C(59)-C(60)-C(61)-O(62)	-179.0(4)
C(59)-C(60)-C(61)-C(56)	-0.6(7)
C(41)-O(42)-C(43)-C(44)	166.0(4)
C(53)-N(32)-C(33)-N(34)	-57.9(4)
C(52)-N(32)-C(33)-N(34)	165.3(3)
C(53)-N(32)-C(33)-C(56)	69.1(4)
C(52)-N(32)-C(33)-C(56)	-67.7(5)
C(55)-N(34)-C(33)-N(32)	55.7(4)
C(35)-N(34)-C(33)-N(32)	-70.1(4)
C(55)-N(34)-C(33)-C(56)	-76.4(4)
C(35)-N(34)-C(33)-C(56)	157.8(3)
C(29)-C(28)-C(27)-C(26)	1.9(7)
O(31)-C(26)-C(27)-C(28)	179.6(4)
C(25)-C(26)-C(27)-C(28)	0.9(7)
O(14)-C(15)-C(16)-C(17)	179.3(4)
C(20)-C(15)-C(16)-C(17)	-2.0(6)
C(33)-N(32)-C(53)-C(54)	56.3(4)
C(52)-N(32)-C(53)-C(54)	-165.9(3)
C(55)-C(54)-C(53)-N(32)	-52.3(5)
C(15)-C(16)-C(17)-C(18)	2.1(7)
C(46)-C(47)-C(48)-C(49)	-1.3(7)
C(47)-C(48)-C(49)-C(50)	-1.2(7)
C(40)-C(39)-C(38)-C(37)	1.4(7)
C(36)-C(37)-C(38)-C(39)	-1.0(7)
C(46)-C(51)-C(50)-C(49)	-3.0(7)
C(52)-C(51)-C(50)-C(49)	-178.5(4)
C(48)-C(49)-C(50)-C(51)	3.5(7)
C(55)-N(34)-C(35)-C(36)	146.0(4)
C(33)-N(34)-C(35)-C(36)	-90.0(4)
C(37)-C(36)-C(35)-N(34)	-63.7(5)
C(41)-C(36)-C(35)-N(34)	112.5(4)

C(44)-O(45)-C(46)-C(47)	13.2(6)
C(44)-O(45)-C(46)-C(51)	-167.8(4)
C(48)-C(47)-C(46)-O(45)	-179.3(4)
C(48)-C(47)-C(46)-C(51)	1.7(6)
C(50)-C(51)-C(46)-O(45)	-178.6(4)
C(52)-C(51)-C(46)-O(45)	-3.1(6)
C(50)-C(51)-C(46)-C(47)	0.4(6)
C(52)-C(51)-C(46)-C(47)	175.9(4)
C(10)-C(9)-C(8)-C(7)	-0.5(7)
C(6)-C(7)-C(8)-C(9)	-1.4(7)
C(46)-O(45)-C(44)-C(43)	156.1(4)
O(42)-C(43)-C(44)-O(45)	-62.0(4)
C(33)-N(32)-C(52)-C(51)	-137.9(4)
C(53)-N(32)-C(52)-C(51)	85.1(5)
C(50)-C(51)-C(52)-N(32)	-97.0(5)
C(46)-C(51)-C(52)-N(32)	87.7(5)
C(38)-C(39)-C(40)-C(41)	-0.5(7)
O(42)-C(41)-C(40)-C(39)	175.9(4)
C(36)-C(41)-C(40)-C(39)	-0.9(7)
C(28)-C(29)-C(30)-C(25)	-0.4(7)
C(26)-C(25)-C(30)-C(29)	3.1(6)
C(2)-C(25)-C(30)-C(29)	-168.1(4)
C(21)-N(1)-C(22)-C(23)	166.5(3)
C(2)-N(1)-C(22)-C(23)	-55.9(5)
C(24)-C(23)-C(22)-N(1)	54.3(5)
C(22)-N(1)-C(21)-C(20)	-87.4(4)
C(2)-N(1)-C(21)-C(20)	136.0(4)
C(15)-C(20)-C(21)-N(1)	-83.6(5)
C(19)-C(20)-C(21)-N(1)	100.4(4)
C(15)-C(20)-C(19)-C(18)	2.0(6)
C(21)-C(20)-C(19)-C(18)	178.0(4)
C(58)-C(57)-C(56)-C(61)	-2.9(7)
C(58)-C(57)-C(56)-C(33)	169.2(4)
O(62)-C(61)-C(56)-C(57)	-177.7(4)
C(60)-C(61)-C(56)-C(57)	4.0(6)
O(62)-C(61)-C(56)-C(33)	10.0(6)

C(60)-C(61)-C(56)-C(33)	-168.3(4)
N(32)-C(33)-C(56)-C(57)	17.1(6)
N(34)-C(33)-C(56)-C(57)	144.5(4)
N(32)-C(33)-C(56)-C(61)	-171.0(4)
N(34)-C(33)-C(56)-C(61)	-43.6(5)
C(20)-C(19)-C(18)-C(17)	-1.8(6)
C(16)-C(17)-C(18)-C(19)	-0.3(7)
C(21)-N(1)-C(2)-N(3)	-166.8(3)
C(22)-N(1)-C(2)-N(3)	56.7(4)
C(21)-N(1)-C(2)-C(25)	65.9(5)
C(22)-N(1)-C(2)-C(25)	-70.5(4)
C(24)-N(3)-C(2)-N(1)	-56.1(4)
C(4)-N(3)-C(2)-N(1)	69.8(4)
C(24)-N(3)-C(2)-C(25)	76.3(4)
C(4)-N(3)-C(2)-C(25)	-157.8(3)
C(30)-C(25)-C(2)-N(1)	-17.3(6)
C(26)-C(25)-C(2)-N(1)	171.7(3)
C(30)-C(25)-C(2)-N(3)	-145.1(4)
C(26)-C(25)-C(2)-N(3)	43.9(5)
C(24)-N(3)-C(4)-C(5)	-144.1(4)
C(2)-N(3)-C(4)-C(5)	91.5(4)
C(6)-C(5)-C(4)-N(3)	64.2(5)
C(10)-C(5)-C(4)-N(3)	-112.2(4)
C(10)-O(11)-C(12)-C(13)	-165.6(4)
C(15)-O(14)-C(13)-C(12)	-159.5(3)
O(11)-C(12)-C(13)-O(14)	61.2(4)

Symmetry transformations used to generate equivalent atoms:

Table 1. **Crystal data and structure refinement for 2**

Identification code	2	
Empirical formula	C27 H30 N2 O3	
Formula weight	430.53	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.42318(14) Å	α= 90°
	b = 7.17490(10) Å	β= 101.1273(12)°
	c = 26.7283(4) Å	γ= 90°
Volume	2149.47(5) $Å^3$	
Z	4	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	920	
Crystal size	0.30 x 0.30 x 0.20 mm^3	
Theta range for data collection	3.37 to 27.00°	
Index ranges	-14<=h<=14, -9<=k<=9, -34<=l<=34	
Reflections collected	47309	
Independent reflections	4695 [R(int) = 0.0299]	
Completeness to theta = 25.00°	99.8 %	
Max. and min. transmission	0.9829 and 0.9745	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4695 / 0 / 289	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0397, wR2 = 0.0978	
R indices (all data)	R1 = 0.0462, wR2 = 0.1023	
Largest diff. peak and hole	0.592 and -0.197 $e.Å^{-3}$	

Table 2. Bond lengths [!] and angles [°] for ?.

O(11)-C(10)	1.3683(15)
O(11)-C(12)	1.4418(15)
O(15)-C(16)	1.3666(15)
O(15)-C(14)	1.4191(15)
N(3)-C(2)	1.4628(15)
N(3)-C(23)	1.4721(16)
N(3)-C(4)	1.4794(15)
O(32)-C(27)	1.3507(15)
O(32)-H(32)	0.9401
N(1)-C(22)	1.4753(15)
N(1)-C(25)	1.4838(16)
N(1)-C(2)	1.4940(15)
C(26)-C(31)	1.3979(17)
C(26)-C(27)	1.4093(17)
C(26)-C(2)	1.5329(16)
C(6)-C(7)	1.3887(19)
C(6)-C(5)	1.3917(18)
C(6)-H(6)	0.9500
C(7)-C(8)	1.384(2)
C(7)-H(7)	0.9500
C(5)-C(10)	1.4088(17)
C(5)-C(4)	1.5156(17)
C(16)-C(17)	1.3861(17)
C(16)-C(21)	1.4022(17)
C(14)-C(13)	1.5188(18)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(9)-C(8)	1.389(2)
C(9)-C(10)	1.4004(18)
C(9)-H(9)	0.9500
C(25)-C(24)	1.5259(18)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(27)-C(28)	1.3952(19)

C(18)-C(19)	1.3813(19)
C(18)-C(17)	1.3951(18)
C(18)-H(18)	0.9500
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(21)-C(20)	1.3821(17)
C(21)-C(22)	1.5066(16)
C(19)-C(20)	1.3963(18)
C(19)-H(19)	0.9500
C(13)-C(12)	1.5186(19)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(2)-H(2)	1.0000
C(31)-C(30)	1.3906(18)
C(31)-H(31)	0.9500
C(17)-H(17)	0.9500
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.5266(18)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(8)-H(8)	0.9500
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(28)-C(29)	1.384(2)
C(28)-H(28)	0.9500
C(20)-H(20)	0.9500
C(30)-C(29)	1.387(2)
C(30)-H(30)	0.9500
C(29)-H(29)	0.9500
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900

C(10)-O(11)-C(12)	116.94(10)
C(16)-O(15)-C(14)	120.69(10)
C(2)-N(3)-C(23)	111.23(9)

C(2)-N(3)-C(4)	115.00(9)
C(23)-N(3)-C(4)	112.80(10)
C(27)-O(32)-H(32)	102.5
C(22)-N(1)-C(25)	112.27(10)
C(22)-N(1)-C(2)	111.57(9)
C(25)-N(1)-C(2)	110.93(9)
C(31)-C(26)-C(27)	117.96(11)
C(31)-C(26)-C(2)	120.65(11)
C(27)-C(26)-C(2)	120.67(11)
C(7)-C(6)-C(5)	122.05(12)
C(7)-C(6)-H(6)	119.0
C(5)-C(6)-H(6)	119.0
C(8)-C(7)-C(6)	119.03(13)
C(8)-C(7)-H(7)	120.5
C(6)-C(7)-H(7)	120.5
C(6)-C(5)-C(10)	118.41(11)
C(6)-C(5)-C(4)	119.27(11)
C(10)-C(5)-C(4)	122.30(11)
O(15)-C(16)-C(17)	125.53(11)
O(15)-C(16)-C(21)	112.88(11)
C(17)-C(16)-C(21)	121.58(11)
O(15)-C(14)-C(13)	105.89(10)
O(15)-C(14)-H(14A)	110.6
C(13)-C(14)-H(14A)	110.6
O(15)-C(14)-H(14B)	110.6
C(13)-C(14)-H(14B)	110.6
H(14A)-C(14)-H(14B)	108.7
C(8)-C(9)-C(10)	120.33(12)
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-H(9)	119.8
N(1)-C(25)-C(24)	112.47(10)
N(1)-C(25)-H(25A)	109.1
C(24)-C(25)-H(25A)	109.1
N(1)-C(25)-H(25B)	109.1
C(24)-C(25)-H(25B)	109.1
H(25A)-C(25)-H(25B)	107.8

O(32)-C(27)-C(28)	117.76(11)
O(32)-C(27)-C(26)	121.86(11)
C(28)-C(27)-C(26)	120.34(12)
C(19)-C(18)-C(17)	120.80(12)
C(19)-C(18)-H(18)	119.6
C(17)-C(18)-H(18)	119.6
N(3)-C(4)-C(5)	111.81(10)
N(3)-C(4)-H(4A)	109.3
C(5)-C(4)-H(4A)	109.3
N(3)-C(4)-H(4B)	109.3
C(5)-C(4)-H(4B)	109.3
H(4A)-C(4)-H(4B)	107.9
C(20)-C(21)-C(16)	118.70(11)
C(20)-C(21)-C(22)	126.26(11)
C(16)-C(21)-C(22)	115.03(11)
C(18)-C(19)-C(20)	119.92(12)
C(18)-C(19)-H(19)	120.0
C(20)-C(19)-H(19)	120.0
C(12)-C(13)-C(14)	113.96(11)
C(12)-C(13)-H(13A)	108.8
C(14)-C(13)-H(13A)	108.8
C(12)-C(13)-H(13B)	108.8
C(14)-C(13)-H(13B)	108.8
H(13A)-C(13)-H(13B)	107.7
N(3)-C(2)-N(1)	115.90(10)
N(3)-C(2)-C(26)	111.36(10)
N(1)-C(2)-C(26)	110.79(9)
N(3)-C(2)-H(2)	106.0
N(1)-C(2)-H(2)	106.0
C(26)-C(2)-H(2)	106.0
C(30)-C(31)-C(26)	121.54(12)
C(30)-C(31)-H(31)	119.2
C(26)-C(31)-H(31)	119.2
C(16)-C(17)-C(18)	118.50(12)
C(16)-C(17)-H(17)	120.7
C(18)-C(17)-H(17)	120.7

N(1)-C(22)-C(21)	115.46(10)
N(1)-C(22)-H(22A)	108.4
C(21)-C(22)-H(22A)	108.4
N(1)-C(22)-H(22B)	108.4
C(21)-C(22)-H(22B)	108.4
H(22A)-C(22)-H(22B)	107.5
N(3)-C(23)-C(24)	113.33(10)
N(3)-C(23)-H(23A)	108.9
C(24)-C(23)-H(23A)	108.9
N(3)-C(23)-H(23B)	108.9
C(24)-C(23)-H(23B)	108.9
H(23A)-C(23)-H(23B)	107.7
C(7)-C(8)-C(9)	120.51(12)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
C(25)-C(24)-C(23)	109.17(11)
C(25)-C(24)-H(24A)	109.8
C(23)-C(24)-H(24A)	109.8
C(25)-C(24)-H(24B)	109.8
C(23)-C(24)-H(24B)	109.8
H(24A)-C(24)-H(24B)	108.3
C(29)-C(28)-C(27)	120.34(12)
C(29)-C(28)-H(28)	119.8
C(27)-C(28)-H(28)	119.8
C(21)-C(20)-C(19)	120.48(12)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(29)-C(30)-C(31)	119.58(13)
C(29)-C(30)-H(30)	120.2
C(31)-C(30)-H(30)	120.2
C(28)-C(29)-C(30)	120.22(12)
C(28)-C(29)-H(29)	119.9
C(30)-C(29)-H(29)	119.9
O(11)-C(12)-C(13)	110.24(11)
O(11)-C(12)-H(12A)	109.6
C(13)-C(12)-H(12A)	109.6

O(11)-C(12)-H(12B)	109.6
C(13)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
O(11)-C(10)-C(9)	123.47(11)
O(11)-C(10)-C(5)	116.87(11)
C(9)-C(10)-C(5)	119.66(12)

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for ?.

C(5)-C(6)-C(7)-C(8)	-0.2(2)
C(7)-C(6)-C(5)-C(10)	1.00(18)
C(7)-C(6)-C(5)-C(4)	179.26(11)
C(14)-O(15)-C(16)-C(17)	3.80(19)
C(14)-O(15)-C(16)-C(21)	-175.88(11)
C(16)-O(15)-C(14)-C(13)	-179.63(11)
C(22)-N(1)-C(25)-C(24)	73.22(13)
C(2)-N(1)-C(25)-C(24)	-52.37(13)
C(31)-C(26)-C(27)-O(32)	179.10(11)
C(2)-C(26)-C(27)-O(32)	8.77(18)
C(31)-C(26)-C(27)-C(28)	1.49(18)
C(2)-C(26)-C(27)-C(28)	-168.84(12)
C(2)-N(3)-C(4)-C(5)	60.50(13)
C(23)-N(3)-C(4)-C(5)	-170.49(10)
C(6)-C(5)-C(4)-N(3)	42.68(15)
C(10)-C(5)-C(4)-N(3)	-139.13(11)
O(15)-C(16)-C(21)-C(20)	-179.15(11)
C(17)-C(16)-C(21)-C(20)	1.16(19)
O(15)-C(16)-C(21)-C(22)	2.00(16)
C(17)-C(16)-C(21)-C(22)	-177.69(12)
C(17)-C(18)-C(19)-C(20)	0.3(2)
O(15)-C(14)-C(13)-C(12)	-62.43(15)
C(23)-N(3)-C(2)-N(1)	-51.00(13)
C(4)-N(3)-C(2)-N(1)	78.79(13)
C(23)-N(3)-C(2)-C(26)	76.85(12)
C(4)-N(3)-C(2)-C(26)	-153.37(10)
C(22)-N(1)-C(2)-N(3)	-74.82(13)
C(25)-N(1)-C(2)-N(3)	51.16(13)
C(22)-N(1)-C(2)-C(26)	157.05(10)
C(25)-N(1)-C(2)-C(26)	-76.97(12)
C(31)-C(26)-C(2)-N(3)	24.20(15)
C(27)-C(26)-C(2)-N(3)	-165.72(11)
C(31)-C(26)-C(2)-N(1)	154.75(11)
C(27)-C(26)-C(2)-N(1)	-35.17(15)

C(27)-C(26)-C(31)-C(30)	-0.90(19)
C(2)-C(26)-C(31)-C(30)	169.44(12)
O(15)-C(16)-C(17)-C(18)	179.83(12)
C(21)-C(16)-C(17)-C(18)	-0.51(19)
C(19)-C(18)-C(17)-C(16)	-0.22(19)
C(25)-N(1)-C(22)-C(21)	90.55(13)
C(2)-N(1)-C(22)-C(21)	-144.21(10)
C(20)-C(21)-C(22)-N(1)	-6.33(18)
C(16)-C(21)-C(22)-N(1)	172.42(11)
C(2)-N(3)-C(23)-C(24)	52.62(14)
C(4)-N(3)-C(23)-C(24)	-78.32(13)
C(6)-C(7)-C(8)-C(9)	-1.1(2)
C(10)-C(9)-C(8)-C(7)	1.5(2)
N(1)-C(25)-C(24)-C(23)	54.29(14)
N(3)-C(23)-C(24)-C(25)	-54.48(14)
O(32)-C(27)-C(28)-C(29)	-178.46(12)
C(26)-C(27)-C(28)-C(29)	-0.8(2)
C(16)-C(21)-C(20)-C(19)	-1.07(19)
C(22)-C(21)-C(20)-C(19)	177.63(12)
C(18)-C(19)-C(20)-C(21)	0.4(2)
C(26)-C(31)-C(30)-C(29)	-0.5(2)
C(27)-C(28)-C(29)-C(30)	-0.6(2)
C(31)-C(30)-C(29)-C(28)	1.2(2)
C(10)-O(11)-C(12)-C(13)	-169.92(10)
C(14)-C(13)-C(12)-O(11)	85.27(14)
C(12)-O(11)-C(10)-C(9)	-2.38(17)
C(12)-O(11)-C(10)-C(5)	177.31(10)
C(8)-C(9)-C(10)-O(11)	178.95(12)
C(8)-C(9)-C(10)-C(5)	-0.73(19)
C(6)-C(5)-C(10)-O(11)	179.79(11)
C(4)-C(5)-C(10)-O(11)	1.58(16)
C(6)-C(5)-C(10)-C(9)	-0.51(17)
C(4)-C(5)-C(10)-C(9)	-178.72(11)

Symmetry transformations used to generate equivalent atoms:

Table 1. **Crystal data and structure refinement for 4.**

Identification code	4	
Empirical formula	C29 H34 N2 O3	
Formula weight	458.58	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/n$	
Unit cell dimensions	a = 11.4570(2) Å	α= 90°
	b = 19.2880(3) Å	β= 114.522(1)°
	c = 11.9570(2) Å	γ= 90°
Volume	2403.96(7) $Å^3$	
Z	4	
Density (calculated)	1.267 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	984	
Crystal size	0.550 x 0.500 x 0.400 mm^3	
Theta range for data collection	2.958 to 27.489°	
Index ranges	-14<=h<=14, -24<=k<=25, -15<=l<=15	
Reflections collected	43294	
Independent reflections	5506 [R(int) = 0.0586]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.972 and 0.868	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5506 / 0 / 307	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.1343	
R indices (all data)	R1 = 0.0778, wR2 = 0.1485	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.036 and -0.312 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for ?.

O(1)-C(6)	1.3789(19)
O(1)-C(7)	1.435(2)
O(2)-C(12)	1.385(2)
O(2)-C(11)	1.431(2)
O(3)-C(29)	1.336(2)
O(3)-H(3)	0.9853
N(1)-C(22)	1.474(2)
N(1)-C(21)	1.483(2)
N(1)-C(23)	1.498(2)
N(2)-C(23)	1.462(2)
N(2)-C(18)	1.465(2)
N(2)-C(19)	1.472(2)
C(1)-C(2)	1.393(2)
C(1)-C(6)	1.398(2)
C(1)-C(22)	1.515(2)
C(2)-C(3)	1.391(2)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.380(3)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.384(2)
C(4)-H(4A)	0.9300
C(5)-C(6)	1.390(2)
C(5)-H(5A)	0.9300
C(7)-C(8)	1.511(2)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-C(9)	1.523(2)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-C(10)	1.524(2)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(11)	1.512(2)
C(10)-H(10A)	0.9700

C(10)-H(10B)	0.9700
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.391(2)
C(12)-C(17)	1.399(2)
C(13)-C(14)	1.383(3)
C(13)-H(13A)	0.9300
C(14)-C(15)	1.390(3)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.384(2)
C(15)-H(15A)	0.9300
C(16)-C(17)	1.391(2)
C(16)-H(16A)	0.9300
C(17)-C(18)	1.518(2)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-C(20)	1.525(2)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-C(21)	1.526(2)
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(24)	1.534(2)
C(23)-H(23A)	0.9800
C(24)-C(29)	1.403(2)
C(24)-C(25)	1.404(3)
C(25)-C(26)	1.390(3)
C(25)-H(25A)	0.9300
C(26)-C(27)	1.376(3)
C(26)-H(26A)	0.9300
C(27)-C(28)	1.377(3)
C(27)-H(27A)	0.9300

C(28)-C(29)	1.407(3)
C(28)-H(28A)	0.9300

C(6)-O(1)-C(7)	116.94(13)
C(12)-O(2)-C(11)	116.33(13)
C(29)-O(3)-H(3)	101.3
C(22)-N(1)-C(21)	112.44(13)
C(22)-N(1)-C(23)	112.53(12)
C(21)-N(1)-C(23)	110.11(12)
C(23)-N(2)-C(18)	115.93(13)
C(23)-N(2)-C(19)	111.98(12)
C(18)-N(2)-C(19)	113.36(13)
C(2)-C(1)-C(6)	117.73(15)
C(2)-C(1)-C(22)	123.51(15)
C(6)-C(1)-C(22)	118.76(14)
C(3)-C(2)-C(1)	121.29(16)
C(3)-C(2)-H(2A)	119.4
C(1)-C(2)-H(2A)	119.4
C(4)-C(3)-C(2)	120.00(16)
C(4)-C(3)-H(3A)	120.0
C(2)-C(3)-H(3A)	120.0
C(3)-C(4)-C(5)	119.83(16)
C(3)-C(4)-H(4A)	120.1
C(5)-C(4)-H(4A)	120.1
C(4)-C(5)-C(6)	120.05(16)
C(4)-C(5)-H(5A)	120.0
C(6)-C(5)-H(5A)	120.0
O(1)-C(6)-C(5)	122.71(15)
O(1)-C(6)-C(1)	116.20(14)
C(5)-C(6)-C(1)	121.08(15)
O(1)-C(7)-C(8)	108.01(13)
O(1)-C(7)-H(7A)	110.1
C(8)-C(7)-H(7A)	110.1
O(1)-C(7)-H(7B)	110.1
C(8)-C(7)-H(7B)	110.1
H(7A)-C(7)-H(7B)	108.4

C(7)-C(8)-C(9)	113.27(14)
C(7)-C(8)-H(8A)	108.9
C(9)-C(8)-H(8A)	108.9
C(7)-C(8)-H(8B)	108.9
C(9)-C(8)-H(8B)	108.9
H(8A)-C(8)-H(8B)	107.7
C(8)-C(9)-C(10)	112.78(14)
C(8)-C(9)-H(9A)	109.0
C(10)-C(9)-H(9A)	109.0
C(8)-C(9)-H(9B)	109.0
C(10)-C(9)-H(9B)	109.0
H(9A)-C(9)-H(9B)	107.8
C(11)-C(10)-C(9)	113.57(15)
C(11)-C(10)-H(10A)	108.9
C(9)-C(10)-H(10A)	108.9
C(11)-C(10)-H(10B)	108.9
C(9)-C(10)-H(10B)	108.9
H(10A)-C(10)-H(10B)	107.7
O(2)-C(11)-C(10)	107.77(14)
O(2)-C(11)-H(11A)	110.2
C(10)-C(11)-H(11A)	110.2
O(2)-C(11)-H(11B)	110.2
C(10)-C(11)-H(11B)	110.2
H(11A)-C(11)-H(11B)	108.5
O(2)-C(12)-C(13)	121.73(15)
O(2)-C(12)-C(17)	117.07(14)
C(13)-C(12)-C(17)	121.16(16)
C(14)-C(13)-C(12)	120.01(17)
C(14)-C(13)-H(13A)	120.0
C(12)-C(13)-H(13A)	120.0
C(13)-C(14)-C(15)	119.64(16)
C(13)-C(14)-H(14A)	120.2
C(15)-C(14)-H(14A)	120.2
C(16)-C(15)-C(14)	119.87(16)
C(16)-C(15)-H(15A)	120.1
C(14)-C(15)-H(15A)	120.1

C(15)-C(16)-C(17)	121.67(16)
C(15)-C(16)-H(16A)	119.2
C(17)-C(16)-H(16A)	119.2
C(16)-C(17)-C(12)	117.59(15)
C(16)-C(17)-C(18)	122.36(15)
C(12)-C(17)-C(18)	120.04(15)
N(2)-C(18)-C(17)	112.57(13)
N(2)-C(18)-H(18A)	109.1
C(17)-C(18)-H(18A)	109.1
N(2)-C(18)-H(18B)	109.1
C(17)-C(18)-H(18B)	109.1
H(18A)-C(18)-H(18B)	107.8
N(2)-C(19)-C(20)	113.05(14)
N(2)-C(19)-H(19A)	109.0
C(20)-C(19)-H(19A)	109.0
N(2)-C(19)-H(19B)	109.0
C(20)-C(19)-H(19B)	109.0
H(19A)-C(19)-H(19B)	107.8
C(19)-C(20)-C(21)	109.53(14)
C(19)-C(20)-H(20A)	109.8
C(21)-C(20)-H(20A)	109.8
C(19)-C(20)-H(20B)	109.8
C(21)-C(20)-H(20B)	109.8
H(20A)-C(20)-H(20B)	108.2
N(1)-C(21)-C(20)	112.53(13)
N(1)-C(21)-H(21A)	109.1
C(20)-C(21)-H(21A)	109.1
N(1)-C(21)-H(21B)	109.1
C(20)-C(21)-H(21B)	109.1
H(21A)-C(21)-H(21B)	107.8
N(1)-C(22)-C(1)	113.58(13)
N(1)-C(22)-H(22A)	108.9
C(1)-C(22)-H(22A)	108.9
N(1)-C(22)-H(22B)	108.9
C(1)-C(22)-H(22B)	108.9
H(22A)-C(22)-H(22B)	107.7

N(2)-C(23)-N(1)	116.07(13)
N(2)-C(23)-C(24)	110.27(13)
N(1)-C(23)-C(24)	109.90(13)
N(2)-C(23)-H(23A)	106.7
N(1)-C(23)-H(23A)	106.7
C(24)-C(23)-H(23A)	106.7
C(29)-C(24)-C(25)	117.62(16)
C(29)-C(24)-C(23)	121.12(16)
C(25)-C(24)-C(23)	121.12(15)
C(26)-C(25)-C(24)	122.08(19)
C(26)-C(25)-H(25A)	119.0
C(24)-C(25)-H(25A)	119.0
C(27)-C(26)-C(25)	119.1(2)
C(27)-C(26)-H(26A)	120.4
C(25)-C(26)-H(26A)	120.4
C(26)-C(27)-C(28)	120.83(19)
C(26)-C(27)-H(27A)	119.6
C(28)-C(27)-H(27A)	119.6
C(27)-C(28)-C(29)	120.37(19)
C(27)-C(28)-H(28A)	119.8
C(29)-C(28)-H(28A)	119.8
O(3)-C(29)-C(24)	121.33(16)
O(3)-C(29)-C(28)	118.72(17)
C(24)-C(29)-C(28)	119.94(18)

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for ?.

C(6)-C(1)-C(2)-C(3)	-1.2(3)
C(22)-C(1)-C(2)-C(3)	179.30(17)
C(1)-C(2)-C(3)-C(4)	0.2(3)
C(2)-C(3)-C(4)-C(5)	0.1(3)
C(3)-C(4)-C(5)-C(6)	0.6(3)
C(7)-O(1)-C(6)-C(5)	36.1(2)
C(7)-O(1)-C(6)-C(1)	-145.58(16)
C(4)-C(5)-C(6)-O(1)	176.61(17)
C(4)-C(5)-C(6)-C(1)	-1.7(3)
C(2)-C(1)-C(6)-O(1)	-176.49(15)
C(22)-C(1)-C(6)-O(1)	3.1(2)
C(2)-C(1)-C(6)-C(5)	1.9(3)
C(22)-C(1)-C(6)-C(5)	-178.54(16)
C(6)-O(1)-C(7)-C(8)	174.64(14)
O(1)-C(7)-C(8)-C(9)	-54.8(2)
C(7)-C(8)-C(9)-C(10)	-175.81(15)
C(8)-C(9)-C(10)-C(11)	-177.53(15)
C(12)-O(2)-C(11)-C(10)	-168.31(14)
C(9)-C(10)-C(11)-O(2)	56.4(2)
C(11)-O(2)-C(12)-C(13)	-50.7(2)
C(11)-O(2)-C(12)-C(17)	131.74(16)
O(2)-C(12)-C(13)-C(14)	-179.18(16)
C(17)-C(12)-C(13)-C(14)	-1.7(3)
C(12)-C(13)-C(14)-C(15)	0.1(3)
C(13)-C(14)-C(15)-C(16)	1.7(3)
C(14)-C(15)-C(16)-C(17)	-1.8(3)
C(15)-C(16)-C(17)-C(12)	0.2(3)
C(15)-C(16)-C(17)-C(18)	179.81(16)
O(2)-C(12)-C(17)-C(16)	179.14(15)
C(13)-C(12)-C(17)-C(16)	1.6(2)
O(2)-C(12)-C(17)-C(18)	-0.5(2)
C(13)-C(12)-C(17)-C(18)	-178.04(16)
C(23)-N(2)-C(18)-C(17)	-155.58(14)
C(19)-N(2)-C(18)-C(17)	72.86(18)

C(16)-C(17)-C(18)-N(2)	22.9(2)
C(12)-C(17)-C(18)-N(2)	-157.52(15)
C(23)-N(2)-C(19)-C(20)	-51.14(18)
C(18)-N(2)-C(19)-C(20)	82.33(17)
N(2)-C(19)-C(20)-C(21)	53.52(19)
C(22)-N(1)-C(21)-C(20)	-73.04(17)
C(23)-N(1)-C(21)-C(20)	53.31(17)
C(19)-C(20)-C(21)-N(1)	-55.15(19)
C(21)-N(1)-C(22)-C(1)	-68.95(17)
C(23)-N(1)-C(22)-C(1)	166.02(13)
C(2)-C(1)-C(22)-N(1)	-26.3(2)
C(6)-C(1)-C(22)-N(1)	154.12(15)
C(18)-N(2)-C(23)-N(1)	-81.70(17)
C(19)-N(2)-C(23)-N(1)	50.50(18)
C(18)-N(2)-C(23)-C(24)	152.53(14)
C(19)-N(2)-C(23)-C(24)	-75.27(16)
C(22)-N(1)-C(23)-N(2)	74.87(17)
C(21)-N(1)-C(23)-N(2)	-51.42(17)
C(22)-N(1)-C(23)-C(24)	-159.17(13)
C(21)-N(1)-C(23)-C(24)	74.54(16)
N(2)-C(23)-C(24)-C(29)	163.89(15)
N(1)-C(23)-C(24)-C(29)	34.7(2)
N(2)-C(23)-C(24)-C(25)	-20.4(2)
N(1)-C(23)-C(24)-C(25)	-149.60(16)
C(29)-C(24)-C(25)-C(26)	-2.6(3)
C(23)-C(24)-C(25)-C(26)	-178.45(17)
C(24)-C(25)-C(26)-C(27)	0.9(3)
C(25)-C(26)-C(27)-C(28)	0.5(3)
C(26)-C(27)-C(28)-C(29)	-0.1(3)
C(25)-C(24)-C(29)-O(3)	-175.97(17)
C(23)-C(24)-C(29)-O(3)	-0.1(3)
C(25)-C(24)-C(29)-C(28)	2.9(3)
C(23)-C(24)-C(29)-C(28)	178.78(16)
C(27)-C(28)-C(29)-O(3)	177.26(18)
C(27)-C(28)-C(29)-C(24)	-1.7(3)