Supporting Information

for

Inclusion complexes of β-cyclodextrin with tricyclic drugs: an X-ray diffraction, NMR and molecular dynamics study

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Crystallographic data for cyclobenzaprine (1) and amitryptiline (2)

Crystallographic data for cyclobenzaprine **(1)**

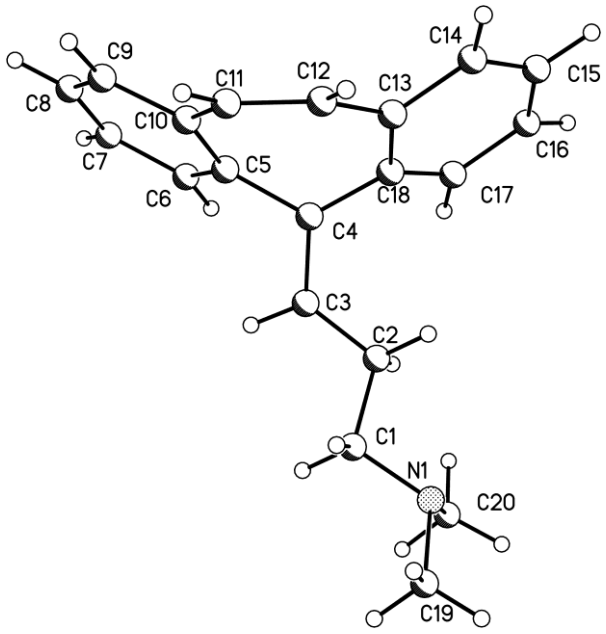

Figure S1: The structure of compound **1** in the inclusion complex with the atom numbering scheme from the X-ray results.

Table S1: Crystal data and structure refinement for cdbzp-16.

Identification code	cdbzp-16
Empirical formula	C62 H91 N O50.10
Formula weight	1651.96
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system, space group	orthorhombic, P212121
Unit cell dimensions	a = 15.361(12)Å alpha = 90 deg. b = 17.609(12)Å beta = 90 deg. c = 27.316(16)Å gamma = 90 deg.
Volume	7389(9) A^3
Z, Calculated density	4, 1.485 Mg/m^3
Absorption coefficient	1.139 mm^-1
F(000)	3483
Crystal size	0.25 x 0.15 x 0.08 mm
Theta range for data collection	6.61 to 87.64 deg.
Limiting indices	0<=h<=18, 0<=k<=22, 0<=l<=35
Reflections collected / unique	8189 / 8189 [R(int) = 0.0000]
Completeness to theta	87.64 89.3 %
Refinement method	Full-matrix-block least-squares on F^2
Data / restraints / parameters	8189 / 0 / 1087
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0780, wR2 = 0.1952
R indices (all data)	R1 = 0.1473, wR2 = 0.2413
Absolute structure parameter	1.2(4)
Extinction coefficient	0.00021(12)
Largest diff. peak and hole	0.421 and -0.305 e.A^-3

Table S2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cdbzp-16. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1A)	2520(5)	983(5)	7759(3)	38(2)
C(2A)	2584(5)	359(5)	8079(3)	41(2)
O(2A)	3036(4)	-217(4)	7854(2)	50(2)
C(3A)	1677(5)	127(4)	8248(3)	35(2)
O(3A)	1806(4)	-411(4)	8601(2)	53(2)
C(4A)	1167(5)	754(5)	8419(3)	38(2)
O(4A)	310(3)	504(3)	8547(2)	34(1)
C(5A)	1116(6)	1322(5)	8046(3)	41(2)
O(5A)	1998(4)	1542(3)	7938(2)	43(1)
C(6A)	590(8)	1983(5)	8174(4)	59(3)
O(6A)	875(6)	2290(5)	8596(3)	84(3)
C(1B)	2555(5)	940(5)	5981(3)	36(2)
C(2B)	2912(6)	275(5)	6205(3)	42(2)
O(2B)	2712(4)	-349(4)	5935(2)	54(2)
C(3B)	2501(5)	185(4)	6663(3)	32(2)
O(3B)	2881(4)	-421(3)	6893(2)	43(1)
C(4B)	2634(5)	854(4)	6944(2)	27(2)
O(4B)	2134(3)	748(3)	7345(2)	33(1)
C(5B)	2333(5)	1523(4)	6687(3)	32(2)
O(5B)	2742(3)	1557(3)	6250(2)	36(1)
C(6B)	2545(6)	2225(5)	6918(3)	42(2)
O(6B)	3462(4)	2285(3)	7008(2)	49(2)
C(1C)	-447(5)	1043(5)	5066(3)	34(2)
C(2C)	194(6)	439(5)	4944(3)	37(2)
O(2C)	-283(4)	-203(3)	4847(2)	51(2)
C(3C)	807(6)	320(5)	5350(3)	38(2)
O(3C)	1434(5)	-213(4)	5234(2)	55(2)
C(4C)	1255(5)	1015(4)	5485(3)	34(2)
O(4C)	1640(4)	859(3)	5921(2)	35(1)
C(5C)	582(6)	1611(5)	5551(3)	40(2)
O(5C)	6(4)	1673(3)	5163(2)	37(1)
C(6C)	1009(7)	2351(5)	5582(4)	51(2)
O(6C)	391(6)	2870(4)	5689(3)	73(2)
C(1D)	-3654(6)	787(6)	5757(3)	54(3)
C(2D)	-3355(6)	289(6)	5382(3)	51(2)
O(2D)	-3784(5)	-362(5)	5402(3)	74(2)
C(3D)	-2360(6)	205(5)	5394(3)	43(2)
O(3D)	-2099(4)	-231(4)	5016(2)	57(2)
O(4D)	-987(3)	813(3)	5426(2)	35(1)
C(4D)	-1924(5)	937(5)	5385(3)	42(2)
C(5D)	-2255(6)	1394(6)	5776(3)	49(2)
O(5D)	-3187(4)	1457(4)	5756(2)	55(2)
C(6D)	-1916(7)	2139(5)	5787(4)	56(2)
O(6OD)	-2218(5)	2540(4)	5404(3)	70(2)
C(1E)	-5011(5)	-98(5)	7297(3)	37(2)
C(2E)	-4903(6)	-669(5)	6935(3)	46(2)
O(2OE)	-4779(5)	-1358(3)	7148(3)	59(2)
C(3E)	-4134(6)	-492(5)	6624(3)	45(2)
O(3E)	-4068(6)	-1016(4)	6273(3)	78(2)
C(4E)	-4254(5)	267(5)	6434(3)	41(2)
O(4E)	-3499(4)	430(4)	6172(2)	47(2)
C(5E)	-4360(6)	797(5)	6831(3)	40(2)
O(5E)	-5103(4)	591(3)	7098(2)	38(1)

C(6E)	-4526(6)	1563(6)	6677(3)	52(2)
O(6E)	-5293(5)	1604(4)	6390(2)	58(2)
C(1F)	-3387(5)	-1(4)	8884(3)	33(2)
C(2F)	-3813(6)	-712(5)	8756(3)	36(2)
O(2F)	-3283(4)	-1276(3)	8933(2)	49(2)
C(3F)	-3904(5)	-750(4)	8256(3)	33(2)
O(3F)	-4392(4)	-1390(3)	8123(2)	48(2)
C(4F)	-4380(5)	-98(4)	8063(2)	33(2)
O(4F)	-4256(4)	-123(3)	7584(2)	38(1)
C(5F)	-3995(6)	604(5)	8235(3)	40(2)
O(5F)	-3908(4)	580(3)	8719(2)	39(1)
C(6F)	-4533(6)	1261(5)	8127(3)	45(2)
O(6F)	-5394(4)	1196(4)	8309(3)	57(2)
C(1G)	18(5)	639(4)	8983(3)	31(2)
C(2G)	-324(5)	-57(5)	9193(3)	38(2)
O(2G)	329(4)	-601(4)	9177(2)	51(2)
C(3G)	-1139(5)	-302(4)	8944(3)	32(2)
O(3G)	-1485(4)	-934(3)	9159(2)	48(2)
C(4G)	-1814(5)	282(4)	8943(3)	32(2)
O(4G)	-2544(3)	26(3)	8676(2)	32(1)
C(5G)	-1416(5)	961(4)	8731(3)	37(2)
O(5G)	-654(4)	1172(3)	8983(2)	40(1)
C(6G)	-2041(6)	1616(5)	8746(4)	56(3)
O(6G)	-1568(5)	2222(4)	8572(3)	77(2)
O(1W)	-5477(5)	2709(4)	5781(2)	62(2)
O(2W)	-5792(6)	1843(6)	5006(3)	87(3)
O(3W)	2936(6)	-1857(4)	6622(3)	85(3)
O(4W)	-3758(6)	-2576(5)	7046(3)	90(3)
O(5W)	-3672(6)	3254(5)	5781(3)	82(2)
O(6W)	3719(7)	-1423(6)	8286(4)	100(3)
O(7W)	740(9)	-971(9)	4239(4)	169(6)
O(8W)	3696(9)	-2185(7)	7449(4)	125(4)
O(9W)	2570(8)	2973(8)	8675(6)	154(6)
O(10W)	-5756(6)	153(6)	5232(3)	94(3)
O(11W)	-5673(8)	-689(8)	5331(5)	92(4)
O(12W)	2963(12)	-341(10)	9271(6)	116(6)
O(13W)	2519(15)	-3305(7)	4933(7)	123(7)
O(14W)	-1042(14)	-1784(10)	4418(6)	105(7)
O(15A)	4120(20)	-1601(19)	5906(12)	80(9)
O(15W)	4420(20)	-2015(17)	6032(9)	156(12)
O(16W)	-6508(15)	525(13)	4857(8)	92(7)
O(17W)	-5770(20)	1385(18)	5028(11)	38(8)
O(18W)	2730(30)	1920(50)	9396(14)	210(40)
O(18A)	3170(30)	2190(30)	9357(18)	118(15)
O(20A)	2340(30)	-380(20)	4436(15)	128(13)
O(20C)	2920(30)	-940(30)	4654(18)	93(13)
O(20D)	3330(40)	-1250(40)	4950(20)	130(20)
O(21W)	2990(30)	-1690(30)	8258(16)	82(12)
N(1)	371(9)	-2195(6)	5687(4)	88(3)
C(1)	-112(10)	-1551(7)	5833(4)	81(4)
C(2)	337(12)	-1269(9)	6264(5)	111(5)
C(3)	-78(9)	-639(7)	6426(6)	94(4)
C(4)	-285(8)	-512(7)	6901(4)	72(3)
C(5)	-693(8)	205(7)	6987(4)	66(3)
C(6)	-297(9)	821(8)	6805(5)	86(4)
C(7)	-678(13)	1511(9)	6878(7)	118(6)
C(8)	-1427(11)	1537(9)	7113(6)	100(5)
C(9)	-1832(9)	946(7)	7285(5)	77(3)
C(10)	-1449(7)	257(7)	7228(4)	63(3)
C(11)	-1920(8)	-360(7)	7438(4)	71(3)
C(12)	-1545(8)	-977(8)	7606(4)	78(4)
C(13)	-621(8)	-1127(6)	7611(5)	72(3)

C(14)	-354(10)	-1519(7)	8006(6)	87(4)
C(15)	526(16)	-1686(7)	8037(8)	133(9)
C(16)	1164(9)	-1488(7)	7715(7)	86(4)
C(17)	868(10)	-1119(8)	7317(7)	101(5)
C(18)	14(6)	-959(5)	7272(5)	59(3)
C(19)	-151(14)	-2624(8)	5364(5)	122(7)
C(20)	1220(13)	-2035(9)	5493(6)	119(6)

Table S3: Bond lengths [A] and angles [deg] for cdbzp-16.

C(1A)-O(4B)	1.342(9)
C(1A)-O(5A)	1.360(10)
C(1A)-C(2A)	1.408(11)
C(2A)-O(2A)	1.375(10)
C(2A)-C(3A)	1.523(11)
C(3A)-O(3A)	1.367(9)
C(3A)-C(4A)	1.434(11)
C(4A)-C(5A)	1.429(11)
C(4A)-O(4A)	1.430(10)
O(4A)-C(1G)	1.297(9)
C(5A)-O(5A)	1.441(11)
C(5A)-C(6A)	1.459(12)
C(6A)-O(6A)	1.347(13)
C(1B)-O(5B)	1.343(9)
C(1B)-O(4C)	1.423(10)
C(1B)-C(2B)	1.431(12)
C(2B)-O(2B)	1.359(10)
C(2B)-C(3B)	1.410(11)
C(3B)-O(3B)	1.368(9)
C(3B)-C(4B)	1.420(10)
C(4B)-O(4B)	1.351(8)
C(4B)-C(5B)	1.447(10)
C(5B)-O(5B)	1.351(9)
C(5B)-C(6B)	1.425(11)
C(6B)-O(6B)	1.433(11)
C(1C)-O(5C)	1.335(9)
C(1C)-O(4D)	1.349(9)
C(1C)-C(2C)	1.488(11)
C(2C)-O(2C)	1.372(10)
C(2C)-C(3C)	1.470(11)
C(3C)-O(3C)	1.381(10)
C(3C)-C(4C)	1.451(11)
C(4C)-O(4C)	1.359(9)
C(4C)-C(5C)	1.485(12)
C(5C)-O(5C)	1.385(10)
C(5C)-C(6C)	1.460(12)
C(6C)-O(6C)	1.350(12)
C(1D)-O(4E)	1.319(10)
C(1D)-O(5D)	1.380(12)
C(1D)-C(2D)	1.424(14)
C(2D)-O(2D)	1.325(11)
C(2D)-C(3D)	1.536(13)
C(3D)-O(3D)	1.349(10)
C(3D)-C(4D)	1.453(13)
O(4D)-C(4D)	1.461(10)
C(4D)-C(5D)	1.432(12)
C(5D)-C(6D)	1.410(13)
C(5D)-O(5D)	1.437(11)
C(6D)-O(6OD)	1.345(12)
C(1E)-O(5E)	1.336(10)
C(1E)-O(4F)	1.401(9)
C(1E)-C(2E)	1.420(12)
C(2E)-O(2OE)	1.358(11)
C(2E)-C(3E)	1.488(13)
C(3E)-O(3E)	1.334(10)
C(3E)-C(4E)	1.446(12)
C(4E)-O(4E)	1.392(10)
C(4E)-C(5E)	1.440(12)
C(5E)-O(5E)	1.402(10)

C(5E)-C(6E)	1.437(13)
C(6E)-O(6E)	1.416(11)
C(1F)-O(5F)	1.375(9)
C(1F)-O(4G)	1.415(9)
C(1F)-C(2F)	1.454(11)
C(2F)-O(2F)	1.373(9)
C(2F)-C(3F)	1.376(10)
C(3F)-O(3F)	1.402(10)
C(3F)-C(4F)	1.460(11)
C(4F)-O(4F)	1.323(8)
C(4F)-C(5F)	1.449(12)
C(5F)-O(5F)	1.330(9)
C(5F)-C(6F)	1.451(12)
C(6F)-O(6F)	1.417(11)
C(1G)-O(5G)	1.394(9)
C(1G)-C(2G)	1.452(11)
C(2G)-O(2G)	1.386(10)
C(2G)-C(3G)	1.491(11)
C(3G)-O(3G)	1.366(9)
C(3G)-C(4G)	1.460(11)
C(4G)-O(4G)	1.411(9)
C(4G)-C(5G)	1.463(11)
C(5G)-O(5G)	1.407(10)
C(5G)-C(6G)	1.502(12)
C(6G)-O(6G)	1.376(11)
O(2W)-O(17W)	0.81(3)
O(6W)-O(21W)	1.22(5)
O(10W)-O(11W)	1.512(17)
O(10W)-O(16W)	1.68(2)
O(12W)-O(20A)#1	1.42(4)
O(15A)-O(15W)	0.93(4)
O(18W)-O(18A)	0.84(8)
O(20A)-O(12W)#2	1.42(4)
O(20A)-O(20C)	1.45(6)
O(20C)-O(20D)	1.18(7)
N(1)-C(19)	1.411(18)
N(1)-C(1)	1.413(17)
N(1)-C(20)	1.44(2)
C(1)-C(2)	1.451(18)
C(2)-C(3)	1.354(19)
C(3)-C(4)	1.353(18)
C(4)-C(18)	1.364(16)
C(4)-C(5)	1.429(17)
C(5)-C(10)	1.339(15)
C(5)-C(6)	1.339(16)
C(6)-C(7)	1.36(2)
C(7)-C(8)	1.32(2)
C(8)-C(9)	1.301(17)
C(9)-C(10)	1.357(16)
C(10)-C(11)	1.427(15)
C(11)-C(12)	1.312(16)
C(12)-C(13)	1.444(17)
C(13)-C(14)	1.346(18)
C(13)-C(18)	1.377(17)
C(14)-C(15)	1.39(2)
C(15)-C(16)	1.36(3)
C(16)-C(17)	1.34(2)
C(17)-C(18)	1.347(17)

O(4B)-C(1A)-O(5A)	105.5(6)
O(4B)-C(1A)-C(2A)	108.2(7)
O(5A)-C(1A)-C(2A)	112.5(7)

O(2A)-C(2A)-C(1A)	109.5(7)
O(2A)-C(2A)-C(3A)	113.5(7)
C(1A)-C(2A)-C(3A)	109.5(7)
O(3A)-C(3A)-C(4A)	112.4(6)
O(3A)-C(3A)-C(2A)	105.6(6)
C(4A)-C(3A)-C(2A)	113.0(7)
C(5A)-C(4A)-O(4A)	109.7(7)
C(5A)-C(4A)-C(3A)	109.6(7)
O(4A)-C(4A)-C(3A)	110.2(7)
C(1G)-O(4A)-C(4A)	119.0(6)
C(4A)-C(5A)-O(5A)	106.4(7)
C(4A)-C(5A)-C(6A)	114.7(7)
O(5A)-C(5A)-C(6A)	110.7(8)
C(1A)-O(5A)-C(5A)	115.6(6)
O(6A)-C(6A)-C(5A)	110.2(9)
O(5B)-C(1B)-O(4C)	110.8(6)
O(5B)-C(1B)-C(2B)	110.2(6)
O(4C)-C(1B)-C(2B)	110.2(7)
O(2B)-C(2B)-C(3B)	106.9(7)
O(2B)-C(2B)-C(1B)	109.9(7)
C(3B)-C(2B)-C(1B)	107.6(7)
O(3B)-C(3B)-C(2B)	107.7(7)
O(3B)-C(3B)-C(4B)	109.7(6)
C(2B)-C(3B)-C(4B)	108.8(7)
O(4B)-C(4B)-C(3B)	104.0(6)
O(4B)-C(4B)-C(5B)	108.9(6)
C(3B)-C(4B)-C(5B)	111.7(6)
C(1A)-O(4B)-C(4B)	112.9(6)
O(5B)-C(5B)-C(6B)	104.3(6)
O(5B)-C(5B)-C(4B)	108.4(6)
C(6B)-C(5B)-C(4B)	114.8(6)
C(1B)-O(5B)-C(5B)	110.5(6)
C(5B)-C(6B)-O(6B)	111.3(7)
O(5C)-C(1C)-O(4D)	115.3(6)
O(5C)-C(1C)-C(2C)	107.1(6)
O(4D)-C(1C)-C(2C)	110.7(7)
O(2C)-C(2C)-C(3C)	111.8(7)
O(2C)-C(2C)-C(1C)	106.2(7)
C(3C)-C(2C)-C(1C)	110.9(6)
O(3C)-C(3C)-C(4C)	107.5(7)
O(3C)-C(3C)-C(2C)	111.7(6)
C(4C)-C(3C)-C(2C)	112.0(7)
O(4C)-C(4C)-C(3C)	104.9(6)
O(4C)-C(4C)-C(5C)	109.8(6)
C(3C)-C(4C)-C(5C)	107.3(7)
C(4C)-O(4C)-C(1B)	120.6(6)
O(5C)-C(5C)-C(6C)	105.2(7)
O(5C)-C(5C)-C(4C)	114.0(6)
C(6C)-C(5C)-C(4C)	109.0(7)
C(1C)-O(5C)-C(5C)	114.8(6)
O(6C)-C(6C)-C(5C)	107.5(8)
O(4E)-C(1D)-O(5D)	108.4(7)
O(4E)-C(1D)-C(2D)	105.5(9)
O(5D)-C(1D)-C(2D)	110.9(8)
O(2D)-C(2D)-C(1D)	110.0(8)
O(2D)-C(2D)-C(3D)	114.2(9)
C(1D)-C(2D)-C(3D)	111.4(8)
O(3D)-C(3D)-C(4D)	110.8(7)
O(3D)-C(3D)-C(2D)	109.5(7)
C(4D)-C(3D)-C(2D)	111.8(8)
C(1C)-O(4D)-C(4D)	120.3(6)
C(5D)-C(4D)-C(3D)	108.8(7)

C(5D)-C(4D)-O(4D)	112.1(7)
C(3D)-C(4D)-O(4D)	108.6(7)
C(6D)-C(5D)-C(4D)	114.0(9)
C(6D)-C(5D)-O(5D)	107.3(8)
C(4D)-C(5D)-O(5D)	111.5(8)
C(1D)-O(5D)-C(5D)	116.9(8)
O(6OD)-C(6D)-C(5D)	110.2(9)
O(5E)-C(1E)-O(4F)	110.1(7)
O(5E)-C(1E)-C(2E)	111.9(6)
O(4F)-C(1E)-C(2E)	105.7(7)
O(2OE)-C(2E)-C(1E)	110.6(7)
O(2OE)-C(2E)-C(3E)	108.7(8)
C(1E)-C(2E)-C(3E)	110.0(8)
O(3E)-C(3E)-C(4E)	113.0(7)
O(3E)-C(3E)-C(2E)	109.0(8)
C(4E)-C(3E)-C(2E)	107.3(7)
O(4E)-C(4E)-C(5E)	110.4(7)
O(4E)-C(4E)-C(3E)	105.6(7)
C(5E)-C(4E)-C(3E)	110.1(7)
C(1D)-O(4E)-C(4E)	113.0(7)
O(5E)-C(5E)-C(6E)	104.5(7)
O(5E)-C(5E)-C(4E)	108.5(7)
C(6E)-C(5E)-C(4E)	114.1(7)
C(1E)-O(5E)-C(5E)	111.1(6)
O(6E)-C(6E)-C(5E)	110.9(8)
O(5F)-C(1F)-O(4G)	112.1(6)
O(5F)-C(1F)-C(2F)	107.4(6)
O(4G)-C(1F)-C(2F)	110.2(6)
O(2F)-C(2F)-C(3F)	112.0(7)
O(2F)-C(2F)-C(1F)	105.8(6)
C(3F)-C(2F)-C(1F)	109.0(7)
C(2F)-C(3F)-O(3F)	110.5(7)
C(2F)-C(3F)-C(4F)	111.7(7)
O(3F)-C(3F)-C(4F)	105.7(6)
O(4F)-C(4F)-C(5F)	106.9(7)
O(4F)-C(4F)-C(3F)	104.9(6)
C(5F)-C(4F)-C(3F)	110.4(7)
C(4F)-O(4F)-C(1E)	115.7(6)
O(5F)-C(5F)-C(4F)	109.6(7)
O(5F)-C(5F)-C(6F)	106.5(7)
C(4F)-C(5F)-C(6F)	112.4(7)
C(5F)-O(5F)-C(1F)	114.0(6)
O(6F)-C(6F)-C(5F)	113.4(7)
O(4A)-C(1G)-O(5G)	112.2(6)
O(4A)-C(1G)-C(2G)	109.5(7)
O(5G)-C(1G)-C(2G)	107.5(6)
O(2G)-C(2G)-C(1G)	108.0(7)
O(2G)-C(2G)-C(3G)	113.1(7)
C(1G)-C(2G)-C(3G)	111.6(6)
O(3G)-C(3G)-C(4G)	107.3(6)
O(3G)-C(3G)-C(2G)	111.4(6)
C(4G)-C(3G)-C(2G)	113.1(7)
O(4G)-C(4G)-C(3G)	109.9(6)
O(4G)-C(4G)-C(5G)	112.9(6)
C(3G)-C(4G)-C(5G)	106.2(6)
C(4G)-O(4G)-C(1F)	122.0(5)
O(5G)-C(5G)-C(4G)	111.8(6)
O(5G)-C(5G)-C(6G)	108.4(7)
C(4G)-C(5G)-C(6G)	110.5(7)
C(1G)-O(5G)-C(5G)	116.0(6)
O(6G)-C(6G)-C(5G)	104.4(7)
O(11W)-O(10W)-O(16W)	123.4(12)

O(12W)#2-O(20A)-O(20C)	159(4)
O(20D)-O(20C)-O(20A)	159(6)
C(19)-N(1)-C(1)	107.9(13)
C(19)-N(1)-C(20)	113.0(13)
C(1)-N(1)-C(20)	115.0(12)
N(1)-C(1)-C(2)	104.7(13)
C(3)-C(2)-C(1)	108.8(16)
C(4)-C(3)-C(2)	124.1(15)
C(3)-C(4)-C(18)	122.5(13)
C(3)-C(4)-C(5)	114.0(12)
C(18)-C(4)-C(5)	122.4(11)
C(10)-C(5)-C(6)	121.4(13)
C(10)-C(5)-C(4)	121.5(11)
C(6)-C(5)-C(4)	117.1(12)
C(5)-C(6)-C(7)	118.2(14)
C(8)-C(7)-C(6)	118.5(16)
C(9)-C(8)-C(7)	124.4(16)
C(8)-C(9)-C(10)	117.8(13)
C(5)-C(10)-C(9)	119.6(11)
C(5)-C(10)-C(11)	125.9(12)
C(9)-C(10)-C(11)	114.5(11)
C(12)-C(11)-C(10)	123.2(11)
C(11)-C(12)-C(13)	126.0(11)
C(14)-C(13)-C(18)	115.7(12)
C(14)-C(13)-C(12)	113.7(13)
C(18)-C(13)-C(12)	130.6(12)
C(13)-C(14)-C(15)	117.0(17)
C(16)-C(15)-C(14)	127.5(16)
C(17)-C(16)-C(15)	113.7(15)
C(16)-C(17)-C(18)	120.3(17)
C(17)-C(18)-C(4)	121.1(14)
C(17)-C(18)-C(13)	125.7(14)
C(4)-C(18)-C(13)	112.7(10)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y,z+1/2 #2 -x+1/2,-y,z-1/2

Table S4: Anisotropic displacement parameters (A^2 x 10^3) for cdbzp-16. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1A)	32(4)	44(5)	38(4)	-2(4)	-2(4)	-5(4)
C(2A)	37(5)	51(5)	35(4)	2(4)	8(4)	0(4)
O(2A)	46(4)	55(4)	48(3)	15(3)	13(3)	15(3)
C(3A)	37(4)	35(4)	34(4)	6(3)	5(4)	5(4)
O(3A)	53(4)	56(4)	50(4)	18(3)	10(3)	15(3)
C(4A)	41(5)	41(5)	30(4)	3(3)	1(4)	-3(4)
O(4A)	35(3)	39(3)	28(3)	1(2)	4(2)	-3(3)
C(5A)	53(5)	35(4)	37(4)	2(3)	12(4)	4(4)
O(5A)	64(4)	32(3)	33(3)	-1(2)	12(3)	-7(3)
C(6A)	76(7)	42(5)	59(6)	10(5)	28(6)	14(5)
O(6A)	117(7)	54(4)	81(6)	-22(4)	36(5)	-6(5)
C(1B)	31(4)	46(5)	30(4)	-5(4)	4(3)	1(4)
C(2B)	45(5)	48(5)	32(4)	-7(4)	0(4)	7(4)
O(2B)	71(5)	52(4)	38(3)	-14(3)	-3(3)	22(3)
C(3B)	33(4)	23(4)	39(4)	0(3)	5(3)	-1(3)
O(3B)	58(4)	33(3)	38(3)	1(2)	-5(3)	5(3)
C(4B)	23(4)	32(4)	26(3)	1(3)	-1(3)	3(3)
O(4B)	30(3)	38(3)	30(3)	1(2)	2(2)	1(2)
C(5B)	35(4)	33(4)	28(4)	1(3)	3(3)	-2(4)
O(5B)	36(3)	40(3)	32(3)	2(2)	-3(2)	-9(3)
C(6B)	59(6)	32(4)	35(4)	4(3)	-2(4)	1(4)
O(6B)	61(4)	40(3)	46(3)	-4(3)	-14(3)	-12(3)
C(1C)	37(5)	43(5)	22(3)	1(3)	0(3)	-3(4)
C(2C)	44(5)	40(4)	28(4)	-5(3)	-6(4)	-4(4)
O(2C)	52(4)	45(4)	55(4)	-19(3)	-5(3)	-4(3)
C(3C)	49(5)	37(4)	29(4)	-5(3)	-6(4)	1(4)
O(3C)	66(4)	47(4)	53(4)	-20(3)	-14(3)	18(3)
C(4C)	39(4)	36(4)	28(4)	2(3)	0(3)	-5(4)
O(4C)	38(3)	44(3)	23(2)	2(2)	-2(2)	1(3)
C(5C)	41(5)	43(5)	35(4)	-5(4)	2(4)	-4(4)
O(5C)	48(3)	34(3)	28(2)	4(2)	-8(2)	-4(3)
C(6C)	60(6)	28(4)	67(6)	-7(4)	-12(5)	-6(4)
O(6C)	87(6)	38(4)	95(6)	-23(4)	-14(5)	9(4)
C(1D)	40(5)	85(7)	36(5)	10(5)	-3(4)	-9(5)
C(2D)	43(5)	71(6)	37(4)	-3(4)	-2(4)	-21(5)
O(2D)	76(5)	98(6)	47(4)	-4(4)	9(4)	-44(5)
C(3D)	48(5)	58(6)	24(4)	-6(4)	2(4)	-4(5)
O(3D)	57(4)	77(5)	39(3)	-19(3)	7(3)	-15(4)
O(4D)	41(3)	43(3)	21(2)	-1(2)	0(2)	-4(3)
C(4D)	33(5)	61(6)	30(4)	6(4)	1(3)	1(4)
C(5D)	43(5)	62(6)	42(5)	-4(4)	3(4)	8(5)
O(5D)	44(4)	77(5)	43(3)	4(3)	8(3)	10(4)
C(6D)	47(6)	47(5)	74(7)	-7(5)	7(5)	4(5)
O(6OD)	71(5)	59(4)	80(5)	13(4)	3(4)	-2(4)
C(1E)	28(4)	55(5)	27(4)	7(4)	-1(3)	7(4)
C(2E)	47(5)	54(5)	36(4)	5(4)	-5(4)	-6(4)
O(2OE)	81(5)	41(3)	56(4)	8(3)	-3(4)	-5(4)
C(3E)	56(6)	48(5)	31(4)	-7(4)	-2(4)	7(5)
O(3E)	109(7)	67(5)	57(4)	-17(4)	17(5)	10(5)
C(4E)	28(4)	60(6)	36(4)	-1(4)	0(3)	6(4)
O(4E)	36(3)	82(4)	23(3)	10(3)	6(2)	3(3)
C(5E)	42(5)	51(5)	25(4)	2(4)	1(4)	-1(4)
O(5E)	39(3)	52(3)	24(2)	7(2)	0(2)	10(3)
C(6E)	47(6)	65(6)	44(5)	9(5)	-5(4)	-7(5)

O(6E)	62(4)	60(4)	51(4)	27(3)	-3(3)	6(4)
C(1F)	37(4)	36(4)	26(3)	2(3)	-3(3)	3(4)
C(2F)	39(4)	44(5)	25(4)	8(3)	-4(3)	6(4)
O(2F)	55(4)	41(3)	50(3)	22(3)	-17(3)	-6(3)
C(3F)	31(4)	38(4)	30(4)	-1(3)	-1(3)	7(4)
O(3F)	61(4)	37(3)	47(3)	-4(3)	-14(3)	5(3)
C(4F)	35(4)	43(4)	22(3)	2(3)	3(3)	10(4)
O(4F)	37(3)	54(3)	24(2)	9(2)	7(2)	12(3)
C(5F)	48(5)	44(5)	30(4)	6(4)	-3(4)	3(4)
O(5F)	43(3)	45(3)	28(3)	-3(2)	3(2)	4(3)
C(6F)	53(6)	34(4)	48(5)	2(4)	-4(4)	11(4)
O(6F)	58(4)	46(4)	65(4)	4(3)	-13(4)	12(3)
C(1G)	25(4)	36(4)	31(4)	-1(3)	-5(3)	-2(3)
C(2G)	34(4)	48(5)	33(4)	14(4)	-2(4)	-1(4)
O(2G)	43(4)	54(4)	56(4)	18(3)	-10(3)	5(3)
C(3G)	38(4)	34(4)	24(3)	7(3)	3(3)	-1(4)
O(3G)	40(3)	38(3)	65(4)	24(3)	-4(3)	1(3)
C(4G)	33(4)	30(4)	32(4)	-1(3)	-3(3)	1(3)
O(4G)	30(3)	38(3)	28(2)	1(2)	1(2)	2(2)
C(5G)	42(5)	30(4)	39(4)	1(3)	-5(4)	9(4)
O(5G)	39(3)	33(3)	47(3)	-9(2)	6(3)	-8(3)
C(6G)	45(5)	37(5)	87(7)	15(5)	4(5)	0(4)
O(6G)	72(5)	36(4)	122(7)	12(4)	-10(5)	2(4)
O(1W)	99(6)	42(3)	44(3)	-1(3)	-1(4)	12(4)
O(2W)	96(7)	95(7)	71(5)	-7(5)	8(5)	-23(6)
O(3W)	103(6)	43(4)	110(6)	-9(4)	-24(5)	-14(4)
O(4W)	96(6)	74(5)	100(6)	-18(5)	-27(5)	14(5)
O(5W)	89(6)	84(5)	72(5)	-9(4)	-11(5)	14(5)
O(6W)	102(7)	97(7)	100(7)	28(5)	11(6)	18(6)
O(7W)	169(11)	265(16)	74(6)	-58(9)	-32(7)	114(12)
O(8W)	149(11)	125(9)	101(8)	7(7)	-36(8)	26(9)
O(9W)	106(9)	134(11)	223(16)	5(11)	19(10)	-66(9)
O(10W)	79(6)	130(8)	72(5)	-22(6)	9(5)	-6(6)
O(11W)	59(7)	116(11)	101(9)	-13(8)	11(7)	16(8)
O(12W)	132(14)	112(13)	104(11)	-12(10)	-76(11)	25(12)
O(13W)	190(18)	38(7)	142(14)	-13(8)	-16(14)	23(10)
O(14W)	154(18)	83(12)	78(11)	33(9)	-48(12)	-22(12)
O(15W)	230(30)	140(20)	106(18)	9(17)	50(20)	-60(20)
O(16W)	93(15)	101(16)	83(14)	14(13)	35(13)	4(14)
O(18W)	80(30)	490(120)	60(20)	-30(40)	0(20)	60(50)
N(1)	143(11)	65(6)	58(6)	3(5)	8(7)	-5(7)
C(1)	133(12)	57(7)	53(6)	8(5)	5(7)	-7(8)
C(2)	156(15)	96(11)	81(9)	-36(8)	8(10)	-14(11)
C(3)	91(10)	57(7)	132(13)	13(8)	5(9)	7(7)
C(4)	71(8)	82(8)	63(7)	-1(7)	5(6)	-29(7)
C(5)	64(7)	78(8)	58(6)	-12(6)	-6(6)	-9(6)
C(6)	73(8)	104(11)	82(8)	23(8)	8(7)	-38(8)
C(7)	132(15)	58(8)	162(17)	-5(10)	-28(14)	-4(10)
C(8)	98(11)	82(10)	121(12)	30(9)	14(10)	-1(9)
C(9)	79(8)	76(8)	77(8)	13(7)	9(7)	6(7)
C(10)	51(6)	83(8)	53(6)	6(6)	4(5)	-12(6)
C(11)	61(7)	79(8)	74(7)	-2(6)	6(6)	-9(7)
C(12)	66(8)	87(9)	80(8)	14(7)	33(7)	-10(7)
C(13)	77(8)	36(5)	102(9)	-7(6)	-14(8)	6(6)
C(14)	91(10)	61(7)	109(10)	-13(7)	-25(9)	21(7)
C(15)	200(20)	37(7)	160(18)	-8(9)	-102(17)	6(11)
C(16)	67(8)	50(7)	141(14)	-19(8)	-29(9)	2(7)
C(17)	86(10)	82(9)	135(13)	-35(10)	-36(10)	4(8)
C(18)	41(6)	35(5)	100(8)	-30(5)	-1(6)	1(5)
C(19)	230(20)	75(9)	64(7)	4(7)	-25(11)	5(12)
C(20)	170(18)	92(11)	93(11)	9(9)	17(12)	26(12)

Table S5: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for cdbzp-16.

	x	y	z	U(eq)
H(1A)	3100	1186	7687	46
H(2A)	2916	520	8367	49
H(2OA)	3158	-545	8056	74
H(3A)	1373	-110	7972	42
H(3OA)	1359	-461	8762	79
H(4A)	1446	972	8710	45
H(5A)	866	1088	7752	50
H(6A1)	626	2357	7914	71
H(6A2)	-15	1833	8209	71
H(6OA)	1392	2398	8570	126
H(1B)	2820	1000	5656	43
H(2B)	3543	323	6245	50
H(2OB)	3113	-443	5746	80
H(3B)	1877	92	6619	38
H(3OB)	2863	-357	7190	65
H(4B)	3248	906	7035	33
H(5B)	1703	1492	6637	38
H(6B1)	2234	2263	7226	51
H(6B2)	2360	2642	6711	51
H(6OB)	3546	2549	7250	74
H(1C)	-799	1139	4774	41
H(2C)	518	586	4650	45
H(2OC)	28	-518	4713	76
H(3C)	481	138	5635	46
H(3OC)	1775	-303	5459	83
H(4C)	1684	1162	5237	41
H(5C)	257	1515	5854	47
H(6C1)	1451	2344	5836	62
H(6C2)	1286	2474	5273	62
H(6OC)	153	3201	5878	110
H(1D)	-4277	888	5719	65
H(2D)	-3503	527	5068	61
H(2OD)	-4252	-297	5539	111
H(3D)	-2200	-53	5699	52
H(3OD)	-1570	-194	4982	86
H(4D)	-2048	1189	5072	50
H(5D)	-2102	1146	6086	59
H(6D1)	-2085	2386	6090	67
H(6D2)	-1286	2119	5776	67
H(6D)	-1890	2898	5350	105
H(1E)	-5520	-215	7499	44
H(2E)	-5425	-689	6729	55
H(2E)	-5234	-1498	7277	89
H(3E)	-3608	-505	6827	54
H(3OE)	-4324	-869	6027	117
H(4E)	-4761	283	6217	50
H(5E)	-3847	783	7044	47
H(6E1)	-4589	1886	6963	62
H(6E2)	-4036	1748	6487	62
H(6OE)	-5317	2018	6254	87
H(1F)	-3337	32	9241	40
H(2F)	-4385	-740	8913	43
H(2OF)	-3582	-1611	9057	73
H(3F)	-3328	-776	8102	40
H(3OF)	-4066	-1755	8088	72

H(4F)	-5000	-126	8146	40
H(5F)	-3421	670	8084	48
H(6F1)	-4264	1708	8269	54
H(6F2)	-4556	1331	7776	54
H(6OF)	-5692	1543	8200	85
H(1G)	496	826	9188	37
H(2G)	-461	41	9538	46
H(2OG)	682	-545	9398	77
H(3G)	-998	-427	8603	38
H(3OG)	-1105	-1258	9190	71
H(4G)	-1990	389	9281	38
H(5G)	-1266	856	8389	44
H(6G1)	-2543	1518	8540	68
H(6G2)	-2238	1710	9078	68
H(6OG)	-1900	2572	8503	115
H(1C1)	-707	-1689	5911	97
H(2C1)	-118	-1171	5576	97
H(1C2)	339	-1655	6517	134
H(2C2)	936	-1147	6182	134
H(3)	-231	-272	6198	112
H(6)	224	779	6633	103
H(7)	-415	1953	6765	141
H(8)	-1684	2010	7158	120
H(9)	-2367	993	7442	92
H(11)	-2523	-324	7457	86
H(12)	-1907	-1351	7733	93
H(14)	-742	-1671	8249	104
H(15)	701	-1966	8308	159
H(16)	1750	-1597	7766	103
H(17)	1255	-974	7073	121
H(191)	-704	-2725	5515	183
H(192)	134	-3095	5290	183
H(193)	-240	-2343	5067	183
H(201)	1540	-1732	5724	178
H(202)	1164	-1763	5191	178
H(203)	1524	-2503	5437	178

Table S6: Torsion angles [deg] for cdbzp-16.

O(4B)-C(1A)-C(2A)-O(2A)	57.1(9)
O(5A)-C(1A)-C(2A)-O(2A)	173.3(7)
O(4B)-C(1A)-C(2A)-C(3A)	-68.0(8)
O(5A)-C(1A)-C(2A)-C(3A)	48.2(9)
O(2A)-C(2A)-C(3A)-O(3A)	64.9(8)
C(1A)-C(2A)-C(3A)-O(3A)	-172.4(7)
O(2A)-C(2A)-C(3A)-C(4A)	-171.8(7)
C(1A)-C(2A)-C(3A)-C(4A)	-49.1(9)
O(3A)-C(3A)-C(4A)-C(5A)	175.4(7)
C(2A)-C(3A)-C(4A)-C(5A)	56.0(10)
O(3A)-C(3A)-C(4A)-O(4A)	-63.8(9)
C(2A)-C(3A)-C(4A)-O(4A)	176.8(6)
C(5A)-C(4A)-O(4A)-C(1G)	-114.8(8)
C(3A)-C(4A)-O(4A)-C(1G)	124.4(7)
O(4A)-C(4A)-C(5A)-O(5A)	-179.9(6)
C(3A)-C(4A)-C(5A)-O(5A)	-58.8(9)
O(4A)-C(4A)-C(5A)-C(6A)	57.2(11)
C(3A)-C(4A)-C(5A)-C(6A)	178.4(8)
O(4B)-C(1A)-O(5A)-C(5A)	59.4(8)
C(2A)-C(1A)-O(5A)-C(5A)	-58.4(9)
C(4A)-C(5A)-O(5A)-C(1A)	62.2(8)
C(6A)-C(5A)-O(5A)-C(1A)	-172.5(7)
C(4A)-C(5A)-C(6A)-O(6A)	54.8(12)
O(5A)-C(5A)-C(6A)-O(6A)	-65.7(10)
O(5B)-C(1B)-C(2B)-O(2B)	179.2(7)
O(4C)-C(1B)-C(2B)-O(2B)	56.7(9)
O(5B)-C(1B)-C(2B)-C(3B)	63.2(9)
O(4C)-C(1B)-C(2B)-C(3B)	-59.3(8)
O(2B)-C(2B)-C(3B)-O(3B)	65.9(8)
C(1B)-C(2B)-C(3B)-O(3B)	-176.0(7)
O(2B)-C(2B)-C(3B)-C(4B)	-175.2(7)
C(1B)-C(2B)-C(3B)-C(4B)	-57.2(9)
O(3B)-C(3B)-C(4B)-O(4B)	-69.6(8)
C(2B)-C(3B)-C(4B)-O(4B)	172.8(6)
O(3B)-C(3B)-C(4B)-C(5B)	173.2(7)
C(2B)-C(3B)-C(4B)-C(5B)	55.6(9)
O(5A)-C(1A)-O(4B)-C(4B)	118.5(6)
C(2A)-C(1A)-O(4B)-C(4B)	-120.9(7)
C(3B)-C(4B)-O(4B)-C(1A)	139.6(7)
C(5B)-C(4B)-O(4B)-C(1A)	-101.3(7)
O(4B)-C(4B)-C(5B)-O(5B)	-170.4(6)
C(3B)-C(4B)-C(5B)-O(5B)	-56.2(8)
O(4B)-C(4B)-C(5B)-C(6B)	73.4(8)
C(3B)-C(4B)-C(5B)-C(6B)	-172.3(7)
O(4C)-C(1B)-O(5B)-C(5B)	56.2(8)
C(2B)-C(1B)-O(5B)-C(5B)	-66.0(8)
C(6B)-C(5B)-O(5B)-C(1B)	-176.6(7)
C(4B)-C(5B)-O(5B)-C(1B)	60.6(8)
O(5B)-C(5B)-C(6B)-O(6B)	-63.7(8)
C(4B)-C(5B)-C(6B)-O(6B)	54.7(9)
O(5C)-C(1C)-C(2C)-O(2C)	179.9(6)
O(4D)-C(1C)-C(2C)-O(2C)	53.5(8)
O(5C)-C(1C)-C(2C)-C(3C)	58.2(8)
O(4D)-C(1C)-C(2C)-C(3C)	-68.2(9)
O(2C)-C(2C)-C(3C)-O(3C)	64.7(9)
C(1C)-C(2C)-C(3C)-O(3C)	-177.0(7)
O(2C)-C(2C)-C(3C)-C(4C)	-174.6(7)
C(1C)-C(2C)-C(3C)-C(4C)	-56.3(9)
O(3C)-C(3C)-C(4C)-O(4C)	-69.9(8)

C(2C)-C(3C)-C(4C)-O(4C)	167.0(7)
O(3C)-C(3C)-C(4C)-C(5C)	173.3(6)
C(2C)-C(3C)-C(4C)-C(5C)	50.2(9)
C(3C)-C(4C)-O(4C)-C(1B)	122.8(7)
C(5C)-C(4C)-O(4C)-C(1B)	-122.2(7)
O(5B)-C(1B)-O(4C)-C(4C)	106.6(7)
C(2B)-C(1B)-O(4C)-C(4C)	-131.2(7)
O(4C)-C(4C)-C(5C)-O(5C)	-164.3(6)
C(3C)-C(4C)-C(5C)-O(5C)	-50.8(9)
O(4C)-C(4C)-C(5C)-C(6C)	78.6(9)
C(3C)-C(4C)-C(5C)-C(6C)	-167.9(7)
O(4D)-C(1C)-O(5C)-C(5C)	63.4(9)
C(2C)-C(1C)-O(5C)-C(5C)	-60.3(8)
C(6C)-C(5C)-O(5C)-C(1C)	178.9(7)
C(4C)-C(5C)-O(5C)-C(1C)	59.6(9)
O(5C)-C(5C)-C(6C)-O(6C)	63.2(9)
C(4C)-C(5C)-C(6C)-O(6C)	-174.2(8)
O(4E)-C(1D)-C(2D)-O(2D)	60.1(10)
O(5D)-C(1D)-C(2D)-O(2D)	177.3(8)
O(4E)-C(1D)-C(2D)-C(3D)	-67.6(10)
O(5D)-C(1D)-C(2D)-C(3D)	49.6(11)
O(2D)-C(2D)-C(3D)-O(3D)	58.3(10)
C(1D)-C(2D)-C(3D)-O(3D)	-176.2(8)
O(2D)-C(2D)-C(3D)-C(4D)	-178.4(7)
C(1D)-C(2D)-C(3D)-C(4D)	-53.0(10)
O(5C)-C(1C)-O(4D)-C(4D)	104.0(8)
C(2C)-C(1C)-O(4D)-C(4D)	-134.3(7)
O(3D)-C(3D)-C(4D)-C(5D)	176.9(8)
C(2D)-C(3D)-C(4D)-C(5D)	54.5(9)
O(3D)-C(3D)-C(4D)-O(4D)	-60.8(9)
C(2D)-C(3D)-C(4D)-O(4D)	176.7(6)
C(1C)-O(4D)-C(4D)-C(5D)	-120.3(8)
C(1C)-O(4D)-C(4D)-C(3D)	119.5(7)
C(3D)-C(4D)-C(5D)-C(6D)	-176.5(8)
O(4D)-C(4D)-C(5D)-C(6D)	63.4(11)
C(3D)-C(4D)-C(5D)-O(5D)	-54.7(10)
O(4D)-C(4D)-C(5D)-O(5D)	-174.8(7)
O(4E)-C(1D)-O(5D)-C(5D)	62.4(10)
C(2D)-C(1D)-O(5D)-C(5D)	-53.0(10)
C(6D)-C(5D)-O(5D)-C(1D)	-178.2(8)
C(4D)-C(5D)-O(5D)-C(1D)	56.3(10)
C(4D)-C(5D)-C(6D)-O(6OD)	69.2(11)
O(5D)-C(5D)-C(6D)-O(6OD)	-54.8(11)
O(5E)-C(1E)-C(2E)-O(2OE)	177.8(7)
O(4F)-C(1E)-C(2E)-O(2OE)	57.9(9)
O(5E)-C(1E)-C(2E)-C(3E)	57.7(9)
O(4F)-C(1E)-C(2E)-C(3E)	-62.1(8)
O(2OE)-C(2E)-C(3E)-O(3E)	61.7(9)
C(1E)-C(2E)-C(3E)-O(3E)	-177.1(7)
O(2OE)-C(2E)-C(3E)-C(4E)	-175.6(7)
C(1E)-C(2E)-C(3E)-C(4E)	-54.4(9)
O(3E)-C(3E)-C(4E)-O(4E)	-63.5(10)
C(2E)-C(3E)-C(4E)-O(4E)	176.3(7)
O(3E)-C(3E)-C(4E)-C(5E)	177.3(8)
C(2E)-C(3E)-C(4E)-C(5E)	57.1(9)
O(5D)-C(1D)-O(4E)-C(4E)	123.8(8)
C(2D)-C(1D)-O(4E)-C(4E)	-117.3(8)
C(5E)-C(4E)-O(4E)-C(1D)	-102.2(9)
C(3E)-C(4E)-O(4E)-C(1D)	138.8(8)
O(4E)-C(4E)-C(5E)-O(5E)	-177.2(6)
C(3E)-C(4E)-C(5E)-O(5E)	-61.0(9)
O(4E)-C(4E)-C(5E)-C(6E)	66.7(10)

C(3E)-C(4E)-C(5E)-C(6E)	-177.1(8)
O(4F)-C(1E)-O(5E)-C(5E)	55.4(7)
C(2E)-C(1E)-O(5E)-C(5E)	-61.8(9)
C(6E)-C(5E)-O(5E)-C(1E)	-175.4(7)
C(4E)-C(5E)-O(5E)-C(1E)	62.5(8)
O(5E)-C(5E)-C(6E)-O(6E)	-59.1(9)
C(4E)-C(5E)-C(6E)-O(6E)	59.3(11)
O(5F)-C(1F)-C(2F)-O(2F)	-179.0(6)
O(4G)-C(1F)-C(2F)-O(2F)	58.6(7)
O(5F)-C(1F)-C(2F)-C(3F)	60.4(8)
O(4G)-C(1F)-C(2F)-C(3F)	-62.0(8)
O(2F)-C(2F)-C(3F)-O(3F)	69.4(9)
C(1F)-C(2F)-C(3F)-O(3F)	-173.9(6)
O(2F)-C(2F)-C(3F)-C(4F)	-173.2(7)
C(1F)-C(2F)-C(3F)-C(4F)	-56.4(9)
C(2F)-C(3F)-C(4F)-O(4F)	167.0(7)
O(3F)-C(3F)-C(4F)-O(4F)	-72.8(8)
C(2F)-C(3F)-C(4F)-C(5F)	52.1(9)
O(3F)-C(3F)-C(4F)-C(5F)	172.3(7)
C(5F)-C(4F)-O(4F)-C(1E)	-115.2(8)
C(3F)-C(4F)-O(4F)-C(1E)	127.5(7)
O(5E)-C(1E)-O(4F)-C(4F)	104.1(7)
C(2E)-C(1E)-O(4F)-C(4F)	-134.8(7)
O(4F)-C(4F)-C(5F)-O(5F)	-165.0(7)
C(3F)-C(4F)-C(5F)-O(5F)	-51.4(9)
O(4F)-C(4F)-C(5F)-C(6F)	76.8(9)
C(3F)-C(4F)-C(5F)-C(6F)	-169.6(7)
C(4F)-C(5F)-O(5F)-C(1F)	60.2(9)
C(6F)-C(5F)-O(5F)-C(1F)	-177.9(7)
O(4G)-C(1F)-O(5F)-C(5F)	56.8(9)
C(2F)-C(1F)-O(5F)-C(5F)	-64.3(8)
O(5F)-C(5F)-C(6F)-O(6F)	-65.1(10)
C(4F)-C(5F)-C(6F)-O(6F)	55.0(10)
C(4A)-O(4A)-C(1G)-O(5G)	111.0(7)
C(4A)-O(4A)-C(1G)-C(2G)	-129.7(7)
O(4A)-C(1G)-C(2G)-O(2G)	55.4(8)
O(5G)-C(1G)-C(2G)-O(2G)	177.6(6)
O(4A)-C(1G)-C(2G)-C(3G)	-69.6(8)
O(5G)-C(1G)-C(2G)-C(3G)	52.6(8)
O(2G)-C(2G)-C(3G)-O(3G)	61.3(9)
C(1G)-C(2G)-C(3G)-O(3G)	-176.6(7)
O(2G)-C(2G)-C(3G)-C(4G)	-177.6(6)
C(1G)-C(2G)-C(3G)-C(4G)	-55.5(9)
O(3G)-C(3G)-C(4G)-O(4G)	-60.2(8)
C(2G)-C(3G)-C(4G)-O(4G)	176.5(6)
O(3G)-C(3G)-C(4G)-C(5G)	177.4(6)
C(2G)-C(3G)-C(4G)-C(5G)	54.1(8)
C(3G)-C(4G)-O(4G)-C(1F)	123.9(7)
C(5G)-C(4G)-O(4G)-C(1F)	-117.7(7)
O(5F)-C(1F)-O(4G)-C(4G)	104.4(7)
C(2F)-C(1F)-O(4G)-C(4G)	-136.0(7)
O(4G)-C(4G)-C(5G)-O(5G)	-175.7(6)
C(3G)-C(4G)-C(5G)-O(5G)	-55.2(8)
O(4G)-C(4G)-C(5G)-C(6G)	63.5(9)
C(3G)-C(4G)-C(5G)-C(6G)	-176.0(7)
O(4A)-C(1G)-O(5G)-C(5G)	63.1(8)
C(2G)-C(1G)-O(5G)-C(5G)	-57.3(8)
C(4G)-C(5G)-O(5G)-C(1G)	61.1(8)
C(6G)-C(5G)-O(5G)-C(1G)	-176.9(7)
O(5G)-C(5G)-C(6G)-O(6G)	53.0(10)
C(4G)-C(5G)-C(6G)-O(6G)	175.8(8)
O(12W)#2-O(20A)-O(20C)-O(20D)	65(21)

C(19)-N(1)-C(1)-C(2)	163.4(12)
C(20)-N(1)-C(1)-C(2)	-69.4(14)
N(1)-C(1)-C(2)-C(3)	179.2(12)
C(1)-C(2)-C(3)-C(4)	133.7(15)
C(2)-C(3)-C(4)-C(18)	9(2)
C(2)-C(3)-C(4)-C(5)	177.8(14)
C(3)-C(4)-C(5)-C(10)	127.5(13)
C(18)-C(4)-C(5)-C(10)	-64.1(16)
C(3)-C(4)-C(5)-C(6)	-51.0(16)
C(18)-C(4)-C(5)-C(6)	117.5(13)
C(10)-C(5)-C(6)-C(7)	1(2)
C(4)-C(5)-C(6)-C(7)	179.4(13)
C(5)-C(6)-C(7)-C(8)	-2(2)
C(6)-C(7)-C(8)-C(9)	1(3)
C(7)-C(8)-C(9)-C(10)	1(2)
C(6)-C(5)-C(10)-C(9)	1.0(18)
C(4)-C(5)-C(10)-C(9)	-177.4(12)
C(6)-C(5)-C(10)-C(11)	-179.6(12)
C(4)-C(5)-C(10)-C(11)	2.0(18)
C(8)-C(9)-C(10)-C(5)	-2.2(19)
C(8)-C(9)-C(10)-C(11)	178.4(13)
C(5)-C(10)-C(11)-C(12)	30.0(19)
C(9)-C(10)-C(11)-C(12)	-150.6(13)
C(10)-C(11)-C(12)-C(13)	1(2)
C(11)-C(12)-C(13)-C(14)	144.4(13)
C(11)-C(12)-C(13)-C(18)	-38(2)
C(18)-C(13)-C(14)-C(15)	2.1(17)
C(12)-C(13)-C(14)-C(15)	179.9(12)
C(13)-C(14)-C(15)-C(16)	1(2)
C(14)-C(15)-C(16)-C(17)	-3(2)
C(15)-C(16)-C(17)-C(18)	1.9(19)
C(16)-C(17)-C(18)-C(4)	172.4(12)
C(16)-C(17)-C(18)-C(13)	1.4(19)
C(3)-C(4)-C(18)-C(17)	51.2(17)
C(5)-C(4)-C(18)-C(17)	-116.3(14)
C(3)-C(4)-C(18)-C(13)	-136.8(13)
C(5)-C(4)-C(18)-C(13)	55.8(14)
C(14)-C(13)-C(18)-C(17)	-3.5(17)
C(12)-C(13)-C(18)-C(17)	179.1(13)
C(14)-C(13)-C(18)-C(4)	-175.2(10)
C(12)-C(13)-C(18)-C(4)	7.5(18)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y,z+1/2 #2 -x+1/2,-y,z-1/2

Table S7: Hydrogen bonds for cdbzp-16 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3A)-H(3OA)...O(2G)	0.82	1.96	2.781(9)	176.9
O(3A)-H(3OA)...O(4A)	0.82	2.42	2.811(8)	110.5
O(3B)-H(3OB)...O(2A)	0.82	1.85	2.659(8)	169.7
O(3B)-H(3OB)...O(4B)	0.82	2.28	2.660(8)	108.4
O(3C)-H(3OC)...O(2B)	0.82	1.94	2.752(9)	168.5
O(6C)-H(6OC)...O(2G)#3	0.86	2.24	2.933(10)	137.7
O(3D)-H(3OD)...O(2C)	0.82	2.01	2.827(10)	173.4
O(3D)-H(3OD)...O(4D)	0.82	2.33	2.748(8)	112.6
O(3E)-H(3OE)...O(2D)	0.82	2.10	2.680(11)	127.7
O(3F)-H(3OF)...O(6B)#4	0.82	1.95	2.759(8)	170.8
O(3G)-H(3OG)...O(6C)#4	0.82	1.92	2.725(10)	169.2
C(4B)-H(4B)...O(5E)#5	0.98	2.60	3.532(9)	159.2
C(1E)-H(1E)...O(2A)#6	0.98	2.42	3.369(10)	163.2
C(1F)-H(1F)...O(3D)#7	0.98	2.25	3.207(10)	165.9
C(1)-H(1C1)...O(6A)#4	0.97	2.26	2.823(14)	116.0

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y,z+1/2 #2 -x+1/2,-y,z-1/2 #3 -x,y+1/2,-z+3/2
#4 -x,y-1/2,-z+3/2 #5 x+1,y,z #6 x-1,y,z
#7 -x-1/2,-y,z+1/2

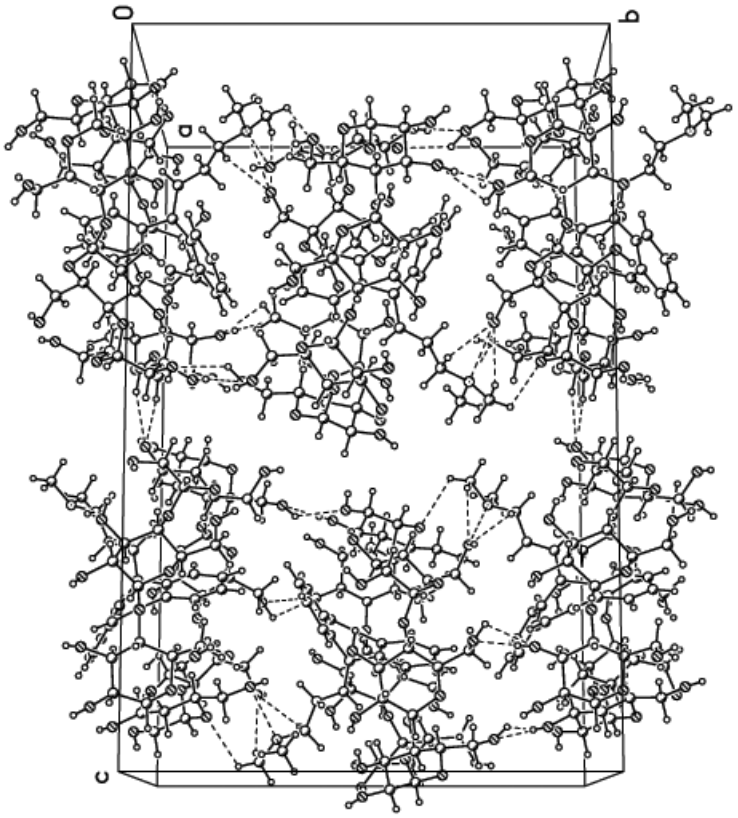

Figure S2: Packing diagram of complex **1**.

Crystallographic data for amitryptiline (**2**)

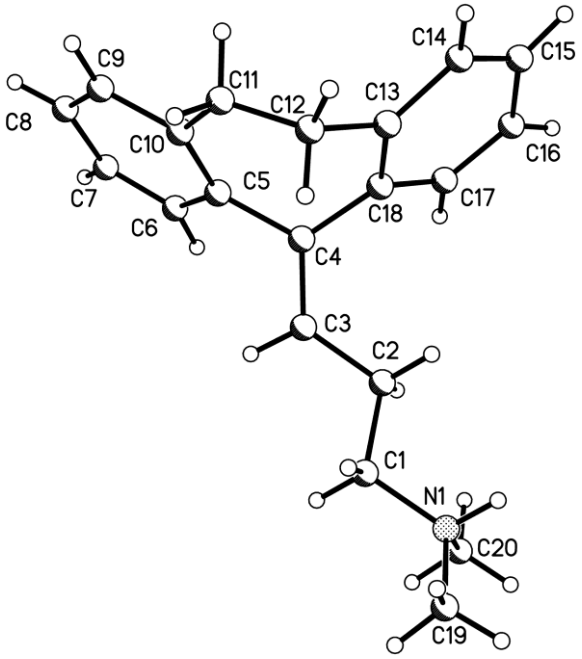

Figure S3: The structure of compound **2** in the inclusion complex with the atom numbering scheme from the X-ray results.

Table S8: Crystal data and structure refinement for cdamtr-16.

Identification code	cdamtr-16
Empirical formula	C62 H93 N O48.10
Formula weight	1621.97
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	orthorhombic, P212121
Unit cell dimensions	a = 15.1868(15)Å alpha = 90 deg. b = 18.5587(18)Å beta = 90 deg. c = 29.501(3) Å gamma = 90 deg.
Volume	8314.7(14) A^3
Z, Calculated density	4, 1.296 Mg/m^3
Absorption coefficient	0.113 mm^-1
F(000)	3427
Crystal size	0.38 x 0.35 x 0.06 mm
Theta range for data collection	1.76 to 30.00 deg.
Limiting indices	-21<=h<=21, -26<=k<=26, -26<=l<=26
Reflections collected / unique	110431 / 20064 [R(int) = 0.0527]
Completeness to theta	30.00 82.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	20064 / 0 / 1102
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0680, wR2 = 0.1830
R indices (all data)	R1 = 0.0895, wR2 = 0.1972
Absolute structure parameter	0.4(7)
Largest diff. peak and hole	0.551 and -0.348 e.A^-3

Table S9: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cdamtr-16. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1A)	2507(2)	990(2)	7765(1)	39(1)
C(2A)	2577(2)	355(2)	8092(1)	40(1)
O(2A)	3024(1)	-218(1)	7864(1)	52(1)
C(3A)	1679(2)	122(1)	8262(1)	38(1)
O(3A)	1802(1)	-403(1)	8606(1)	54(1)
C(4A)	1169(2)	769(1)	8436(1)	34(1)
O(4A)	311(1)	513(1)	8558(1)	35(1)
C(5A)	1114(2)	1332(1)	8068(1)	40(1)
O(5A)	2002(1)	1546(1)	7954(1)	46(1)
C(6A)	603(3)	1999(2)	8197(1)	59(1)
O(6A)	877(2)	2296(2)	8611(1)	82(1)
C(1B)	2554(2)	950(2)	5983(1)	40(1)
C(2B)	2900(2)	267(2)	6212(1)	43(1)
O(2B)	2705(2)	-350(1)	5939(1)	57(1)
C(3B)	2485(2)	182(1)	6673(1)	36(1)
O(3B)	2860(1)	-420(1)	6901(1)	46(1)
C(4B)	2623(2)	858(1)	6949(1)	32(1)
O(4B)	2125(1)	757(1)	7357(1)	37(1)
C(5B)	2323(2)	1531(1)	6696(1)	35(1)
O(5B)	2736(1)	1556(1)	6258(1)	41(1)
C(6B)	2556(2)	2232(1)	6927(1)	44(1)
O(6B)	3465(2)	2289(1)	7017(1)	52(1)
C(1C)	-457(2)	1037(1)	5065(1)	36(1)
C(2C)	191(2)	447(2)	4951(1)	41(1)
O(2C)	-295(2)	-193(1)	4849(1)	54(1)
C(3C)	807(2)	322(1)	5345(1)	38(1)
O(3C)	1449(2)	-205(1)	5227(1)	57(1)
C(4C)	1251(2)	1018(1)	5495(1)	36(1)
O(4C)	1638(1)	868(1)	5923(1)	39(1)
C(5C)	580(2)	1624(1)	5553(1)	37(1)
O(5C)	9(1)	1678(1)	5170(1)	41(1)
C(6C)	1031(2)	2356(2)	5598(1)	53(1)
O(6C)	386(2)	2876(1)	5704(1)	69(1)
C(1D)	-3645(2)	812(2)	5768(1)	52(1)
C(2D)	-3361(2)	321(2)	5372(1)	56(1)
O(2D)	-3828(2)	-325(2)	5380(1)	82(1)
C(3D)	-2369(2)	214(2)	5393(1)	44(1)
O(3D)	-2101(2)	-211(2)	5017(1)	58(1)
O(4D)	-987(1)	817(1)	5430(1)	39(1)
C(4D)	-1924(2)	943(2)	5392(1)	40(1)
C(5D)	-2243(2)	1387(2)	5791(1)	46(1)
O(5D)	-3182(1)	1459(1)	5769(1)	56(1)
C(6D)	-1900(2)	2148(2)	5801(2)	62(1)
O(6OD)	-2206(2)	2542(2)	5419(1)	79(1)
C(1E)	-5027(2)	-99(2)	7297(1)	39(1)
C(2E)	-4934(2)	-678(2)	6935(1)	44(1)
O(2OE)	-4813(2)	-1360(1)	7141(1)	64(1)
C(3E)	-4168(2)	-501(2)	6617(1)	45(1)
O(3E)	-4147(2)	-1003(2)	6251(1)	73(1)
C(4E)	-4280(2)	263(2)	6438(1)	40(1)
O(4E)	-3520(1)	422(1)	6174(1)	50(1)
C(5E)	-4376(2)	798(2)	6828(1)	40(1)
O(5E)	-5112(1)	586(1)	7101(1)	41(1)
C(6E)	-4532(2)	1563(2)	6683(1)	49(1)

O(6E)	-5289(2)	1624(1)	6396(1)	58(1)
C(1F)	-3378(2)	3(1)	8878(1)	35(1)
C(2F)	-3803(2)	-714(1)	8755(1)	38(1)
O(2F)	-3276(1)	-1281(1)	8928(1)	51(1)
C(3F)	-3909(2)	-765(1)	8251(1)	38(1)
O(3F)	-4394(1)	-1398(1)	8125(1)	51(1)
C(4F)	-4387(2)	-109(1)	8059(1)	34(1)
O(4F)	-4274(1)	-137(1)	7579(1)	40(1)
C(5F)	-3990(2)	592(1)	8237(1)	39(1)
O(5F)	-3903(1)	578(1)	8717(1)	39(1)
C(6F)	-4522(2)	1257(2)	8118(1)	48(1)
O(6F)	-5383(2)	1201(1)	8303(1)	58(1)
C(1G)	14(2)	658(1)	8999(1)	36(1)
C(2G)	-322(2)	-47(2)	9207(1)	39(1)
O(2G)	343(1)	-583(1)	9198(1)	53(1)
C(3G)	-1128(2)	-307(1)	8956(1)	35(1)
O(3G)	-1481(1)	-929(1)	9175(1)	49(1)
C(4G)	-1814(2)	286(1)	8948(1)	33(1)
O(4G)	-2537(1)	22(1)	8677(1)	36(1)
C(5G)	-1421(2)	968(1)	8736(1)	37(1)
O(5G)	-661(1)	1174(1)	9001(1)	41(1)
C(6G)	-2044(2)	1601(2)	8757(2)	62(1)
O(6G)	-1581(2)	2217(1)	8584(1)	75(1)
O(1W)	3777(2)	2430(2)	7958(1)	86(1)
O(2W)	4523(2)	2719(1)	5782(1)	64(1)
O(3W)	6329(2)	3268(2)	5774(1)	83(1)
O(4W)	2916(2)	-1851(2)	6622(2)	97(1)
O(5W)	3735(3)	-1422(2)	8295(1)	71(1)
O(6W)	3709(4)	-2151(3)	7451(2)	81(1)
O(7W)	4006(6)	6798(5)	5603(3)	88(2)
O(8W)	4061(8)	-1514(10)	5890(6)	111(6)
O(9W)	4244(7)	1507(7)	5026(4)	62(3)
O(9')	4194(4)	1871(2)	5018(2)	63(1)
O(10W)	7442(2)	8082(2)	6203(3)	73(2)
O(10')	7318(9)	7905(8)	6446(7)	62(4)
O(11W)	2050(5)	355(4)	4282(3)	133(2)
O(12W)	7524(16)	8321(6)	5017(4)	97(4)
O(12A)	7730(20)	8252(16)	5144(13)	83(8)
O(12B)	7290(20)	8299(15)	5265(12)	116(9)
O(13W)	5801(4)	5891(4)	5777(2)	81(2)
O(13')	5382(9)	6289(7)	5719(5)	59(3)
O(14W)	4244(2)	165(3)	5239(2)	77(1)
O(14B)	3405(11)	504(9)	4847(6)	68(4)
O(14C)	4306(9)	-743(8)	5355(5)	50(3)
O(15W)	4253(14)	8166(11)	5948(7)	102(6)
O(15')	4508(13)	7900(12)	6070(7)	89(5)
O(16W)	7053(10)	7057(9)	5608(5)	75(4)
O(16')	7273(13)	6559(12)	5662(7)	100(5)
O(17W)	4349(13)	-487(13)	5327(7)	79(5)
O(18W)	2326(15)	-360(12)	4393(8)	108(6)
O(19W)	3691(14)	440(11)	4988(7)	86(5)
O(20W)	3045(16)	-1598(13)	8303(8)	55(5)
O(21W)	3370(30)	-1270(20)	5032(13)	94(10)
O(14')	3020(20)	-978(18)	4715(12)	82(8)
N(1)	441(3)	-2199(2)	5670(1)	82(1)
C(1)	-34(3)	-1546(2)	5830(2)	75(1)
C(2)	394(3)	-1267(2)	6255(2)	75(1)
C(3)	-85(3)	-616(2)	6434(2)	74(1)
C(4)	-288(2)	-472(2)	6867(1)	59(1)
C(5)	-697(2)	229(2)	6975(1)	60(1)
C(6)	-288(3)	845(2)	6808(2)	91(2)
C(7)	-566(5)	1517(3)	6908(3)	135(3)

C(8)	-1318(6)	1605(3)	7158(3)	142(3)
C(9)	-1725(4)	1019(3)	7332(2)	104(2)
C(10)	-1448(3)	319(3)	7240(2)	72(1)
C(11)	-1935(3)	-262(4)	7469(3)	109(2)
C(12)	-1681(3)	-997(3)	7445(3)	119(3)
C(13)	-697(3)	-1158(2)	7565(2)	72(1)
C(14)	-463(4)	-1495(2)	7963(2)	90(2)
C(15)	425(6)	-1633(3)	8050(3)	122(3)
C(16)	1065(4)	-1446(3)	7720(2)	95(2)
C(17)	819(3)	-1104(2)	7356(2)	76(1)
C(18)	-49(2)	-934(2)	7252(2)	63(1)
C(19)	-81(6)	-2588(3)	5346(2)	128(3)
C(20)	1336(5)	-2019(3)	5476(2)	119(2)

Table S10: Bond lengths [A] and angles [deg] for cdamtr-16.

C(1A)-O(5A)	1.401(3)
C(1A)-O(4B)	1.405(3)
C(1A)-C(2A)	1.527(4)
C(2A)-O(2A)	1.431(4)
C(2A)-C(3A)	1.516(4)
C(3A)-O(3A)	1.419(3)
C(3A)-C(4A)	1.517(4)
C(4A)-O(4A)	1.433(3)
C(4A)-C(5A)	1.508(4)
O(4A)-C(1G)	1.403(3)
C(5A)-O(5A)	1.445(3)
C(5A)-C(6A)	1.509(4)
C(6A)-O(6A)	1.405(5)
C(1B)-O(4C)	1.411(3)
C(1B)-O(5B)	1.416(4)
C(1B)-C(2B)	1.530(4)
C(2B)-O(2B)	1.431(4)
C(2B)-C(3B)	1.506(4)
C(3B)-O(3B)	1.422(3)
C(3B)-C(4B)	1.510(4)
C(4B)-O(4B)	1.433(3)
C(4B)-C(5B)	1.525(4)
C(5B)-O(5B)	1.436(4)
C(5B)-C(6B)	1.510(4)
C(6B)-O(6B)	1.411(4)
C(1C)-O(4D)	1.404(3)
C(1C)-O(5C)	1.418(3)
C(1C)-C(2C)	1.510(4)
C(2C)-O(2C)	1.430(3)
C(2C)-C(3C)	1.511(4)
C(3C)-O(3C)	1.426(3)
C(3C)-C(4C)	1.522(4)
C(4C)-O(4C)	1.419(3)
C(4C)-C(5C)	1.528(4)
C(5C)-O(5C)	1.429(3)
C(5C)-C(6C)	1.527(4)
C(6C)-O(6C)	1.410(4)
C(1D)-O(5D)	1.391(4)
C(1D)-O(4E)	1.413(4)
C(1D)-C(2D)	1.542(5)
C(2D)-O(2D)	1.393(5)
C(2D)-C(3D)	1.522(4)
C(3D)-O(3D)	1.422(4)
C(3D)-C(4D)	1.512(4)
O(4D)-C(4D)	1.447(3)
C(4D)-C(5D)	1.516(4)
C(5D)-O(5D)	1.433(4)
C(5D)-C(6D)	1.506(5)
C(6D)-O(6OD)	1.421(5)
C(1E)-O(5E)	1.402(3)
C(1E)-O(4F)	1.417(3)
C(1E)-C(2E)	1.522(4)
C(2E)-O(2OE)	1.415(4)
C(2E)-C(3E)	1.531(4)
C(3E)-O(3E)	1.427(4)
C(3E)-C(4E)	1.522(4)
C(4E)-O(4E)	1.423(3)
C(4E)-C(5E)	1.525(4)
C(5E)-O(5E)	1.433(3)

C(5E)-C(6E)	1.501(4)
C(6E)-O(6E)	1.434(4)
C(1F)-O(4G)	1.410(3)
C(1F)-O(5F)	1.414(3)
C(1F)-C(2F)	1.524(4)
C(2F)-O(2F)	1.417(3)
C(2F)-C(3F)	1.499(5)
C(3F)-O(3F)	1.436(3)
C(3F)-C(4F)	1.526(4)
C(4F)-O(4F)	1.427(4)
C(4F)-C(5F)	1.526(4)
C(5F)-O(5F)	1.422(4)
C(5F)-C(6F)	1.516(4)
C(6F)-O(6F)	1.420(4)
C(1G)-O(5G)	1.402(3)
C(1G)-C(2G)	1.532(4)
C(2G)-O(2G)	1.418(3)
C(2G)-C(3G)	1.509(4)
C(3G)-O(3G)	1.428(3)
C(3G)-C(4G)	1.515(3)
C(4G)-O(4G)	1.444(3)
C(4G)-C(5G)	1.533(3)
C(5G)-O(5G)	1.447(3)
C(5G)-C(6G)	1.510(4)
C(6G)-O(6G)	1.437(4)
O(5W)-O(20W)	1.10(2)
O(8W)-O(15W)#1	0.68(2)
O(8W)-O(15')#1	1.39(3)
O(9W)-O(9')	0.680(11)
O(10W)-O(10')	0.811(17)
O(11W)-O(18W)	1.43(2)
O(12W)-O(12A)	0.51(3)
O(12W)-O(12B)	0.81(3)
O(12A)-O(12B)	0.77(4)
O(13W)-O(13')	0.990(13)
O(14W)-O(19W)	1.23(2)
O(14W)-O(17W)	1.25(2)
O(14W)-O(14C)	1.722(16)
O(14B)-O(19W)	0.61(2)
O(15W)-O(8W)#2	0.68(2)
O(15W)-O(15')	0.72(2)
O(15')-O(8W)#2	1.39(3)
O(16W)-O(16')	0.99(2)
O(21W)-O(14')	1.21(5)
N(1)-C(19)	1.435(8)
N(1)-C(1)	1.488(6)
N(1)-C(20)	1.512(8)
C(1)-C(2)	1.506(7)
C(2)-C(3)	1.506(5)
C(3)-C(4)	1.340(6)
C(4)-C(18)	1.470(6)
C(4)-C(5)	1.476(5)
C(5)-C(6)	1.390(6)
C(5)-C(10)	1.394(5)
C(6)-C(7)	1.350(7)
C(7)-C(8)	1.370(10)
C(8)-C(9)	1.353(9)
C(9)-C(10)	1.394(7)
C(10)-C(11)	1.471(7)
C(11)-C(12)	1.420(8)
C(12)-C(13)	1.563(8)
C(13)-C(14)	1.379(8)

C(13)-C(18)	1.411(6)
C(14)-C(15)	1.396(10)
C(15)-C(16)	1.418(11)
C(16)-C(17)	1.300(8)
C(17)-C(18)	1.390(6)
O(5A)-C(1A)-O(4B)	110.1(2)
O(5A)-C(1A)-C(2A)	110.8(2)
O(4B)-C(1A)-C(2A)	109.4(2)
O(2A)-C(2A)-C(3A)	111.8(2)
O(2A)-C(2A)-C(1A)	108.0(2)
C(3A)-C(2A)-C(1A)	111.5(2)
O(3A)-C(3A)-C(2A)	108.3(2)
O(3A)-C(3A)-C(4A)	111.7(2)
C(2A)-C(3A)-C(4A)	110.2(2)
O(4A)-C(4A)-C(5A)	111.2(2)
O(4A)-C(4A)-C(3A)	106.7(2)
C(5A)-C(4A)-C(3A)	109.5(2)
C(1G)-O(4A)-C(4A)	117.6(2)
O(5A)-C(5A)-C(4A)	107.9(2)
O(5A)-C(5A)-C(6A)	108.2(2)
C(4A)-C(5A)-C(6A)	114.5(2)
C(1A)-O(5A)-C(5A)	113.6(2)
O(6A)-C(6A)-C(5A)	112.9(3)
O(4C)-C(1B)-O(5B)	110.6(2)
O(4C)-C(1B)-C(2B)	107.7(2)
O(5B)-C(1B)-C(2B)	109.7(2)
O(2B)-C(2B)-C(3B)	109.8(2)
O(2B)-C(2B)-C(1B)	110.1(2)
C(3B)-C(2B)-C(1B)	110.0(2)
O(3B)-C(3B)-C(2B)	109.9(2)
O(3B)-C(3B)-C(4B)	110.0(2)
C(2B)-C(3B)-C(4B)	110.0(2)
O(4B)-C(4B)-C(3B)	105.71(19)
O(4B)-C(4B)-C(5B)	111.15(19)
C(3B)-C(4B)-C(5B)	112.0(2)
C(1A)-O(4B)-C(4B)	117.42(18)
O(5B)-C(5B)-C(6B)	105.9(2)
O(5B)-C(5B)-C(4B)	109.7(2)
C(6B)-C(5B)-C(4B)	114.5(2)
C(1B)-O(5B)-C(5B)	113.86(19)
O(6B)-C(6B)-C(5B)	112.3(2)
O(4D)-C(1C)-O(5C)	111.3(2)
O(4D)-C(1C)-C(2C)	109.5(2)
O(5C)-C(1C)-C(2C)	109.4(2)
O(2C)-C(2C)-C(1C)	108.2(2)
O(2C)-C(2C)-C(3C)	110.7(2)
C(1C)-C(2C)-C(3C)	110.0(2)
O(3C)-C(3C)-C(2C)	109.9(2)
O(3C)-C(3C)-C(4C)	110.5(2)
C(2C)-C(3C)-C(4C)	111.6(2)
O(4C)-C(4C)-C(3C)	106.0(2)
O(4C)-C(4C)-C(5C)	108.7(2)
C(3C)-C(4C)-C(5C)	111.1(2)
C(1B)-O(4C)-C(4C)	119.9(2)
O(5C)-C(5C)-C(6C)	106.2(2)
O(5C)-C(5C)-C(4C)	111.6(2)
C(6C)-C(5C)-C(4C)	111.4(2)
C(1C)-O(5C)-C(5C)	114.5(2)
O(6C)-C(6C)-C(5C)	108.5(3)
O(5D)-C(1D)-O(4E)	111.8(3)
O(5D)-C(1D)-C(2D)	111.8(2)
O(4E)-C(1D)-C(2D)	107.6(3)

O(2D)-C(2D)-C(3D)	113.0(4)
O(2D)-C(2D)-C(1D)	110.7(3)
C(3D)-C(2D)-C(1D)	108.8(3)
O(3D)-C(3D)-C(4D)	111.5(2)
O(3D)-C(3D)-C(2D)	108.9(3)
C(4D)-C(3D)-C(2D)	109.0(3)
C(1C)-O(4D)-C(4D)	117.2(2)
O(4D)-C(4D)-C(3D)	107.2(2)
O(4D)-C(4D)-C(5D)	110.0(2)
C(3D)-C(4D)-C(5D)	109.9(2)
O(5D)-C(5D)-C(6D)	104.9(3)
O(5D)-C(5D)-C(4D)	109.5(3)
C(6D)-C(5D)-C(4D)	114.5(3)
C(1D)-O(5D)-C(5D)	115.0(2)
O(6OD)-C(6D)-C(5D)	110.8(3)
O(5E)-C(1E)-O(4F)	111.3(2)
O(5E)-C(1E)-C(2E)	111.1(2)
O(4F)-C(1E)-C(2E)	107.6(2)
O(2OE)-C(2E)-C(1E)	110.1(3)
O(2OE)-C(2E)-C(3E)	110.8(2)
C(1E)-C(2E)-C(3E)	110.4(2)
O(3E)-C(3E)-C(4E)	110.4(3)
O(3E)-C(3E)-C(2E)	110.0(3)
C(4E)-C(3E)-C(2E)	109.1(2)
O(4E)-C(4E)-C(3E)	107.0(2)
O(4E)-C(4E)-C(5E)	110.8(2)
C(3E)-C(4E)-C(5E)	110.9(2)
C(1D)-O(4E)-C(4E)	117.4(2)
O(5E)-C(5E)-C(6E)	107.2(2)
O(5E)-C(5E)-C(4E)	108.6(2)
C(6E)-C(5E)-C(4E)	114.7(3)
C(1E)-O(5E)-C(5E)	114.1(2)
O(6E)-C(6E)-C(5E)	111.7(3)
O(4G)-C(1F)-O(5F)	110.5(2)
O(4G)-C(1F)-C(2F)	107.7(2)
O(5F)-C(1F)-C(2F)	109.9(2)
O(2F)-C(2F)-C(3F)	111.8(2)
O(2F)-C(2F)-C(1F)	108.9(2)
C(3F)-C(2F)-C(1F)	109.7(2)
O(3F)-C(3F)-C(2F)	111.3(2)
O(3F)-C(3F)-C(4F)	108.2(2)
C(2F)-C(3F)-C(4F)	111.6(2)
O(4F)-C(4F)-C(5F)	108.9(2)
O(4F)-C(4F)-C(3F)	106.3(2)
C(5F)-C(4F)-C(3F)	111.4(2)
C(1E)-O(4F)-C(4F)	118.98(19)
O(5F)-C(5F)-C(6F)	107.1(2)
O(5F)-C(5F)-C(4F)	111.3(2)
C(6F)-C(5F)-C(4F)	113.8(2)
C(1F)-O(5F)-C(5F)	113.7(2)
O(6F)-C(6F)-C(5F)	110.0(2)
O(5G)-C(1G)-O(4A)	111.7(2)
O(5G)-C(1G)-C(2G)	109.7(2)
O(4A)-C(1G)-C(2G)	108.3(2)
O(2G)-C(2G)-C(3G)	110.2(2)
O(2G)-C(2G)-C(1G)	110.7(2)
C(3G)-C(2G)-C(1G)	110.3(2)
O(3G)-C(3G)-C(2G)	109.9(2)
O(3G)-C(3G)-C(4G)	109.7(2)
C(2G)-C(3G)-C(4G)	109.5(2)
O(4G)-C(4G)-C(3G)	106.6(2)
O(4G)-C(4G)-C(5G)	110.5(2)

C(3G)-C(4G)-C(5G)	109.8(2)
C(1F)-O(4G)-C(4G)	117.6(2)
O(5G)-C(5G)-C(6G)	105.8(2)
O(5G)-C(5G)-C(4G)	108.0(2)
C(6G)-C(5G)-C(4G)	112.4(2)
C(1G)-O(5G)-C(5G)	113.59(19)
O(6G)-C(6G)-C(5G)	107.3(2)
O(15W)#1-O(8W)-O(15')#1	10(2)
O(12A)-O(12W)-O(12B)	66(4)
O(12W)-O(12A)-O(12B)	77(5)
O(12A)-O(12B)-O(12W)	37(3)
O(19W)-O(14W)-O(17W)	127.9(14)
O(19W)-O(14W)-O(14C)	124.2(11)
O(17W)-O(14W)-O(14C)	4.2(12)
O(8W)#2-O(15W)-O(15')	161(5)
O(15W)-O(15')-O(8W)#2	9(2)
O(14B)-O(19W)-O(14W)	166(4)
C(19)-N(1)-C(1)	110.6(5)
C(19)-N(1)-C(20)	110.9(5)
C(1)-N(1)-C(20)	112.1(4)
N(1)-C(1)-C(2)	109.5(4)
C(1)-C(2)-C(3)	111.0(4)
C(4)-C(3)-C(2)	127.2(4)
C(3)-C(4)-C(18)	124.3(3)
C(3)-C(4)-C(5)	118.5(4)
C(18)-C(4)-C(5)	116.8(3)
C(6)-C(5)-C(10)	117.8(4)
C(6)-C(5)-C(4)	117.4(3)
C(10)-C(5)-C(4)	124.8(4)
C(7)-C(6)-C(5)	122.9(5)
C(6)-C(7)-C(8)	119.2(6)
C(9)-C(8)-C(7)	119.3(5)
C(8)-C(9)-C(10)	122.5(5)
C(9)-C(10)-C(5)	118.0(4)
C(9)-C(10)-C(11)	116.2(5)
C(5)-C(10)-C(11)	125.6(4)
C(12)-C(11)-C(10)	123.0(5)
C(11)-C(12)-C(13)	115.6(4)
C(14)-C(13)-C(18)	120.7(5)
C(14)-C(13)-C(12)	121.7(4)
C(18)-C(13)-C(12)	117.6(5)
C(13)-C(14)-C(15)	119.2(5)
C(14)-C(15)-C(16)	119.4(6)
C(17)-C(16)-C(15)	119.2(6)
C(16)-C(17)-C(18)	124.5(5)
C(17)-C(18)-C(13)	116.7(5)
C(17)-C(18)-C(4)	122.5(4)
C(13)-C(18)-C(4)	120.3(3)

Symmetry transformations used to generate equivalent atoms:
#1 x,y-1,z #2 x,y+1,z

Table S11: Anisotropic displacement parameters (A^2 x 10^3) for cdamtr-16. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1A)	36(1)	40(1)	40(2)	-1(1)	4(1)	-9(1)
C(2A)	31(1)	50(1)	40(2)	5(1)	4(1)	3(1)
O(2A)	45(1)	52(1)	60(2)	11(1)	15(1)	18(1)
C(3A)	32(1)	39(1)	43(2)	5(1)	4(1)	4(1)
O(3A)	45(1)	55(1)	62(2)	24(1)	11(1)	13(1)
C(4A)	32(1)	35(1)	36(2)	-1(1)	4(1)	-3(1)
O(4A)	31(1)	38(1)	36(1)	-2(1)	2(1)	-2(1)
C(5A)	46(1)	34(1)	40(2)	1(1)	12(1)	3(1)
O(5A)	53(1)	34(1)	51(1)	-3(1)	15(1)	-9(1)
C(6A)	73(2)	37(1)	66(2)	9(1)	25(2)	14(1)
O(6A)	99(2)	56(2)	90(2)	-26(2)	29(2)	1(2)
C(1B)	33(1)	46(1)	40(2)	0(1)	5(1)	-1(1)
C(2B)	36(1)	45(1)	48(2)	-8(1)	-1(1)	9(1)
O(2B)	68(1)	54(1)	50(2)	-19(1)	-3(1)	18(1)
C(3B)	32(1)	31(1)	45(2)	2(1)	-1(1)	3(1)
O(3B)	52(1)	31(1)	56(1)	2(1)	-3(1)	6(1)
C(4B)	28(1)	32(1)	36(2)	-2(1)	1(1)	-1(1)
O(4B)	34(1)	39(1)	37(1)	1(1)	4(1)	-6(1)
C(5B)	31(1)	33(1)	42(2)	1(1)	0(1)	2(1)
O(5B)	37(1)	42(1)	43(1)	3(1)	2(1)	-7(1)
C(6B)	52(2)	29(1)	52(2)	3(1)	-2(1)	4(1)
O(6B)	54(1)	41(1)	63(2)	0(1)	-10(1)	-10(1)
C(1C)	35(1)	40(1)	34(2)	1(1)	0(1)	-6(1)
C(2C)	38(1)	44(1)	40(2)	-5(1)	3(1)	-5(1)
O(2C)	49(1)	49(1)	65(2)	-22(1)	-1(1)	-6(1)
C(3C)	41(1)	35(1)	37(2)	-1(1)	2(1)	2(1)
O(3C)	58(1)	48(1)	64(2)	-16(1)	-7(1)	16(1)
C(4C)	36(1)	37(1)	34(2)	4(1)	1(1)	-4(1)
O(4C)	33(1)	48(1)	35(1)	2(1)	1(1)	0(1)
C(5C)	37(1)	31(1)	43(2)	-1(1)	-1(1)	-4(1)
O(5C)	40(1)	33(1)	48(1)	4(1)	-4(1)	-5(1)
C(6C)	53(2)	35(1)	69(2)	-3(1)	-14(2)	-6(1)
O(6C)	74(2)	35(1)	96(2)	-17(1)	-8(2)	4(1)
C(1D)	31(1)	85(2)	41(2)	11(2)	2(1)	-4(1)
C(2D)	42(1)	89(3)	38(2)	4(2)	0(1)	-20(2)
O(2D)	68(2)	114(2)	64(2)	-18(2)	7(1)	-50(2)
C(3D)	42(1)	57(2)	33(2)	-1(1)	-1(1)	-9(1)
O(3D)	53(1)	76(2)	44(1)	-18(1)	7(1)	-19(1)
O(4D)	34(1)	46(1)	36(1)	1(1)	2(1)	-4(1)
C(4D)	34(1)	54(2)	33(2)	-1(1)	2(1)	-2(1)
C(5D)	40(1)	59(2)	41(2)	-1(1)	8(1)	0(1)
O(5D)	40(1)	70(2)	58(2)	7(1)	13(1)	5(1)
C(6D)	51(2)	58(2)	78(3)	-15(2)	12(2)	3(2)
O(6OD)	68(2)	69(2)	100(2)	14(2)	13(2)	2(1)
C(1E)	30(1)	48(1)	40(2)	8(1)	2(1)	4(1)
C(2E)	39(1)	49(2)	45(2)	3(1)	-3(1)	0(1)
O(2OE)	71(2)	49(1)	74(2)	12(1)	4(1)	0(1)
C(3E)	45(1)	51(2)	38(2)	-1(1)	5(1)	7(1)
O(3E)	91(2)	63(2)	66(2)	-15(1)	19(2)	5(1)
C(4E)	32(1)	51(2)	36(2)	6(1)	5(1)	1(1)
O(4E)	32(1)	85(2)	34(1)	9(1)	4(1)	3(1)
C(5E)	33(1)	55(2)	32(2)	5(1)	3(1)	-1(1)
O(5E)	35(1)	50(1)	38(1)	9(1)	6(1)	9(1)
C(6E)	51(2)	52(2)	45(2)	5(1)	4(1)	-2(1)

O(6E)	52(1)	61(1)	62(2)	22(1)	2(1)	10(1)
C(1F)	32(1)	42(1)	31(2)	5(1)	2(1)	2(1)
C(2F)	35(1)	39(1)	39(2)	10(1)	2(1)	-2(1)
O(2F)	47(1)	43(1)	62(2)	22(1)	-12(1)	-6(1)
C(3F)	36(1)	35(1)	43(2)	1(1)	1(1)	6(1)
O(3F)	52(1)	36(1)	66(2)	-6(1)	-15(1)	4(1)
C(4F)	31(1)	41(1)	31(2)	3(1)	4(1)	6(1)
O(4F)	30(1)	58(1)	33(1)	6(1)	3(1)	8(1)
C(5F)	39(1)	37(1)	41(2)	6(1)	4(1)	2(1)
O(5F)	39(1)	38(1)	42(1)	1(1)	1(1)	9(1)
C(6F)	56(2)	36(1)	53(2)	8(1)	-3(1)	7(1)
O(6F)	54(1)	55(1)	66(2)	10(1)	-1(1)	16(1)
C(1G)	31(1)	41(1)	37(2)	-1(1)	-1(1)	-3(1)
C(2G)	37(1)	44(1)	36(2)	7(1)	0(1)	-1(1)
O(2G)	36(1)	54(1)	70(2)	23(1)	-4(1)	4(1)
C(3G)	36(1)	30(1)	40(2)	7(1)	0(1)	3(1)
O(3G)	38(1)	36(1)	74(2)	21(1)	-5(1)	0(1)
C(4G)	29(1)	31(1)	39(2)	-1(1)	-1(1)	-1(1)
O(4G)	30(1)	38(1)	38(1)	1(1)	0(1)	1(1)
C(5G)	35(1)	30(1)	48(2)	3(1)	1(1)	-1(1)
O(5G)	37(1)	36(1)	51(1)	-9(1)	4(1)	-1(1)
C(6G)	40(1)	31(1)	116(3)	8(2)	7(2)	3(1)
O(6G)	60(1)	35(1)	130(3)	21(1)	-1(2)	2(1)
O(1W)	80(2)	59(2)	118(3)	9(2)	-17(2)	-8(1)
O(2W)	87(2)	51(1)	55(2)	6(1)	3(1)	12(1)
O(3W)	81(2)	84(2)	86(2)	-14(2)	-15(2)	17(2)
O(4W)	91(2)	49(2)	149(3)	-19(2)	-20(2)	-11(2)
O(5W)	71(2)	70(2)	70(3)	21(2)	13(2)	14(2)
O(6W)	84(3)	86(3)	72(3)	5(3)	-2(3)	5(3)
O(7W)	99(6)	105(6)	60(5)	16(4)	27(4)	-16(5)
O(8W)	64(6)	120(12)	150(14)	-71(11)	-16(7)	8(7)
O(9W)	58(5)	81(8)	47(6)	-19(6)	6(4)	7(6)
O(9')	74(3)	47(2)	69(3)	0(2)	-2(2)	-5(2)
O(10W)	47(2)	71(2)	101(5)	6(3)	10(2)	31(2)
O(11W)	111(4)	149(6)	140(6)	14(5)	58(4)	10(4)
O(12W)	184(13)	60(5)	48(8)	-2(4)	-9(8)	-26(6)
O(13W)	80(4)	125(5)	39(3)	-32(3)	4(3)	-19(4)
O(14W)	48(2)	118(4)	65(3)	-20(2)	16(2)	3(2)
N(1)	138(4)	47(2)	60(2)	4(2)	7(2)	8(2)
C(1)	105(3)	56(2)	65(3)	13(2)	24(2)	-1(2)
C(2)	87(3)	54(2)	85(3)	-10(2)	36(2)	-2(2)
C(3)	85(3)	46(2)	90(3)	9(2)	41(2)	4(2)
C(4)	54(2)	50(2)	72(3)	3(2)	21(2)	-11(1)
C(5)	55(2)	60(2)	64(2)	-2(2)	11(2)	-5(2)
C(6)	74(3)	62(2)	137(5)	11(3)	26(3)	-8(2)
C(7)	124(5)	53(3)	229(9)	-19(4)	61(6)	-7(3)
C(8)	189(8)	54(3)	184(7)	-16(4)	63(7)	12(4)
C(9)	109(4)	98(4)	104(4)	-6(3)	34(3)	39(3)
C(10)	56(2)	88(3)	71(3)	11(2)	15(2)	4(2)
C(11)	59(2)	118(4)	149(5)	50(4)	28(3)	5(3)
C(12)	66(3)	73(3)	217(7)	-22(4)	69(4)	-30(2)
C(13)	82(3)	40(2)	95(3)	3(2)	29(2)	-2(2)
C(14)	117(4)	53(2)	100(4)	-8(2)	33(3)	-11(2)
C(15)	190(8)	48(2)	130(5)	-6(3)	-48(5)	-7(4)
C(16)	91(3)	55(2)	140(5)	-9(3)	-16(3)	-11(2)
C(17)	67(2)	52(2)	107(4)	-4(2)	7(2)	-7(2)
C(18)	49(2)	41(2)	100(3)	-17(2)	16(2)	-7(1)
C(19)	220(8)	73(3)	90(4)	-8(3)	-32(5)	6(4)
C(20)	150(6)	88(4)	119(5)	14(3)	54(4)	41(4)

Table S12: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for cdamtr-16.

	x	y	z	U(eq)
H(1A)	3099	1173	7702	46
H(2A)	2933	504	8353	48
H(2OA)	2973	-591	8011	78
H(3A)	1351	-96	8011	46
H(3OA)	1332	-481	8734	81
H(4A)	1464	970	8703	41
H(5A)	841	1116	7800	48
H(6A1)	671	2357	7960	70
H(6A2)	-17	1878	8217	70
H(6OA)	743	2024	8819	122
H(1B)	2839	1009	5687	48
H(2B)	3539	306	6248	52
H(2OB)	3084	-395	5743	86
H(3B)	1851	100	6636	43
H(3OB)	2805	-368	7175	69
H(4B)	3248	904	7026	38
H(5B)	1683	1509	6655	43
H(6B1)	2377	2630	6735	53
H(6B2)	2232	2268	7209	53
H(6OB)	3540	2365	7288	79
H(1C)	-834	1125	4801	43
H(2C)	534	590	4684	49
H(2OC)	43	-506	4759	82
H(3C)	461	136	5600	45
H(3OC)	1839	-287	5445	85
H(4C)	1705	1159	5276	43
H(5C)	227	1532	5825	44
H(6C1)	1471	2338	5836	63
H(6C2)	1321	2481	5316	63
H(6OC)	167	3262	5875	103
H(1D)	-4274	919	5735	63
H(2D)	-3501	569	5088	68
H(2OD)	-3710	-546	5613	123
H(3D)	-2219	-39	5674	53
H(3OD)	-1562	-219	5003	86
H(4D)	-2053	1195	5108	48
H(5D)	-2081	1143	6073	55
H(6D1)	-2094	2383	6077	75
H(6D2)	-1261	2141	5801	75
H(6OD)	-1868	2482	5206	119
H(1E)	-5552	-200	7479	47
H(2E)	-5478	-692	6757	53
H(2E)	-5291	-1519	7223	97
H(3E)	-3614	-532	6786	54
H(3OE)	-4054	-787	6013	110
H(4E)	-4804	286	6245	48
H(5E)	-3842	780	7014	48
H(6E1)	-4616	1861	6950	59
H(6E2)	-4018	1739	6523	59
H(6OE)	-5694	1812	6537	87
H(1F)	-3320	39	9208	42
H(2F)	-4386	-739	8896	45
H(2OF)	-3587	-1564	9069	76
H(3F)	-3323	-791	8113	45
H(3OF)	-4054	-1737	8094	77

H(4F)	-5014	-132	8135	41
H(5F)	-3401	646	8105	47
H(6F1)	-4232	1682	8239	58
H(6F2)	-4558	1307	7792	58
H(6OF)	-5349	1112	8575	88
H(1G)	508	837	9181	44
H(2G)	-485	44	9523	47
H(2OG)	826	-389	9173	80
H(3G)	-964	-431	8644	42
H(3OG)	-1095	-1236	9200	74
H(4G)	-2017	388	9256	40
H(5G)	-1248	875	8421	45
H(6G1)	-2564	1506	8575	75
H(6G2)	-2228	1686	9067	75
H(6OG)	-1922	2558	8562	113
H(11)	-646	-1664	5890	90
H(12)	-18	-1177	5597	90
H(21)	1001	-1141	6192	90
H(22)	392	-1643	6484	90
H(3)	-260	-277	6220	89
H(6)	198	791	6619	109
H(7)	-249	1916	6808	162
H(8)	-1548	2063	7207	171
H(9)	-2208	1086	7521	124
H(11A)	-1953	-137	7788	130
H(11B)	-2536	-237	7360	130
H(12A)	-1795	-1170	7141	143
H(12B)	-2052	-1271	7650	143
H(14)	-891	-1629	8172	108
H(15)	596	-1846	8321	147
H(16)	1653	-1567	7763	114
H(17)	1253	-963	7153	91
H(19A)	-640	-2707	5479	192
H(19B)	220	-3022	5261	192
H(19C)	-172	-2295	5083	192
H(20A)	1624	-2454	5381	179
H(20B)	1686	-1785	5704	179
H(20C)	1268	-1703	5221	179

Table S13: Torsion angles [deg] for cdamtr-16.

O(5A)-C(1A)-C(2A)-O(2A)	174.5(2)
O(4B)-C(1A)-C(2A)-O(2A)	53.0(3)
O(5A)-C(1A)-C(2A)-C(3A)	51.3(3)
O(4B)-C(1A)-C(2A)-C(3A)	-70.2(3)
O(2A)-C(2A)-C(3A)-O(3A)	66.4(3)
C(1A)-C(2A)-C(3A)-O(3A)	-172.5(2)
O(2A)-C(2A)-C(3A)-C(4A)	-171.2(2)
C(1A)-C(2A)-C(3A)-C(4A)	-50.1(3)
O(3A)-C(3A)-C(4A)-O(4A)	-63.7(3)
C(2A)-C(3A)-C(4A)-O(4A)	175.9(2)
O(3A)-C(3A)-C(4A)-C(5A)	175.8(2)
C(2A)-C(3A)-C(4A)-C(5A)	55.5(3)
C(5A)-C(4A)-O(4A)-C(1G)	-114.9(3)
C(3A)-C(4A)-O(4A)-C(1G)	125.7(2)
O(4A)-C(4A)-C(5A)-O(5A)	-178.3(2)
C(3A)-C(4A)-C(5A)-O(5A)	-60.7(3)
O(4A)-C(4A)-C(5A)-C(6A)	61.1(3)
C(3A)-C(4A)-C(5A)-C(6A)	178.7(3)
O(4B)-C(1A)-O(5A)-C(5A)	61.7(3)
C(2A)-C(1A)-O(5A)-C(5A)	-59.4(3)
C(4A)-C(5A)-O(5A)-C(1A)	64.4(3)
C(6A)-C(5A)-O(5A)-C(1A)	-171.1(3)
O(5A)-C(5A)-C(6A)-O(6A)	-69.6(3)
C(4A)-C(5A)-C(6A)-O(6A)	50.7(4)
O(4C)-C(1B)-C(2B)-O(2B)	58.6(3)
O(5B)-C(1B)-C(2B)-O(2B)	179.0(2)
O(4C)-C(1B)-C(2B)-C(3B)	-62.4(3)
O(5B)-C(1B)-C(2B)-C(3B)	58.0(3)
O(2B)-C(2B)-C(3B)-O(3B)	63.6(3)
C(1B)-C(2B)-C(3B)-O(3B)	-175.2(2)
O(2B)-C(2B)-C(3B)-C(4B)	-175.2(2)
C(1B)-C(2B)-C(3B)-C(4B)	-54.0(3)
O(3B)-C(3B)-C(4B)-O(4B)	-65.2(2)
C(2B)-C(3B)-C(4B)-O(4B)	173.63(19)
O(3B)-C(3B)-C(4B)-C(5B)	173.6(2)
C(2B)-C(3B)-C(4B)-C(5B)	52.4(3)
O(5A)-C(1A)-O(4B)-C(4B)	116.2(2)
C(2A)-C(1A)-O(4B)-C(4B)	-121.8(2)
C(3B)-C(4B)-O(4B)-C(1A)	139.7(2)
C(5B)-C(4B)-O(4B)-C(1A)	-98.6(2)
O(4B)-C(4B)-C(5B)-O(5B)	-171.17(18)
C(3B)-C(4B)-C(5B)-O(5B)	-53.2(3)
O(4B)-C(4B)-C(5B)-C(6B)	69.9(3)
C(3B)-C(4B)-C(5B)-C(6B)	-172.1(2)
O(4C)-C(1B)-O(5B)-C(5B)	57.3(3)
C(2B)-C(1B)-O(5B)-C(5B)	-61.4(3)
C(6B)-C(5B)-O(5B)-C(1B)	-177.2(2)
C(4B)-C(5B)-O(5B)-C(1B)	58.7(3)
O(5B)-C(5B)-C(6B)-O(6B)	-65.9(3)
C(4B)-C(5B)-C(6B)-O(6B)	55.1(3)
O(4D)-C(1C)-C(2C)-O(2C)	57.6(3)
O(5C)-C(1C)-C(2C)-O(2C)	179.7(2)
O(4D)-C(1C)-C(2C)-C(3C)	-63.5(3)
O(5C)-C(1C)-C(2C)-C(3C)	58.7(3)
O(2C)-C(2C)-C(3C)-O(3C)	63.8(3)
C(1C)-C(2C)-C(3C)-O(3C)	-176.6(2)
O(2C)-C(2C)-C(3C)-C(4C)	-173.3(2)
C(1C)-C(2C)-C(3C)-C(4C)	-53.7(3)
O(3C)-C(3C)-C(4C)-O(4C)	-70.8(3)

C(2C)-C(3C)-C(4C)-O(4C)	166.6(2)
O(3C)-C(3C)-C(4C)-C(5C)	171.2(2)
C(2C)-C(3C)-C(4C)-C(5C)	48.7(3)
O(5B)-C(1B)-O(4C)-C(4C)	108.7(3)
C(2B)-C(1B)-O(4C)-C(4C)	-131.4(2)
C(3C)-C(4C)-O(4C)-C(1B)	121.0(2)
C(5C)-C(4C)-O(4C)-C(1B)	-119.5(2)
O(4C)-C(4C)-C(5C)-O(5C)	-165.0(2)
C(3C)-C(4C)-C(5C)-O(5C)	-48.7(3)
O(4C)-C(4C)-C(5C)-C(6C)	76.5(3)
C(3C)-C(4C)-C(5C)-C(6C)	-167.3(3)
O(4D)-C(1C)-O(5C)-C(5C)	59.5(3)
C(2C)-C(1C)-O(5C)-C(5C)	-61.6(3)
C(6C)-C(5C)-O(5C)-C(1C)	178.5(2)
C(4C)-C(5C)-O(5C)-C(1C)	56.9(3)
O(5C)-C(5C)-C(6C)-O(6C)	65.1(3)
C(4C)-C(5C)-C(6C)-O(6C)	-173.1(3)
O(5D)-C(1D)-C(2D)-O(2D)	179.4(3)
O(4E)-C(1D)-C(2D)-O(2D)	56.4(3)
O(5D)-C(1D)-C(2D)-C(3D)	54.7(4)
O(4E)-C(1D)-C(2D)-C(3D)	-68.4(3)
O(2D)-C(2D)-C(3D)-O(3D)	59.2(4)
C(1D)-C(2D)-C(3D)-O(3D)	-177.4(3)
O(2D)-C(2D)-C(3D)-C(4D)	-178.9(3)
C(1D)-C(2D)-C(3D)-C(4D)	-55.5(4)
O(5C)-C(1C)-O(4D)-C(4D)	104.4(3)
C(2C)-C(1C)-O(4D)-C(4D)	-134.5(2)
C(1C)-O(4D)-C(4D)-C(3D)	116.8(3)
C(1C)-O(4D)-C(4D)-C(5D)	-123.7(3)
O(3D)-C(3D)-C(4D)-O(4D)	-61.9(3)
C(2D)-C(3D)-C(4D)-O(4D)	177.8(2)
O(3D)-C(3D)-C(4D)-C(5D)	178.6(2)
C(2D)-C(3D)-C(4D)-C(5D)	58.3(3)
O(4D)-C(4D)-C(5D)-O(5D)	-175.3(2)
C(3D)-C(4D)-C(5D)-O(5D)	-57.6(3)
O(4D)-C(4D)-C(5D)-C(6D)	67.2(4)
C(3D)-C(4D)-C(5D)-C(6D)	-175.1(3)
O(4E)-C(1D)-O(5D)-C(5D)	63.5(3)
C(2D)-C(1D)-O(5D)-C(5D)	-57.2(4)
C(6D)-C(5D)-O(5D)-C(1D)	-178.5(3)
C(4D)-C(5D)-O(5D)-C(1D)	58.1(4)
O(5D)-C(5D)-C(6D)-O(6OD)	-56.4(3)
C(4D)-C(5D)-C(6D)-O(6OD)	63.7(4)
O(5E)-C(1E)-C(2E)-O(2OE)	177.6(2)
O(4F)-C(1E)-C(2E)-O(2OE)	55.6(3)
O(5E)-C(1E)-C(2E)-C(3E)	54.9(3)
O(4F)-C(1E)-C(2E)-C(3E)	-67.1(3)
O(2OE)-C(2E)-C(3E)-O(3E)	64.1(3)
C(1E)-C(2E)-C(3E)-O(3E)	-173.6(3)
O(2OE)-C(2E)-C(3E)-C(4E)	-174.7(3)
C(1E)-C(2E)-C(3E)-C(4E)	-52.4(3)
O(3E)-C(3E)-C(4E)-O(4E)	-63.6(3)
C(2E)-C(3E)-C(4E)-O(4E)	175.4(2)
O(3E)-C(3E)-C(4E)-C(5E)	175.6(2)
C(2E)-C(3E)-C(4E)-C(5E)	54.6(3)
O(5D)-C(1D)-O(4E)-C(4E)	120.4(3)
C(2D)-C(1D)-O(4E)-C(4E)	-116.6(3)
C(3E)-C(4E)-O(4E)-C(1D)	140.1(3)
C(5E)-C(4E)-O(4E)-C(1D)	-99.0(3)
O(4E)-C(4E)-C(5E)-O(5E)	-176.0(2)
C(3E)-C(4E)-C(5E)-O(5E)	-57.4(3)
O(4E)-C(4E)-C(5E)-C(6E)	64.1(3)

C(3E)-C(4E)-C(5E)-C(6E)	-177.3(2)
O(4F)-C(1E)-O(5E)-C(5E)	59.4(3)
C(2E)-C(1E)-O(5E)-C(5E)	-60.5(3)
C(6E)-C(5E)-O(5E)-C(1E)	-174.5(2)
C(4E)-C(5E)-O(5E)-C(1E)	61.1(3)
O(5E)-C(5E)-C(6E)-O(6E)	-64.6(3)
C(4E)-C(5E)-C(6E)-O(6E)	56.0(3)
O(4G)-C(1F)-C(2F)-O(2F)	60.8(3)
O(5F)-C(1F)-C(2F)-O(2F)	-178.8(2)
O(4G)-C(1F)-C(2F)-C(3F)	-61.9(3)
O(5F)-C(1F)-C(2F)-C(3F)	58.5(3)
O(2F)-C(2F)-C(3F)-O(3F)	65.5(3)
C(1F)-C(2F)-C(3F)-O(3F)	-173.61(19)
O(2F)-C(2F)-C(3F)-C(4F)	-173.5(2)
C(1F)-C(2F)-C(3F)-C(4F)	-52.6(3)
O(3F)-C(3F)-C(4F)-O(4F)	-69.9(3)
C(2F)-C(3F)-C(4F)-O(4F)	167.3(2)
O(3F)-C(3F)-C(4F)-C(5F)	171.5(2)
C(2F)-C(3F)-C(4F)-C(5F)	48.7(3)
O(5E)-C(1E)-O(4F)-C(4F)	103.5(3)
C(2E)-C(1E)-O(4F)-C(4F)	-134.6(2)
C(5F)-C(4F)-O(4F)-C(1E)	-112.9(2)
C(3F)-C(4F)-O(4F)-C(1E)	127.0(2)
O(4F)-C(4F)-C(5F)-O(5F)	-166.79(19)
C(3F)-C(4F)-C(5F)-O(5F)	-49.8(3)
O(4F)-C(4F)-C(5F)-C(6F)	72.1(3)
C(3F)-C(4F)-C(5F)-C(6F)	-170.9(2)
O(4G)-C(1F)-O(5F)-C(5F)	56.2(3)
C(2F)-C(1F)-O(5F)-C(5F)	-62.5(3)
C(6F)-C(5F)-O(5F)-C(1F)	-176.8(2)
C(4F)-C(5F)-O(5F)-C(1F)	58.2(3)
O(5F)-C(5F)-C(6F)-O(6F)	-63.7(3)
C(4F)-C(5F)-C(6F)-O(6F)	59.8(3)
C(4A)-O(4A)-C(1G)-O(5G)	108.9(2)
C(4A)-O(4A)-C(1G)-C(2G)	-130.1(2)
O(5G)-C(1G)-C(2G)-O(2G)	178.6(2)
O(4A)-C(1G)-C(2G)-O(2G)	56.3(3)
O(5G)-C(1G)-C(2G)-C(3G)	56.4(3)
O(4A)-C(1G)-C(2G)-C(3G)	-65.9(3)
O(2G)-C(2G)-C(3G)-O(3G)	62.4(3)
C(1G)-C(2G)-C(3G)-O(3G)	-175.1(2)
O(2G)-C(2G)-C(3G)-C(4G)	-177.1(2)
C(1G)-C(2G)-C(3G)-C(4G)	-54.6(3)
O(3G)-C(3G)-C(4G)-O(4G)	-63.3(3)
C(2G)-C(3G)-C(4G)-O(4G)	176.0(2)
O(3G)-C(3G)-C(4G)-C(5G)	177.0(2)
C(2G)-C(3G)-C(4G)-C(5G)	56.3(3)
O(5F)-C(1F)-O(4G)-C(4G)	103.8(2)
C(2F)-C(1F)-O(4G)-C(4G)	-136.3(2)
C(3G)-C(4G)-O(4G)-C(1F)	123.3(2)
C(5G)-C(4G)-O(4G)-C(1F)	-117.5(2)
O(4G)-C(4G)-C(5G)-O(5G)	-175.60(19)
C(3G)-C(4G)-C(5G)-O(5G)	-58.3(3)
O(4G)-C(4G)-C(5G)-C(6G)	68.1(3)
C(3G)-C(4G)-C(5G)-C(6G)	-174.7(3)
O(4A)-C(1G)-O(5G)-C(5G)	58.6(3)
C(2G)-C(1G)-O(5G)-C(5G)	-61.6(3)
C(6G)-C(5G)-O(5G)-C(1G)	-176.8(2)
C(4G)-C(5G)-O(5G)-C(1G)	62.6(3)
O(5G)-C(5G)-C(6G)-O(6G)	57.8(4)
C(4G)-C(5G)-C(6G)-O(6G)	175.4(3)
O(17W)-O(14W)-O(19W)-O(14B)	-15(16)

O(14C)-O(14W)-O(19W)-O(14B)	-18(16)
C(19)-N(1)-C(1)-C(2)	164.0(4)
C(20)-N(1)-C(1)-C(2)	-71.7(5)
N(1)-C(1)-C(2)-C(3)	-178.5(3)
C(1)-C(2)-C(3)-C(4)	137.4(5)
C(2)-C(3)-C(4)-C(18)	1.5(7)
C(2)-C(3)-C(4)-C(5)	174.9(4)
C(3)-C(4)-C(5)-C(6)	-50.5(6)
C(18)-C(4)-C(5)-C(6)	123.4(4)
C(3)-C(4)-C(5)-C(10)	131.1(5)
C(18)-C(4)-C(5)-C(10)	-55.0(5)
C(10)-C(5)-C(6)-C(7)	2.9(10)
C(4)-C(5)-C(6)-C(7)	-175.6(7)
C(5)-C(6)-C(7)-C(8)	-4.8(13)
C(6)-C(7)-C(8)-C(9)	5.7(14)
C(7)-C(8)-C(9)-C(10)	-5.0(13)
C(8)-C(9)-C(10)-C(5)	3.1(10)
C(8)-C(9)-C(10)-C(11)	177.7(7)
C(6)-C(5)-C(10)-C(9)	-1.9(7)
C(4)-C(5)-C(10)-C(9)	176.4(5)
C(6)-C(5)-C(10)-C(11)	-175.9(6)
C(4)-C(5)-C(10)-C(11)	2.5(8)
C(9)-C(10)-C(11)-C(12)	-173.7(7)
C(5)-C(10)-C(11)-C(12)	0.3(10)
C(10)-C(11)-C(12)-C(13)	51.3(10)
C(11)-C(12)-C(13)-C(14)	108.0(6)
C(11)-C(12)-C(13)-C(18)	-70.9(7)
C(18)-C(13)-C(14)-C(15)	-1.9(7)
C(12)-C(13)-C(14)-C(15)	179.3(5)
C(13)-C(14)-C(15)-C(16)	-2.1(7)
C(14)-C(15)-C(16)-C(17)	4.8(8)
C(15)-C(16)-C(17)-C(18)	-3.5(7)
C(16)-C(17)-C(18)-C(13)	-0.5(6)
C(16)-C(17)-C(18)-C(4)	172.4(4)
C(14)-C(13)-C(18)-C(17)	3.2(6)
C(12)-C(13)-C(18)-C(17)	-177.9(4)
C(14)-C(13)-C(18)-C(4)	-169.9(4)
C(12)-C(13)-C(18)-C(4)	9.1(6)
C(3)-C(4)-C(18)-C(17)	59.3(6)
C(5)-C(4)-C(18)-C(17)	-114.2(4)
C(3)-C(4)-C(18)-C(13)	-128.0(4)
C(5)-C(4)-C(18)-C(13)	58.5(5)

Symmetry transformations used to generate equivalent atoms:
#1 x,y-1,z #2 x,y+1,z

Table S14: Hydrogen bonds for cdamtr-16 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3A)-H(3OA)...O(2G)	0.82	2.04	2.840(3)	164.7
O(6A)-H(6OA)...O(5G)	0.82	2.71	3.335(4)	134.8
O(6A)-H(6OA)...O(4A)	0.82	2.98	3.423(3)	116.3
O(3B)-H(3OB)...O(2A)	0.82	2.08	2.876(3)	164.8
O(3B)-H(3OB)...O(4B)	0.82	2.39	2.797(3)	111.6
O(3C)-H(3OC)...O(2B)	0.89	1.97	2.850(4)	173.5
O(6C)-H(6OC)...O(2G)#3	0.94	2.29	3.082(3)	141.7
O(2D)-H(2OD)...O(3E)	0.82	2.17	2.899(4)	148.9
O(3D)-H(3OD)...O(2C)	0.82	1.98	2.788(3)	169.3
O(3E)-H(3OE)...O(2D)	0.82	2.08	2.899(4)	175.0
O(6E)-H(6OE)...O(6B)#4	0.82	2.10	2.909(4)	167.5
O(3F)-H(3OF)...O(6B)#5	0.82	2.04	2.848(3)	166.7
O(3G)-H(3OG)...O(6C)#5	0.82	1.99	2.796(3)	167.0
C(1)-H(11)...O(6A)#5	0.97	2.45	2.997(5)	115.1
C(1E)-H(1E)...O(2A)#4	0.98	2.44	3.407(3)	168.0

Symmetry transformations used to generate equivalent atoms:
#1 x,y-1,z #2 x,y+1,z #3 -x,y+1/2,-z+3/2
#4 x-1,y,z #5 -x,y-1/2,-z+3/2

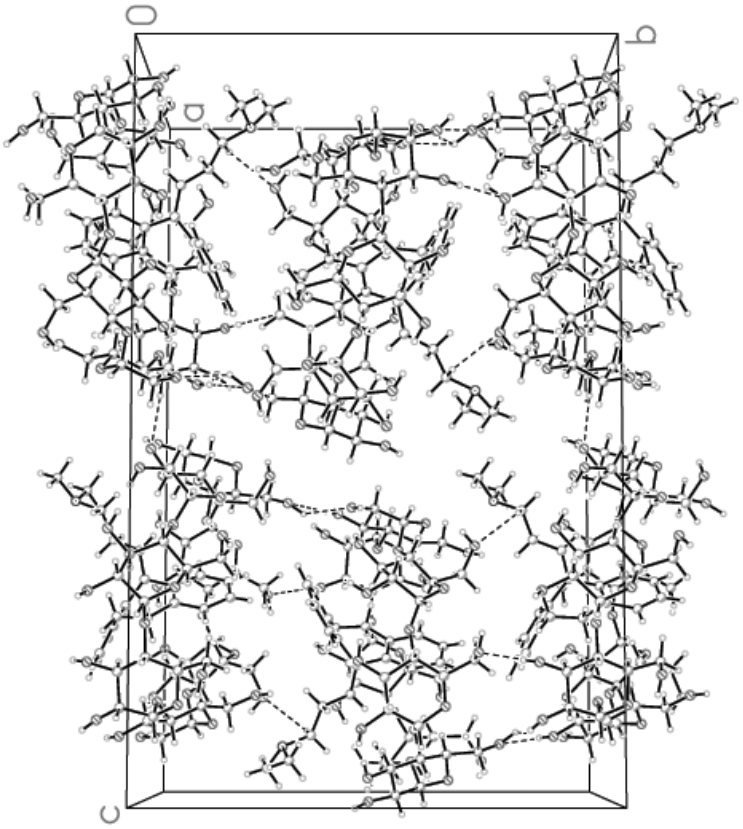

Figure S4: Packing diagram of complex **2**.