Supplementary Material (ESI) for Chemical Communications

Supramolecular stabilization of hydroxylamine TEMPOH by complexation with an amphiphilic calixarene

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Table 1. Crystal data and structure refinement for Gena34.

Identification code	gena34	
Empirical formula	C63 H91 N O11	
Formula weight	1038.37	
Temperature	125(2) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.4572(18) Å	α= 90°.
	b = 22.041(4) Å	β= 95.870(3)°.
	c = 24.899(4) Å	γ = 90°.
Volume	5708.8(17) $Å^3$	
Z	4	
Density (calculated)	1.208 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	2256	
Crystal size	0.50 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.64 to 29.57°.	
Index ranges	-14<=h<=14, -30<=k<=30, -34<=l<=34	
Reflections collected	70995	
Independent reflections	15946 [R(int) = 0.0425]	
Completeness to theta = 29.57°	99.5 %	
Absorption correction	Multiscan	
Max. and min. transmission	0.9919 and 0.9605	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15946 / 9 / 729	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0513, wR2 = 0.1338	
R indices (all data)	R1 = 0.0801, wR2 = 0.1559	
Largest diff. peak and hole	0.952 and -0.522 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Gena34. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(11)	-1474(2)	7467(1)	6921(1)	45(1)
C(62)	-2762(3)	7741(1)	6955(1)	47(1)
C(63)	-3602(3)	7680(1)	6430(1)	44(1)
O(11A)	-2253(9)	8215(3)	7191(3)	45(1)
C(62A)	-2499(13)	7697(7)	6856(5)	47(1)
C(63A)	-3786(14)	7790(7)	6532(6)	44(1)
O(11B)	-404(8)	7424(4)	6990(3)	45(1)
C(62B)	-1699(11)	7526(9)	6860(6)	47(1)
C(63B)	-2981(12)	7753(6)	7088(6)	44(1)
O(1)	3224(1)	8377(1)	9344(1)	27(1)
O(2)	3365(1)	8444(1)	10507(1)	23(1)
O(3)	3280(1)	7232(1)	10275(1)	23(1)
O(4)	3595(1)	7259(1)	9251(1)	21(1)
O(5)	-1208(1)	9272(1)	7632(1)	47(1)
O(6)	-2544(1)	9109(1)	10301(1)	27(1)
O(7)	-879(1)	5227(1)	10637(1)	36(1)
O(8)	-897(1)	6336(1)	7533(1)	39(1)
O(9)	-4237(1)	7151(1)	8848(1)	31(1)
O(10)	-4332(1)	8255(1)	9871(1)	32(1)
N(1)	-3246(1)	7445(1)	9184(1)	21(1)
C(1)	2087(1)	7262(1)	8456(1)	20(1)
C(2)	2537(1)	7878(1)	8280(1)	22(1)
C(3)	1859(1)	8416(1)	8508(1)	20(1)
C(4)	878(1)	8716(1)	8203(1)	21(1)
C(5)	297(1)	9233(1)	8395(1)	20(1)
C(6)	706(1)	9444(1)	8914(1)	20(1)
C(7)	1669(1)	9145(1)	9239(1)	19(1)
C(8)	2108(1)	9348(1)	9810(1)	19(1)
C(9)	1451(1)	8990(1)	10225(1)	18(1)
C(10)	167(1)	9098(1)	10283(1)	19(1)
C(11)	-489(1)	8779(1)	10652(1)	20(1)
C(12)	144(1)	8311(1)	10949(1)	20(1)

C(13)	1411(1)	8164(1)	10881(1)	19(1)
C(14)	2023(1)	7611(1)	11167(1)	21(1)
C(15)	1681(1)	7026(1)	10859(1)	20(1)
C(16)	706(1)	6653(1)	11008(1)	21(1)
C(17)	357(1)	6123(1)	10722(1)	20(1)
C(18)	1007(1)	5971(1)	10277(1)	20(1)
C(19)	1981(1)	6330(1)	10115(1)	20(1)
C(20)	2678(1)	6138(1)	9634(1)	21(1)
C(21)	2157(1)	6424(1)	9105(1)	20(1)
C(22)	1183(1)	6138(1)	8778(1)	21(1)
C(23)	656(1)	6395(1)	8291(1)	22(1)
C(24)	1121(1)	6959(1)	8141(1)	22(1)
C(25)	2249(1)	8636(1)	9029(1)	20(1)
C(26)	2079(1)	8525(1)	10537(1)	19(1)
C(27)	2309(1)	6862(1)	10408(1)	20(1)
C(28)	2629(1)	6986(1)	8941(1)	19(1)
C(29)	-743(1)	9530(1)	8037(1)	25(1)
C(30)	-1210(1)	10157(1)	8173(1)	25(1)
C(31)	-2275(1)	10385(1)	7759(1)	24(1)
C(32)	-2774(1)	11013(1)	7878(1)	25(1)
C(33)	-3841(1)	11213(1)	7452(1)	28(1)
C(34)	-4361(2)	11839(1)	7559(1)	35(1)
C(35)	-1862(1)	8928(1)	10699(1)	22(1)
C(36)	-2364(1)	8858(1)	11240(1)	34(1)
C(37)	-3706(1)	9119(1)	11278(1)	33(1)
C(38)	-3698(1)	9814(1)	11259(1)	34(1)
C(39)	-4967(2)	10122(1)	11333(1)	38(1)
C(40)	-5975(2)	10033(1)	10862(1)	46(1)
C(41)	-684(1)	5711(1)	10870(1)	24(1)
C(42)	-1479(1)	5903(1)	11313(1)	26(1)
C(43)	-2566(1)	5469(1)	11415(1)	25(1)
C(44)	-3720(1)	5482(1)	10990(1)	25(1)
C(45)	-4747(1)	5025(1)	11108(1)	28(1)
C(46)	-5957(2)	5070(1)	10714(1)	42(1)
C(47)	-388(1)	6092(1)	7941(1)	25(1)
C(48)	-811(1)	5467(1)	8105(1)	26(1)
C(49)	-1938(1)	5195(1)	7754(1)	30(1)

C(50)	-2312(1)	4577(1)	7964(1)	30(1)
C(51)	-3474(2)	4289(1)	7644(1)	36(1)
C(52)	-3906(2)	3708(1)	7900(1)	55(1)
C(53)	-2486(1)	7851(1)	8827(1)	26(1)
C(54)	-1411(1)	8144(1)	9199(1)	27(1)
C(55)	-593(1)	7692(1)	9545(1)	26(1)
C(56)	-1444(1)	7334(1)	9891(1)	25(1)
C(57)	-2517(1)	6984(1)	9565(1)	23(1)
C(58)	-1975(1)	7489(1)	8374(1)	37(1)
C(59)	-3430(2)	8331(1)	8586(1)	40(1)
C(60)	-2007(1)	6455(1)	9255(1)	35(1)
C(61)	-3490(1)	6749(1)	9929(1)	32(1)

Table 3. Bond lengths [Å] and angles [°] for Gena34.

O(11)-C(62)	1.486(3)
C(62)-C(63)	1.504(3)
O(11A)-C(62A)	1.422(13)
C(62A)-C(63A)	1.511(15)
O(11B)-C(62B)	1.379(13)
C(62B)-C(63B)	1.589(14)
O(1)-C(25)	1.3478(14)
O(2)-C(26)	1.3655(15)
O(3)-C(27)	1.3690(15)
O(4)-C(28)	1.3475(14)
O(5)-C(29)	1.2151(16)
O(6)-C(35)	1.2263(15)
O(7)-C(41)	1.2194(16)
O(8)-C(47)	1.2234(16)
O(9)-N(1)	1.4199(13)
N(1)-C(57)	1.5371(16)
N(1)-C(53)	1.5388(17)
C(1)-C(24)	1.3857(17)
C(1)-C(28)	1.4169(17)
C(1)-C(2)	1.5184(16)
C(2)-C(3)	1.5200(16)
C(3)-C(4)	1.3818(17)
C(3)-C(25)	1.4043(16)
C(4)-C(5)	1.4002(17)
C(5)-C(6)	1.3981(16)
C(5)-C(29)	1.4868(17)
C(6)-C(7)	1.3920(16)
C(7)-C(25)	1.4020(16)
C(7)-C(8)	1.5157(16)
C(8)-C(9)	1.5198(16)
C(9)-C(10)	1.3852(17)
C(9)-C(26)	1.4071(16)
C(10)-C(11)	1.3931(17)
C(11)-C(12)	1.3960(16)
C(11)-C(35)	1.4892(17)

C(12)-C(13)	1.3905(17)
C(13)-C(26)	1.4055(17)
C(13)-C(14)	1.5209(16)
C(14)-C(15)	1.5232(16)
C(15)-C(16)	1.3890(17)
C(15)-C(27)	1.4048(17)
C(16)-C(17)	1.3987(16)
C(17)-C(18)	1.3973(17)
C(17)-C(41)	1.4927(17)
C(18)-C(19)	1.3845(17)
C(19)-C(27)	1.4056(16)
C(19)-C(20)	1.5238(17)
C(20)-C(21)	1.5113(17)
C(21)-C(22)	1.3887(16)
C(21)-C(28)	1.4075(17)
C(22)-C(23)	1.3980(17)
C(23)-C(24)	1.4001(17)
C(23)-C(47)	1.4851(17)
C(29)-C(30)	1.5150(18)
C(30)-C(31)	1.5250(17)
C(31)-C(32)	1.5193(18)
C(32)-C(33)	1.5245(18)
C(33)-C(34)	1.516(2)
C(35)-C(36)	1.5016(19)
C(36)-C(37)	1.529(2)
C(37)-C(38)	1.533(2)
C(38)-C(39)	1.519(2)
C(39)-C(40)	1.508(2)
C(41)-C(42)	1.5088(18)
C(42)-C(43)	1.5264(18)
C(43)-C(44)	1.5225(18)
C(44)-C(45)	1.5228(18)
C(45)-C(46)	1.524(2)
C(47)-C(48)	1.5154(19)
C(48)-C(49)	1.5161(18)
C(49)-C(50)	1.5262(19)
C(50)-C(51)	1.521(2)

C(51)-C(52)	1.519(2)
C(53)-C(58)	1.521(2)
C(53)-C(54)	1.5248(18)
C(53)-C(59)	1.528(2)
C(54)-C(55)	1.5219(19)
C(55)-C(56)	1.5205(19)
C(56)-C(57)	1.5254(17)
C(57)-C(61)	1.5224(19)
C(57)-C(60)	1.5243(19)

O(11)-C(62)-C(63)	111.54(19)
O(11A)-C(62A)-C(63A)	107.6(11)
O(11B)-C(62B)-C(63B)	144.2(13)
O(9)-N(1)-C(57)	110.35(9)
O(9)-N(1)-C(53)	108.26(9)
C(57)-N(1)-C(53)	119.17(9)
C(24)-C(1)-C(28)	118.80(11)
C(24)-C(1)-C(2)	119.76(11)
C(28)-C(1)-C(2)	121.44(11)
C(1)-C(2)-C(3)	114.80(10)
C(4)-C(3)-C(25)	118.11(11)
C(4)-C(3)-C(2)	121.06(11)
C(25)-C(3)-C(2)	120.79(11)
C(3)-C(4)-C(5)	121.72(11)
C(6)-C(5)-C(4)	118.98(11)
C(6)-C(5)-C(29)	123.03(11)
C(4)-C(5)-C(29)	117.98(10)
C(7)-C(6)-C(5)	120.95(11)
C(6)-C(7)-C(25)	118.48(11)
C(6)-C(7)-C(8)	122.42(10)
C(25)-C(7)-C(8)	119.10(10)
C(7)-C(8)-C(9)	111.71(9)
C(10)-C(9)-C(26)	118.10(11)
C(10)-C(9)-C(8)	119.41(10)
C(26)-C(9)-C(8)	122.39(11)
C(9)-C(10)-C(11)	121.99(11)
C(10)-C(11)-C(12)	118.89(11)

C(10)-C(11)-C(35)	118.96(10)
C(12)-C(11)-C(35)	122.08(11)
C(13)-C(12)-C(11)	120.89(11)
C(12)-C(13)-C(26)	118.84(11)
C(12)-C(13)-C(14)	119.27(11)
C(26)-C(13)-C(14)	121.87(11)
C(13)-C(14)-C(15)	112.06(9)
C(16)-C(15)-C(27)	118.54(11)
C(16)-C(15)-C(14)	120.41(11)
C(27)-C(15)-C(14)	121.02(11)
C(15)-C(16)-C(17)	121.27(11)
C(18)-C(17)-C(16)	118.78(11)
C(18)-C(17)-C(41)	118.40(11)
C(16)-C(17)-C(41)	122.82(11)
C(19)-C(18)-C(17)	121.76(11)
C(18)-C(19)-C(27)	118.29(11)
C(18)-C(19)-C(20)	119.71(10)
C(27)-C(19)-C(20)	122.00(11)
C(21)-C(20)-C(19)	114.12(10)
C(22)-C(21)-C(28)	119.13(11)
C(22)-C(21)-C(20)	119.89(11)
C(28)-C(21)-C(20)	120.97(10)
C(21)-C(22)-C(23)	121.68(11)
C(22)-C(23)-C(24)	118.32(11)
C(22)-C(23)-C(47)	121.88(11)
C(24)-C(23)-C(47)	119.79(11)
C(1)-C(24)-C(23)	121.87(11)
O(1)-C(25)-C(7)	116.80(10)
O(1)-C(25)-C(3)	121.44(11)
C(7)-C(25)-C(3)	121.73(11)
O(2)-C(26)-C(13)	120.90(10)
O(2)-C(26)-C(9)	118.12(11)
C(13)-C(26)-C(9)	120.96(11)
O(3)-C(27)-C(15)	117.39(10)
O(3)-C(27)-C(19)	121.23(11)
C(15)-C(27)-C(19)	121.35(11)
O(4)-C(28)-C(21)	119.39(10)

O(4)-C(28)-C(1)	120.45(10)
C(21)-C(28)-C(1)	120.16(11)
O(5)-C(29)-C(5)	119.84(12)
O(5)-C(29)-C(30)	120.25(12)
C(5)-C(29)-C(30)	119.90(10)
C(29)-C(30)-C(31)	112.21(10)
C(32)-C(31)-C(30)	114.16(10)
C(31)-C(32)-C(33)	111.61(10)
C(34)-C(33)-C(32)	112.98(11)
O(6)-C(35)-C(11)	119.61(11)
O(6)-C(35)-C(36)	122.02(12)
C(11)-C(35)-C(36)	118.36(11)
C(35)-C(36)-C(37)	115.09(12)
C(36)-C(37)-C(38)	111.48(12)
C(39)-C(38)-C(37)	115.78(13)
C(40)-C(39)-C(38)	113.30(13)
O(7)-C(41)-C(17)	120.33(12)
O(7)-C(41)-C(42)	120.97(12)
C(17)-C(41)-C(42)	118.70(11)
C(41)-C(42)-C(43)	114.90(11)
C(44)-C(43)-C(42)	115.03(10)
C(43)-C(44)-C(45)	112.13(10)
C(44)-C(45)-C(46)	112.81(12)
O(8)-C(47)-C(23)	121.45(12)
O(8)-C(47)-C(48)	120.63(12)
C(23)-C(47)-C(48)	117.92(11)
C(47)-C(48)-C(49)	115.72(11)
C(48)-C(49)-C(50)	111.47(11)
C(51)-C(50)-C(49)	114.36(12)
C(52)-C(51)-C(50)	112.82(13)
C(58)-C(53)-C(54)	112.24(11)
C(58)-C(53)-C(59)	109.47(12)
C(54)-C(53)-C(59)	110.58(12)
C(58)-C(53)-N(1)	111.43(12)
C(54)-C(53)-N(1)	106.74(10)
C(59)-C(53)-N(1)	106.20(11)
C(55)-C(54)-C(53)	113.80(11)

C(56)-C(55)-C(54)	109.44(11)
C(55)-C(56)-C(57)	113.76(11)
C(61)-C(57)-C(60)	109.34(11)
C(61)-C(57)-C(56)	110.80(11)
C(60)-C(57)-C(56)	112.36(11)
C(61)-C(57)-N(1)	105.83(10)
C(60)-C(57)-N(1)	111.76(11)
C(56)-C(57)-N(1)	106.54(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Gena34. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(11)	53(1)	33(1)	49(1)	7(1)	10(1)	5(1)
C(62)	59(1)	58(1)	30(1)	3(1)	31(1)	5(1)
C(63)	58(1)	32(1)	41(1)	5(1)	3(1)	-1(1)
O(11A)	53(1)	33(1)	49(1)	7(1)	10(1)	5(1)
C(62A)	59(1)	58(1)	30(1)	3(1)	31(1)	5(1)
C(63A)	58(1)	32(1)	41(1)	5(1)	3(1)	-1(1)
O(11B)	53(1)	33(1)	49(1)	7(1)	10(1)	5(1)
C(62B)	59(1)	58(1)	30(1)	3(1)	31(1)	5(1)
C(63B)	58(1)	32(1)	41(1)	5(1)	3(1)	-1(1)
O(1)	25(1)	20(1)	33(1)	-6(1)	-7(1)	5(1)
O(2)	17(1)	19(1)	33(1)	1(1)	-2(1)	0(1)
O(3)	22(1)	20(1)	29(1)	-3(1)	3(1)	-5(1)
O(4)	15(1)	19(1)	30(1)	-3(1)	1(1)	-2(1)
O(5)	63(1)	38(1)	35(1)	-14(1)	-21(1)	23(1)
O(6)	22(1)	30(1)	28(1)	0(1)	-2(1)	0(1)
O(7)	42(1)	23(1)	44(1)	-8(1)	17(1)	-11(1)
O(8)	48(1)	36(1)	31(1)	1(1)	-11(1)	-10(1)
O(9)	14(1)	52(1)	26(1)	-12(1)	-1(1)	-5(1)
O(10)	18(1)	36(1)	40(1)	-12(1)	0(1)	1(1)
N(1)	14(1)	29(1)	20(1)	-3(1)	0(1)	0(1)
C(1)	19(1)	17(1)	25(1)	-3(1)	7(1)	2(1)
C(2)	22(1)	19(1)	25(1)	-1(1)	7(1)	0(1)
C(3)	20(1)	17(1)	23(1)	0(1)	6(1)	-2(1)
C(4)	25(1)	19(1)	19(1)	0(1)	4(1)	-1(1)
C(5)	23(1)	18(1)	20(1)	1(1)	3(1)	0(1)
C(6)	21(1)	16(1)	22(1)	1(1)	3(1)	-1(1)
C(7)	19(1)	16(1)	22(1)	0(1)	2(1)	-3(1)
C(8)	20(1)	15(1)	22(1)	-1(1)	1(1)	-1(1)
C(9)	21(1)	14(1)	20(1)	-3(1)	-1(1)	-2(1)
C(10)	21(1)	17(1)	20(1)	-2(1)	-2(1)	1(1)
C(11)	20(1)	18(1)	21(1)	-4(1)	0(1)	-1(1)
C(12)	22(1)	19(1)	20(1)	-2(1)	0(1)	-2(1)

C(13)	22(1)	15(1)	18(1)	-2(1)	-3(1)	-1(1)
C(14)	24(1)	16(1)	21(1)	-1(1)	-3(1)	0(1)
C(15)	21(1)	16(1)	21(1)	1(1)	-4(1)	1(1)
C(16)	23(1)	19(1)	20(1)	2(1)	-2(1)	1(1)
C(17)	21(1)	17(1)	23(1)	2(1)	0(1)	0(1)
C(18)	22(1)	15(1)	23(1)	-1(1)	-2(1)	0(1)
C(19)	19(1)	16(1)	23(1)	0(1)	-1(1)	2(1)
C(20)	19(1)	16(1)	27(1)	-2(1)	1(1)	1(1)
C(21)	17(1)	17(1)	25(1)	-3(1)	3(1)	1(1)
C(22)	18(1)	18(1)	26(1)	-4(1)	5(1)	-1(1)
C(23)	19(1)	22(1)	24(1)	-5(1)	4(1)	0(1)
C(24)	21(1)	22(1)	23(1)	-3(1)	3(1)	3(1)
C(25)	18(1)	18(1)	23(1)	1(1)	1(1)	-2(1)
C(26)	18(1)	17(1)	22(1)	-4(1)	-2(1)	-2(1)
C(27)	17(1)	17(1)	25(1)	2(1)	-2(1)	0(1)
C(28)	14(1)	18(1)	26(1)	-5(1)	4(1)	1(1)
C(29)	29(1)	23(1)	22(1)	0(1)	0(1)	4(1)
C(30)	28(1)	23(1)	24(1)	0(1)	-2(1)	6(1)
C(31)	25(1)	22(1)	23(1)	1(1)	0(1)	3(1)
C(32)	27(1)	24(1)	23(1)	1(1)	0(1)	4(1)
C(33)	27(1)	28(1)	28(1)	3(1)	-1(1)	4(1)
C(34)	36(1)	32(1)	38(1)	8(1)	4(1)	11(1)
C(35)	21(1)	18(1)	26(1)	-1(1)	1(1)	-2(1)
C(36)	27(1)	43(1)	34(1)	12(1)	8(1)	7(1)
C(37)	24(1)	42(1)	36(1)	9(1)	10(1)	0(1)
C(38)	29(1)	41(1)	34(1)	-1(1)	6(1)	-2(1)
C(39)	36(1)	39(1)	39(1)	-6(1)	4(1)	0(1)
C(40)	41(1)	42(1)	52(1)	-6(1)	-8(1)	1(1)
C(41)	25(1)	19(1)	26(1)	2(1)	1(1)	-1(1)
C(42)	28(1)	25(1)	24(1)	0(1)	3(1)	-4(1)
C(43)	27(1)	27(1)	22(1)	3(1)	2(1)	-3(1)
C(44)	26(1)	24(1)	23(1)	2(1)	2(1)	-2(1)
C(45)	28(1)	26(1)	31(1)	2(1)	4(1)	-3(1)
C(46)	32(1)	53(1)	39(1)	0(1)	-1(1)	-12(1)
C(47)	26(1)	26(1)	25(1)	-6(1)	2(1)	-2(1)
C(48)	25(1)	27(1)	27(1)	-4(1)	0(1)	-5(1)
C(49)	28(1)	29(1)	31(1)	-4(1)	-2(1)	-7(1)

C(50)	32(1)	28(1)	29(1)	-2(1)	0(1)	-7(1)
C(51)	39(1)	35(1)	33(1)	-7(1)	3(1)	-13(1)
C(52)	74(1)	46(1)	46(1)	-10(1)	10(1)	-29(1)
C(53)	19(1)	36(1)	22(1)	4(1)	4(1)	1(1)
C(54)	23(1)	28(1)	30(1)	3(1)	4(1)	-3(1)
C(55)	18(1)	29(1)	32(1)	-4(1)	-1(1)	-3(1)
C(56)	20(1)	27(1)	25(1)	2(1)	-4(1)	-1(1)
C(57)	19(1)	23(1)	28(1)	1(1)	0(1)	0(1)
C(58)	25(1)	60(1)	25(1)	-5(1)	7(1)	-1(1)
C(59)	33(1)	50(1)	36(1)	18(1)	4(1)	10(1)
C(60)	27(1)	27(1)	51(1)	-10(1)	5(1)	0(1)
C(61)	28(1)	34(1)	34(1)	6(1)	5(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Gena34.

	x	y	z	U(eq)
H(11)	-1290(30)	7130(13)	7134(12)	61(8)
H(62A)	-2661	8176	7049	56
H(62B)	-3182	7539	7245	56
H(63A)	-3116	7802	6131	53
H(63B)	-4358	7942	6436	53
H(63C)	-3878	7257	6380	53
H(11A)	-1591	8154	7405	67
H(62C)	-2518	7326	7080	56
H(62D)	-1816	7650	6612	56
H(63D)	-4183	8162	6652	53
H(63E)	-4346	7444	6585	53
H(63F)	-3663	7826	6148	53
H(11B)	-232	7061	6924	67
H(62E)	-1978	7125	6710	56
H(62F)	-1683	7790	6539	56
H(63G)	-3681	7468	6979	53
H(63H)	-3207	8156	6942	53
H(63I)	-2846	7773	7483	53
H(4)	3314(18)	8015(9)	9270(8)	49(5)
H(6)	3514(16)	8065(8)	10490(7)	35(4)
H(3)	3398(18)	7202(8)	9926(8)	45(5)
H(5)	-4940(20)	7171(10)	9016(9)	68(7)
H(101)	-5110(20)	8381(9)	9802(8)	56(6)
H(102)	-3880(20)	8559(10)	10013(9)	72(7)
H(2)	-3629(15)	7709(7)	9403(6)	24(4)
H(2A)	2409	7899	7881	26
H(2B)	3471	7914	8390	26
H(4)	590	8567	7853	25
H(6)	321	9797	9047	24
H(8A)	1913	9785	9847	23
H(8B)	3050	9295	9880	23

H(10)	-279	9399	10064	23
H(12)	-296	8089	11201	24
H(14A)	1730	7581	11532	25
H(14B)	2968	7660	11210	25
H(16)	268	6761	11310	25
H(18)	773	5610	10081	24
H(20A)	3599	6244	9708	25
H(20B)	2620	5691	9597	25
H(22)	867	5759	8888	25
H(24)	765	7139	7812	26
H(30A)	-479	10444	8192	30
H(30B)	-1533	10145	8533	30
H(31A)	-1948	10392	7399	28
H(31B)	-3000	10095	7740	28
H(32A)	-2057	11308	7891	30
H(32B)	-3106	11010	8237	30
H(33A)	-3505	11213	7094	33
H(33B)	-4553	10916	7439	33
H(34A)	-5027	11947	7269	42
H(34B)	-3661	12136	7573	42
H(34C)	-4731	11837	7905	42
H(36A)	-1756	9059	11515	41
H(36B)	-2377	8421	11330	41
H(37A)	-4024	8984	11619	40
H(37B)	-4301	8962	10975	40
H(38A)	-3042	9963	11543	41
H(38B)	-3427	9942	10906	41
H(39A)	-5298	9960	11663	45
H(39B)	-4815	10562	11388	45
H(40A)	-6741	10271	10919	55
H(40B)	-6204	9602	10831	55
H(40C)	-5634	10167	10529	55
H(42A)	-1854	6307	11221	31
H(42B)	-904	5947	11652	31
H(43A)	-2219	5051	11438	30
H(43B)	-2863	5568	11770	30
H(44A)	-3431	5392	10632	29

H(44B)	-4098	5894	10974	29
H(45A)	-4978	5093	11479	34
H(45B)	-4389	4611	11093	34
H(46A)	-6582	4766	10807	50
H(46B)	-5737	4995	10346	50
H(46C)	-6329	5476	10734	50
H(48A)	-1041	5489	8481	32
H(48B)	-70	5187	8104	32
H(49A)	-1707	5152	7380	36
H(49B)	-2683	5473	7746	36
H(50A)	-1569	4298	7959	36
H(50B)	-2494	4621	8344	36
H(51A)	-4193	4583	7615	43
H(51B)	-3259	4198	7274	43
H(52A)	-4667	3548	7684	66
H(52B)	-4118	3794	8267	66
H(52C)	-3212	3408	7915	66
H(54A)	-848	8375	8976	32
H(54B)	-1794	8436	9438	32
H(55A)	-160	7412	9311	31
H(55B)	76	7911	9780	31
H(56A)	-1832	7618	10136	30
H(56B)	-903	7044	10116	30
H(58A)	-2647	7215	8214	44
H(58B)	-1227	7251	8520	44
H(58C)	-1722	7768	8097	44
H(59A)	-3854	8523	8875	48
H(59B)	-4077	8139	8328	48
H(59C)	-2963	8639	8399	48
H(60A)	-2665	6327	8969	42
H(60B)	-1796	6116	9502	42
H(60C)	-1234	6583	9094	42
H(61A)	-4147	6509	9715	38
H(61B)	-3899	7093	10094	38
H(61C)	-3051	6494	10213	38

Table 6. Hydrogen bonds for Gena34 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(10)-H(101)...O(1)#1	0.86(2)	1.98(2)	2.7644(14)	150.5(19)
O(11A)-H(11A)...O(5)	0.84	2.55	2.753(8)	95.0
O(11B)-H(11B)...O(8)	0.84	2.36	2.825(8)	115.9
O(11)-H(11)...O(8)	0.92(3)	2.03(3)	2.952(2)	174(3)
N(1)-H(2)...O(10)	0.917(15)	1.877(15)	2.7929(15)	177.1(14)
O(10)-H(102)...O(6)	0.87(2)	1.93(2)	2.7892(14)	167(2)
O(9)-H(5)...O(4)	0.89(2)	1.70(15)	2.581(8)	171.2(18)
O(2)-H(6)...O(3)	0.852(17)	1.920(17)	2.7320(13)	158.8(16)
O(3)-H(3)...O(4)	0.891(19)	1.720(19)	2.6047(13)	171.5(18)
O(1)-H(4)...O(4)	0.83(2)	1.70(2)	2.5108(13)	168.7(19)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z