APPENDIX

Table A-1.1. Crystal data and structure refinement for HEDP·H_2O.

Identification code	HEDP·H_2O	
Empirical formula	$C_2 H_{10} O_8 P_2$	
Formula weight	224.04	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 6.9878(7) Å	a = 90º
	b = 17.5810(18) Å	b = 108.451(2)º
	c = 7.1140(8) Å	g = 90º
Volume	829.05(15) $Å^3$	
Z	4	
Density (calculated)	1.795 Mg/m^3	
Absorption coefficient	0.535 mm^{-1}	
F(000)	464	
Crystal size	0.68 x 0.32 x 0.30 mm^3	
Theta range for data collection	3.07 to 26.60º.	
Index ranges	-7<=h<=8, -21<=k<=8, -8<=l<=8	
Reflections collected	4 313	
Independent reflections	1 571 [R(int) = 0.0292]	
Completeness to theta = 25.00º	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.852 and 0.746	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1571 / 0 / 150	
Goodness-of-fit on F^2	1.094	
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0844	
R indices (all data)	R1 = 0.0319, wR2 = 0.0846	
Extinction coefficient	0.015(3)	
Largest diff. peak and hole	0.422 and -0.389 e.$Å^{-3}$	

Table A-1.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for HEDP·H_2O. U(eq) is defined as one-third of the trace of the orthogonalised U^{ij} tensor

	x	y	z	U(eq)
P(1)	1978(1)	5911(1)	5422(1)	21(1)
P(2)	3784(1)	6334(1)	2130(1)	22(1)
O(1)	2564(2)	5093(1)	5381(2)	28(1)
O(2)	-11(2)	6021(1)	5933(2)	31(1)
O(3)	3580(2)	6406(1)	6881(2)	29(1)
O(4)	4302(3)	5491(1)	1918(2)	34(1)
O(5)	3244(2)	6724(1)	163(2)	29(1)
O(6)	5505(2)	6730(1)	3730(2)	31(1)
O(7)	996(2)	7129(1)	3063(2)	27(1)
O(8)	7375(3)	7743(1)	2758(3)	36(1)
C(1)	1572(3)	6349(1)	2991(3)	21(1)
C(2)	-187(3)	5943(1)	1466(3)	30(1)

Table A-1.3. Bond lengths [Å] and angles [º] for HEDP·H_2O

LENGTHS:			
P(1)-O(1)	1.4980(13)	O(5)-P(2)-O(6)	113.12(8)
P(1)-O(3)	1.5337(14)	O(5)-P(2)-O(4)	110.22(8)
P(1)-O(2)	1.5559(14)	O(6)-P(2)-O(4)	110.73(9)
P(1)-C(1)	1.8309(18)	O(5)-P(2)-C(1)	108.47(8)
P(2)-O(5)	1.4952(13)	O(6)-P(2)-C(1)	106.92(8)
P(2)-O(6)	1.5361(14)	O(4)-P(2)-C(1)	107.12(8)
P(2)-O(4)	1.5445(15)	P(1)-O(2)-H(2)	112(2)
P(2)-C(1)	1.8342(19)	P(1)-O(3)-H(3)	113(3)
O(2)-H(2)	0.77(3)	P(2)-O(4)-H(4)	113(3)
O(3)-H(3)	0.77(4)	P(2)-O(6)-H(6)	115(2)
O(4)-H(4)	0.73(4)	C(1)-O(7)-H(7)	115.9(19)
O(6)-H(6)	1.04(4)	H(6)-O(8)-H(8A)	111(3)
O(7)-C(1)	1.435(2)	H(6)-O(8)-H(8B)	107(3)
O(7)-H(7)	0.79(3)	H(8A)-O(8)-H(8B)	113(3)
O(8)-H(6)	1.40(4)	O(7)-C(1)-C(2)	107.36(14)
O(8)-H(8A)	0.76(3)	O(7)-C(1)-P(1)	109.25(12)
O(8)-H(8B)	0.73(4)	C(2)-C(1)-P(1)	108.83(13)
C(1)-C(2)	1.534(2)	O(7)-C(1)-P(2)	107.47(11)
C(2)-H(2A)	0.98(3)	C(2)-C(1)-P(2)	109.19(13)
C(2)-H(2B)	1.01(3)	P(1)-C(1)-P(2)	114.50(9)
C(2)-H(2C)	0.93(3)	C(1)-C(2)-H(2A)	110.7(15)
		C(1)-C(2)-H(2B)	109.5(16)
ANGLES:		H(2A)-C(2)-H(2B)	108(2)
O(1)-P(1)-O(3)	114.35(8)	C(1)-C(2)-H(2C)	108.3(17)
O(1)-P(1)-O(2)	113.19(8)	H(2A)-C(2)-H(2C)	105(2)
O(3)-P(1)-O(2)	106.60(8)	H(2B)-C(2)-H(2C)	115(2)
O(1)-P(1)-C(1)	110.29(8)		
O(3)-P(1)-C(1)	105.21(8)		
O(2)-P(1)-C(1)	106.61(8)		

Table A-1.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $HEDP{\cdot}H_2O$. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	22(1)	21(1)	21(1)	0(1)	7(1)	-2(1)
P(2)	24(1)	24(1)	18(1)	1(1)	7(1)	3(1)
O(1)	28(1)	23(1)	33(1)	4(1)	7(1)	1(1)
O(2)	28(1)	31(1)	39(1)	-7(1)	17(1)	-5(1)
O(3)	30(1)	38(1)	22(1)	-6(1)	10(1)	-10(1)
O(4)	39(1)	30(1)	33(1)	-1(1)	9(1)	12(1)
O(5)	38(1)	30(1)	21(1)	3(1)	10(1)	5(1)
O(6)	26(1)	43(1)	24(1)	-1(1)	6(1)	-6(1)
O(7)	24(1)	20(1)	33(1)	-2(1)	5(1)	2(1)
O(8)	25(1)	39(1)	43(1)	5(1)	9(1)	1(1)
C(1)	22(1)	18(1)	21(1)	0(1)	5(1)	2(1)
C(2)	28(1)	30(1)	27(1)	-3(1)	0(1)	-4(1)

Table A-1.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for HEDP·H_2O

	x	y	z	U(eq)
H(2)	-740(50)	5683(18)	5580(50)	56(9)
H(2A)	-430(40)	6162(14)	150(40)	42(7)
H(2B)	-1460(40)	6008(15)	1840(40)	50(7)
H(2C)	190(40)	5440(16)	1360(40)	48(7)
H(3)	3390(60)	6450(20)	7880(60)	80(12)
H(4)	5120(60)	5350(20)	2760(50)	67(11)
H(6)	6230(60)	7160(20)	3210(50)	93(12)
H(7)	1780(40)	7388(15)	3830(40)	39(7)
H(8A)	8350(50)	7586(15)	2650(40)	42(8)
H(8B)	6730(50)	7930(20)	1860(50)	63(10)

Table A-1.6. Torsion angles [º] for HEDP·H_2O

O(1)-P(1)-C(1)-O(7)	179.52(11)
O(3)-P(1)-C(1)-O(7)	-56.70(13)
O(2)-P(1)-C(1)-O(7)	56.26(13)
O(1)-P(1)-C(1)-C(2)	62.57(14)
O(3)-P(1)-C(1)-C(2)	-173.64(13)
O(2)-P(1)-C(1)-C(2)	-60.68(14)
O(1)-P(1)-C(1)-P(2)	-59.91(11)
O(3)-P(1)-C(1)-P(2)	63.88(11)
O(2)-P(1)-C(1)-P(2)	176.84(9)
O(5)-P(2)-C(1)-O(7)	-57.17(13)
O(6)-P(2)-C(1)-O(7)	65.12(13)
O(4)-P(2)-C(1)-O(7)	-176.13(11)
O(5)-P(2)-C(1)-C(2)	58.98(14)
O(6)-P(2)-C(1)-C(2)	-178.72(12)
O(4)-P(2)-C(1)-C(2)	-59.98(14)
O(5)-P(2)-C(1)-P(1)	-178.73(8)
O(6)-P(2)-C(1)-P(1)	-56.43(11)
O(4)-P(2)-C(1)-P(1)	62.31(12)

Table A-1.7. Hydrogen bonds for HEDP·H_2O [Å and º]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)#1	0.77(3)	1.84(3)	2.615(2)	177(3)
O(3)-H(3)...O(5)#2	0.77(4)	1.72(4)	2.4832(19)	169(4)
O(4)-H(4)...O(1)#3	0.73(4)	1.90(4)	2.623(2)	170(4)
O(6)-H(6)...O(8)	1.04(4)	1.40(4)	2.435(2)	173(3)
O(7)-H(7)...O(5)#4	0.79(3)	1.94(3)	2.699(2)	162(3)
O(8)-H(8A)...O(7)#5	0.76(3)	1.95(3)	2.696(2)	166(3)
O(8)-H(8B)...O(6)#6	0.73(4)	2.20(4)	2.899(2)	160(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 x,y,z+1 #3 -x+1,-y+1,-z+1

#4 x,-y+3/2,z+1/2 #5 x+1,y,z #6 x,-y+3/2,z-1/2

Table A-2.1. Crystal data and structure refinement for $CaHEDP{\cdot}2H_2O$

Identification code	$CaHEDP{\cdot}2H_2O$	
Empirical formula	$C_2\ H_{10}\ Ca\ O_9\ P_2$	
Formula weight	280.12	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P$\bar{1}$	
Unit cell dimensions	a = 6.9499(6) Å	a = 92.7330(10)º
	b = 7.5961(6) Å	b = 106.3140(10)º
	c = 9.7000(8) Å	g = 112.4250(10)º
Volume	447.33(6) $Å^3$	
Z	2	
Density (calculated)	2.080 Mg/m^3	
Absorption coefficient	1.087 mm^{-1}	
F(000)	288	
Crystal size	0.30 x 0.22 x 0.18 mm^3	
Theta range for data collection	2.95 to 26.41º.	
Index ranges	-5<=h<=8, -9<=k<=4, -11<=l<=10	
Reflections collected	2 442	
Independent reflections	1622 [R(int) = 0.0200]	
Completeness to theta = 25.00º	97.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.822 and 0.707	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1622 / 0 / 163	
Goodness-of-fit on F^2	1.115	
Final R indices [I>2sigma(I)]	R1 = 0.0339, wR2 = 0.0942	
R indices (all data)	R1 = 0.0344, wR2 = 0.0947	
Extinction coefficient	0	
Largest diff. peak and hole	0.841 and -0.537 $e.Å^{-3}$	

Table A-2.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CaHEDP·2H_2O. U(eq) is defined as one-third of the trace of the orthogonalised U^{ij} tensor

	x	y	z	U(eq)
Ca(1)	4077(1)	7051(1)	-147(1)	14(1)
P(1)	-166(1)	7575(1)	1252(1)	13(1)
O(1)	1074(3)	7498(3)	230(2)	19(1)
O(2)	-2637(3)	6484(2)	654(2)	17(1)
O(3)	335(3)	9740(3)	1828(2)	20(1)
P(2)	3609(1)	7030(1)	3444(1)	16(1)
O(4)	4035(3)	6130(2)	2211(2)	18(1)
O(5)	4829(3)	9255(2)	3765(2)	21(1)
O(6)	4106(3)	6190(3)	4844(2)	22(1)
C(1)	677(4)	6522(3)	2864(3)	16(1)
C(2)	-40(5)	7133(4)	4086(3)	21(1)
O(7)	-531(3)	4433(2)	2392(2)	20(1)
O(8)	3569(4)	9773(3)	-1459(2)	19(1)
O(9)	5753(3)	7331(3)	-2133(2)	20(1)

Table A-2.3. Bond lengths [Å] and angles [º] for CaHEDP·2H_2O

LENGTHS:

Ca(1)-O(1)	2.3580(17)	O(7)-Ca(1)#2	2.5919(18)
Ca(1)-O(2)#1	2.4064(16)	O(7)-H(7)	0.82(4)
Ca(1)-O(4)	2.4277(18)	O(8)-Ca(1)#3	2.4743(19)
Ca(1)-O(2)#2	2.4498(17)	O(8)-H(8A)	0.66(4)
Ca(1)-O(8)#3	2.4743(19)	O(8)-H(8B)	0.72(4)
Ca(1)-O(9)	2.4956(19)	O(9)-H(9A)	0.82(4)
Ca(1)-O(8)	2.564(2)	O(9)-H(9B)	0.73(4)
Ca(1)-O(7)#2	2.5919(18)		
Ca(1)-P(1)#2	3.4061(7)	ANGLES:	
Ca(1)-Ca(1)#4	3.7906(9)	O(1)-Ca(1)-O(2)#1	152.91(6)
Ca(1)-Ca(1)#3	4.1334(9)	O(1)-Ca(1)-O(4)	75.61(6)
Ca(1)-H(9A)	2.70(4)	O(2)#1-Ca(1)-O(4)	77.87(6)
P(1)-O(1)	1.4974(17)	O(1)-Ca(1)-O(2)#2	101.40(6)
P(1)-O(2)	1.5103(17)	O(2)#1-Ca(1)-O(2)#2	77.38(6)
P(1)-O(3)	1.5828(18)	O(4)-Ca(1)-O(2)#2	76.37(6)
P(1)-C(1)	1.842(2)	O(1)-Ca(1)-O(8)#3	86.48(7)
P(1)-Ca(1)#2	3.4061(7)	O(2)#1-Ca(1)-O(8)#3	83.63(6)
O(2)-Ca(1)#5	2.4064(16)	O(4)-Ca(1)-O(8)#3	80.04(7)
O(2)-Ca(1)#2	2.4498(17)	O(2)#2-Ca(1)-O(8)#3	152.27(6)
O(3)-H(3)	0.79(4)	O(1)-Ca(1)-O(9)	136.47(7)
P(2)-O(4)	1.5042(17)	O(2)#1-Ca(1)-O(9)	70.40(7)
P(2)-O(6)	1.5353(18)	O(4)-Ca(1)-O(9)	147.81(7)
P(2)-O(5)	1.5432(18)	O(2)#2-Ca(1)-O(9)	91.28(6)
P(2)-C(1)	1.831(2)	O(8)#3-Ca(1)-O(9)	101.24(7)
O(6)-H(6)	0.8200	O(1)-Ca(1)-O(8)	71.29(7)
C(1)-O(7)	1.460(3)	O(2)#1-Ca(1)-O(8)	127.47(7)
C(1)-C(2)	1.524(3)	O(4)-Ca(1)-O(8)	135.91(7)
C(2)-H(2A)	0.92(4)	O(2)#2-Ca(1)-O(8)	137.96(6)
C(2)-H(2B)	0.93(4)	O(8)#3-Ca(1)-O(8)	69.77(8)
C(2)-H(2C)	0.89(4)	O(9)-Ca(1)-O(8)	71.60(7)

O(1)-Ca(1)-O(7)#2 66.70(6)
O(2)#1-Ca(1)-O(7)#2 133.89(6)
O(4)-Ca(1)-O(7)#2 120.31(6)
O(2)#2-Ca(1)-O(7)#2 68.27(6)
O(8)#3-Ca(1)-O(7)#2 137.91(6)
O(9)-Ca(1)-O(7)#2 80.35(7)
O(8)-Ca(1)-O(7)#2 71.09(6)
O(1)-Ca(1)-P(1)#2 80.17(5)
O(2)#1-Ca(1)-P(1)#2 100.70(4)
O(4)-Ca(1)-P(1)#2 80.21(4)
O(2)#2-Ca(1)-P(1)#2 23.35(4)
O(8)#3-Ca(1)-P(1)#2 158.38(6)
O(9)-Ca(1)-P(1)#2 100.15(5)
O(8)-Ca(1)-P(1)#2 120.68(5)
O(7)#2-Ca(1)-P(1)#2 49.84(4)
O(1)-Ca(1)-Ca(1)#4 133.87(5)
O(2)#1-Ca(1)-Ca(1)#4 39.10(4)
O(4)-Ca(1)-Ca(1)#4 73.40(4)
O(2)#2-Ca(1)-Ca(1)#4 38.28(4)
O(8)#3-Ca(1)-Ca(1)#4 120.10(5)
O(9)-Ca(1)-Ca(1)#4 78.55(5)
O(8)-Ca(1)-Ca(1)#4 150.02(6)
O(7)#2-Ca(1)-Ca(1)#4 101.59(4)
P(1)#2-Ca(1)-Ca(1)#4 61.608(16)
O(1)-Ca(1)-Ca(1)#3 76.36(5)
O(2)#1-Ca(1)-Ca(1)#3 108.11(4)
O(4)-Ca(1)-Ca(1)#3 110.00(4)
O(2)#2-Ca(1)-Ca(1)#3 172.13(5)
O(8)#3-Ca(1)-Ca(1)#3 35.60(5)
O(9)-Ca(1)-Ca(1)#3 85.46(5)
O(8)-Ca(1)-Ca(1)#3 34.17(4)
O(7)#2-Ca(1)-Ca(1)#3 104.07(4)
P(1)#2-Ca(1)-Ca(1)#3 150.81(2)
Ca(1)#4-Ca(1)-Ca(1)#3 146.88(2)
O(1)-Ca(1)-H(9A) 148.2(9)
O(2)#1-Ca(1)-H(9A) 58.5(9)
O(4)-Ca(1)-H(9A) 132.4(9)
O(2)#2-Ca(1)-H(9A) 76.5(9)
O(8)#3-Ca(1)-H(9A) 110.3(8)
O(9)-Ca(1)-H(9A) 17.5(9)
O(8)-Ca(1)-H(9A) 88.9(9)
O(7)#2-Ca(1)-H(9A) 83.7(8)
P(1)#2-Ca(1)-H(9A) 89.6(8)
Ca(1)#4-Ca(1)-H(9A) 61.1(9)
Ca(1)#3-Ca(1)-H(9A) 101.3(9)
O(1)-P(1)-O(2) 116.26(10)
O(1)-P(1)-O(3) 110.84(11)
O(2)-P(1)-O(3) 107.13(10)
O(1)-P(1)-C(1) 110.61(10)
O(2)-P(1)-C(1) 104.59(10)
O(3)-P(1)-C(1) 106.85(10)
O(1)-P(1)-Ca(1)#2 97.26(7)
O(2)-P(1)-Ca(1)#2 40.00(6)
O(3)-P(1)-Ca(1)#2 145.53(7)
C(1)-P(1)-Ca(1)#2 80.00(8)
P(1)-O(1)-Ca(1) 147.91(10)
P(1)-O(2)-Ca(1)#5 140.64(10)
P(1)-O(2)-Ca(1)#2 116.65(9)
Ca(1)#5-O(2)-Ca(1)#2 102.62(6)
P(1)-O(3)-H(3) 113(3)
O(4)-P(2)-O(6) 113.28(10)
O(4)-P(2)-O(5) 112.30(10)
O(6)-P(2)-O(5) 110.56(10)
O(4)-P(2)-C(1) 107.60(11)
O(6)-P(2)-C(1) 107.14(11)
O(5)-P(2)-C(1) 105.47(10)
P(2)-O(4)-Ca(1) 130.26(10)
P(2)-O(6)-H(6) 109.5

O(7)-C(1)-C(2)	108.30(19)	C(1)-O(7)-Ca(1)#2	121.59(14)
O(7)-C(1)-P(2)	106.92(16)	C(1)-O(7)-H(7)	110(2)
C(2)-C(1)-P(2)	113.00(17)	Ca(1)#2-O(7)-H(7)	92(2)
O(7)-C(1)-P(1)	105.19(15)	Ca(1)#3-O(8)-Ca(1)	110.23(8)
C(2)-C(1)-P(1)	110.16(17)	Ca(1)#3-O(8)-H(8A)	104(3)
P(2)-C(1)-P(1)	112.81(12)	Ca(1)-O(8)-H(8A)	121(3)
C(1)-C(2)-H(2A)	108(2)	Ca(1)#3-O(8)-H(8B)	104(3)
C(1)-C(2)-H(2B)	111(2)	Ca(1)-O(8)-H(8B)	110(3)
H(2A)-C(2)-H(2B)	107(3)	H(8A)-O(8)-H(8B)	105(4)
C(1)-C(2)-H(2C)	111(2)	Ca(1)-O(9)-H(9A)	96(3)
H(2A)-C(2)-H(2C)	109(3)	Ca(1)-O(9)-H(9B)	116(3)
H(2B)-C(2)-H(2C)	111(3)	H(9A)-O(9)-H(9B)	105(4)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 -x,-y+1,-z #3 -x+1,-y+2,-z #4 -x+1,-y+1,-z #5 x-1,y,z

Table A-2.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $CaHEDP{\cdot}2H_2O$. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ca(1)	14(1)	14(1)	16(1)	2(1)	6(1)	6(1)
P(1)	11(1)	14(1)	14(1)	3(1)	5(1)	6(1)
O(1)	18(1)	26(1)	19(1)	7(1)	9(1)	12(1)
O(2)	12(1)	18(1)	19(1)	2(1)	4(1)	5(1)
O(3)	17(1)	14(1)	29(1)	2(1)	8(1)	6(1)
P(2)	14(1)	18(1)	15(1)	1(1)	4(1)	7(1)
O(4)	20(1)	19(1)	17(1)	3(1)	6(1)	12(1)
O(5)	22(1)	18(1)	20(1)	1(1)	8(1)	5(1)
O(6)	29(1)	29(1)	18(1)	7(1)	9(1)	19(1)
C(1)	16(1)	15(1)	17(1)	3(1)	6(1)	5(1)
C(2)	23(1)	27(1)	19(1)	5(1)	11(1)	13(1)
O(7)	19(1)	14(1)	24(1)	2(1)	6(1)	4(1)
O(8)	18(1)	19(1)	22(1)	5(1)	9(1)	8(1)
O(9)	24(1)	18(1)	18(1)	2(1)	5(1)	11(1)

Table A-2.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for CaHEDP·2H_2O

	x	y	z	U(eq)
H(3)	1490(70)	10490(60)	1840(40)	39(10)
H(6)	4677	5449	4739	34
H(2A)	690(60)	8450(60)	4350(40)	37(9)
H(2B)	-1540(60)	6860(50)	3760(40)	30(8)
H(2C)	300(60)	6580(50)	4850(40)	34(9)
H(7)	140(60)	4000(50)	2000(40)	24(8)
H(8A)	3760(60)	9890(60)	-2090(50)	33(12)
H(8B)	2470(70)	9700(50)	-1590(40)	33(11)
H(9A)	6010(60)	6370(60)	-2050(40)	40(10)
H(9B)	5000(60)	7130(50)	-2880(50)	31(10)

Table A-2.6. Torsion angles [º] for CaHEDP·2H_2O

O(2)-P(1)-O(1)-Ca(1)	-133.98(19)
O(3)-P(1)-O(1)-Ca(1)	103.4(2)
C(1)-P(1)-O(1)-Ca(1)	-14.9(2)
Ca(1)#2-P(1)-O(1)-Ca(1)	-96.94(19)
O(2)#1-Ca(1)-O(1)-P(1)	-2.3(3)
O(4)-Ca(1)-O(1)-P(1)	9.68(19)
O(2)#2-Ca(1)-O(1)-P(1)	82.2(2)
O(8)#3-Ca(1)-O(1)-P(1)	-70.9(2)
O(9)-Ca(1)-O(1)-P(1)	-173.57(17)
O(8)-Ca(1)-O(1)-P(1)	-140.7(2)
O(7)#2-Ca(1)-O(1)-P(1)	142.4(2)
P(1)#2-Ca(1)-O(1)-P(1)	92.0(2)
Ca(1)#4-Ca(1)-O(1)-P(1)	58.7(2)
Ca(1)#3-Ca(1)-O(1)-P(1)	-105.5(2)
O(1)-P(1)-O(2)-Ca(1)#5	-107.44(16)
O(3)-P(1)-O(2)-Ca(1)#5	17.11(18)
C(1)-P(1)-O(2)-Ca(1)#5	130.29(15)
Ca(1)#2-P(1)-O(2)-Ca(1)#5	-175.8(2)
O(1)-P(1)-O(2)-Ca(1)#2	68.36(13)
O(3)-P(1)-O(2)-Ca(1)#2	-167.09(10)
C(1)-P(1)-O(2)-Ca(1)#2	-53.91(12)
O(6)-P(2)-O(4)-Ca(1)	-170.67(11)
O(5)-P(2)-O(4)-Ca(1)	-44.54(16)
C(1)-P(2)-O(4)-Ca(1)	71.09(15)
O(1)-Ca(1)-O(4)-P(2)	-40.26(12)
O(2)#1-Ca(1)-O(4)-P(2)	134.19(14)
O(2)#2-Ca(1)-O(4)-P(2)	-146.06(14)
O(8)#3-Ca(1)-O(4)-P(2)	48.63(13)
O(9)-Ca(1)-O(4)-P(2)	143.94(12)
O(8)-Ca(1)-O(4)-P(2)	1.94(18)
O(7)#2-Ca(1)-O(4)-P(2)	-91.72(14)

P(1)#2-Ca(1)-O(4)-P(2)	-122.53(13)
Ca(1)#4-Ca(1)-O(4)-P(2)	174.35(14)
Ca(1)#3-Ca(1)-O(4)-P(2)	29.11(14)
O(4)-P(2)-C(1)-O(7)	53.61(17)
O(6)-P(2)-C(1)-O(7)	-68.52(17)
O(5)-P(2)-C(1)-O(7)	173.67(14)
O(4)-P(2)-C(1)-C(2)	172.67(17)
O(6)-P(2)-C(1)-C(2)	50.5(2)
O(5)-P(2)-C(1)-C(2)	-67.27(19)
O(4)-P(2)-C(1)-P(1)	-61.54(15)
O(6)-P(2)-C(1)-P(1)	176.33(11)
O(5)-P(2)-C(1)-P(1)	58.51(14)
O(1)-P(1)-C(1)-O(7)	-80.41(17)
O(2)-P(1)-C(1)-O(7)	45.48(17)
O(3)-P(1)-C(1)-O(7)	158.86(15)
Ca(1)#2-P(1)-C(1)-O(7)	13.65(13)
O(1)-P(1)-C(1)-C(2)	163.08(17)
O(2)-P(1)-C(1)-C(2)	-71.03(18)
O(3)-P(1)-C(1)-C(2)	42.3(2)
Ca(1)#2-P(1)-C(1)-C(2)	-102.86(17)
O(1)-P(1)-C(1)-P(2)	35.78(16)
O(2)-P(1)-C(1)-P(2)	161.67(12)
O(3)-P(1)-C(1)-P(2)	-84.95(14)
Ca(1)#2-P(1)-C(1)-P(2)	129.84(12)
C(2)-C(1)-O(7)-Ca(1)#2	96.8(2)
P(2)-C(1)-O(7)-Ca(1)#2	-141.17(11)
P(1)-C(1)-O(7)-Ca(1)#2	-21.0(2)
O(1)-Ca(1)-O(8)-Ca(1)#3	93.19(10)
O(2)#1-Ca(1)-O(8)-Ca(1)#3	-64.44(12)
O(4)-Ca(1)-O(8)-Ca(1)#3	49.80(14)
O(2)#2-Ca(1)-O(8)-Ca(1)#3	179.53(7)
O(8)#3-Ca(1)-O(8)-Ca(1)#3	0.0
O(9)-Ca(1)-O(8)-Ca(1)#3	-109.98(10)
O(7)#2-Ca(1)-O(8)-Ca(1)#3	164.20(11)

P(1)#2-Ca(1)-O(8)-Ca(1)#3 158.96(6)

Ca(1)#4-Ca(1)-O(8)-Ca(1)#3 -115.52(9)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 -x,-y+1,-z #3 -x+1,-y+2,-z

#4 -x+1,-y+1,-z #5 x-1,y,z

Table A-2.7. Hydrogen bonds for CaHEDP·2H_2O [Å and º]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)...O(9)#3	0.79(4)	1.93(4)	2.702(3)	168(4)
O(6)-H(6)...O(6)#6	0.82	1.76	2.542(3)	159.4
O(7)-H(7)...O(1)#2	0.82(4)	2.17(3)	2.728(3)	126(3)
O(7)-H(7)...O(4)	0.82(4)	2.51(3)	2.996(3)	119(3)
O(8)-H(8A)...O(5)#3	0.66(4)	2.13(5)	2.778(3)	166(4)
O(8)-H(8B)...O(3)#7	0.72(4)	2.10(5)	2.803(3)	165(4)
O(9)-H(9A)...O(4)#4	0.82(4)	1.89(4)	2.687(3)	166(4)
O(9)-H(9B)...O(6)#8	0.73(4)	2.13(4)	2.788(3)	151(4)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 -x,-y+1,-z #3 -x+1,-y+2,-z

#4 -x+1,-y+1,-z #5 x-1,y,z #6 -x+1,-y+1,-z+1

#7 -x,-y+2,-z #8 x,y,z-1