APPENDIX 2: Atomic positions, equivalent isotropic U values, and occupancies for atoms in synthetic F-OH apatites.

TABLE 2a. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for DHAPS68. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**	**Occ.**
Ca1	2/3	1/3	0.99891(5)	0.00800(8)	$Ca_{1.00}$
Ca2	0.24210(3)	0.99295(3)	1/4	0.00664(7)	$Ca_{1.00}$
P	0.63130(4)	0.02944(4)	1/4	0.00437(8)	$P_{1.00}$
O1	0.51559(12)	0.84203(12)	1/4	0.00873(17)	$O_{1.00}$
O2	0.53346(12)	0.12139(12)	1/4	0.01029(18)	$O_{1.00}$
O3	0.74312(9)	0.08460(9)	0.07061(11)	0.01203(14)	$O_{1.00}$
F	0	0	1/4	0.0097(12)	$F_{0.66(5)}$*
O(H)	0	0	0.205(4)	0.006(3)	$O_{0.19(3)}$*

*Total column occupancy, per unit cell = $[F_{1.33}(OH)_{0.75}]_{\Sigma 2.08}$.

TABLE 2b. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for DHAPS69. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**	**Occ.**
Ca1	2/3	1/3	0.99883(4)	0.00842(7)	$Ca_{1.00}$
Ca2	0.24369(3)	0.99309(3)	1/4	0.00707(6)	$Ca_{1.00}$
P	0.63134(3)	0.02969(3)	1/4	0.00469(7)	$P_{1.00}$
O1	0.51551(11)	0.84265(10)	1/4	0.00919(15)	$O_{1.00}$
O2	0.53398(11)	0.12186(11)	1/4	0.01117(16)	$O_{1.00}$
O3	0.74285(8)	0.08491(8)	0.07045(9)	0.01296(13)	$O_{1.00}$
F	0	0	1/4	0.0098(13)	$F_{0.48(3)}$
O(H)	0	0	0.1995(19)	0.0096(17)	$O_{0.27(2)}$

*Total column occupancy, per unit cell = $[F_{0.97}(OH)_{1.10}]_{\Sigma 2.07}$.

TABLE 1c. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for DHAPS70. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)	Occ.
Ca1	2/3	1/3	0.99879(4)	0.00844(6)	$Ca_{1.00}$
Ca2	0.24393(2)	0.99312(2)	1/4	0.00708(6)	$Ca_{1.00}$
P	0.63132(3)	0.02972(3)	1/4	0.00474(6)	$P_{1.00}$
O1	0.51548(10)	0.84277(9)	1/4	0.00915(13)	$O_{1.00}$
O2	0.53408(10)	0.12197(10)	1/4	0.01118(15)	$O_{1.00}$
O3	0.74279(7)	0.08497(7)	0.07039(9)	0.01313(12)	$O_{1.00}$
F	0	0	1/4	0.0095(13)	$F_{0.45(3)}$
O(H)	0	0	0.1989(16)	0.0098(15)	$O_{0.29(2)}$

*Total column occupancy, per unit cell = $[F_{0.91}(OH)_{1.15}]_{\Sigma 2.06}$.

TABLE 2d. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for DHAPS77. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)	Occ.
Ca1	2/3	1/3	0.99876(4)	0.00856(7)	$Ca_{1.00}$
Ca2	0.24453(3)	0.99318(3)	1/4	0.00717(6)	$Ca_{1.00}$
P	0.63138(3)	0.02984(3)	1/4	0.00481(6)	$P_{1.00}$
O1	0.51550(10)	0.84302(10)	1/4	0.00931(14)	$O_{1.00}$
O2	0.53422(10)	0.12204(10)	1/4	0.01148(15)	$O_{1.00}$
O3	0.74269(7)	0.08510(7)	0.07036(9)	0.01352(12)	$O_{1.00}$
F	0	0	1/4	0.0103(14)	$F_{0.41(3)}$
O(H)	0	0	0.1967(14)	0.0097(14)	$O_{0.30(2)}$

*Total column occupancy, per unit cell = $[F_{0.82}(OH)_{1.22}]_{\Sigma 2.04}$.

TABLE 2e. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for DHAPS84. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)	Occ.
Ca1	2/3	1/3	0.99890(4)	0.00808(6)	$Ca_{1.00}$
Ca2	0.24268(3)	0.99301(3)	1/4	0.00674(6)	$Ca_{1.00}$
P	0.63132(3)	0.02952(3)	1/4	0.00441(6)	$P_{1.00}$
O1	0.51552(10)	0.84224(10)	1/4	0.00877(14)	$O_{1.00}$
O2	0.53363(10)	0.12160(10)	1/4	0.01061(15)	$O_{1.00}$
O3	0.74298(7)	0.08469(7)	0.07055(9)	0.01227(12)	$O_{1.00}$
F	0	0	1/4	0.0091(11)	$F_{0.59(4)}$
O(H)	0	0	0.202(2)	0.008(2)	$O_{0.22(2)}$

*Total column occupancy, per unit cell = $[F_{1.17}(OH)_{0.90}]_{\Sigma 2.07}$.

TABLE 2f. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for DHAPS85. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)	Occ.
Ca1	2/3	1/3	0.99881(4)	0.00829(7)	$Ca_{1.00}$
Ca2	0.24390(3)	0.99309(3)	1/4	0.00691(6)	$Ca_{1.00}$
P	0.63133(3)	0.02972(3)	1/4	0.00468(7)	$P_{1.00}$
O1	0.51549(11)	0.84282(11)	1/4	0.00902(15)	$O_{1.00}$
O2	0.53402(11)	0.12190(11)	1/4	0.01105(17)	$O_{1.00}$
O3	0.74278(8)	0.08503(8)	0.07036(10)	0.01305(13)	$O_{1.00}$
F	0	0	1/4	0.0087(15)	$F_{0.45(3)}$
O(H)	0	0	0.1983(18)	0.0096(17)	$O_{0.29(2)}$

*Total column occupancy, per unit cell = $[F_{0.91}(OH)_{1.14}]_{\Sigma 2.05}$.

TABLE 2g. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for DHAPS86. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)	Occ.
Ca1	2/3	1/3	0.99890(4)	0.00816(7)	$Ca_{1.00}$
Ca2	0.24233(3)	0.99295(3)	1/4	0.00680(6)	$Ca_{1.00}$
P	0.63129(3)	0.02947(3)	1/4	0.00454(6)	$P_{1.00}$
O1	0.51554(11)	0.84216(10)	1/4	0.00887(14)	$O_{1.00}$
O2	0.53354(11)	0.12154(11)	1/4	0.01052(16)	$O_{1.00}$
O3	0.74307(7)	0.08464(8)	0.07051(9)	0.01221(12)	$O_{1.00}$
F	0	0	1/4	0.0094(11)	$F_{0.63(4)}$
O(H)	0	0	0.203(3)	0.007(2)	$O_{0.20(3)}$

*Total column occupancy, per unit cell = $[F_{1.27}(OH)_{0.81}]_{\Sigma 2.08}$.

TABLE 2h. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for DHAPS87. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)	Occ.
Ca1	2/3	1/3	0.99893(4)	0.00801(7)	$Ca_{1.00}$
Ca2	0.24182(3)	0.99291(3)	1/4	0.00663(6)	$Ca_{1.00}$
P	0.63126(3)	0.02937(3)	1/4	0.00438(7)	$P_{1.00}$
O1	0.51550(11)	0.84197(10)	1/4	0.00873(15)	$O_{1.00}$
O2	0.53340(11)	0.12138(11)	1/4	0.01030(16)	$O_{1.00}$
O3	0.74315(8)	0.08457(8)	0.07058(9)	0.01192(12)	$O_{1.00}$
F	0	0	1/4	0.0097(10)	$F_{0.70(5)}$
O(H)	0	0	0.207(4)	0.005(3)	$O_{0.17(3)}$

*Total column occupancy, per unit cell = $[F_{1.39}(OH)_{0.68}]_{\Sigma 2.07}$.