Supplementary Table 3. Single-crystal structure refinement and refined atomic parameters for FAp-II at 43.4 GPa and room temperature.

Beamline	13-BM-C (PX^2), GSECARS, APS, ANL
Pressure (GPa)	43.4
Wavelength (Å)	0.4343
Temperature (K)	295
Composition*	$Ca_5(PO_4)_3F$ (nominal)
Symmetry	Triclinic, $P\bar{1}$
Lattice Parameters: *a, b, c* (Å)	See table 3
Volume (Å^3)	See table 3
Z	4
R_{int}	0.0505
Reflection range	$-10 \leq h \leq 10$, $-16 \leq k \leq 16$, $-16 \leq l \leq 16$
Maximum 2θ (°)	39
Total reflections collected	20105
Independent reflections	1922
Completeness	31.7 %
Number independent parameters	173
Refinement method	F^2
R1	0.0537
wR2	0.1513
Goodness of fit	1.095

Atom	Site occupancy	*x/a*	*y/b*	*z/c*	U_{iso}
Ca1A	1	0.0133(6)	0.32900(17)	0.6593(3)	0.0070(3)
Ca1B	1	0.2627(5)	0.41377(16)	0.0775(3)	0.0048(3)
Ca1C	1	0.4856(6)	0.14367(18)	0.8541(3)	0.0098(3)
Ca1D	1	0.2262(6)	0.07255(17)	0.4271(3)	0.0072(3)
Ca2A	1	0.7750(6)	0.24388(17)	0.0058(3)	0.0053(3)
Ca2B	1	0.9072(5)	0.88319(16)	0.8739(3)	0.0041(2)
Ca2C	1	0.2397(5)	0.52635(16)	0.7385(3)	0.0045(2)
Ca2D	1	0.2494(5)	0.97582(16)	0.7617(3)	0.0043(2)
Ca2E	1	0.3948(5)	0.39608(16)	0.3717(3)	0.0046(2)
Ca2F	1	0.2796(5)	0.73389(16)	0.5126(3)	0.0047(2)
P1A	1	0.0984(7)	0.3135(2)	0.9310(4)	0.0034(3)
P1B	1	0.9724(7)	0.6462(2)	0.6168(4)	0.0041(3)
P1C	1	0.4178(7)	0.1933(2)	0.5665(4)	0.0042(3)
P1D	1	0.9382(7)	0.0796(2)	0.6842(4)	0.0028(3)
P1E	1	0.4472(7)	0.5825(2)	0.1769(4)	0.0028(3)
P1F	1	0.5186(7)	0.8530(2)	0.8700(4)	0.0041(3)
F1A	0.5	0.025(8)	0.9904(18)	0.983(4)	0.0041(14)

F1B	0.5	0.479(7)	0.5097(17)	0.515(3)	0.0028(14)
F1C	1	0.2364(15)	0.7509(5)	0.7696(8)	0.0100(8)
O1A	1	0.959(2)	0.5460(6)	0.7159(11)	0.0087(9)
O1B	1	0.552(2)	0.1473(6)	0.6338(10)	0.0080(9)
O1C	1	0.283(2)	0.5458(6)	0.2178(11)	0.0087(9)
O1D	1	0.953(2)	0.3710(6)	0.8776(10)	0.0071(9)
O1E	1	0.530(2)	0.9417(6)	0.7558(11)	0.0095(9)
O1F	1	0.785(2)	0.0319(6)	0.7429(11)	0.0101(9)
O2A	1	0.676(2)	0.8213(6)	0.9133(11)	0.0093(9)
O2B	1	0.300(2)	0.1120(6)	0.5978(11)	0.0093(9)
O2C	1	0.808(2)	0.7043(6)	0.5781(11)	0.0092(9)
O2D	1	0.425(2)	0.7032(6)	0.0956(10)	0.0080(9)
O2E	1	0.251(2)	0.3633(6)	0.8753(10)	0.0072(9)
O2F	1	0.911(2)	0.1844(6)	0.5882(10)	0.0085(9)
O3A	1	0.342(2)	0.9294(7)	0.9890(12)	0.0131(10)
O3B	1	0.539(2)	0.1829(7)	0.4133(11)	0.0120(10)
O3C	1	0.459(2)	0.6094(7)	0.3100(11)	0.0137(10)
O3D	1	0.1913(19)	0.1556(6)	0.8979(10)	0.0045(8)
O3E	1	0.991(2)	0.7645(6)	0.6755(10)	0.0069(9)
O3F	1	0.521(2)	0.7193(6)	0.8270(10)	0.0067(9)
O3G	1	0.960(2)	0.1401(7)	0.7983(11)	0.0117(10)
O3H	1	0.2893(19)	0.3467(6)	0.6102(10)	0.0054(8)
O3I	1	0.625(2)	0.4618(6)	0.0921(11)	0.0082(9)
O3J	1	0.122(2)	0.9547(6)	0.6071(11)	0.0073(9)
O3K	1	0.008(2)	0.3494(7)	0.0868(11)	0.0123(10)
O3L	1	0.148(2)	0.5761(6)	0.4869(11)	0.0099(9)