$Ca_5[PO_4]_3Cl_{0.83}F_{0.17}$	*hP*50	(176) $P6_3/m$ – ih^4fe^2a

$Ca_5(PO_4)_3(Cl,F)$ [1], apatite family
Structural features: Infinite columns of base-linked CaO_6O_3 tricapped trigonal prisms share atoms with PO_4 tetrahedra to form a 3D-framework; Cl (near octahedron centers) and F (in and near trigonal voids) in infinite columns of face-linked Ca_6 octahedra parallel to [001] (partial disorder).

Mackie P.E., Young R.A. (1974) [1]
$Ca_5Cl_{0.86}F_{0.17}O_{12}P_3$
$a = 0.96205$, $c = 0.67761$ nm, $c/a = 0.704$, $V = 0.5431$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	12*i*	1	0.3534	0.0873	0.0671		single atom P
O2	6*h*	*m*..	0.1494	0.4911	$^1/_4$		single atom P
Ca3	6*h*	*m*..	0.2594	0.2567	$^1/_4$		
P4	6*h*	*m*..	0.4063	0.0322	$^1/_4$		tetrahedron O_4
O5	6*h*	*m*..	0.592	0.1269	$^1/_4$		single atom P
Ca6	4*f*	3..	$^1/_3$	$^2/_3$	0.0033		trigonal prism O_6
Cl7	4*e*	3..	0	0	0.0568	0.429	
F8	4*e*	3..	0	0	0.1595	0.06	
F9	2*a*	-6..	0	0	$^1/_4$	0.051	

Transformation from published data: *y*,*x*,-*z*
Experimental: single crystal, diffractometer, X-rays, wR = 0.042

Remarks: Refinement of the site occupancies showed no significant deviation from unity except for the sites on the c-axis. Short interatomic distances for partly occupied site(s). In table II of [1] the occupancies of former F(2) and Cl are misprinted as 0.119 and 0.858 instead of 0.0595 and 0.429, respectively (agreement with the notation used for the other sites).

References: [1] Mackie P.E., Young R.A. (1974), J. Solid State Chem. 11, 319-329.