$Ca_5[PO_4]_3Br$	*hP*46	(176) $P6_3/m$ – ih^4feb

$Ca_5(PO_4)_3Br$ [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; infinite columns of face-linked $BrCa_6$ octahedra parallel to [001] (Br in part displaced along the column axis).

Elliott J.C. et al. (1981) [1]
$Br_{1.01}Ca_5O_{12}P_3$
$a = 0.9761$, $c = 0.6739$ nm, $c/a = 0.690$, $V = 0.5561$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	12*i*	1	0.3572	0.0859	0.0662		single atom P
O2	6*h*	*m*..	0.1439	0.4972	$^1/_4$		single atom P
Ca3	6*h*	*m*..	0.2672	0.2551	$^1/_4$		monocapped trigonal prism O_5Br_2
P4	6*h*	*m*..	0.4124	0.0339	$^1/_4$		tetrahedron O_4
O5	6*h*	*m*..	0.5954	0.1312	$^1/_4$		single atom P
Ca6	4*f*	3..	$^1/_3$	$^2/_3$	0.0045		tricapped trigonal prism O_9
Br7	4*e*	3..	0	0	0.1032	0.03	
Br8	2*b*	-3..	0	0	0	0.952	

Transformation from published data: *y*,*x*,-*z*
Experimental: single crystal, diffractometer, X-rays, wR = 0.031

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Elliott J.C., Dykes E., Mackie P.E. (1981), Acta Crystallogr. B 37, 435-438.