$Rb_5BeZr_6Br_{15}$	*hP*68	(182) $P6_322 - i^3h^3gedc$

$Rb_5Zr_6Br_{15}Be$ [1]
Structural features: $BeZr_6Br_{18}$ units (a central Be atom surrounded by a Zr_6 octahedron, a Br_{12} cuboctahedron and a Br_6 octahedron) share vertices of the Br_6 octahedron to form a 3D-framework; Rb mainly in large channels parallel to [001] (partial disorder).

Qi R.Y., Corbett J.D. (1995) [1]
$BeBr_{15}Rb_{5.05}Zr_6$
a = 1.3009, c = 1.206 nm, c/a = 0.927, V = 1.7675 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Zr1	12*i*	1	0.1831	0.5184	0.1359		octahedron $BeBr_5$
Rb2	12*i*	1	0.194	0.166	0.054	0.31	
Br3	12*i*	1	0.4966	0.3297	0.0088		non-colinear Zr_2
Br4	6*h*	..2	0.1647	0.3294	$^1/_4$		non-colinear Zr_2
Br5	6*h*	..2	0.5031	0.0062	$^1/_4$		non-colinear Zr_2
Rb6	6*h*	..2	0.8425	0.685	$^1/_4$	0.64	non-colinear Rb_2
Br7	6*g*	.2.	0.3287	0	0		non-colinear Zr_2
Rb8	4*e*	3..	0	0	0.179	0.49	
Rb9	2*d*	3.2	$^1/_3$	$^2/_3$	$^3/_4$	0.29	cuboctahedron Br_9Rb_3
Be10	2*c*	3.2	$^1/_3$	$^2/_3$	$^1/_4$		octahedron Zr_6

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.044
Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Qi R.Y., Corbett J.D. (1995), Inorg. Chem. 34, 1646-1651.