$AlBi_4Cl_4$	*hP*124	(176) $P6_3/m$ – $i^6h^5f^3e^2d$

$Bi_8(AlCl_4)_2$ [1]
Structural features: $AlCl_4$ tetrahedra (partial orientational disorder) and Bi_8 clusters (square antiprism).

Beck J. et al. (1996) [1]
$AlBi_4Cl_4$
a = 1.7854, c = 1.2953 nm, c/a = 0.725, V = 3.5758 nm^3, Z = 12

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	12*i*	1	0.028	0.126	0.05	0.5	
Cl2	12*i*	1	0.127	0.443	0.124		single atom Al
Bi3	12*i*	1	0.2678	0.3212	0.0847		non-coplanar square Bi_4
Bi4	12*i*	1	0.3693	0.2245	0.1312		non-coplanar square Bi_4
Cl5	12*i*	1	0.559	0.218	0.014		non-colinear Al_2
Bi6	12*i*	1	0.576	0.04	0.1304		non-coplanar square Bi_4
Cl7	6*h*	*m*..	0.044	0.25	$^1/_4$		single atom Al
Al8	6*h*	*m*..	0.056	0.36	$^1/_4$		tetrahedron Cl_4
Bi9	6*h*	*m*..	0.1992	0.1776	$^1/_4$		non-coplanar square Bi_4
Bi10	6*h*	*m*..	0.338	0.4649	$^1/_4$		non-coplanar square Bi_4
Cl11	6*h*	*m*..	0.417	0.07	$^1/_4$		single atom Al
Al12	4*f*	3..	$^1/_3$	$^2/_3$	0.034	0.5	trigonal bipyramid $AlCl_4$
Cl13	4*f*	3..	$^1/_3$	$^2/_3$	0.203	0.5	single atom Cl
Al14	4*f*	3..	$^1/_3$	$^2/_3$	0.591	0.5	trigonal bipyramid $AlCl_4$
Al15	4*e*	3..	0	0	0.024	0.5	
Cl16	4*e*	3..	0	0	0.164	0.5	single atom Al
Cl17	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		colinear Al_2

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, wR = 0.062, T = 293 K

Remarks: We deduced probable occupancies of the Al and Cl sites from the drawing in fig. 3. Space group (173) $P6_3$ was tested and rejected. Short interatomic distances for partly occupied site(s).

References: [1] Beck J., Brendel C.J., Bengtsson Kloo L., Krebs B., Mummert M., Stankowski A., Ulvenlund S. (1996), Chem. Ber. 129, 1219-1226.