$Cr_{24.5}Ni_{0.5}Al_{88.5}$	*hP*238	(176) $P6_3/m$ – $i^{13}h^{11}fe^3$

$Al_{177}Cr_{49}Ni$ κ-phase [1]
Structural features: A dense 3D-framework with mainly icosahedral coordination; $Cr(Al_{11}Cr)$ icosahedra are interconnected along [001] via common faces ($CrAl_2$) and double empty Al_6 trigonal antiprisms.

Marsh R.E. (1998) [1]
$Al_{88.50}Cr_{24.50}Ni_{0.50}$
a = 1.7674, c = 1.2516 nm, c/a = 0.708, V = 3.3858 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cr1	12*i*	1	0.00908	0.13942	0.05036		
Al2	12*i*	1	0.03529	0.27634	0.13523		14-vertex Frank-Kasper Cr_3Al_{11}
Al3	12*i*	1	0.06077	0.43593	0.06432		pseudo Frank-Kasper $Al_{10}Cr_3$
Al4	12*i*	1	0.08755	0.60312	0.06964		12-vertex polyhedron Cr_2Al_{10}
Al5	12*i*	1	0.12231	0.14114	0.13675		
Al6	12*i*	1	0.20513	0.41243	0.07009		12-vertex polyhedron Cr_2Al_{10}
Al7	12*i*	1	0.22628	0.57614	0.1367		single atom Ni
Al8	12*i*	1	0.26164	0.13073	0.05933		14-vertex Frank-Kasper Cr_4Al_{10}
Al9	12*i*	1	0.27786	0.29496	0.06803		tricapped pentagonal prism Cr_3Al_{10}
Cr10	12*i*	1	0.40289	0.10866	0.07749		icosahedron $Al_{11}Cr$
Al11	12*i*	1	0.42233	0.26831	0.13648		pseudo Frank-Kasper $Al_{10}Cr_3$
Al12	12*i*	1	0.53822	0.08024	0.13636		pseudo Frank-Kasper $Al_{10}Cr_3$
Al13	12*i*	1	0.56425	0.24593	0.05757		single atom Ni
Cr14	6*h*	*m*..	0.08028	0.53589	$^1/_4$		icosahedron $Al_{11}Cr$
Cr15	6*h*	*m*..	0.14663	0.42386	$^1/_4$		icosahedron $Al_{11}Cr$
Al16	6*h*	*m*..	0.15168	0.02892	$^1/_4$		
Al17	6*h*	*m*..	0.18987	0.30951	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Cr18	6*h*	*m*..	0.26463	0.22396	$^1/_4$		icosahedron Al_{12}
Al19	6*h*	*m*..	0.30793	0.49875	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al20	6*h*	*m*..	0.32793	0.12278	$^1/_4$		icosahedron Cr_4Al_8
Al21	6*h*	*m*..	0.38228	0.38147	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Al22	6*h*	*m*..	0.39011	0.01879	$^1/_4$		icosahedron Cr_5Al_7
Cr23	6*h*	*m*..	0.49372	0.18527	$^1/_4$		icosahedron $Al_{10}Cr_2$
Al24	6*h*	*m*..	0.58098	0.34776	$^1/_4$		12-vertex polyhedron Cr_2Al_{10}
Ni25	4*f*	3..	$^1/_3$	$^2/_3$	0.0419	0.25	octahedron Al_6
Al26	4*e*	3..	0	0	0.0148	0.5	
Al27	4*e*	3..	0	0	0.1767	0.25	
Cr28	4*e*	3..	0	0	0.2313	0.25	

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.041

Remarks: Short interatomic distances for partly occupied site(s). Short interatomic distances: d(Ni25-Al7) = 0.213 nm; refinement considering O in site Ni25 led to negative displacement parameters. Supersedes a refinement on the same diffraction data in space group (173) $P6_3$ [2], which does not take into consideration all symmetry elements of the proposed structure.

References: [1] Marsh R.E. (1998), Acta Crystallogr. B 54, 925-926. [2] Sato A., Yamamoto A., Li X.Z., Hiraga K., Haibach T., Steurer W. (1997), Acta Crystallogr. C 53, 1531-1533.