$Tl_{0.36}V_3(P_{0.78}Se_{0.22})Se_3$	*hP*16	(176) $P6_3/m - h^2da$

$Tl_{0.72}V_6Se_{6.45}P_{1.55}$ [1]; $Tl_{0.77}V_6S_{6.9}P_{1.1}$ [2]
Structural features: Units of three face-linked $V[(P,Se)_2Se_4]$ octahedra share edges to form a 3D-framework; Tl in channels of hexagonal cross-section parallel to [001] (partial disorder with maximum probability for trigonal coordination). Ordering variant of rt-$Tl_{0.78}V_6S_8$.

Bensch W. et al. (1992) [1]
$P_{0.77}Se_{3.22}Tl_{0.36}V_3$
$a = 0.9505$, $c = 0.3413$ nm, $c/a = 0.359$, $V = 0.2670$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
V1	6*h*	*m*..	0.1327	0.4986	$^1/_4$		octahedron P_2Se_4
Se2	6*h*	*m*..	0.2957	0.3422	$^1/_4$		4-vertex polyhedron V_4
M3	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		trigonal prism V_6
Tl4	2*a*	-6..	0	0	$^1/_4$	0.36	colinear Tl_2

M3 = 0.775P + 0.225Se
Experimental: single crystal, diffractometer, X-rays, wR = 0.018, T = 295 K

Remarks: We derived approximate values for the refinable atom coordinates from interatomic distances. The authors state that Tl is delocalized along [001] with maximum probability in Wyckoff position 2*a*. Short interatomic distances for partly occupied site(s).

References: [1] Bensch W., Koy J., Biberacher W. (1992), Solid State Commun. 82, 851-855. [2] Bensch W., Koy J., Biberacher W. (1994), Eur. J. Solid State Inorg. Chem. 31, 371-379.