

Table 3. Volumes of mutation-induced internal cavities

Structure	Probe radius, Å	Center of cavity gravity (x,y,z), Å	Volume, Å ³ *	No. of lining atoms [†]	Lining residues
<i>T</i> -p53C-V143A	1.4	93.81 85.87 -28.67	46.6 (1.6)	35 (27)	113, 124, 133, 141, 142, 143, 234, 236, 270
<i>T</i> -p53C-V143A	1.2	94.86 86.91 -34.52	19.3 (1.6)	18 (16)	111, 143, 145, 157, 232, 234, 255
<i>T</i> -p53C-V143A	1.2	93.77 86.11 -28.40	62.2 (2.2)	33 (25)	113, 124, 133, 141, 142, 143, 234, 236, 270
<i>T</i> -p53C-F270L	1.4	96.30 85.30 -29.97	50.8 (0.9)	29 (27)	111, 113, 133, 143, 159, 234, 236, 253, 255, 270, 272
<i>T</i> -p53C-F270L	1.2	95.58 84.70 -30.02	89.4 (3.1)	40 (35)	111, 113, 133, 141, 143, 159, 195, 234, 236, 253, 255, 270, 272

*Cavity volumes were calculated with VOIDOO using different probe sizes (1.2-Å and 1.4-Å radius; cf. *Materials and Methods*). The numbers given are the averages of the size of a mutation-induced cavity (volume occupied by the probe) calculated for 10 random orientations of the molecule. Standard deviations are given in parentheses. In both mutants, the cavity calculated with a probe radius of 1.2 Å is substantially enlarged, because the smaller probe better delineates the shape of the cavity and because of leaking into smaller cavities preexisting in *T*-p53C. In *T*-p53C-V143A, for example, the large cavity at the mutation site includes two preexisting cavities, which have a volume of 16 Å³ and 19 Å³ in *T*-p53C. In *T*-p53C-F270L, the cavity comprises two smaller preexisting cavities, with a volume of 19 Å³ and 22 Å³ in *T*-p53C. With a probe radius of 1.4 Å, which mimics the size of a water molecule, no cavities next to Val-143 or Phe-270 were detected in *T*-p53C.

[†]The number of carbon atoms lining the cavity is given in parentheses. The high percentage of carbon atoms illustrates the hydrophobic nature of these cavities.