

Table 2. Hot-spot* residues of selected robust modes of *Thermus aquaticus* DNA polymerase I

Mode # †	Residue numbers
4	461, 464, 516, 532, 533, 537, 538, 541, 545, 570, 571, 590, 591, 610, 611, 612, 613, 614 ‡, 615, 616, 617, 619, 622, 626 , 632, 638, 666 , 667 , 669 , 670 , 672, 697, 720, 721, 723, 725, 747, 749, 754, 785, 809, 810, 812, 813, 814
7	463, 464, 468, 506, 514, 515, 516, 532, 533, 537, 538, 541, 542, 545, 546, 584, 590, 591, 613, 615, 616, 617, 632, 637, 638, 662 , 664 , 665, 666 , 667 , 668, 672, 673, 692, 697, 745, 783, 816, 817, 818, 819, 820, 832
10	613, 627, 628, 638, 642, 643, 655, 659 , 660 , 663 , 664 , 667 , 669 , 670 , 671, 672, 673, 675, 690 , 693, 694, 695 , 696 , 699 , 700, 704, 707 , 708 , 711, 727, 728, 729, 730, 731, 732, 733, 734, 737, 740, 741, 742, 743, 744, 745, 747, 748

* The hot-spot residues that introduce most significant site-specific perturbation have high- $\delta\omega$ values. The details of the calculations are given in ref. 1.

† These modes describe allosteric transitions and are also robust to sequence variations.

‡ Residues in bold have already been experimentally identified to be significant.

1. Zheng, W., Brooks, B. R., Doniach, S. & Thirumalai, D. (2005) *Structure (London)* **13**, 565-577.