

**Supplementary Table-7:** Active residues of four cavities in Acetate kinase (ack) protein.

<b>Cavity Number</b>	<b>Cavity Volume</b>	<b>Cavity coordinates</b>	<b>Cavity Residues</b>
1(A chain)	335.87	-17.67 36.31 20.10	Ala109, Arg230, Asn258, Glu254, Gly16, His83, His112, His259, Leu111, Leu219, Pro110, Pro221, Ser17, Ser18, Ser19, Thr220, Val82, Phe168
2(B chain)	296.96	-18.42 -4.09 10.14	Ala116, Arg80, Arg230, Asn14, Asn113, Asn200, Asn258, Gly16, Gly201, Gly228, His83, His112, Leu111, Met227, Pro114, Pro115, Ser15, Ser17, Ser19, Thr229, Val81, Val82, Val117
4(B chain)	44.03	-18.77 14.38 24.58	Ala303, Arg165, Arg296, Asp233, Glu214, Glu223, Gly224, His295, Leu234, Lys299, Thr215, Ser216, Tyr300, Tyr304, Ala147, Ala148, Ala303, Arg165, Arg296, Asp233, Glu214, Glu223, Leu234, Lys299, Ser216, Thr150, Tyr151, Tyr300, Tyr304
5(B chain)	32.25	-34.83 -3.79 17.27	Arg165, Arg296, Asp233, Asp235, Glu214, Glu223, Gly224, Leu234, Lys299, Pro236, Ser216, Thr215, Tyr300, Tyr304, Ala303, Arg165, Arg296, Asp233, Asp235, Glu223, Gly224, Leu234, Lys299, Pro236, Ser216, Tyr151, Tyr300