Supporting Information

Theoretical identification on the role of Lys15 for Sulfolobus tokodaii hexokinase

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The atomic coordinates of these atoms (QM part) for the ATP-bound StHK.

ATOM	61	N	LYS	15	-6.406	-7.181	4.486	1.00	18.96	N
ATOM	62	HN	LYS	15	-6.584	-6.526	3.721	1.00	0.00	H
ATOM	63	CA	LYS	15	-6.947	-6.868	5.810	1.00	27.33	C
ATOM	64	HA	LYS	15	-6.741	-7.693	6.506	1.00	0.00	H
ATOM	65	CB	LYS	15	-6.376	-5.555	6.392	1.00	31.73	C
ATOM	66	HB1	LYS	15	-6.640	-4.762	5.683	1.00	0.00	H
ATOM	67	HB2	LYS	15	-6.916	-5.314	7.318	1.00	0.00	H
ATOM	68	CG	LYS	15	-4.855	-5.573	6.658	1.00	46.58	C
ATOM	69	HG1	LYS	15	-4.671	-5.553	7.738	1.00	0.00	H
ATOM	70	HG2	LYS	15	-4.418	-6.512	6.288	1.00	0.00	H
ATOM	71	CD	LYS	15	-4.112	-4.391	6.017	1.00	52.98	C
ATOM	72	HD1	LYS	15	-4.645	-3.456	6.234	1.00	0.00	H
ATOM	73	HD2	LYS	15	-3.117	-4.281	6.469	1.00	0.00	H
ATOM	74	CE	LYS	15	-3.948	-4.552	4.507	1.00	55.66	C
ATOM	75	HE1	LYS	15	-3.367	-5.443	4.266	1.00	0.00	H
ATOM	76	HE2	LYS	15	-4.907	-4.644	3.995	1.00	0.00	H
ATOM	77	NZ	LYS	15	-3.255	-3.362	3.914	1.00	52.51	N
ATOM	78	HZ1	LYS	15	-2.818	-3.506	2.982	1.00	0.00	H
ATOM	79	HZ2	LYS	15	-3.977	-2.607	3.775	1.00	0.00	H
ATOM	80	HZ3	LYS	15	-2.459	-3.002	4.482	1.00	0.00	H
ATOM	81	C	LYS	15	-8.476	-6.701	5.629	1.00	26.81	C
ATOM	82	O	LYS	15	-8.867	-5.810	4.884	1.00	22.30	O
TER	83		LYS	15						
ATOM	84	N	ASP	71	-4.763	-1.672	-12.390	1.00	30.04	N
ATOM	85	HN	ASP	71	-4.335	-2.597	-12.310	1.00	0.00	H
ATOM	86	CA	ASP	71	-3.932	-0.599	-12.945	1.00	32.00	C
ATOM	87	HA	ASP	71	-4.120	0.363	-12.457	1.00	0.00	H
ATOM	88	CB	ASP	71	-2.438	-0.932	-12.728	1.00	28.61	C
ATOM	89	HB1	ASP	71	-2.193	-1.901	-13.179	1.00	0.00	H
ATOM	90	HB2	ASP	71	-1.807	-0.181	-13.225	1.00	0.00	H
ATOM	91	CG	ASP	71	-2.073	-0.963	-11.236	1.00	28.31	C
ATOM	92	OD1	ASP	71	-1.207	-1.813	-10.906	1.00	20.80	O
ATOM	93	OD2	ASP	71	-2.663	-0.140	-10.478	1.00	22.40	O

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ATOM     94  C    ASP     71      -4.161  -0.378 -14.449  1.00 37.73           C
ATOM     95  O    ASP     71      -4.172   0.787 -14.873  1.00 40.83           O
TER      96       ASP     71
ATOM     97  N    ASP     95      -7.567   0.144  -4.299  1.00 17.31           N
ATOM     98  HN   ASP     95      -6.790   0.208  -4.954  1.00  0.00           H
ATOM     99  CA   ASP     95      -7.229   0.571  -2.923  1.00 21.42           C
ATOM    100  HA   ASP     95      -7.983   0.167  -2.238  1.00  0.00           H
ATOM    101  CB   ASP     95      -5.893  -0.102  -2.537  1.00 22.01           C
ATOM    102  HB1  ASP     95      -5.712   0.058  -1.467  1.00  0.00           H
ATOM    103  HB2  ASP     95      -6.005  -1.185  -2.676  1.00  0.00           H
ATOM    104  CG   ASP     95      -4.662   0.364  -3.349  1.00 25.03           C
ATOM    105  OD1  ASP     95      -4.861   1.012  -4.414  1.00 18.38           O
ATOM    106  OD2  ASP     95      -3.547   0.021  -2.870  1.00 33.04           O
ATOM    107  C    ASP     95      -7.182   2.098  -2.641  1.00 20.21           C
ATOM    108  O    ASP     95      -7.736   2.533  -1.634  1.00 19.04           O
TER     109       ASP     95
ATOM    110  N    THR    116       3.460  -1.219   0.044  1.00 22.49           N
ATOM    111  HN   THR    116       2.461  -1.329  -0.001  1.00  0.00           H
ATOM    112  CA   THR    116       4.280  -2.186  -0.681  1.00 17.24           C
ATOM    113  HA   THR    116       5.198  -2.340  -0.136  1.00  0.00           H
ATOM    114  CB   THR    116       3.616  -3.525  -0.893  1.00 23.75           C
ATOM    115  HB   THR    116       2.823  -3.475  -1.671  1.00  0.00           H
ATOM    116  OG1  THR    116       3.040  -3.947   0.327  1.00 20.76           O
ATOM    117  HG1  THR    116       2.192  -3.454   0.384  1.00  0.00           H
ATOM    118  CG2  THR    116       4.640  -4.586  -1.300  1.00 21.59           C
ATOM    119 HG21  THR    116       4.134  -5.553  -1.499  1.00  0.00           H
ATOM    120 HG22  THR    116       5.180  -4.288  -2.223  1.00  0.00           H
ATOM    121 HG23  THR    116       5.365  -4.747  -0.484  1.00  0.00           H
ATOM    122  C    THR    116       4.620  -1.641  -2.036  1.00 24.46           C
ATOM    123  O    THR    116       5.774  -1.687  -2.468  1.00 18.70           O
TER     124       THR    116
ATOM    125  N    ASP    140       6.608   2.468  -8.569  1.00 18.27           N
ATOM    126  HN   ASP    140       5.695   2.394  -9.003  1.00  0.00           H
ATOM    127  CA   ASP    140       6.633   2.187  -7.124  1.00 22.74           C
ATOM    128  HA   ASP    140       5.654   2.589  -6.814  1.00  0.00           H
ATOM    129  CB   ASP    140       6.562   0.716  -6.701  1.00 16.60           C
ATOM    130  HB1  ASP    140       7.312   0.109  -7.222  1.00  0.00           H
ATOM    131  HB2  ASP    140       6.799   0.660  -5.633  1.00  0.00           H
ATOM    132  CG   ASP    140       5.152   0.106  -6.919  1.00 24.88           C
ATOM    133  OD1  ASP    140       4.200   0.911  -7.169  1.00 22.74           O
ATOM    134  OD2  ASP    140       5.034  -1.130  -6.755  1.00 19.30           O
ATOM    135  C    ASP    140       7.599   3.088  -6.322  1.00 15.06           C
ATOM    136  O    ASP    140       7.826   2.827  -5.145  1.00 16.59           O
TER     137       ASP    140
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HETATM 138 C1 GLO 1 1.320 -0.736 -6.864 1.00 12.70 C
HETATM 139 H1 GLO 1 1.738 0.224 -7.206 1.00 0.00 H
HETATM 140 O1 GLO 1 2.289 -1.734 -6.918 1.00 18.41 O
HETATM 141 H1A GLO 1 3.200 -1.348 -6.853 1.00 0.00 H
HETATM 142 C2 GLO 1 0.122 -1.127 -7.727 1.00 13.93 C
HETATM 143 H2 GLO 1 -0.149 -2.160 -7.449 1.00 0.00 H
HETATM 144 O2 GLO 1 0.544 -1.040 -9.072 1.00 17.69 O
HETATM 145 H2A GLO 1 -0.180 -1.370 -9.663 1.00 0.00 H
HETATM 146 C3 GLO 1 -1.113 -0.235 -7.485 1.00 14.37 C
HETATM 147 H3 GLO 1 -0.947 0.698 -8.043 1.00 0.00 H
HETATM 148 O3 GLO 1 -2.297 -0.859 -7.952 1.00 15.82 O
HETATM 149 H3A GLO 1 -2.452 -0.578 -8.889 1.00 0.00 H
HETATM 150 C4 GLO 1 -1.348 0.161 -6.034 1.00 12.99 C
HETATM 151 H4 GLO 1 -1.788 -0.693 -5.505 1.00 0.00 H
HETATM 152 O4 GLO 1 -2.180 1.299 -5.943 1.00 16.09 O
HETATM 153 H4A GLO 1 -3.105 1.043 -6.131 1.00 0.00 H
HETATM 154 C5 GLO 1 -0.037 0.494 -5.326 1.00 13.50 C
HETATM 155 H5 GLO 1 0.391 1.417 -5.762 1.00 0.00 H
HETATM 156 O5 GLO 1 0.884 -0.586 -5.504 1.00 13.60 O
HETATM 157 C6 GLO 1 -0.263 0.710 -3.830 1.00 14.16 C
HETATM 158 H6A GLO 1 0.695 0.852 -3.318 1.00 0.00 H
HETATM 159 H6B GLO 1 -0.858 1.628 -3.721 1.00 0.00 H
HETATM 160 O6 GLO 1 -0.899 -0.396 -3.238 1.00 15.87 O
HETATM 161 H6C GLO 1 -1.873 -0.243 -3.226 1.00 0.00 H
HETATM 162 C5 ATP 1 4.040 -2.461 4.310 1.00 22.91 C
HETATM 163 H5 ATP 1 3.833 -2.246 3.257 1.00 0.00 H
HETATM 164 O5 ATP 1 4.450 -1.237 4.964 1.00 24.49 O
HETATM 165 C8 ATP 1 5.781 -1.306 5.396 1.00 24.51 C
HETATM 166 H8 ATP 1 6.473 -0.791 4.718 1.00 0.00 H
HETATM 167 C10 ATP 1 6.716 0.541 8.397 1.00 28.07 C
HETATM 168 N9 ATP 1 5.472 0.042 8.795 1.00 30.76 N
HETATM 169 C9 ATP 1 5.026 -0.620 7.737 1.00 25.92 C
HETATM 170 H9 ATP 1 4.065 -1.113 7.677 1.00 0.00 H
HETATM 171 N8 ATP 1 5.881 -0.595 6.673 1.00 24.23 N
HETATM 172 N12 ATP 1 8.865 1.513 8.292 1.00 31.20 N

HETATM 173 C12 ATP 1 8.949 1.104 7.019 1.00 30.86 C
HETATM 174 H12 ATP 1 9.870 1.359 6.498 1.00 0.00 H
HETATM 175 N11 ATP 1 8.048 0.406 6.331 1.00 25.68 N
HETATM 176 C11 ATP 1 6.969 0.149 7.068 1.00 27.55 C
HETATM 177 C13 ATP 1 7.761 1.266 9.016 1.00 34.82 C
HETATM 178 N13 ATP 1 7.775 1.694 10.342 1.00 33.87 N
HETATM 179 H13B ATP 1 8.700 2.103 10.558 1.00 0.00 H
HETATM 180 H13A ATP 1 7.066 2.411 10.550 1.00 0.00 H
HETATM 181 C7 ATP 1 6.144 -2.807 5.503 1.00 25.14 C
HETATM 182 H7 ATP 1 5.890 -3.172 6.504 1.00 0.00
H
HETATM 183 O7 ATP 1 7.503 -3.080 5.294 1.00 22.96 O
HETATM 184 H7A ATP 1 7.632 -3.081 4.325 1.00 0.00
H
HETATM 185 C6 ATP 1 5.210 -3.447 4.440 1.00 21.74 C
HETATM 186 H6 ATP 1 4.851 -4.428 4.766 1.00 0.00
H
HETATM 187 O6 ATP 1 5.926 -3.570 3.215 1.00 20.39 O
HETATM 188 H6A ATP 1 6.256 -4.486 3.184 1.00 0.00
H
HETATM 189 C4 ATP 1 2.775 -2.978 4.999 1.00 17.35 C
HETATM 190 H4A ATP 1 2.388 -3.830 4.432 1.00 0.00
H
HETATM 191 H4B ATP 1 3.032 -3.311 6.017 1.00 0.00 H
HETATM 192 O3 ATP 1 1.799 -1.955 5.122 1.00 25.21 O
HETATM 193 P3 ATP 1 0.402 -1.865 4.210 1.00 25.58 P
HETATM 194 O3A ATP 1 0.347 -0.415 3.749 1.00 19.33 O
HETATM 195 O3B ATP 1 -0.762 -2.370 5.027 1.00 27.75 O
HETATM 196 O2 ATP 1 0.815 -2.895 3.046 1.00 23.57 O
HETATM 197 P2 ATP 1 -0.166 -3.242 1.700 1.00 22.77 P
HETATM 198 O2A ATP 1 -1.498 -2.530 1.993 1.00 24.45 O
HETATM 199 O2B ATP 1 -0.169 -4.735 1.570 1.00 18.45 O
HETATM 200 O1 ATP 1 0.690 -2.503 0.600 1.00 23.12 O
HETATM 201 P1 ATP 1 0.117 -1.678 -0.952 1.00 0.00 P
HETATM 202 O1C ATP 1 -1.397 -1.794 -0.746 1.00 0.00 O
HETATM 203 O1B ATP 1 0.761 -2.597 -1.952 1.00 0.00 O
HETATM 204 O1A ATP 1 0.756 -0.316 -0.692 1.00 0.00 O
HETATM 205 MG MGL 1 -2.365 -0.985 0.812 1.00 27.88
LP
HETATM 206 OH2 TIP3 1 -0.776 0.362 1.346 1.00 18.54 O
HETATM 207 H1 TIP3 1 -0.133 0.237 0.571 1.00 0.00 H
HETATM 208 H2 TIP3 1 -0.312 0.004 2.137 1.00 0.00 H
HETATM 209 OH2 TIP3 5 -3.488 -0.178 2.472 1.00 21.67 O
HETATM 210 H1 TIP3 5 -2.984 0.016 3.293 1.00 0.00 H

HETATM	211	H2	TIP3	5	-4.287	-0.708	2.749	1.00	0.00	H
HETATM	212	OH2	TIP3	6	-2.993	0.431	-0.356	1.00	23.98	O
HETATM	213	H1	TIP3	6	-3.246	0.157	-1.281	1.00	0.00	H
HETATM	214	H2	TIP3	6	-2.553	1.267	-0.555	1.00	0.00	H
HETATM	215	OH2	TIP3	7	-3.940	-2.062	0.430	1.00	26.17	O
HETATM	216	H1	TIP3	7	-4.861	-1.862	0.766	1.00	0.00	H
HETATM	217	H2	TIP3	7	-4.155	-2.573	-0.368	1.00	0.00	H

The atomic coordinates of these atoms (QM part) for ATP-bound K15A mutant

ATOM	200	N	ALA	15	-8.326	-5.518	-3.313	1.00	0.00	N
ATOM	201	HN	ALA	15	-7.710	-4.895	-3.821	1.00	0.00	H
ATOM	202	CA	ALA	15	-9.640	-4.989	-3.061	1.00	0.00	C
ATOM	203	HA	ALA	15	-10.270	-5.731	-2.577	1.00	0.00	H
ATOM	204	CB	ALA	15	-9.555	-3.714	-2.201	1.00	0.00	C
ATOM	205	HB1	ALA	15	-8.944	-2.939	-2.718	1.00	0.00	H
ATOM	206	HB2	ALA	15	-10.559	-3.282	-2.003	1.00	0.00	H
ATOM	207	HB3	ALA	15	-9.066	-3.927	-1.228	1.00	0.00	H
ATOM	208	C	ALA	15	-10.284	-4.620	-4.395	1.00	0.00	C
ATOM	209	O	ALA	15	-9.725	-3.792	-5.139	1.00	0.00	O
ATOM	972	N	ASP	71	7.210	-1.891	-11.093	1.00	30.04	N
ATOM	973	HN	ASP	71	7.216	-2.855	-10.754	1.00	0.00	H
ATOM	974	CA	ASP	71	8.264	-0.995	-10.626	1.00	32.00	C
ATOM	975	HA	ASP	71	7.887	0.004	-10.375	1.00	0.00	H
ATOM	976	CB	ASP	71	8.874	-1.582	-9.332	1.00	28.61	C
ATOM	977	HB1	ASP	71	9.245	-2.593	-9.526	1.00	0.00	H
ATOM	978	HB2	ASP	71	9.735	-0.986	-9.006	1.00	0.00	H
ATOM	979	CG	ASP	71	7.833	-1.617	-8.204	1.00	28.31	C
ATOM	980	OD1	ASP	71	7.834	-2.658	-7.505	1.00	20.80	O
ATOM	981	OD2	ASP	71	7.083	-0.603	-8.097	1.00	22.40	O
ATOM	982	C	ASP	71	9.421	-0.813	-11.617	1.00	37.73	C
ATOM	983	O	ASP	71	9.916	0.321	-11.732	1.00	40.83	O
ATOM	1362	N	ASP	95	-0.606	1.089	-8.456	1.00	17.31	N
ATOM	1363	HN	ASP	95	0.377	0.895	-8.283	1.00	0.00	H
ATOM	1364	CA	ASP	95	-1.345	1.592	-7.272	1.00	21.42	C
ATOM	1365	HA	ASP	95	-2.412	1.388	-7.414	1.00	0.00	H
ATOM	1366	CB	ASP	95	-0.906	0.734	-6.065	1.00	22.01	C
ATOM	1367	HB1	ASP	95	-1.517	1.016	-5.200	1.00	0.00	H
ATOM	1368	HB2	ASP	95	-1.156	-0.312	-6.276	1.00	0.00	H
ATOM	1369	CG	ASP	95	0.584	0.799	-5.665	1.00	25.03	C
ATOM	1370	OD1	ASP	95	1.400	1.458	-6.383	1.00	18.38	O
ATOM	1371	OD2	ASP	95	0.874	0.142	-4.630	1.00	33.04	O
ATOM	1372	C	ASP	95	-1.229	3.114	-6.984	1.00	20.21	C
ATOM	1373	O	ASP	95	-2.254	3.775	-6.826	1.00	19.04	O

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ATOM   1650  N   THR   116      1.752  -2.109   3.325  1.00 22.49           N
ATOM   1651  HN  THR   116      1.019  -2.206   2.632  1.00  0.00           H
ATOM   1652  CA  THR   116      2.883  -3.040   3.214  1.00 17.24           C
ATOM   1653  HA  THR   116      3.181  -3.379   4.218  1.00  0.00           H
ATOM   1654  CB  THR   116      2.411  -4.313   2.377  1.00 23.75           C
ATOM   1655  HB  THR   116      2.958  -4.294   1.425  1.00  0.00           H
ATOM   1656  OG1 THR   116      1.038  -4.268   2.090  1.00 20.76           O
ATOM   1657  HG1 THR   116      0.962  -3.706   1.272  1.00  0.00           H
ATOM   1658  CG2 THR   116      2.729  -5.620   3.076  1.00 21.59           C
ATOM   1659 HG21 THR   116      2.556  -6.463   2.400  1.00  0.00           H
ATOM   1660 HG22 THR   116      3.773  -5.639   3.410  1.00  0.00           H
ATOM   1661 HG23 THR   116      2.070  -5.751   3.938  1.00  0.00           H
ATOM   1662  C   THR   116      4.187  -2.542   2.540  1.00 24.46           C
ATOM   1663  O   THR   116      5.244  -2.708   3.160  1.00 18.70           O
ATOM   2012  N   ASP   140     11.528   0.228   0.719  1.00 18.27           N
ATOM   2013  HN  ASP   140     11.680   0.435  -0.244  1.00  0.00           H
ATOM   2014  CA  ASP   140     10.241   0.680   1.186  1.00 22.74           C
ATOM   2015  HA  ASP   140      9.931   1.469   0.522  1.00  0.00           H
ATOM   2016  CB  ASP   140      9.189  -0.430   1.028  1.00 16.60           C
ATOM   2017  HB1 ASP   140      9.493  -1.331   1.598  1.00  0.00           H
ATOM   2018  HB2 ASP   140      8.206  -0.087   1.409  1.00  0.00           H
ATOM   2019  CG  ASP   140      9.019  -0.822  -0.434  1.00 24.88           C
ATOM   2020  OD1 ASP   140      9.649  -0.242  -1.367  1.00 22.74           O
ATOM   2021  OD2 ASP   140      8.217  -1.760  -0.658  1.00 19.30           O
ATOM   2022  C   ASP   140     10.376   1.364   2.542  1.00 15.06           C
ATOM   2023  O   ASP   140      9.816   0.963   3.562  1.00 16.59           O
TER    4533       ILE   297
HETATM 4534  C1  GLO     1      6.298  -1.677  -3.194  1.00 12.70           C
HETATM 4535  H1  GLO     1      7.194  -1.052  -3.386  1.00  0.00           H
HETATM 4536  O1  GLO     1      6.627  -2.727  -2.344  1.00 18.41           O
HETATM 4537  H1A GLO     1      7.238  -2.363  -1.642  1.00  0.00           H
HETATM 4538  C2  GLO     1      5.771  -2.211  -4.524  1.00 13.93           C
HETATM 4539  H2  GLO     1      4.836  -2.751  -4.300  1.00  0.00           H
HETATM 4540  O2  GLO     1      6.709  -3.101  -5.090  1.00 17.69           O
HETATM 4541  H2A GLO     1      6.934  -2.820  -6.007  1.00  0.00           H
HETATM 4542  C3  GLO     1      5.450  -0.990  -5.398  1.00 14.37           C
HETATM 4543  H3  GLO     1      6.379  -0.406  -5.518  1.00  0.00           H
HETATM 4544  O3  GLO     1      4.988  -1.368  -6.676  1.00 15.82           O
HETATM 4545  H3A GLO     1      5.640  -1.005  -7.320  1.00  0.00           H
HETATM 4546  C4  GLO     1      4.400  -0.112  -4.722  1.00 12.99           C
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HETATM 4547 H4 GLO 1 3.463 -0.680 -4.723 1.00 0.00 H
HETATM 4548 O4 GLO 1 4.234 1.129 -5.382 1.00 16.09 O
HETATM 4549 H4A GLO 1 3.432 1.084 -5.945 1.00 0.00 H
HETATM 4550 C5 GLO 1 4.773 0.221 -3.274 1.00 13.50 C
HETATM 4551 H5 GLO 1 5.517 1.043 -3.305 1.00 0.00 H
HETATM 4552 O5 GLO 1 5.305 -0.883 -2.551 1.00 13.60 O
HETATM 4553 C6 GLO 1 3.525 0.705 -2.526 1.00 14.16 C
HETATM 4554 H6A GLO 1 3.766 0.929 -1.482 1.00 0.00 H
HETATM 4555 H6B GLO 1 3.189 1.631 -3.012 1.00 0.00 H
HETATM 4556 O6 GLO 1 2.505 -0.267 -2.516 1.00 15.87 O
HETATM 4557 H6C GLO 1 1.966 -0.158 -3.333 1.00 0.00 H
HETATM 4558 C5 ATP 1 -0.728 -2.609 5.866 1.00 22.91 C
HETATM 4559 H5 ATP 1 0.310 -2.196 5.812 1.00 0.00 H
HETATM 4560 O5 ATP 1 -1.523 -1.659 6.608 1.00 24.49 O
HETATM 4561 C8 ATP 1 -1.259 -1.894 7.945 1.00 24.51 C
HETATM 4562 H8 ATP 1 -0.215 -1.538 8.119 1.00 0.00 H
HETATM 4563 C10 ATP 1 -2.994 -0.050 10.480 1.00 28.07 C
HETATM 4564 N9 ATP 1 -4.111 -0.372 9.690 1.00 30.76 N
HETATM 4565 C9 ATP 1 -3.572 -1.040 8.682 1.00 25.92 C
HETATM 4566 H9 ATP 1 -4.112 -1.435 7.815 1.00 0.00 H
HETATM 4567 N8 ATP 1 -2.209 -1.202 8.794 1.00 24.23 N
HETATM 4568 N12 ATP 1 -1.581 0.707 12.216 1.00 31.20 N
HETATM 4569 C12 ATP 1 -0.561 0.204 11.533 1.00 30.86 C
HETATM 4570 H12 ATP 1 0.424 0.311 11.998 1.00 0.00 H
HETATM 4571 N11 ATP 1 -0.586 -0.483 10.402 1.00 25.68 N
HETATM 4572 C11 ATP 1 -1.833 -0.561 9.921 1.00 27.55 C
HETATM 4573 C13 ATP 1 -2.826 0.620 11.715 1.00 34.82 C
HETATM 4574 N13 ATP 1 -3.772 1.143 12.502 1.00 33.87 N
HETATM 4575 H13B ATP 1 -3.377 1.403 13.405 1.00 0.00 H
HETATM 4576 H13A ATP 1 -4.277 1.932 12.149 1.00 0.00 H
HETATM 4577 C7 ATP 1 -1.317 -3.387 8.102 1.00 25.14 C
HETATM 4578 H7 ATP 1 -2.363 -3.752 8.201 1.00 0.00 H
HETATM 4579 O7 ATP 1 -0.530 -3.837 9.191 1.00 22.96 O
HETATM 4580 H7A ATP 1 0.356 -4.014 8.824 1.00 0.00 H
HETATM 4581 C6 ATP 1 -0.746 -3.848 6.750 1.00 21.74 C
HETATM 4582 H6 ATP 1 -1.455 -4.573 6.294 1.00 0.00 H
HETATM 4583 O6 ATP 1 0.555 -4.431 6.814 1.00 20.39 O
HETATM 4584 H6A ATP 1 0.453 -5.398 6.688 1.00 0.00 H
HETATM 4585 C4 ATP 1 -1.301 -2.860 4.479 1.00 17.35 C
HETATM 4586 H4A ATP 1 -0.568 -3.399 3.879 1.00 0.00 H
HETATM 4587 H4B ATP 1 -2.194 -3.485 4.609 1.00 0.00 H
HETATM 4588 O3 ATP 1 -1.643 -1.634 3.862 1.00 25.21 O
HETATM 4589 P3 ATP 1 -3.083 -1.587 3.090 1.00 25.58 P
HETATM 4590 O3A ATP 1 -3.119 -0.201 2.489 1.00 19.33 O

HETATM 4591 O3B ATP 1 -4.152 -2.054 4.051 1.00 27.75 O
HETATM 4592 O2 ATP 1 -2.935 -2.789 2.003 1.00 23.57 O
HETATM 4593 P2 ATP 1 -2.110 -2.835 0.554 1.00 22.77 P
HETATM 4594 O2A ATP 1 -2.869 -1.940 -0.411 1.00 24.45 O
HETATM 4595 O2B ATP 1 -1.938 -4.292 0.242 1.00 18.45 O
HETATM 4596 O1 ATP 1 -0.710 -2.124 1.020 1.00 23.12 O
HETATM 4597 P1 ATP 1 0.491 -1.569 -0.099 1.00 0.00 P
HETATM 4598 O1C ATP 1 -0.238 -1.703 -1.435 1.00 0.00 O
HETATM 4599 O1B ATP 1 1.630 -2.585 0.167 1.00 0.00 O
HETATM 4600 O1A ATP 1 0.823 -0.143 0.333 1.00 0.00 O
HETATM 4601 MG MGL 1 -2.019 -0.449 -1.528 1.00 27.88 LP
HETATM 4602 OH2 TIP3 1 -1.649 0.720 0.249 1.00 18.54 O
HETATM 4603 H1 TIP3 1 -2.118 0.303 1.008 1.00 0.00 H
HETATM 4604 H2 TIP3 1 -0.677 0.552 0.423 1.00 0.00 H
HETATM 4614 OH2 TIP3 5 -3.758 0.721 -1.634 1.00 21.67 O
HETATM 4615 H1 TIP3 5 -4.123 0.804 -0.720 1.00 0.00 H
HETATM 4616 H2 TIP3 5 -4.469 0.188 -2.114 1.00 0.00 H
HETATM 4617 OH2 TIP3 6 -0.627 0.815 -2.464 1.00 23.98 O
HETATM 4618 H1 TIP3 6 -0.260 0.399 -3.287 1.00 0.00 H
HETATM 4619 H2 TIP3 6 0.113 0.695 -1.833 1.00 0.00 H
HETATM 4620 OH2 TIP3 7 -2.644 -1.325 -3.335 1.00 26.17 O
HETATM 4621 H1 TIP3 7 -3.349 -0.858 -3.885 1.00 0.00 H
HETATM 4622 H2 TIP3 7 -3.117 -2.106 -2.997 1.00 0.00 H

The atomic coordinates of these atoms (QM part) for ATPγS-bound StHK.

ATOM 200 N LYS 15 -8.346 -5.502 -3.328 1.00 18.96 N
ATOM 201 HN LYS 15 -7.712 -4.933 -3.892 1.00 0.00 H
ATOM 202 CA LYS 15 -9.674 -4.964 -3.021 1.00 27.33 C
ATOM 203 HA LYS 15 -10.271 -5.711 -2.479 1.00 0.00 H
ATOM 204 CB LYS 15 -9.577 -3.672 -2.177 1.00 31.73 C
ATOM 205 HB1 LYS 15 -9.002 -2.955 -2.774 1.00 0.00 H
ATOM 206 HB2 LYS 15 -10.574 -3.224 -2.074 1.00 0.00 H
ATOM 207 CG LYS 15 -8.939 -3.869 -0.784 1.00 46.58 C
ATOM 208 HG1 LYS 15 -9.699 -3.695 -0.013 1.00 0.00 H
ATOM 209 HG2 LYS 15 -8.607 -4.912 -0.669 1.00 0.00 H
ATOM 210 CD LYS 15 -7.748 -2.937 -0.500 1.00 52.98 C
ATOM 211 HD1 LYS 15 -8.025 -1.902 -0.733 1.00 0.00 H
ATOM 212 HD2 LYS 15 -7.512 -2.957 0.573 1.00 0.00 H
ATOM 213 CE LYS 15 -6.489 -3.319 -1.277 1.00 55.66 C
ATOM 214 HE1 LYS 15 -6.206 -4.358 -1.104 1.00 0.00 H
ATOM 215 HE2 LYS 15 -6.623 -3.200 -2.352 1.00 0.00 H
ATOM 216 NZ LYS 15 -5.333 -2.436 -0.895 1.00 52.51 N
ATOM 217 HZ1 LYS 15 -4.402 -2.801 -1.153 1.00 0.00 H
ATOM 218 HZ2 LYS 15 -5.447 -1.544 -1.439 1.00 0.00 H

ATOM 219 HZ3 LYS 15 -5.245 -2.235 0.128 1.00 0.00 H
ATOM 220 C LYS 15 -10.349 -4.620 -4.372 1.00 26.81 C
ATOM 221 O LYS 15 -9.776 -3.796 -5.077 1.00 22.30 O
ATOM 984 N ASP 71 7.157 -1.842 -11.081 1.00 30.04 N
ATOM 985 HN ASP 71 7.206 -2.822 -10.797 1.00 0.00 H
ATOM 986 CA ASP 71 8.214 -0.955 -10.591 1.00 32.00 C
ATOM 987 HA ASP 71 7.838 0.043 -10.343 1.00 0.00 H
ATOM 988 CB ASP 71 8.823 -1.553 -9.299 1.00 28.61 C
ATOM 989 HB1 ASP 71 9.201 -2.561 -9.500 1.00 0.00 H
ATOM 990 HB2 ASP 71 9.680 -0.952 -8.968 1.00 0.00 H
ATOM 991 CG ASP 71 7.789 -1.603 -8.166 1.00 28.31 C
ATOM 992 OD1 ASP 71 7.831 -2.614 -7.425 1.00 20.80 O
ATOM 993 OD2 ASP 71 6.993 -0.620 -8.088 1.00 22.40 O
ATOM 994 C ASP 71 9.392 -0.765 -11.559 1.00 37.73 C
ATOM 995 O ASP 71 9.998 0.316 -11.537 1.00 40.83 O
ATOM 1374 N ASP 95 -0.470 1.121 -8.518 1.00 17.31 N
ATOM 1375 HN ASP 95 0.519 1.014 -8.301 1.00 0.00 H
ATOM 1376 CA ASP 95 -1.278 1.618 -7.379 1.00 21.42 C
ATOM 1377 HA ASP 95 -2.329 1.372 -7.566 1.00 0.00 H
ATOM 1378 CB ASP 95 -0.859 0.813 -6.124 1.00 22.01 C
ATOM 1379 HB1 ASP 95 -1.589 1.001 -5.330 1.00 0.00 H
ATOM 1380 HB2 ASP 95 -0.925 -0.254 -6.375 1.00 0.00 H
ATOM 1381 CG ASP 95 0.570 1.097 -5.599 1.00 25.03 C
ATOM 1382 OD1 ASP 95 1.398 1.640 -6.378 1.00 18.38 O
ATOM 1383 OD2 ASP 95 0.801 0.739 -4.407 1.00 33.04 O
ATOM 1384 C ASP 95 -1.239 3.148 -7.101 1.00 20.21 C
ATOM 1385 O ASP 95 -2.298 3.753 -6.945 1.00 19.04 O
ATOM 1662 N THR 116 1.719 -1.920 2.950 1.00 22.49 N
ATOM 1663 HN THR 116 1.423 -1.633 2.008 1.00 0.00
H
ATOM 1664 CA THR 116 2.789 -2.939 3.054 1.00 17.24 C
ATOM 1665 HA THR 116 2.962 -3.167 4.113 1.00 0.00
H
ATOM 1666 CB THR 116 2.161 -4.228 2.456 1.00 23.75 C
ATOM 1667 HB THR 116 1.941 -4.041 1.402 1.00 0.00
H
ATOM 1668 OG1 THR 116 0.953 -4.450 3.172 1.00 20.76 O
ATOM 1669 HG1 THR 116 0.555 -3.558 3.225 1.00 0.00 H
ATOM 1670 CG2 THR 116 3.074 -5.431 2.582 1.00 21.59 C
ATOM 1671 HG21 THR 116 2.509 -6.355 2.419 1.00 0.00 H
ATOM 1672 HG22 THR 116 3.872 -5.376 1.832 1.00 0.00 H
ATOM 1673 HG23 THR 116 3.540 -5.489 3.570 1.00 0.00 H
ATOM 1674 C THR 116 4.179 -2.586 2.474 1.00 24.46 C
ATOM 1675 O THR 116 5.145 -2.794 3.218 1.00 18.70 O

ATOM 2024 N ASP 140 11.582 0.397 0.814 1.00 18.27 N
ATOM 2025 HN ASP 140 11.790 0.754 -0.092 1.00 0.00 H
ATOM 2026 CA ASP 140 10.240 0.689 1.238 1.00 22.74 C
ATOM 2027 HA ASP 140 9.882 1.475 0.591 1.00 0.00
H
ATOM 2028 CB ASP 140 9.312 -0.519 1.007 1.00 16.60 C
ATOM 2029 HB1 ASP 140 9.705 -1.412 1.532 1.00 0.00 H
ATOM 2030 HB2 ASP 140 8.302 -0.299 1.407 1.00 0.00 H
ATOM 2031 CG ASP 140 9.165 -0.859 -0.469 1.00 24.88 C
ATOM 2032 OD1 ASP 140 9.801 -0.251 -1.376 1.00 22.74 O
ATOM 2033 OD2 ASP 140 8.360 -1.786 -0.728 1.00 19.30 O
ATOM 2034 C ASP 140 10.202 1.314 2.628 1.00 15.06 C
ATOM 2035 O ASP 140 9.388 0.991 3.494 1.00 16.59 O
HETATM 4546 C1 GLO 1 6.332 -1.711 -3.160 1.00 12.70 C
HETATM 4547 H1 GLO 1 7.234 -1.103 -3.378 1.00 0.00 H
HETATM 4548 O1 GLO 1 6.659 -2.748 -2.298 1.00 18.41 O
HETATM 4549 H1A GLO 1 7.327 -2.390 -1.645 1.00 0.00 H
HETATM 4550 C2 GLO 1 5.760 -2.253 -4.472 1.00 13.93 C
HETATM 4551 H2 GLO 1 4.802 -2.730 -4.216 1.00 0.00 H
HETATM 4552 O2 GLO 1 6.616 -3.215 -5.054 1.00 17.69 O
HETATM 4553 H2A GLO 1 6.934 -2.892 -5.929 1.00 0.00 H
HETATM 4554 C3 GLO 1 5.512 -1.033 -5.362 1.00 14.37 C
HETATM 4555 H3 GLO 1 6.486 -0.544 -5.527 1.00 0.00 H
HETATM 4556 O3 GLO 1 4.964 -1.373 -6.621 1.00 15.82 O
HETATM 4557 H3A GLO 1 5.628 -1.060 -7.286 1.00 0.00 H
HETATM 4558 C4 GLO 1 4.591 -0.017 -4.695 1.00 12.99 C
HETATM 4559 H4 GLO 1 3.575 -0.436 -4.688 1.00 0.00 H
HETATM 4560 O4 GLO 1 4.625 1.215 -5.397 1.00 16.09 O
HETATM 4561 H4A GLO 1 4.192 1.071 -6.269 1.00 0.00 H
HETATM 4562 C5 GLO 1 5.003 0.292 -3.257 1.00 13.50 C
HETATM 4563 H5 GLO 1 5.871 0.979 -3.300 1.00 0.00 H
HETATM 4564 O5 GLO 1 5.356 -0.877 -2.531 1.00 13.60 O
HETATM 4565 C6 GLO 1 3.867 1.018 -2.522 1.00 14.16 C
HETATM 4566 H6A GLO 1 4.194 1.263 -1.508 1.00 0.00 H
HETATM 4567 H6B GLO 1 3.695 1.956 -3.065 1.00 0.00 H
HETATM 4568 O6 GLO 1 2.696 0.264 -2.390 1.00 15.87 O
HETATM 4569 H6C GLO 1 2.126 0.383 -3.180 1.00 0.00 H
HETATM 4570 C5 ATP 1 -1.492 -2.686 5.485 1.00 22.91 C
HETATM 4571 H5 ATP 1 -0.617 -2.501 4.811 1.00 0.00 H
HETATM 4572 O5 ATP 1 -1.641 -1.533 6.359 1.00 24.49 O
HETATM 4573 C8 ATP 1 -1.406 -1.909 7.690 1.00 24.51 C
HETATM 4574 H8 ATP 1 -0.326 -1.699 7.877 1.00 0.00 H
HETATM 4575 C10 ATP 1 -2.954 -0.036 10.361 1.00 28.07 C
HETATM 4576 N9 ATP 1 -4.104 -0.292 9.594 1.00 30.76 N

HETATM 4577 C9 ATP 1 -3.622 -0.950 8.553 1.00 25.92 C
HETATM 4578 H9 ATP 1 -4.206 -1.297 7.695 1.00 0.00 H
HETATM 4579 N8 ATP 1 -2.264 -1.165 8.609 1.00 24.23 N
HETATM 4580 N12 ATP 1 -1.471 0.630 12.082 1.00 31.20 N
HETATM 4581 C12 ATP 1 -0.490 0.106 11.353 1.00 30.86 C
HETATM 4582 H12 ATP 1 0.510 0.169 11.793 1.00 0.00 H
HETATM 4583 N11 ATP 1 -0.570 -0.561 10.208 1.00 25.68 N
HETATM 4584 C11 ATP 1 -1.829 -0.576 9.753 1.00 27.55 C
HETATM 4585 C13 ATP 1 -2.734 0.595 11.612 1.00 34.82 C
HETATM 4586 N13 ATP 1 -3.661 1.120 12.429 1.00 33.87 N
HETATM 4587 H13B ATP 1 -3.267 1.375 13.332 1.00 0.00 H
HETATM 4588 H13A ATP 1 -4.198 1.892 12.089 1.00 0.00 H
HETATM 4589 C7 ATP 1 -1.661 -3.387 7.786 1.00 25.14 C
HETATM 4590 H7 ATP 1 -2.744 -3.620 7.879 1.00 0.00 H
HETATM 4591 O7 ATP 1 -0.938 -3.965 8.859 1.00 22.96 O
HETATM 4592 H7A ATP 1 -0.025 -4.066 8.540 1.00 0.00 H
HETATM 4593 C6 ATP 1 -1.161 -3.859 6.422 1.00 21.74 C
HETATM 4594 H6 ATP 1 -1.755 -4.739 6.093 1.00 0.00 H
HETATM 4595 O6 ATP 1 0.229 -4.204 6.425 1.00 20.39 O
HETATM 4596 H6A ATP 1 0.295 -5.180 6.381 1.00 0.00 H
HETATM 4597 C4 ATP 1 -2.768 -2.920 4.655 1.00 17.35 C
HETATM 4598 H4A ATP 1 -2.565 -3.702 3.918 1.00 0.00 H
HETATM 4599 H4B ATP 1 -3.542 -3.288 5.352 1.00 0.00 H
HETATM 4600 O3 ATP 1 -3.234 -1.725 4.063 1.00 25.21 O
HETATM 4601 P3 ATP 1 -3.311 -1.510 2.424 1.00 25.58 P
HETATM 4602 O3A ATP 1 -3.022 -0.031 2.224 1.00 19.33 O
HETATM 4603 O3B ATP 1 -4.597 -2.099 1.899 1.00 27.75 O
HETATM 4604 O2 ATP 1 -2.003 -2.383 1.977 1.00 23.57 O
HETATM 4605 P2 ATP 1 -1.832 -3.068 0.457 1.00 22.77 P
HETATM 4606 O2A ATP 1 -2.527 -2.112 -0.517 1.00 24.45 O
HETATM 4607 O2B ATP 1 -2.294 -4.491 0.508 1.00 18.45 O
HETATM 4608 O1 ATP 1 -0.236 -3.059 0.308 1.00 23.12 O
HETATM 4609 P1 ATP 1 0.915 -1.961 -0.423 1.00 0.00 P
HETATM 4610 S1 ATP 1 0.260 -1.750 -2.314 1.00 0.00 S
HETATM 4611 O1B ATP 1 2.199 -2.764 -0.270 1.00 0.00 O
HETATM 4612 O1A ATP 1 0.825 -0.717 0.464 1.00 0.00 O
HETATM 4613 MG MGL 1 -1.970 -0.507 -1.731 1.00 27.88 LP
HETATM 4614 OH2 TIP3 1 -1.386 0.583 -0.000 1.00 18.54 O
HETATM 4615 H1 TIP3 1 -1.956 0.346 0.769 1.00 0.00 H
HETATM 4616 H2 TIP3 1 -0.485 0.186 0.226 1.00 0.00 H
HETATM 4626 OH2 TIP3 5 -3.784 0.568 -1.615 1.00 21.67 O
HETATM 4627 H1 TIP3 5 -4.200 0.727 -0.733 1.00 0.00 H
HETATM 4628 H2 TIP3 5 -4.537 0.252 -2.189 1.00 0.00 H
HETATM 4629 OH2 TIP3 6 -1.221 1.129 -2.784 1.00 23.98 O

HETATM 4630	H1	TIP3	6	-0.423	0.908	-3.368	1.00	0.00 H
HETATM 4631	H2	TIP3	6	-0.891	1.706	-2.076	1.00	0.00 H
HETATM 4632	OH2	TIP3	7	-2.764	-1.399	-3.460	1.00	26.17 O
HETATM 4633	H1	TIP3	7	-3.492	-0.911	-3.957	1.00	0.00 H
HETATM 4634	H2	TIP3	7	-2.153	-1.757	-4.123	1.00	0.00 H

Fig. S 1 The relative energies of the optimized structures obtained at B3LYP/6-31G(d)/CHARMM22 level in the phosphate transfer process and the proton transfer process. The curves colored in black, red and blue denotes the relative energies in ATP-bound StHK, ATP-bound K15A mutant, and ATPγS-bound StHK complexes, respectively.