

Cationic state distribution over the P700 chlorophyll pair in
Photosystem I

Keisuke Saito and Hiroshi Ishikita

Table S1. Atomic charges of Table 1 (**ESP: unrestricted DFT**).

| | atom | wild type | wild type, vacuum | wild type, $\Delta(\text{Arg-A750}$ $/\text{Ser-B734})$ | wild type, $\Delta(\text{Arg-A750}$ $/\text{Ser-B734})$ |
|----|------|-----------|----------------------|---|---|
| PA | MG | 1.35547 | 1.09021 | 1.35482 | 1.35768 |
| PA | CHA | 0.21113 | 0.16956 | 0.2106 | 0.2125 |
| PA | CHB | -0.4912 | -0.45658 | -0.48988 | -0.55482 |
| PA | HHB | 0.18743 | 0.17357 | 0.18537 | 0.17808 |
| PA | CHC | -0.38634 | -0.30492 | -0.38582 | -0.38307 |
| PA | HHC | 0.13862 | 0.12726 | 0.13726 | 0.14347 |
| PA | CHD | -0.5302 | -0.46312 | -0.53629 | -0.52875 |
| PA | HHD | 0.22576 | 0.20466 | 0.23061 | 0.22635 |
| PA | NA | -0.34823 | -0.29126 | -0.34261 | -0.33797 |
| PA | C1A | -0.23261 | -0.20778 | -0.23414 | -0.23464 |
| PA | C2A | 0.40008 | 0.38518 | 0.40054 | 0.37957 |
| PA | H2A | -0.02631 | -0.01067 | -0.02639 | -0.01838 |
| PA | C3A | 0.06662 | -0.01607 | 0.06941 | 0.07146 |
| PA | H3A | 0.03986 | 0.07684 | 0.03779 | 0.03993 |
| PA | C4A | 0.32392 | 0.27399 | 0.31598 | 0.31968 |
| PA | CMA | -0.42324 | -0.38014 | -0.42321 | -0.40562 |
| PA | HMA1 | 0.09253 | 0.11194 | 0.09033 | 0.09498 |
| PA | HMA2 | 0.13027 | 0.10078 | 0.13143 | 0.12669 |
| PA | HMA3 | 0.1156 | 0.11385 | 0.11389 | 0.09918 |
| PA | CAA | 0.01556 | -0.02184 | 0.0143 | 0.01481 |
| PA | HAA1 | 0.02446 | 0.00482 | 0.02405 | 0.02252 |
| PA | HAA2 | -0.007 | 0.01508 | -0.00798 | 0.00098 |
| PA | CBA | -0.61199 | -0.474 | -0.60973 | -0.6242 |
| PA | HBA1 | 0.15418 | 0.14755 | 0.15306 | 0.15756 |
| PA | HBA2 | 0.16968 | 0.09921 | 0.16799 | 0.17431 |
| PA | CGA | 0.8715 | 0.75781 | 0.87158 | 0.86772 |
| PA | O1A | -0.6504 | -0.51537 | -0.65383 | -0.63724 |
| PA | O2A | -0.30004 | -0.28595 | -0.2964 | -0.29961 |
| PA | NB | -0.63623 | -0.54695 | -0.63211 | -0.64985 |
| PA | C1B | 0.26444 | 0.21938 | 0.258 | 0.27296 |
| PA | C2B | 0.23133 | 0.20358 | 0.23263 | 0.1956 |

| | | | | | |
|----|------|----------|----------|----------|----------|
| PA | C3B | -0.29061 | -0.21883 | -0.29347 | -0.28427 |
| PA | C4B | 0.38241 | 0.31378 | 0.37953 | 0.39121 |
| PA | CMB | -0.29415 | -0.33308 | -0.29176 | -0.31864 |
| PA | HMB1 | 0.07044 | 0.09427 | 0.06847 | 0.06699 |
| PA | HMB2 | 0.09042 | 0.10223 | 0.08745 | 0.08984 |
| PA | HMB3 | 0.06796 | 0.10347 | 0.06786 | 0.1089 |
| PA | CAB | 0.08415 | 0.05926 | 0.08762 | 0.10637 |
| PA | HAB | 0.09981 | 0.10634 | 0.10208 | 0.0904 |
| PA | CBB | -0.46526 | -0.44888 | -0.47154 | -0.46195 |
| PA | HBB1 | 0.16713 | 0.17735 | 0.16625 | 0.17159 |
| PA | HBB2 | 0.20099 | 0.20174 | 0.19996 | 0.19687 |
| PA | NC | -0.73739 | -0.6306 | -0.74079 | -0.74584 |
| PA | C1C | 0.33777 | 0.24419 | 0.3378 | 0.34287 |
| PA | C2C | 0.18199 | 0.20962 | 0.18326 | 0.17345 |
| PA | C3C | -0.35219 | -0.3386 | -0.35554 | -0.34222 |
| PA | C4C | 0.53417 | 0.45936 | 0.54383 | 0.5356 |
| PA | CMC | -0.45799 | -0.46301 | -0.45861 | -0.45205 |
| PA | HMC1 | 0.13815 | 0.1409 | 0.1385 | 0.12942 |
| PA | HMC2 | 0.10918 | 0.11828 | 0.10706 | 0.11177 |
| PA | HMC3 | 0.17068 | 0.15583 | 0.17204 | 0.17263 |
| PA | CAC | 0.24828 | 0.23831 | 0.24678 | 0.24004 |
| PA | HAC1 | -0.01493 | -0.01425 | -0.00873 | -0.01229 |
| PA | HAC2 | -0.01128 | -0.00818 | -0.01113 | -0.00899 |
| PA | CBC | -0.37632 | -0.36896 | -0.37692 | -0.37214 |
| PA | HBC1 | 0.07888 | 0.09418 | 0.08062 | 0.07723 |
| PA | HBC2 | 0.12195 | 0.10137 | 0.12917 | 0.12301 |
| PA | HBC3 | 0.12114 | 0.10762 | 0.11784 | 0.12142 |
| PA | ND | -0.59097 | -0.53298 | -0.60291 | -0.60346 |
| PA | C1D | 0.33288 | 0.29241 | 0.35494 | 0.34335 |
| PA | C2D | 0.13526 | 0.17849 | 0.12176 | 0.13117 |
| PA | C3D | -0.31583 | -0.30429 | -0.30219 | -0.31118 |
| PA | C4D | 0.15275 | 0.1541 | 0.15591 | 0.15467 |
| PA | CMD | -0.39934 | -0.38982 | -0.39856 | -0.3998 |
| PA | HMD1 | 0.1243 | 0.11352 | 0.13155 | 0.12593 |
| PA | HMD2 | 0.12394 | 0.12861 | 0.13183 | 0.12533 |
| PA | HMD3 | 0.16348 | 0.14615 | 0.17051 | 0.16508 |

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|----|------|----------|----------|----------|----------|
| PA | CAD | 0.74048 | 0.68283 | 0.73423 | 0.73735 |
| PA | OBD | -0.55761 | -0.45313 | -0.54772 | -0.55323 |
| PA | CBD | -0.77744 | -0.63113 | -0.77961 | -0.77554 |
| PA | HBD1 | 0.20724 | 0.18903 | 0.20698 | 0.20794 |
| PA | CGD | 0.82827 | 0.78205 | 0.83203 | 0.82964 |
| PA | O1D | -0.51448 | -0.49835 | -0.51318 | -0.51646 |
| PA | O2D | -0.36949 | -0.36692 | -0.37077 | -0.37009 |
| PA | CED | -0.07259 | 0.00234 | -0.07155 | -0.06827 |
| PA | HED1 | 0.0387 | 0.0475 | 0.03565 | 0.03493 |
| PA | HED2 | 0.10831 | 0.08183 | 0.11035 | 0.10841 |
| PA | HED3 | 0.14324 | 0.10212 | 0.1419 | 0.14442 |
| PA | C1 | -0.11083 | -0.13187 | -0.11135 | -0.11427 |
| PA | H1 | 0.08074 | 0.09896 | 0.0809 | 0.08477 |
| PA | H2 | 0.10882 | 0.11789 | 0.10676 | 0.11131 |
| PA | H3 | 0.1193 | 0.10102 | 0.11968 | 0.11529 |
| PA | | | | | |
| PB | MG | 1.35866 | 1.11472 | 1.35473 | 1.37558 |
| PB | CHA | -0.02181 | 0.02752 | -0.01974 | -0.02785 |
| PB | CHB | -0.49255 | -0.44837 | -0.49201 | -0.5397 |
| PB | HHB | 0.18925 | 0.17641 | 0.18756 | 0.17141 |
| PB | CHC | -0.40195 | -0.32275 | -0.40055 | -0.39099 |
| PB | HHC | 0.14719 | 0.14175 | 0.14803 | 0.14698 |
| PB | CHD | -0.53921 | -0.43941 | -0.53693 | -0.54109 |
| PB | HHD | 0.22894 | 0.1945 | 0.22965 | 0.22983 |
| PB | NA | -0.31861 | -0.25813 | -0.31215 | -0.32827 |
| PB | C1A | -0.10361 | -0.1788 | -0.11175 | -0.08775 |
| PB | C2A | 0.30105 | 0.40939 | 0.30035 | 0.27306 |
| PB | H2A | -0.01597 | -0.02268 | -0.01772 | -0.00791 |
| PB | C3A | 0.10639 | 0.0244 | 0.11027 | 0.12431 |
| PB | H3A | 0.04012 | 0.05716 | 0.03703 | 0.03555 |
| PB | C4A | 0.30307 | 0.23987 | 0.29528 | 0.31171 |
| PB | CMA | -0.42634 | -0.39464 | -0.42582 | -0.41712 |
| PB | HMA1 | 0.11065 | 0.12054 | 0.10698 | 0.11423 |
| PB | HMA2 | 0.1256 | 0.1063 | 0.1257 | 0.12533 |
| PB | HMA3 | 0.10766 | 0.11363 | 0.10657 | 0.09636 |
| PB | CAA | 0.25084 | 0.09757 | 0.26433 | 0.25311 |

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|----|------|----------|----------|----------|----------|
| PB | HAA1 | -0.07564 | -0.02431 | -0.07775 | -0.08215 |
| PB | HAA2 | -0.0517 | -0.02427 | -0.05471 | -0.04817 |
| PB | CBA | -0.61896 | -0.5508 | -0.6278 | -0.62809 |
| PB | HBA1 | 0.17046 | 0.16367 | 0.16965 | 0.17569 |
| PB | HBA2 | 0.13314 | 0.11206 | 0.13441 | 0.13458 |
| PB | CGA | 0.80025 | 0.76041 | 0.80334 | 0.79446 |
| PB | O1A | -0.57357 | -0.50622 | -0.57624 | -0.55913 |
| PB | O2A | -0.28142 | -0.29511 | -0.28028 | -0.28185 |
| PB | NB | -0.66515 | -0.59837 | -0.66288 | -0.67666 |
| PB | C1B | 0.31505 | 0.26301 | 0.31145 | 0.32722 |
| PB | C2B | 0.15895 | 0.16097 | 0.15933 | 0.14801 |
| PB | C3B | -0.22163 | -0.17209 | -0.22394 | -0.21831 |
| PB | C4B | 0.42619 | 0.37045 | 0.42547 | 0.43796 |
| PB | CMB | -0.28036 | -0.34225 | -0.27832 | -0.33363 |
| PB | HMB1 | 0.07194 | 0.09032 | 0.06981 | 0.08402 |
| PB | HMB2 | 0.08774 | 0.10913 | 0.08501 | 0.08971 |
| PB | HMB3 | 0.06194 | 0.11917 | 0.06252 | 0.11193 |
| PB | CAB | -0.02416 | -0.04771 | -0.02187 | 0.00578 |
| PB | HAB | 0.11718 | 0.12542 | 0.11789 | 0.11555 |
| PB | CBB | -0.36025 | -0.3375 | -0.35943 | -0.39181 |
| PB | HBB1 | 0.16864 | 0.16591 | 0.16826 | 0.1747 |
| PB | HBB2 | 0.16938 | 0.16523 | 0.16755 | 0.16382 |
| PB | NC | -0.69835 | -0.60299 | -0.69961 | -0.71235 |
| PB | C1C | 0.30069 | 0.22714 | 0.3043 | 0.32092 |
| PB | C2C | 0.22874 | 0.23621 | 0.224 | 0.21339 |
| PB | C3C | -0.37195 | -0.34215 | -0.37076 | -0.35604 |
| PB | C4C | 0.53908 | 0.44209 | 0.53975 | 0.54974 |
| PB | CMC | -0.44126 | -0.43601 | -0.43833 | -0.43253 |
| PB | HMC1 | 0.11997 | 0.12812 | 0.11916 | 0.11388 |
| PB | HMC2 | 0.11263 | 0.12353 | 0.11474 | 0.11593 |
| PB | HMC3 | 0.16729 | 0.14988 | 0.17042 | 0.16577 |
| PB | CAC | 0.32461 | 0.28206 | 0.32481 | 0.31209 |
| PB | HAC1 | -0.00683 | -0.02341 | -0.00778 | -0.00252 |
| PB | HAC2 | -0.03653 | -0.02016 | -0.03291 | -0.0325 |
| PB | CBC | -0.39601 | -0.37445 | -0.39496 | -0.39458 |
| PB | HBC1 | 0.07943 | 0.08944 | 0.07611 | 0.0794 |

| | | | | | |
|-------------------------|------|----------|----------|----------|----------|
| PB | HBC2 | 0.15753 | 0.1036 | 0.15906 | 0.1593 |
| PB | HBC3 | 0.10222 | 0.11008 | 0.10337 | 0.10419 |
| PB | ND | -0.75183 | -0.63327 | -0.74694 | -0.77008 |
| PB | C1D | 0.45936 | 0.34739 | 0.45556 | 0.47532 |
| PB | C2D | 0.03884 | 0.09827 | 0.03904 | 0.03821 |
| PB | C3D | -0.22171 | -0.24006 | -0.22117 | -0.22156 |
| PB | C4D | 0.34493 | 0.28779 | 0.33715 | 0.36141 |
| PB | CMD | -0.34924 | -0.35693 | -0.35085 | -0.35105 |
| PB | HMD1 | 0.13113 | 0.11269 | 0.13167 | 0.1336 |
| PB | HMD2 | 0.12901 | 0.12589 | 0.13041 | 0.13095 |
| PB | HMD3 | 0.17045 | 0.14205 | 0.1695 | 0.17285 |
| PB | CAD | 0.62967 | 0.64475 | 0.62997 | 0.6288 |
| PB | OBD | -0.42398 | -0.43502 | -0.4288 | -0.41819 |
| PB | CBD | -0.6503 | -0.62986 | -0.65144 | -0.6478 |
| PB | HBD1 | 0.19526 | 0.1877 | 0.1946 | 0.19576 |
| PB | CGD | 0.79514 | 0.79877 | 0.79634 | 0.794 |
| PB | O1D | -0.49682 | -0.48653 | -0.49843 | -0.49577 |
| PB | O2D | -0.35469 | -0.34845 | -0.35533 | -0.35396 |
| PB | CED | -0.06832 | -0.05297 | -0.06662 | -0.06732 |
| PB | HED1 | 0.11586 | 0.1096 | 0.11353 | 0.11719 |
| PB | HED2 | 0.08628 | 0.07382 | 0.0847 | 0.08633 |
| PB | HED3 | 0.09891 | 0.09368 | 0.09709 | 0.10023 |
| PB | C1 | -0.14602 | -0.14698 | -0.1455 | -0.15119 |
| PB | H1 | 0.1385 | 0.11777 | 0.13686 | 0.14241 |
| PB | H2 | 0.09874 | 0.11437 | 0.09661 | 0.10359 |
| PB | H3 | 0.09296 | 0.10172 | 0.09338 | 0.09138 |
| <hr/> total (PA) | | 0.27916 | 0.41469 | 0.30602 | 0.24039 |
| <hr/> total (PB) | | 0.72078 | 0.58527 | 0.69398 | 0.75961 |
| <hr/> | | | | | |

| | atom | T743V | T743V with $\Delta(\text{Arg-A750}/\text{Ser-B734})$ | [rotated methyl-ester] A _{-1A} | [rotated methyl-ester] A _{-1B} | [rotated methyl-ester] A _{-1A} /A _{-1B} |
|----|------|----------|---|---|---|---|
| PA | MG | 1.36812 | 1.36709 | 1.33677 | 1.3854 | 1.36944 |
| PA | CHA | 0.12917 | 0.1287 | 0.21165 | 0.22768 | 0.22328 |
| PA | CHB | -0.51249 | -0.51061 | -0.51854 | -0.52439 | -0.55317 |
| PA | HHB | 0.18858 | 0.18666 | 0.19219 | 0.19063 | 0.19535 |
| PA | CHC | -0.39299 | -0.39329 | -0.4094 | -0.39813 | -0.42228 |
| PA | HHC | 0.139 | 0.138 | 0.1508 | 0.14254 | 0.15611 |
| PA | CHD | -0.5146 | -0.52118 | -0.52195 | -0.53324 | -0.52928 |
| PA | HHD | 0.21859 | 0.2235 | 0.22481 | 0.22513 | 0.2253 |
| PA | NA | -0.39055 | -0.38357 | -0.34214 | -0.40542 | -0.40155 |
| PA | C1A | -0.15846 | -0.16044 | -0.23803 | -0.21759 | -0.22133 |
| PA | C2A | 0.31003 | 0.30984 | 0.38929 | 0.36245 | 0.36822 |
| PA | H2A | -0.01545 | -0.01527 | -0.0243 | -0.02003 | -0.02163 |
| PA | C3A | 0.1209 | 0.12402 | 0.07651 | 0.0846 | 0.08661 |
| PA | H3A | 0.0193 | 0.01743 | 0.03744 | 0.03104 | 0.03119 |
| PA | C4A | 0.34628 | 0.33756 | 0.3278 | 0.36622 | 0.37498 |
| PA | CMA | -0.43286 | -0.43297 | -0.42473 | -0.42722 | -0.42871 |
| PA | HMA1 | 0.09449 | 0.09252 | 0.09298 | 0.09259 | 0.09361 |
| PA | HMA2 | 0.13255 | 0.13374 | 0.12771 | 0.13166 | 0.12849 |
| PA | HMA3 | 0.11428 | 0.11267 | 0.11363 | 0.11461 | 0.11286 |
| PA | CAA | 0.08311 | 0.08222 | 0.02806 | 0.03891 | 0.02829 |
| PA | HAA1 | 0.02525 | 0.02516 | 0.02291 | 0.03525 | 0.03507 |
| PA | HAA2 | -0.03311 | -0.0342 | -0.00942 | -0.00623 | -0.00217 |
| PA | CBA | -0.62234 | -0.62023 | -0.61675 | -0.65088 | -0.64822 |
| PA | HBA1 | 0.13977 | 0.13871 | 0.1541 | 0.1644 | 0.16455 |
| PA | HBA2 | 0.18113 | 0.17953 | 0.1705 | 0.18238 | 0.18151 |
| PA | CGA | 0.85235 | 0.85228 | 0.87059 | 0.87395 | 0.87457 |
| PA | O1A | -0.63925 | -0.64257 | -0.64938 | -0.64625 | -0.64676 |
| PA | O2A | -0.30834 | -0.30479 | -0.3023 | -0.30603 | -0.30739 |
| PA | NB | -0.65943 | -0.65568 | -0.65742 | -0.66536 | -0.68907 |
| PA | C1B | 0.28235 | 0.27629 | 0.2857 | 0.29883 | 0.31912 |
| PA | C2B | 0.23701 | 0.23805 | 0.23361 | 0.2212 | 0.22694 |

| | | | | | | |
|----|------|----------|----------|----------|----------|----------|
| PA | C3B | -0.31242 | -0.31508 | -0.31415 | -0.29235 | -0.3212 |
| PA | C4B | 0.40341 | 0.40175 | 0.41881 | 0.39027 | 0.4292 |
| PA | CMB | -0.29393 | -0.29195 | -0.29382 | -0.30011 | -0.29499 |
| PA | HMB1 | 0.07033 | 0.06846 | 0.06764 | 0.07239 | 0.06855 |
| PA | HMB2 | 0.08763 | 0.08486 | 0.09278 | 0.09337 | 0.09305 |
| PA | HMB3 | 0.06888 | 0.06928 | 0.06768 | 0.06419 | 0.06321 |
| PA | CAB | 0.094 | 0.09743 | 0.09913 | 0.09195 | 0.11455 |
| PA | HAB | 0.10003 | 0.1024 | 0.08505 | 0.09525 | 0.0774 |
| PA | CBB | -0.46631 | -0.47227 | -0.41861 | -0.46732 | -0.42515 |
| PA | HBB1 | 0.16512 | 0.16444 | 0.15169 | 0.16664 | 0.15243 |
| PA | HBB2 | 0.203 | 0.20192 | 0.2042 | 0.20083 | 0.20454 |
| PA | NC | -0.73486 | -0.73815 | -0.73858 | -0.76269 | -0.76085 |
| PA | C1C | 0.33962 | 0.34038 | 0.34746 | 0.35685 | 0.3624 |
| PA | C2C | 0.18497 | 0.18621 | 0.16571 | 0.16131 | 0.14861 |
| PA | C3C | -0.34863 | -0.35152 | -0.34573 | -0.3429 | -0.34022 |
| PA | C4C | 0.52476 | 0.53475 | 0.523 | 0.54343 | 0.53541 |
| PA | CMC | -0.46995 | -0.47085 | -0.44108 | -0.43744 | -0.42236 |
| PA | HMC1 | 0.14131 | 0.14208 | 0.13437 | 0.12745 | 0.12569 |
| PA | HMC2 | 0.11022 | 0.10824 | 0.10694 | 0.10546 | 0.10299 |
| PA | HMC3 | 0.17639 | 0.17784 | 0.16547 | 0.1667 | 0.16161 |
| PA | CAC | 0.26396 | 0.26154 | 0.24826 | 0.24028 | 0.24187 |
| PA | HAC1 | -0.02074 | -0.01453 | -0.01566 | -0.01274 | -0.01389 |
| PA | HAC2 | -0.01496 | -0.01444 | -0.01101 | -0.00995 | -0.00968 |
| PA | CBC | -0.37424 | -0.37451 | -0.3767 | -0.37135 | -0.37281 |
| PA | HBC1 | 0.07691 | 0.07861 | 0.07807 | 0.07723 | 0.07662 |
| PA | HBC2 | 0.11938 | 0.12667 | 0.12196 | 0.12059 | 0.12086 |
| PA | HBC3 | 0.12056 | 0.11743 | 0.1207 | 0.12014 | 0.12013 |
| PA | ND | -0.61305 | -0.62576 | -0.57814 | -0.61093 | -0.60574 |
| PA | C1D | 0.33635 | 0.36033 | 0.32173 | 0.33932 | 0.33286 |
| PA | C2D | 0.12759 | 0.11301 | 0.13366 | 0.13338 | 0.13026 |
| PA | C3D | -0.31204 | -0.29807 | -0.31313 | -0.32461 | -0.32354 |
| PA | C4D | 0.20338 | 0.20701 | 0.14394 | 0.16239 | 0.16177 |
| PA | CMD | -0.39068 | -0.38936 | -0.39843 | -0.39625 | -0.39415 |
| PA | HMD1 | 0.12493 | 0.13237 | 0.12372 | 0.12208 | 0.12132 |
| PA | HMD2 | 0.12267 | 0.13046 | 0.12244 | 0.12313 | 0.1212 |
| PA | HMD3 | 0.15967 | 0.16663 | 0.16305 | 0.16207 | 0.16174 |

| | | | | | | |
|----|------|----------|----------|----------|----------|----------|
| PA | CAD | 0.69165 | 0.68425 | 0.73665 | 0.74368 | 0.73954 |
| PA | OBD | -0.49495 | -0.48393 | -0.55897 | -0.56079 | -0.56194 |
| PA | CBD | -0.67949 | -0.68108 | -0.77303 | -0.79784 | -0.7948 |
| PA | HBD1 | 0.191 | 0.19085 | 0.20554 | 0.21062 | 0.20951 |
| PA | CGD | 0.79524 | 0.79901 | 0.82857 | 0.83903 | 0.84219 |
| PA | O1D | -0.511 | -0.50943 | -0.51437 | -0.52097 | -0.52127 |
| PA | O2D | -0.35805 | -0.3593 | -0.37079 | -0.37057 | -0.37189 |
| PA | CED | -0.03092 | -0.02991 | -0.0694 | -0.06799 | -0.06918 |
| PA | HED1 | 0.03781 | 0.03498 | 0.03828 | 0.03474 | 0.03512 |
| PA | HED2 | 0.10162 | 0.10372 | 0.10752 | 0.10613 | 0.10655 |
| PA | HED3 | 0.09876 | 0.09724 | 0.14196 | 0.14385 | 0.14349 |
| PA | C1 | -0.09263 | -0.09287 | -0.10572 | -0.1066 | -0.10511 |
| PA | H1 | 0.07445 | 0.0747 | 0.08032 | 0.08162 | 0.0816 |
| PA | H2 | 0.10065 | 0.09853 | 0.10524 | 0.10709 | 0.10659 |
| PA | H3 | 0.12227 | 0.12251 | 0.11926 | 0.11584 | 0.11558 |
| PA | | | | | | |
| PB | MG | 1.36144 | 1.35711 | 1.38975 | 1.39831 | 1.42671 |
| PB | CHA | -0.02528 | -0.02279 | -0.03689 | -0.04485 | -0.06521 |
| PB | CHB | -0.51383 | -0.51287 | -0.5428 | -0.49772 | -0.55591 |
| PB | HHB | 0.18956 | 0.18761 | 0.19271 | 0.18571 | 0.19029 |
| PB | CHC | -0.41738 | -0.41571 | -0.43831 | -0.38043 | -0.41011 |
| PB | HHC | 0.15574 | 0.15645 | 0.15294 | 0.14158 | 0.14562 |
| PB | CHD | -0.52781 | -0.52499 | -0.55196 | -0.5512 | -0.56675 |
| PB | HHD | 0.22584 | 0.22645 | 0.23095 | 0.23007 | 0.23279 |
| PB | NA | -0.34527 | -0.33842 | -0.41224 | -0.38333 | -0.47912 |
| PB | C1A | -0.08612 | -0.09498 | -0.03882 | -0.058 | 0.0104 |
| PB | C2A | 0.27724 | 0.27636 | 0.25068 | 0.28876 | 0.23222 |
| PB | H2A | -0.01357 | -0.01536 | -0.01321 | -0.01762 | -0.01261 |
| PB | C3A | 0.11686 | 0.12133 | 0.13326 | 0.10927 | 0.12895 |
| PB | H3A | 0.03497 | 0.03152 | 0.02766 | 0.03668 | 0.02606 |
| PB | C4A | 0.32948 | 0.32086 | 0.37724 | 0.34471 | 0.43315 |
| PB | CMA | -0.43158 | -0.43103 | -0.4328 | -0.43295 | -0.44061 |
| PB | HMA1 | 0.11135 | 0.1075 | 0.11257 | 0.11154 | 0.11471 |
| PB | HMA2 | 0.12635 | 0.1265 | 0.12577 | 0.1282 | 0.12833 |
| PB | HMA3 | 0.1071 | 0.10593 | 0.10622 | 0.10979 | 0.10876 |
| PB | CAA | 0.26842 | 0.28168 | 0.30457 | 0.2693 | 0.32379 |

| | | | | | | |
|----|------|----------|----------|----------|----------|----------|
| PB | HAA1 | -0.07752 | -0.0796 | -0.09685 | -0.07901 | -0.10209 |
| PB | HAA2 | -0.05496 | -0.05788 | -0.06504 | -0.0566 | -0.06922 |
| PB | CBA | -0.62838 | -0.63723 | -0.63073 | -0.62463 | -0.63476 |
| PB | HBA1 | 0.17223 | 0.17146 | 0.17051 | 0.17118 | 0.17079 |
| PB | HBA2 | 0.13535 | 0.13662 | 0.13497 | 0.13441 | 0.1361 |
| PB | CGA | 0.80046 | 0.80357 | 0.80317 | 0.80027 | 0.80255 |
| PB | O1A | -0.57349 | -0.57623 | -0.57524 | -0.57353 | -0.57532 |
| PB | O2A | -0.28153 | -0.28044 | -0.28221 | -0.28246 | -0.28204 |
| PB | NB | -0.67143 | -0.66823 | -0.71519 | -0.66444 | -0.71683 |
| PB | C1B | 0.32245 | 0.31769 | 0.36961 | 0.32817 | 0.38297 |
| PB | C2B | 0.17307 | 0.17317 | 0.14842 | 0.16882 | 0.16319 |
| PB | C3B | -0.24946 | -0.25183 | -0.24174 | -0.19587 | -0.22248 |
| PB | C4B | 0.43849 | 0.43697 | 0.47388 | 0.42206 | 0.47445 |
| PB | CMB | -0.29214 | -0.28928 | -0.27943 | -0.29643 | -0.2935 |
| PB | HMB1 | 0.07536 | 0.073 | 0.07316 | 0.07794 | 0.07799 |
| PB | HMB2 | 0.08967 | 0.08675 | 0.08807 | 0.0912 | 0.08975 |
| PB | HMB3 | 0.06043 | 0.06032 | 0.0628 | 0.05904 | 0.0608 |
| PB | CAB | -0.00339 | -0.00101 | -0.01481 | -0.02292 | -0.01644 |
| PB | HAB | 0.1084 | 0.10883 | 0.11593 | 0.12395 | 0.12339 |
| PB | CBB | -0.36571 | -0.36515 | -0.3641 | -0.39466 | -0.39398 |
| PB | HBB1 | 0.16726 | 0.16675 | 0.1689 | 0.1661 | 0.16483 |
| PB | HBB2 | 0.16733 | 0.1655 | 0.17159 | 0.15697 | 0.15859 |
| PB | NC | -0.69995 | -0.70078 | -0.72631 | -0.71778 | -0.73851 |
| PB | C1C | 0.31066 | 0.31323 | 0.33887 | 0.3197 | 0.34242 |
| PB | C2C | 0.2303 | 0.22668 | 0.21047 | 0.20812 | 0.20287 |
| PB | C3C | -0.37796 | -0.37737 | -0.36842 | -0.35036 | -0.35598 |
| PB | C4C | 0.53119 | 0.53099 | 0.55565 | 0.55236 | 0.57037 |
| PB | CMC | -0.46634 | -0.46492 | -0.42961 | -0.42905 | -0.42021 |
| PB | HMC1 | 0.12519 | 0.12446 | 0.11663 | 0.1123 | 0.11004 |
| PB | HMC2 | 0.11692 | 0.11924 | 0.11092 | 0.11207 | 0.10998 |
| PB | HMC3 | 0.17973 | 0.18317 | 0.16496 | 0.16374 | 0.1619 |
| PB | CAC | 0.33183 | 0.33277 | 0.32421 | 0.31097 | 0.31252 |
| PB | HAC1 | -0.00869 | -0.00996 | -0.00655 | -0.00338 | -0.00348 |
| PB | HAC2 | -0.04349 | -0.04044 | -0.03586 | -0.03318 | -0.03292 |
| PB | CBC | -0.38645 | -0.38526 | -0.39772 | -0.39664 | -0.39871 |
| PB | HBC1 | 0.07627 | 0.07296 | 0.07971 | 0.08011 | 0.08098 |

| | | | | | | |
|-------------------|------|----------|----------|----------|----------|----------|
| PB | HBC2 | 0.15435 | 0.1557 | 0.15805 | 0.15815 | 0.15876 |
| PB | HBC3 | 0.10012 | 0.10123 | 0.10255 | 0.10308 | 0.10344 |
| PB | ND | -0.74808 | -0.7422 | -0.76449 | -0.78228 | -0.79686 |
| PB | C1D | 0.45254 | 0.44752 | 0.47531 | 0.48017 | 0.49821 |
| PB | C2D | 0.03499 | 0.03556 | 0.03543 | 0.03658 | 0.03179 |
| PB | C3D | -0.22085 | -0.22043 | -0.22365 | -0.22926 | -0.23145 |
| PB | C4D | 0.34203 | 0.33337 | 0.36128 | 0.37561 | 0.39586 |
| PB | CMD | -0.34411 | -0.34594 | -0.34614 | -0.34839 | -0.34424 |
| PB | HMD1 | 0.12834 | 0.12868 | 0.13118 | 0.13101 | 0.13094 |
| PB | HMD2 | 0.12764 | 0.12902 | 0.12757 | 0.12901 | 0.12724 |
| PB | HMD3 | 0.16891 | 0.1679 | 0.17026 | 0.17082 | 0.17055 |
| PB | CAD | 0.62903 | 0.62935 | 0.63393 | 0.63408 | 0.63687 |
| PB | OBD | -0.42533 | -0.43052 | -0.42347 | -0.42427 | -0.42346 |
| PB | CBD | -0.6515 | -0.65253 | -0.6669 | -0.65366 | -0.66516 |
| PB | HBD1 | 0.19583 | 0.19483 | 0.20826 | 0.19707 | 0.20829 |
| PB | CGD | 0.79564 | 0.797 | 0.80005 | 0.79575 | 0.79893 |
| PB | O1D | -0.4971 | -0.4988 | -0.49803 | -0.49637 | -0.49708 |
| PB | O2D | -0.35483 | -0.35553 | -0.35515 | -0.35467 | -0.35526 |
| PB | CED | -0.06953 | -0.06794 | -0.06831 | -0.07028 | -0.06975 |
| PB | HED1 | 0.11584 | 0.11349 | 0.1157 | 0.11647 | 0.11629 |
| PB | HED2 | 0.08613 | 0.08455 | 0.08578 | 0.08666 | 0.08599 |
| PB | HED3 | 0.0987 | 0.09684 | 0.09965 | 0.09948 | 0.09997 |
| PB | C1 | -0.14293 | -0.1424 | -0.14045 | -0.14444 | -0.14048 |
| PB | H1 | 0.13779 | 0.13614 | 0.13666 | 0.13804 | 0.13673 |
| PB | H2 | 0.0974 | 0.09526 | 0.09636 | 0.09831 | 0.09617 |
| PB | H3 | 0.09175 | 0.09211 | 0.09249 | 0.09243 | 0.09267 |
| total (PA) | | 0.32206 | 0.35605 | 0.26617 | 0.2346 | 0.2236 |
| total (PB) | | 0.67798 | 0.64393 | 0.73383 | 0.76546 | 0.77643 |

| | atom | wild type, CH₃COO- deleted | wild type, CH₃COO- deleted, vacuum | T743V, CH₃COO- deleted | T743V, CH₃COO- deleted, Δ(Arg-A750 /Ser-B734) |
|----|-------------|--|--|--|---|
| PA | MG | 1.3556 | 1.09622 | 1.3678 | 1.36713 |
| PA | CHA | 0.25712 | 0.20974 | 0.19641 | 0.19585 |
| PA | CHB | -0.46792 | -0.43392 | -0.49429 | -0.49266 |
| PA | HHB | 0.18776 | 0.17379 | 0.19065 | 0.18875 |
| PA | CHC | -0.41692 | -0.33956 | -0.42067 | -0.42241 |
| PA | HHC | 0.1573 | 0.14652 | 0.15684 | 0.15653 |
| PA | CHD | -0.5058 | -0.43924 | -0.49278 | -0.5004 |
| PA | HHD | 0.22159 | 0.19961 | 0.21482 | 0.21989 |
| PA | NA | -0.27379 | -0.22223 | -0.29767 | -0.29135 |
| PA | C1A | -0.35138 | -0.32123 | -0.31814 | -0.31919 |
| PA | C2A | 0.49326 | 0.47599 | 0.4704 | 0.46828 |
| PA | H2A | -0.04942 | -0.02991 | -0.04902 | -0.04854 |
| PA | C3A | 0.05132 | -0.02506 | 0.08934 | 0.09278 |
| PA | H3A | 0.03955 | 0.0796 | 0.02248 | 0.0205 |
| PA | C4A | 0.27212 | 0.22511 | 0.29175 | 0.28349 |
| PA | CMA | -0.41306 | -0.3776 | -0.42262 | -0.42273 |
| PA | HMA1 | 0.0882 | 0.11001 | 0.08951 | 0.08759 |
| PA | HMA2 | 0.12881 | 0.10098 | 0.13029 | 0.1315 |
| PA | HMA3 | 0.11662 | 0.11556 | 0.11653 | 0.11491 |
| PA | CAA | 0.06006 | -0.01599 | 0.0525 | 0.05424 |
| PA | HAA1 | 0.00514 | 0.00396 | 0.02095 | 0.02029 |
| PA | HAA2 | -0.00062 | 0.02925 | 0.0006 | 0.00066 |
| PA | CBA | -0.7129 | -0.56127 | -0.71205 | -0.71217 |
| PA | HBA1 | 0.17229 | 0.16383 | 0.15556 | 0.15471 |
| PA | HBA2 | 0.18892 | 0.11312 | 0.20008 | 0.19908 |
| PA | CGA | 0.9234 | 0.8131 | 0.9062 | 0.90701 |
| PA | O1A | -0.65689 | -0.52649 | -0.64687 | -0.65014 |
| PA | O2A | -0.32982 | -0.31982 | -0.33322 | -0.3305 |
| PA | NB | -0.64032 | -0.5627 | -0.66921 | -0.66608 |

| | | | | | |
|----|------|----------|----------|----------|----------|
| PA | C1B | 0.25149 | 0.21382 | 0.27987 | 0.2744 |
| PA | C2B | 0.22435 | 0.19643 | 0.21868 | 0.21966 |
| PA | C3B | -0.28333 | -0.21457 | -0.29664 | -0.2998 |
| PA | C4B | 0.40308 | 0.34342 | 0.42347 | 0.42279 |
| PA | CMB | -0.26635 | -0.31186 | -0.26133 | -0.25922 |
| PA | HMB1 | 0.06524 | 0.09053 | 0.06469 | 0.0628 |
| PA | HMB2 | 0.08008 | 0.09398 | 0.07688 | 0.07398 |
| PA | HMB3 | 0.05339 | 0.09239 | 0.05371 | 0.05411 |
| PA | CAB | 0.08524 | 0.05264 | 0.09335 | 0.09758 |
| PA | HAB | 0.08855 | 0.09816 | 0.08805 | 0.08963 |
| PA | CBB | -0.4816 | -0.4508 | -0.48725 | -0.49365 |
| PA | HBB1 | 0.17646 | 0.17909 | 0.17711 | 0.17687 |
| PA | HBB2 | 0.20657 | 0.20437 | 0.20971 | 0.2087 |
| PA | NC | -0.7388 | -0.6355 | -0.73857 | -0.74222 |
| PA | C1C | 0.35666 | 0.26568 | 0.35863 | 0.3605 |
| PA | C2C | 0.17486 | 0.20406 | 0.17456 | 0.17517 |
| PA | C3C | -0.34561 | -0.33436 | -0.33931 | -0.34217 |
| PA | C4C | 0.51973 | 0.44938 | 0.51464 | 0.52517 |
| PA | CMC | -0.45089 | -0.45701 | -0.45995 | -0.4605 |
| PA | HMC1 | 0.14263 | 0.14522 | 0.14461 | 0.14545 |
| PA | HMC2 | 0.10587 | 0.1154 | 0.10633 | 0.10423 |
| PA | HMC3 | 0.169 | 0.15458 | 0.17435 | 0.17575 |
| PA | CAC | 0.24437 | 0.23334 | 0.25564 | 0.25314 |
| PA | HAC1 | -0.01406 | -0.01265 | -0.01913 | -0.01278 |
| PA | HAC2 | -0.01168 | -0.00766 | -0.0139 | -0.01328 |
| PA | CBC | -0.36854 | -0.36076 | -0.36448 | -0.36506 |
| PA | HBC1 | 0.07625 | 0.09128 | 0.07344 | 0.07523 |
| PA | HBC2 | 0.12013 | 0.09959 | 0.11749 | 0.12495 |
| PA | HBC3 | 0.1198 | 0.10635 | 0.11876 | 0.11569 |
| PA | ND | -0.59023 | -0.54381 | -0.61055 | -0.62445 |
| PA | C1D | 0.32799 | 0.29357 | 0.33115 | 0.3568 |
| PA | C2D | 0.10191 | 0.13746 | 0.09745 | 0.08186 |
| PA | C3D | -0.24546 | -0.23374 | -0.24522 | -0.23111 |
| PA | C4D | 0.10174 | 0.12146 | 0.14848 | 0.15287 |
| PA | CMD | -0.39356 | -0.37333 | -0.38527 | -0.38357 |
| PA | HMD1 | 0.12076 | 0.10804 | 0.12127 | 0.12866 |

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|----|------|----------|----------|----------|----------|
| PA | HMD2 | 0.12681 | 0.12909 | 0.12559 | 0.13332 |
| PA | HMD3 | 0.16336 | 0.14208 | 0.1589 | 0.166 |
| PA | CAD | 0.67182 | 0.60958 | 0.62913 | 0.62172 |
| PA | OBD | -0.55813 | -0.45223 | -0.49857 | -0.48735 |
| PA | CBD | -0.67514 | -0.53692 | -0.60269 | -0.60365 |
| PA | HBD1 | 0.17901 | 0.16681 | 0.16848 | 0.16796 |
| PA | C1 | -0.13009 | -0.14639 | -0.12111 | -0.12183 |
| PA | H1 | 0.1022 | 0.11775 | 0.0979 | 0.09838 |
| PA | H2 | 0.1061 | 0.11882 | 0.10115 | 0.0992 |
| PA | H3 | 0.12244 | 0.1001 | 0.12652 | 0.12703 |
| PA | HBD | 0.18688 | 0.17082 | 0.16824 | 0.16923 |
| | | | | | |
| PB | MG | 1.35853 | 1.1124 | 1.3527 | 1.34815 |
| PB | CHA | 0.12088 | 0.15292 | 0.12378 | 0.12901 |
| PB | CHB | -0.51362 | -0.46069 | -0.51867 | -0.51729 |
| PB | HHB | 0.19218 | 0.17763 | 0.19173 | 0.18954 |
| PB | CHC | -0.38849 | -0.30548 | -0.39635 | -0.39395 |
| PB | HHC | 0.13241 | 0.12449 | 0.13872 | 0.13877 |
| PB | CHD | -0.55837 | -0.45312 | -0.54531 | -0.54271 |
| PB | HHD | 0.23664 | 0.20053 | 0.23309 | 0.23365 |
| PB | NA | -0.34272 | -0.26886 | -0.34793 | -0.33942 |
| PB | C1A | -0.22831 | -0.3021 | -0.22575 | -0.23823 |
| PB | C2A | 0.49422 | 0.59141 | 0.47633 | 0.47915 |
| PB | H2A | -0.05042 | -0.05308 | -0.04769 | -0.05049 |
| PB | C3A | 0.0312 | -0.04915 | 0.03789 | 0.04273 |
| PB | H3A | 0.0621 | 0.07952 | 0.05959 | 0.0559 |
| PB | C4A | 0.35467 | 0.27678 | 0.35818 | 0.34828 |
| PB | CMA | -0.42608 | -0.39122 | -0.42757 | -0.42734 |
| PB | HMA1 | 0.10514 | 0.11433 | 0.10461 | 0.10067 |
| PB | HMA2 | 0.12126 | 0.10104 | 0.1222 | 0.12249 |
| PB | HMA3 | 0.1146 | 0.11957 | 0.1133 | 0.11221 |
| PB | CAA | -0.00393 | -0.14371 | 0.00283 | 0.01069 |
| PB | HAA1 | 0.00884 | 0.05364 | 0.01005 | 0.01 |
| PB | HAA2 | 0.02461 | 0.05333 | 0.02449 | 0.02263 |
| PB | CBA | -0.63271 | -0.56224 | -0.63414 | -0.6418 |
| PB | HBA1 | 0.18245 | 0.17408 | 0.18232 | 0.18114 |

| | | | | | |
|----|------|----------|----------|----------|----------|
| PB | HBA2 | 0.13977 | 0.11763 | 0.14035 | 0.14156 |
| PB | CGA | 0.84333 | 0.80129 | 0.84197 | 0.84489 |
| PB | O1A | -0.58279 | -0.51554 | -0.58321 | -0.58592 |
| PB | O2A | -0.3051 | -0.31936 | -0.30537 | -0.30429 |
| PB | NB | -0.66754 | -0.59562 | -0.65138 | -0.64783 |
| PB | C1B | 0.32077 | 0.2612 | 0.31015 | 0.30493 |
| PB | C2B | 0.15838 | 0.16831 | 0.16662 | 0.16699 |
| PB | C3B | -0.23867 | -0.19093 | -0.2533 | -0.25591 |
| PB | C4B | 0.41627 | 0.35637 | 0.4071 | 0.40484 |
| PB | CMB | -0.29649 | -0.35888 | -0.2915 | -0.28883 |
| PB | HMB1 | 0.07598 | 0.09525 | 0.07464 | 0.07222 |
| PB | HMB2 | 0.09513 | 0.11486 | 0.09212 | 0.08915 |
| PB | HMB3 | 0.07184 | 0.12427 | 0.06763 | 0.06742 |
| PB | CAB | 0.02834 | 0.00814 | 0.04768 | 0.05133 |
| PB | HAB | 0.11453 | 0.12387 | 0.10714 | 0.10782 |
| PB | CBB | -0.42622 | -0.41991 | -0.43483 | -0.43622 |
| PB | HBB1 | 0.15344 | 0.16763 | 0.1533 | 0.15405 |
| PB | HBB2 | 0.19801 | 0.19906 | 0.19553 | 0.19404 |
| PB | NC | -0.70413 | -0.60781 | -0.70046 | -0.7013 |
| PB | C1C | 0.29532 | 0.22179 | 0.29988 | 0.30206 |
| PB | C2C | 0.22291 | 0.22709 | 0.22506 | 0.22159 |
| PB | C3C | -0.3708 | -0.33852 | -0.37414 | -0.37329 |
| PB | C4C | 0.54001 | 0.44021 | 0.52765 | 0.52706 |
| PB | CMC | -0.42425 | -0.41528 | -0.45084 | -0.44988 |
| PB | HMC1 | 0.11128 | 0.11881 | 0.11703 | 0.11648 |
| PB | HMC2 | 0.10893 | 0.11861 | 0.11355 | 0.11597 |
| PB | HMC3 | 0.16306 | 0.14423 | 0.17552 | 0.17894 |
| PB | CAC | 0.32611 | 0.2814 | 0.33112 | 0.33209 |
| PB | HAC1 | -0.00848 | -0.0247 | -0.00957 | -0.01091 |
| PB | HAC2 | -0.0372 | -0.0203 | -0.04411 | -0.04109 |
| PB | CBC | -0.39318 | -0.37069 | -0.38244 | -0.3815 |
| PB | HBC1 | 0.07918 | 0.08871 | 0.07589 | 0.07264 |
| PB | HBC2 | 0.15605 | 0.10198 | 0.15276 | 0.15411 |
| PB | HBC3 | 0.10035 | 0.10817 | 0.0978 | 0.09893 |
| PB | ND | -0.71257 | -0.58977 | -0.70449 | -0.69842 |
| PB | C1D | 0.46548 | 0.34271 | 0.45406 | 0.44911 |

| | | | | | |
|-------------------------|------|----------|----------|----------|----------|
| PB | C2D | 0.03655 | 0.1055 | 0.03538 | 0.03615 |
| PB | C3D | -0.19747 | -0.22355 | -0.19595 | -0.19692 |
| PB | C4D | 0.22944 | 0.17668 | 0.21979 | 0.21074 |
| PB | CMD | -0.36285 | -0.37084 | -0.35912 | -0.36105 |
| PB | HMD1 | 0.1329 | 0.11369 | 0.1303 | 0.13047 |
| PB | HMD2 | 0.1293 | 0.12607 | 0.12803 | 0.12939 |
| PB | HMD3 | 0.1747 | 0.14627 | 0.17339 | 0.17233 |
| PB | CAD | 0.60794 | 0.61788 | 0.60586 | 0.60764 |
| PB | OBD | -0.44229 | -0.45118 | -0.44384 | -0.44976 |
| PB | CBD | -0.57808 | -0.53638 | -0.57341 | -0.57379 |
| PB | HBD1 | 0.17478 | 0.16779 | 0.17212 | 0.16916 |
| PB | C1 | -0.13388 | -0.13296 | -0.13236 | -0.13196 |
| PB | H1 | 0.1388 | 0.11722 | 0.13891 | 0.13722 |
| PB | H2 | 0.09599 | 0.11145 | 0.09527 | 0.09322 |
| PB | H3 | 0.09113 | 0.09974 | 0.09033 | 0.09072 |
| PB | HBD | 0.16942 | 0.17122 | 0.16752 | 0.16464 |
| <hr/> total (PA) | | 0.32152 | 0.45507 | 0.37043 | 0.40521 |
| <hr/> total (PB) | | 0.67851 | 0.5449 | 0.62953 | 0.59481 |
| <hr/> | | | | | |