Table S3. Interaction energies for antibody-antigen complexes.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Name | Nativea | | MAPsb | | Name | Native | | MAPs | |
|  | MILPc | Charmmd | MILP | Charmm |  | MILP | Charmm | MILP | Charmm |
| 1ACY | -141 | -206 | -344 | -326 | 2HFG | -129 | -208 | -266 | -217 |
| 1BJ1 | -27 | -180 | -90 | -147 | 2HH0 | -298 | -411 | -355 | -377 |
| 1CE1 | -355 | -429 | -253 | -221 | 2HKF | -397 | -478 | -263 | -283 |
| 1CFS | -194 | -272 | -209 | -260 | 2HRP | -87 | -160 | -271 | -287 |
| 1CFT | -99 | -140 | -319 | -330 | 2HVK | -383 | -505 | -362 | -437 |
| 1CU4 | -394 | -500 | -277 | -386 | 2IFF | 2215 | -399 | -363 | -300 |
| 1DZB | -276 | -408 | -369 | -454 | 2IGF | -231 | -327 | -301 | -355 |
| 1E4W | -19 | -102 | -234 | -248 | 2J4W | -193 | -281 | -330 | -404 |
| 1EGJ | -239 | -304 | -263 | -239 | 2JEL | -122 | -232 | -352 | -354 |
| 1EJO | -176 | -286 | -385 | -337 | 2OQJ | -56 | -129 | -163 | -154 |
| 1F90 | -153 | -193 | -303 | -286 | 2OR9 | -187 | -267 | -113 | -102 |
| 1FBI | -292 | -469 | -258 | -281 | 2OSL | -99 | -157 | -90 | -97 |
| 1FPT | -364 | -474 | -292 | -335 | 2QHR | -353 | -471 | -328 | -330 |
| 1GGI | -252 | -321 | -358 | -268 | 2QR0 | -17 | -99 | -300 | -312 |
| 1HH6 | -117 | -232 | -218 | -175 | 2QSC | -141 | -198 | -313 | -334 |
| 1HIN | -110 | -195 | -192 | -238 | 2R0W | -161 | -240 | -273 | -254 |
| 1I8I | -398 | -474 | -394 | -403 | 2R29 | -198 | -328 | -184 | -206 |
| 1I9R | -104 | -238 | -288 | -325 | 2VWE | -98 | -182 | -113 | -178 |
| 1JHL | -179 | -277 | -330 | -332 | 2VXQ | -280 | -388 | -372 | -441 |
| 1JP5 | -167 | -214 | -179 | -192 | 2VXS | -36 | -92 | -120 | -161 |
| 1JRH | -351 | -464 | -335 | -305 | 2ZPK | -66 | -127 | -143 | -156 |
| 1KC5 | -136 | -188 | -172 | -167 | 2ZUQ | -140 | -213 | -115 | -146 |
| 1KCR | -15 | -97 | -226 | -272 | 3AB0 | -224 | -301 | -407 | -443 |
| 1KIQ | -84 | -171 | -188 | -251 | 3BAE | -92 | -173 | -284 | -307 |
| 1KTR | 50 | -7 | -236 | -216 | 3BDY | -94 | -170 | -247 | -211 |
| 1MLC | -191 | -288 | -230 | -208 | 3BKY | -78 | -131 | -191 | -35 |
| 1MVU | -66 | -116 | -331 | -356 | 3CVH | -134 | -189 | -215 | -153 |
| 1N64 | -114 | -197 | -148 | -192 | 3CXD | -211 | -295 | -271 | -265 |
| 1NAK | -237 | -307 | -227 | -269 | 3D85 | -69 | -181 | -165 | -196 |
| 1NSN | -81 | -210 | -490 | -493 | 3DVG | -90 | -195 | -186 | -222 |
| 1OAZ | 32 | -82 | -217 | -273 | 3E8U | -125 | -200 | -232 | -231 |
| 1OBE | -301 | -373 | -86 | -201 | 3ETB | -461 | -593 | -378 | -410 |
| 1ORS | -151 | -211 | -280 | -297 | 3EYU | -165 | -241 | -320 | -269 |
| 1P4B | -48 | -126 | -146 | -114 | 3F58 | -203 | -286 | -336 | -316 |
| 1PZ5 | -23 | -123 | -122 | -133 | 3FFD | -378 | -512 | -264 | -324 |
| 1QKZ | -75 | -143 | -170 | -192 | 3FN0 | -98 | -176 | -143 | -182 |
| 1QNZ | -148 | -240 | -228 | -322 | 3G5V | -157 | -262 | -230 | -280 |
| 1RJL | -129 | -210 | -208 | -201 | 3G6D | -607 | -729 | -602 | -686 |
| 1SM3 | -67 | -125 | -267 | -278 | 3GGW | -23 | -88 | -194 | -222 |
| 1TET | -152 | -222 | -181 | -159 | 3GHB | -291 | -352 | -111 | -80 |
| 1TQB | -264 | -379 | -364 | -302 | 3GHE | -246 | -387 | -266 | -305 |
| 1TZG | -128 | -220 | -162 | -192 | 3GJG | -6 | -85 | -90 | -114 |
| 1TZH | 21 | -57 | -172 | -201 | 3HR5 | -233 | -340 | -447 | -415 |
| 1TZI | -14 | -37 | -147 | -160 | 3IU3 | -550 | -801 | -110 | -306 |
| 1U8J | -271 | -337 | -297 | -315 | 3KS0 | -58 | -148 | -195 | -248 |
| 1UWX | -65 | -127 | -303 | -305 | 3L5W | -448 | -522 | -497 | -535 |
| 1V7M | -68 | -182 | -193 | -264 | 3L5Y | -422 | -571 | -406 | -476 |
| 1W72 | -158 | -238 | -251 | -274 | 3LQA | -41 | -82 | -210 | -224 |
| 1XGY | -147 | -226 | -353 | -314 | 3MLR | -274 | -345 | -281 | -390 |
| 1XIW | -368 | -478 | -275 | -321 | 3MLS | -290 | -406 | -336 | -402 |
| 1ZTX | -214 | -315 | -410 | -400 | 3MLW | -379 | -490 | -513 | -597 |
| 2A6I | 1888 | -93 | 116 | -191 | 3MLX | -72 | -174 | -132 | -143 |
| 2B1H | -490 | -600 | -286 | -364 | 3MLY | -139 | -246 | -206 | -231 |
| 2BDN | -281 | -407 | -283 | -526 | 3NFP | -165 | -352 | -307 | -415 |
| 2CK0 | -38 | -109 | -111 | -124 | 3NH7 | -620 | -783 | -508 | -569 |
| 2DQJ | -235 | -382 | -272 | -371 | 3O0R | -68 | -120 | -209 | -234 |
| 2EH8 | -178 | -276 | -277 | -210 | 3P30 | -202 | -305 | -244 | -288 |
| 2FJH | -56 | -164 | -345 | -256 | 3QG6 | -28 | -130 | -165 | -183 |
| 2G5B | -109 | -173 | -282 | -257 | 3QWO | -209 | -339 | -495 | -476 |
| 2H1P | -48 | -115 | -172 | -137 | 3RKD | -225 | -348 | -278 | -325 |

aNative indicates the energies are calculated using native antigen and antibody from the X-ray structures

bMAPs indicates the energies are calculated using native antigen from the X-ray structures and antibody from the MAPs databases

cThe energy for MILP selection calculated using pairwise energy function including van der Waals and electrostatic terms

dThe energy calculated using Charmm after minimized the structure including van der Waals, electrostatics, bonds, angles, dihedral angles, improper dihedral angles and generalized Born with molecular volume integration implicit solvation terms.

All energies are in kcal/mol.