# SUPPLEMETARY INFORMATION:
# Large scale motions and electrostatic properties of furin and HIV-1 protease.

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| Atoms | $d$(Å) | | Atoms | $d$(Å) | |
|---|---|---|---|---|---|
| | E-S | E-INT | | E-S | E-INT |
| N@D154–$O_{\delta 2}$@D153 | 2.8(.2)[.0] | 2.8(.1)[.1] | O@R5–N@T367 | 3.1(.2)[.9] | 3.2(.2)[.0] |
| H@D154–$O_{\delta 2}$@D153 | 1.9(.3)[.1] | 1.9(.2)[.1] | O@R5–H@T367 | 2.6(.3)[.9] | 2.8(.3)[.3] |
| $O_{\delta 2}$@D154–N@H194 | 3.0(.2)[.2] | 2.9(.2)[.1] | O@R5–N@S368 | 3.3(.3)[.9] | 2.8(.1)[.0] |
| $O_{\delta 2}$@D154–H@H194 | 2.1(.2)[.2] | 2.0(.2)[.1] | O@R5–H@S368 | 2.4(.3)[.8] | 1.8(.1)[.0] |
| $O_{\delta 1}$@D154–N@H194 | 3.3(.2)[.0] | 3.2(.2)[.0] | O@R5–$N_{\delta}$@N295 | 4.6(.4)[.9] | 2.9(.2)[.3] |
| $O_{\delta 1}$@D154–H@H194 | 2.8(.3)[.1] | 2.8(.3)[.2] | O@R5–$H_{\delta 1}$@N295 | 4.7(.5)[.8] | 2.0(.3)[.4] |
| $O_{\delta 1}$@D154–N@G195 | 2.8(.1)[.0] | 2.8(.1)[.2] | O@R5–$H_{\delta 2}$@N295 | 5.1(.5)[.9] | 3.3(.2)[.7] |
| $O_{\delta 1}$@D154–H@G195 | 1.8(.2)[.1] | 1.8(.1)[.3] | N@R5–O@S253 | 3.1(.2)[.5] | 2.9(.1)[.0] |
| $O_{\delta 2}$@D154–N@G195 | 4.0(.2)[.0] | 3.9(.2)[.7] | H@R5–O@S253 | 2.4(.3)[.6] | 2.0(.2)[.1] |
| $O_{\delta 2}$@D154–H@G195 | 3.2(.2)[.0] | 3.0(.2)[.7] | $O_{\gamma}$@S253–O@S368 | 3.3(.4)[.3] | 2.7(.1)[.1] |
| $O_{\delta 2}$@D153–$N_{\delta 1}$@H194 | 2.9(.2)[.3] | 2.9(.2)[.2] | $H_{\gamma}$@S253–O@S368 | 2.7(.6)[.4] | 1.8(.2)[.1] |
| $O_{\delta 2}$@D153–$H_{\delta 1}$@H194 | 2.0(.3)[.4] | 2.0(.3)[.3] | $N_{\epsilon}$@H194–N@Nme6 | 3.9(.5)[.4] | 3.0(.2)[.0] |
| $O_{\delta 1}$@D153–$N_{\delta 1}$@H194 | 2.9(.2)[.1] | 2.7(.1)[.1] | $C_{\alpha}$@N295–$C_{\alpha}$@T367 | 6.9(.2)[.1] | 6.8(.2)[.4] |
| $O_{\delta 1}$@D153–$H_{\delta 1}$@H194 | 2.0(.3)[.3] | 1.8(.2)[.2] | $C_{\alpha}$@N295–$C_{\alpha}$@S368 | 9.3(.3)[.5] | 8.7(.1)[.1] |
| $C_{\epsilon}$@H194–O@S253 | 3.4(.2)[.4] | 3.3(.1)[.1] | $C_{\alpha}$@N295–$C_{\alpha}$@R5 | 5.5(.2)[.1] | 6.0(.2)[.2] |
| $H_{\epsilon}$@H194–O@S253 | 2.5(.2)[.3] | 2.3(.1)[.0] | $C_{\alpha}$@R5–$C_{\alpha}$@S368 | 5.4(.2)[.6] | 4.4(.1)[.0] |
| $N_{\epsilon}$@H194–$O_{\gamma}$@S368 | 2.8(.1)[.1] | 3.1(.2)[.1] | $C_{\alpha}$@R5–$C_{\alpha}$@H194 | 9.3(.4)[.9] | 9.0(.2)[.2] |
| $N_{\epsilon}$@H194–$H_{\gamma}$@S368 | 1.9(.2)[.1] | - | $C_{\alpha}$@R5–$C_{\alpha}$@S253 | 5.8(.2)[.7] | 5.3(.1)[.2] |
| $N_{\epsilon}$@H194–N@R5 | 3.9(.4)[.7] | 3.8(.3)[.1] | $C_{\alpha}$@H194–$C_{\alpha}$@S368 | 8.0(.2)[.0] | 8.4(.2)[.3] |
| $N_{\epsilon}$@H194–H@R5 | 3.1(.5)[.9] | 3.3(.3)[.1] | $C_{\alpha}$@D153–$C_{\alpha}$@H194 | 6.9(.2)[.8] | 6.9(.2)[.7] |
| $N_{\epsilon}$@H194–H@Nme6 | 3.6(.6)[.9] | 3.1(.2)[.3] | | | |

Table 1: Furin: selected distances (in Å) between active site atoms of furin. Standard deviations from the average are given in parentheses; the deviations from the distances calculated on the initial model are reported in square brackets.