

## Final detected binding pockets

*Table 1. Pockets were obtained by merging results from Fpocket and P2Rank. The pocket with rank 1 is the most probable (best average score over merged pockets).*

Structure	Pocket rank	Residue numbers
7NIO	1	120, 123, 124, 135, 138, 139, 142, 143, 146, 179, 180, 181, 228, 230, 231, 232, 233, 283, 284, 285, 287, 288, 289, 290, 309, 310, 311, 312, 313, 316, 320, 360, 361, 374, 375, 378, 380, 381, 382, 383, 386, 404, 407, 408, 409, 410, 422, 442, 443, 537, 538, 539, 540
	2	175, 177, 178, 179, 406, 407, 408, 409, 412, 415, 416, 417, 485, 514, 515, 516, 532, 534, 553, 554, 557, 560
	3	161, 162, 178, 201, 202, 210, 212, 516, 519, 520, 523, 530, 531, 532, 535
	4	261, 264, 265, 286, 287, 290, 438, 440, 442
	5	281, 402, 419, 429, 430, 434, 456, 458, 460
7NN0	1	284, 285, 284, 285, 285, 287, 288, 289, 375, 404, 442, 443, 538, 540, 567, 285, 287, 288, 375, 404, 443, 538, 567, 285, 287, 288, 289, 443, 538, 540, 567, 286, 287, 288, 289, 290, 312, 313, 316, 320, 374, 375, 404, 442, 443, 537, 538, 540, 567
	2	139, 142, 143, 146, 177, 179, 180, 181, 230, 309, 361, 380, 382, 383, 405, 406, 407, 408, 409, 410, 412, 416, 417, 514, 534, 554, 557, 559, 560
	3	44, 45, 46, 48, 65, 68, 70, 90, 91, 92