**Table S1. Clustering Analysis**

| **Complex** | **6O0K-PSK** | | **6O0K-PSP** | | **2J8B-PSK** | | **5USJ-PSK** | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Model** | **Affinity (Kcal/mol)** | **RMSD** | **Affinity (Kcal/mol)** | **RMSD** | **Affinity (Kcal/mol)** | **RMSD** | **Affinity (Kcal/mol)** | **RMSD** |
| 1 | -7 | 0 | -7.4 | 0 | -6.4 | 0 | -6.3 | 0 |
| 2 | -6.9 | 2.27 | -7.2 | 1.537 | -6 | 2.21 | -6.1 | 5.351 |
| 3 | -6.5 | 1.95 | -7.1 | 3.369 | -5.8 | 2.044 | -6 | 2.429 |
| 4 | -6.4 | 2.406 | -7.1 | 3.613 | -5.6 | 2.452 | -6 | 3.101 |
| 5 | -6.4 | 1.694 | -7.1 | 2.793 | -5.5 | 2.43 | -6 | 1.69 |
| 6 | -6.4 | 1.399 | -7 | 1.761 | -5.5 | 2.007 | -6 | 20.526 |
| 7 | -6.4 | 10.42 | -7 | 3.28 | -5.5 | 3.744 | -5.9 | 2.969 |
| 8 | -6.3 | 10.088 | -7 | 2.778 | -5.5 | 2.684 | -5.9 | 2.809 |
| 9 | -6.2 | 8.051 | -7 | 3.013 | -5.4 | 3.172 | -5.9 | 2.644 |
| 10 | -6.2 | 2.504 | -6.9 | 5.132 | -5.4 | 4.26 | -5.8 | 2.526 |
| 11 | -5.9 | 2.326 | -6.8 | 2.776 | -5.1 | 1.922 | -5.8 | 2.532 |
| 12 | -5.9 | 10.418 | -6.8 | 1.46 | -5 | 2.073 | -5.7 | 2.587 |
| 13 | -5.9 | 2.631 | -6.8 | 4.003 | -4.9 | 2.969 | -5.7 | 2.673 |
| 14 | -5.8 | 2.731 | -6.7 | 3.167 | -4.8 | 3.345 | -5.6 | 5.774 |
| 15 | -5.8 | 9.662 | -6.7 | 4.488 | -4.8 | 3.157 | -5.6 | 2.77 |
| 16 | -5.7 | 2.626 | -6.7 | 4.34 | -4.7 | 3.242 | -5.5 | 19.987 |
| 17 | -5.6 | 11.92 | -6.5 | 4.375 | -4.7 | 1.707 | -5.5 | 8.822 |
| 18 | -5.6 | 2.449 | -6.4 | 5.796 | -4.6 | 2.151 | -5.4 | 19.413 |
| 19 | -5.4 | 2.973 | -6.4 | 4.337 | -4.5 | 1.652 | -5.3 | 2.712 |
| 20 | -5.4 | 9.851 | -6.4 | 5.326 | -4.5 | 4.37 | -5.3 | 16.145 |
| **Acceptable poses** | **13** | | **9** | | **13** | | **13** | |
| **Average threshold (Kcal/mol)** | **-6.2** | | **-7** | | **-5.3** | | **-5.8** | |

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Complex** | | **6L3R-PSK** | | **5VX1-PSK** | | **5VX1-PSP** | | **6Z9B-PSK** | |  |
| **Model** | | **Affinity (Kcal/mol)** | **RMSD** | **Affinity (Kcal/mol)** | **RMSD** | **Affinity (Kcal/mol)** | **RMSD** | **Affinity (Kcal/mol)** | **RMSD** |  |
| 1 | | -7.1 | 0 | -7.6 | 0 | -8.5 | 0 | -6.7 | 0 |  |
| 2 | | -7 | 0.943 | -7.4 | 1.831 | -8.4 | 2.156 | -6.3 | 1.815 |  |
| 3 | | -6.8 | 1.298 | -7.3 | 2.083 | -8.3 | 2.29 | -6.2 | 3.113 |  |
| 4 | | -6.6 | 2.686 | -7.1 | 1.823 | -8 | 2.018 | -6.1 | 2.067 |  |
| 5 | | -6.6 | 2.077 | -6.8 | 2.947 | -8 | 3.058 | -6.1 | 1.565 |  |
| 6 | | -6.4 | 1.729 | -6.3 | 3.046 | -7.9 | 3.595 | -6.1 | 3.494 |  |
| 7 | | -6.3 | 3.429 | -6.2 | 2.793 | -7.9 | 2.002 | -6 | 3.461 |  |
| 8 | | -6.3 | 2.888 | -6.2 | 2.551 | -7.8 | 2.628 | -6 | 3.972 |  |
| 9 | | -6.3 | 1.757 | -6.2 | 2.09 | -7.8 | 2.748 | -5.9 | 2.552 |  |
| 10 | | -6.2 | 1.978 | -6.1 | 2.799 | -7.7 | 3.363 | -5.9 | 2.346 |  |
| 11 | | -6.2 | 1.774 | -6.1 | 2.815 | -7.6 | 3.6 | -5.9 | 2.748 |  |
| 12 | | -6.1 | 2.063 | -6.1 | 3.124 | -7.6 | 3.305 | -5.8 | 3.181 |  |
| 13 | | -6.1 | 2.258 | -6.1 | 2.589 | -7.5 | 1.474 | -5.7 | 3.49 |  |
| 14 | | -6.1 | 3.258 | -6 | 2.764 | -7.5 | 1.679 | -5.6 | 3.313 |  |
| 15 | | -6.1 | 2.465 | -6 | 2.544 | -7.4 | 2.989 | -5.5 | 2.797 |  |
| 16 | | -6 | 2.53 | -5.8 | 2.702 | -7.4 | 2.577 | -5.4 | 2.436 |  |
| 17 | | -6 | 2.836 | -5.7 | 1.426 | -7.4 | 3.299 | -5.3 | 2.762 |  |
| 18 | | -5.9 | 2.1 | -5.6 | 3.257 | -7.4 | 3.75 | -5.3 | 4.09 |  |
| 19 | | -5.9 | 2.182 | -5.6 | 2.905 | -7.3 | 3.438 | -5.2 | 2.314 |  |
| 20 | | -5.8 | 3.187 | -5.5 | 2.855 | 7.3 | 3.431 | -5.1 | 4.212 |  |
| **Acceptable poses** | **17** | | | **17** | | **12** | | **11** | | **Average total threshold (Kcal/mol)** |
| **Average threshold (Kcal/mol)** | | **-6.3** | | **-6.3** | | **-7.9** | | **-5.8** | | **-6.3** |

**Note:** The cells colored in gray represent the values of RMSD ≤ 3.0.

**Information S1 Preparation of the ligands**

**PSK**

**PubChem SID:** 135316798; **Registration of substances:** 134192-05-5; **MW:** 931.52 g/mol, 100kDa; **Composition:** C36H19O30; **SMILES:**[C]1([C](Or[C]([C]([C]1O[C]1[C]([C]([C]([C](O1)[C]Or)Or)Or)Or)Or)Or[C]1[C]([C]([C](Or[C]1[C]Or[C]1[C]([C]([C]([C](O1)[C]Or)Or)Or)Or)Or[C]1[C]([C]([C]Or[C]1[C]Or)Or)Or)Or)Or)[C]Or)Or[C]1[C]([C]([C]([C](O1)[C]Or)Or)Or)Or

**PSP**

**PubChem SID:** Not available; **Registration of substances:** Not available; **MW:** 1102.60 g/mol, 100kDa; **Composition:** C42H22O36; **SMILES:**[C]1([C]([C](Or[C]([C]1O)[C]Or[C]1[C]([C]([C]([C](O1)[C]Or)Or)Or)Or)Or[C]1[C]([C](Or[C]([C]1O)[C]Or)Or[C]1[C]([C](Or[C]([C]1O)[C]Or)Or[C]1[C]([C](Or[C]([C]1O)[C]Or)[Or])Or)Or)Or)Or)Or[C]1[C]([C]([C]([C](O1)[C]Or)Or)Or[C]1[C]([C]([C]([C](O1)[C]Or)Or)Or)Or)Or

**CVG**

**PubChem CID:** 2108; **Registration of substances:** Not available; **MW**: 194.18 g/mol; **Composition:** C7H4O6; **SMILES:** [C]1([C](Or[C]([C]([C]1O)Or)[C]Or)Or[C])Or

**CVP**

**PubChem SID:** Not available; **Registration of substances:** Not available; **MW**: 483.27; g/mol; **Composition:** C18H11O16; **SMILES:**[C]1(Or[C]([C]([C]([C]1O)Or[C]1[C]([C]([C]([C](O1)[C]Or)Or)Or)Or)Or)[C]Or)Or[C]1[C]([C](Or[C](Or)[C]1O)[C]Or)Or

**Reference ligands**

**Venetoclax**

**PubChem CID:** 49846579; **Registration of substances:** Not available; **MW:** 868.4; **Composition**: C45H50CIN7O7S;

**SMILES:**CC1(CCC(=C(C1)C2=CC=C(C=C2)Cl)CN3CCN(CC3)C4=CC(=C(C=C4)C(=Or)NS(=Or)(=Or)C5=CC(=C(C=C5)NCC6CCOCC6)[N+](=Or)[Or-])OC7=CN=C8C(=C7)C=CN8)C

**3144** (**Pan-RAS-IN-1)**

**PubChem CID:** 102004330; **Registration of substances:** Not available; **MW:** 717.66; **Composition**: C36H41CI2F3N6O2;**SMILES:**C1CNCCC1(C(=Or)NCCCN2C=C(C3=C2C=CC(=C3)CN4CCN(CC4)CC5=C(C=CC=C5Cl)Cl)C6=CC=C(C=C6)OC(F)(F)F)N

**AB680**

**PubChem CID:** 155809269; **Registration of substances:** Not available; **MW**: 578.81; **Composition**: [C20H22CIFN4O9P2-2](https://pubchem.ncbi.nlm.nih.gov/#query=C20H22ClFN4O9P2-2); **SMILES:**CC(C1=CC=CC=C1F)NC2=CC(=NC3=C2C=NN3C4C(C(C(O4)COP(=Or)(CP(=Or)(Or)[Or-])[Or-])Or)Or)Cl

**Database S1. Protein database**

1A7S, 1AGW, 1AQV, 1AQW, 1AQX, 1B1E, 1B1I, 1B1J, 1B8Y, 1BD8, 1BHS, 1BJ1, 1BLX, 1BMK, 1BOZ, 1C83, 1C84, 1CAQ, 1CIZ, 1CLL, 1CLU, 1CS3, 1D3G, 1D3H, 1D4A, 1D5R, 1DEB, 1DGB, 1DGF, 1DGG, 1DGH, 1E3G, 1EAX, 1EC6, 1ECV, 1EXA, 1EXX, 1F5K, 1F5L, 1FCX, 1FCY, 1FCZ, 1FDS, 1FDT, 1FH0, 1FVC, 1FVT, 1FY3, 1GMY, 1GS4, 1GUX, 1H00, 1H01, 1H07, 1H08, 1H1P, 1H1R, 1H1S, 1H59, 1H66, 1H69, 1H7S, 1HCK, 1HCL, 1HVY, 1HW3, 1HW4, 1I5R, 1I72, 1I79, 1I7B, 1I7C, 1I7M, 1J55, 1JAH, 1JAI, 1JCQ, 1JCZ, 1JD0, 1JDH, 1JQH, 1JTV, 1K3A, 1K8U, 1K96, 1K9K, 1K9P, 1KBC, 1KHX, 1KI0, 1KLG, 1KLU, 1LGP, 1LGQ, 1LQB, 1MAZ, 1MEJ, 1MEN, 1MEO, 1MMP, 1MMQ, 1MMR, 1MP8, 1MQ4, 1MQB, 1MZC, 1N0W, 1N26, 1N4M, 1N4Q, 1NWU, 1OC0, 1OES, 1OET, 1OEV, 1OKY, 1P5Z, 1P60, 1P61, 1PYE, 1PYO, 1PYX, 1Q0B, 1Q2U, 1Q3D, 1Q3W, 1Q41, 1Q91, 1Q92, 1QIA, 1QIC, 1QR1, 1QX3, 1R0P, 1R1W, 1R2, 1R2D, 1R2E, 1R2I, 1RHJ, 1RV1, 1RVD, 1S1P, 1S1R, 1S2A, 1S2C, 1S63, 1S9W, 1S9Y, 1SA4, 1SC8, 1SPJ, 1SU3, 1T15, 1T29, 1T64, 1T67, 1TN3, 1TSR, 1TTM, 1TUP, 1TVB, 1TVH, 1UNG, 1UNH, 1UNL, 1UOL, 1UPK, 1UU3, 1UU7, 1V1K, 1VJ9, 1VJA, 1VKG, 1VPP, 1VYW, 1VYZ, 1W0X, 1W0Z, 1W10, 1W11, 1W12, 1W13, 1W14, 1W98, 1WCH, 1WER, 1WMA, 1WQ6, 1WYX, 1XF0, 1XI2, 1XJB, 1XKK, 1XOW, 1XPZ, 1XQ0, 1XQ3, 1XQC, 1XRJ, 1XUC, 1XWS, 1YC1, 1YC3, 1YC4, 1YCS, 1YER, 1YES, 1YET, 1YPV, 1YUC, 1YW7, 1YW9, 1YY8, 1YZ1, 1Z5M, 1Z8G, 1Z95, 1ZIV, 1ZQ5, 1ZS0, 1ZSP, 1ZTE, 1ZUA, 1ZUQ, 1ZVX, 2AC0, 2ADQ, 2ADU, 2AHI, 2ANG, 2AO6, 2AOA, 2AOB, 2ARY, 2ASU, 2ATA, 2AX6, 2AX7, 2AX8, 2AX9, 2AXA, 2AXN, 2BBA, 2BDF, 2BDG, 2BIK, 2BIM, 2BIN, 2BIO, 2BIP, 2BIQ, 2BKF, 2BNQ, 2BNR, 2BNU, 2BO9, 2BZH, 2BZI, 2BZJ, 2BZK, 2BZS, 2C3I, 2C6C, 2C6D, 2C6E, 2C6G, 2C6P, 2CBZ, 2CIJ, 2CLX, 2CN5, 2D06, 2D1X, 2D8N, 2DUV, 2E0T, 2ETL, 2F4J, 2F53, 2FBT, 2FBV, 2FBX, 2FBY, 2FC0, 2FGB, 2FMM, 2FVD, 2FWY, 2FWZ, 2G1T, 2G2H, 2G9N, 2GCN, 2GCO, 2GCP, 2GEE, 2GQG, 2GSS, 2GT9, 2GTW, 2GTZ, 2GUO, 2GV6, 2GV7, 2GVG, 2GVJ, 2H55, 2H8H, 2H9G, 2HD5, 2HLE, 2HQU, 2HXK, 2HYI, 2HZ5, 2HZQ, 2HZR, 2I3H, 2I3I, 2I9A, 2IAL, 2IEJ, 2IF5, 2IFQ, 2ILR, 2IMS, 2IMT, 2IOG, 2IOK, 2ITN, 2ITV, 2IUW, 2IW6, 2IW8, 2IW9, 2J0S, 2J1W, 2J1X, 2J1Y, 2J1Z, 2J8B 2J20, 2J21, 2J2I, 2J4Z, 2JAV, 2JCN 2JDO, 2JDR, 2JDS, 2JDT, 2JDV, 2JIH, 2NL9, 2NMN, 2NMO, 2NN8, 2NS2, 2NTE, 2NWG, 2NWN, 2NYR, 2O88, 2OCJ, 2OO0, 2OOT, 2OPM, 2OVH, 2OZ7, 2P1T, 2P1U, 2P1V, 2P4K, 2P5E, 2P5W, 2P85, 2PCU, 2PE4, 2PIO, 2PIP, 2PIQ, 2PIR, 2PIT, 2PIU, 2PIV, 2PIX, 2PJL, 2PKL, 2PL3, 2PN7, 2PQK, 2PSQ, 2PVF, 2PVY, 2PWL, 2PX6, 2PY3, 2PYE, 2PZ1, 2PZ5, 2PZP, 2Q3E, 2Q7I, 2Q7J, 2Q7K, 2Q7L, 2Q81, 2QBX, 2QCC, 2QCD, 2QCE, 2QCF, 2QCG, 2QCH, 2QCL, 2QCM, 2QCN, 2QFO, 2QG0, 2QG2, 2QG4, 2QMS, 2QXH, 2QXI, 2QXJ, 2R2W, 2R3F, 2R3G, 2R3H, 2R3I, 2R3J, 2R3K, 2R3L, 2R3M, 2R3N, 2R3O, 2R3P, 2R3Q, 2R3R, 2R64, 2RA4, 2RBH, 2RF5, 2RFS, 2RH1, 2RIQ, 2RKU, 2TCL, 2UUH, 2UUI, 2UVL, 2UVM, 2UWD, 2UZI, 2UZR, 2UZS, 2V1Y, 2V4B, 2V5Q, 2V5W, 2V5X, 2V8W, 2V8X, 2V8Y, 2V9R, 2V9S, 2V9T, 2VCI, 2VKI, 2VM5, 2VM6, 2VPF, 2VSL, 2VUK, 2VVK, 2VWF, 2VX3, 2W0G, 2W0J, 2W0Z, 2W17, 2W18, 2W1H, 2W3L, 2W5A, 2W5B, 2W5H, 2W7X, 2W83, 2W97, 2WA0, 2WD2, 2WD3, 2WEV, 2WGJ, 2WGP, 2WGX, 2WI1, 2WI2, 2WI3, 2WI4, 2WI5, 2WI6, 2WKM, 2WMQ, 2WMR, 2WMV, 2WMW, 2WMX, 2WND, 2WOG.2X2R, 2WOR, 2WOS, 2WTV, 2X0U, 2X0V, 2X0W, 2X29, 2X39, 2X4Z, 2X7C, 2X7D, 2X7E, 2X7S, 2X7T, 2X7U, 2XAB, 2XBJ, 2XCV, 2XCW, 2XCX, 2XDK, 2XDL, 2XDS, 2XDU, 2XDX, 2XEF, 2XEG, 2XEI, 2XEJ, 2XHR, 2XHT, 2XJB, 2XJC, 2XJD, 2XJE, 2XJF, 2XJG, 2XJJ, 2XJX, 2XK2, 2XMR, 2XMS, 2XOC, 2XOZ, 2XP0, 2XP2, 2XP3, 2XP4, 2XP5, 2XP6, 2XP7, 2XP8, 2XP9, 2XPA, 2XPB, 2XT3, 2XUS, 2XWC, 2XWR, 2Y6E, 2Y6W, 2Y96, 2YAD, 2YBG, 2YGN, 2YGO, 2YGP, 2YHD, 2YI0, 2YI6, 2YI7, 2YIQ, 2YIR, 2YIT, 2YJ1, 2YLP, 2YLQ, 2YXJ, 2Z7Q, 2Z7R, 2Z7S, 2ZGV, 3A99, 3AOX, 3APA, 3ARN, 3AT2, 3AT4, 3AU4, 3AYA, 3AYC, 3AYD, 3AYE, 3B1U, 3B24, 3B25, 3B26, 3B27, 3B28, 3B7G, 3B97, 3B9S, 3BBB, 3BBC, 3BBF, 3BCH, 3BER, 3BET, 3BGM, 3BH8, 3BH9, 3BHB, 3BHT, 3BHU, 3BHV, 3BIN, 3BIY, 3BJF, 3BO8, 3BOR, 3BXM, 3BZ3, 3C0Y, 3C0Z, 3C10, 3C39, 3C3A, 3C3B, 3C3C, 3C4E, 3C4F, 3C4H, 3C5F, 3C5G, 3C5R, 3C7P, 3C7Q, 3CBM, 3CBO, 3CBP, 3CBX, 3CBY, 3CBZ, 3CC0, 3CE4, 3CEK, 3CJF, 3CJG, 3CQV, 3CRY, 3CS4, 3CS6, 3CS9, 3CSH, 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3MB6, 3MB7, 3ME3, 3MHJ, 3MHK, 3MK8, 3MTR, 3MTU, 3MXV, 3MXW, 3MYJ, 3N1F, 3N1G, 3N1M, 3N1V, 3N45, 3N46, 3N5E, 3N5G, 3N5H, 3N5J, 3N5N, 3N6K, 3NBH, 3NBI, 3NBQ, 3NCL, 3NMQ, 3NMW, 3NMX, 3NS9, 3NSZ, 3O0I, 3O33, 3O35, 3O36, 3O37, 3O3A, 3O3B, 3O3D, 3O3E, 3O3U, 3O50, 3O64, 3O7W, 3ODK, 3OGU, 3OOB, 3OSE, 3OVM, 3OWH, 3OWJ, 3OWK, 3OWL, 3OWX, 3OX1, 3OX2, 3OX3, 3OY8, 3OZJ, 3P0N, 3P0P, 3P0Q, 3P0Y, 3P2T, 3P53, 3P5A, 3P8F, 3P8G, 3P8X, 3P92, 3P95, 3PB1, 3PCV, 3PE1, 3PE2, 3PE4, 3PH9, 3PJ8, 3PO6, 3POZ, 3PP0, 3PQZ, 3PY7, 3Q01, 3Q05, 3Q2R, 3Q2U, 3Q6S, 3Q6U, 3Q6W, 3QDJ, 3QF9, 3QFD, 3QI5, 3QIR, 3QKD, 3QQK, 3QQN, 3QR2, 3QRI, 3QRJ, 3QRK, 3QTQ, 3QTR, 3QTS, 3QTU, 3QTW, 3QTX, 3QTZ, 3QU0, 3QX3, 3QXP, 3R0T, 3R43, 3R58, 3R6I, 3R7M, 3R7O, 3R85, 3R8G, 3R8H, 3R8I, 3R8U, 3R8V, 3R8Z, 3R94, 3R9D, 3R9H, 3R9N, 3R9O, 3RAH, 3RAK, 3RAL, 3RDH, 3RGF, 3RHK, 3RHX, 3RI1, 3RJ7, 3RJC, 3RK5, 3RK7, 3RK9, 3RKB, 3RKZ, 3RMF, 3RNI, 3RPR, 3RPV, 3RPY, 3RQD, 3RU0, 3RZ3, 3RZB, 3S00, 3S0O, 3S1H, 3S34, 3S35, 3S98, 3S9D, 3SA0, 3SBD, 3SDE, 3SE2, 3SI5, 3SL9, 3SMI, 3SMJ, 3SP7, 3SPF, 3SQQ, 3SWZ, 3SZ9, 3SZA, 3SZB, 3T1L, 3T1M, 3T2T, 3T6A, 3TB3, 3TE7, 3TEM, 3TF3, 3TH5, 3TH7, 3THE, 3THH, 3THJ, 3TJM, 3TNW, 3TSO, 3TUO, 3TZB, 3U15, 3U2Z, 3U5J, 3U5K, 3U5L, 3U6H, 3U6I, 3U6J, 3U9H, 3U9Y, 3UA9, 3UD1, 3UD2, 3UFY, 3UG8, 3UGC, 3UGR, 3ULI, 3UMW, 3UPA, 3UW4, 3UWP, 3V3B, 3V42, 3V5Q, 3V8S, 3VHA, 3VHC, 3VHD, 3VHE, 3VJN, 3VKX, 3VO3, 3VQU, 3VSO, 3W2O, 3W2P, 3W2Q, 3W2R, 3W2S, 3W51, 3WE4, 3WF5, 3WF6, 3WF7, 3WF8, 3WF9, 3WHA, 3WIX, 3WIY, 3WIZ, 3WUT, 3WZK, 3X01, 3X02, 3ZC6, 3ZCW, 3ZEP, 3ZFM, 3ZFY, 3ZGO, 3ZJB, 3ZK6, 3ZLN, 3ZLR, 3ZM0, 3ZM1, 3ZM2, 3ZM3, 3ZME, 3ZOS, 3ZVY, 3ZVZ, 3ZXE, 3ZXF, 3ZXZ, 3ZZE, 4A14, 4A1U, 4A1W, 4A5Y, 4A63, 4A69, 4A82, 4AG8, 4AGC, 4AGL, 4AGM, 4AGN, 4AGO, 4AGP, 4AGQ, 4AJP, 4AL0, 4AL1, 4AN3, 4ANB, 4AOI, 4AOW, 4AP7, 4APC, 4AQ3, 4AQC, 4AQI, 4AQJ, 4AS7, 4ASD, 4ASE, 4ASZ, 4AT3, 4AT4, 4AT5, 4AUV, 4AVM, 4AVP, 4AVU, 4AVW, 4AW9, 4AXA, 4AY1, 4AZA, 4B04, 4B2D, 4B36, 4B7P, 4B87, 4B9D, 4BCK, 4BCM, 4BCN, 4BCO, 4BCP, 4BCQ, 4BD8, 4BF2, 4BFP, 4BGH, 4BHN, 4BIB, 4BIE, 4BJ9, 4BJB, 4BJC, 4BJX, 4BKJ, 4BPM, 4BS4, 4BU3, 4BU5, 4BU6, 4BU7, 4BU8, 4BU9, 4BUA, 4BUE, 4BUI, 4BUS, 4BUT, 4BUU, 4BUV, 4BUW, 4BUX, 4BUY, 4C41, 4C4P, 4C52, 4C5D, 4CEG, 4CG8, 4CG9, 4CGA, 4CGB, 4CIM, 4CKR, 4CLI, 4CLJ, 4CMH, 4CMM, 4CMO, 4CMT, 4CMU, 4CNC, 4CNH, 4CNM, 4CQ0, 4CTB, 4CTC, 4D0N, 4D0W, 4D0X, 4D1S, 4D4M, 4DA5, 4DBS, 4DBW, 4DD8, 4DEA, 4DEE, 4DRA, 4DRH, 4DRI, 4DRJ, 4DRK, 4DRM, 4DRN, 4DRO, 4DRP, 4DSN, 4DSO, 4DST, 4DSU, 4E28, 4EDW, 4EEH, 4EEV, 4EEY, 4EFT, 4EFU, 4EGC, 4EHR, 4EJH, 4EJI, 4EJJ, 4EOI, 4EOJ, 4EOL, 4EOM, 4EON, 4EOO, 4EOP, 4EOQ, 4EOR, 4EQC, 4EQZ, 4ER3, 4ER6, 4ER7, 4EWI, 4F0E, 4F0I, 4F1L, 4FA3, 4FAL, 4FAM, 4FBX, 4FCJ, 4FCP, 4FCQ, 4FCR, 4FHH, 4FHI, 4FIA, 4FLP, 4FNW, 4FNX, 4FNY, 4FOB, 4FOC, 4FOD, 4FUL, 4FVL, 4FYQ, 4FYR, 4FYS, 4FYT, 4G1N, 4G31, 4GCJ, 4GDX, 4GG2, 4GJY, 4GJZ, 4GKS, 4GMX, 4GOS, 4GOV, 4GOY, 4GP3, 4GPZ, 4GS6, 4GS9, 4GT4, 4GT5, 4GV1, 4GWG, 4GWK, 4GZL, 4H1S, 4H1Y, 4H2B, 4H2F, 4H2G, 4H2I, 4H5S, 4H75, 4H7Y, 4H87, 4HBM, 4HC4, 4HG7, 4HJG, 4HKZ, 4HRF, 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6FNM, 6FO8, 6FQ1, 6FQR, 6FR3, 6FR4, 6FR5, 6FR7, 6FR8, 6FR9, 6FRA, 6FRB, 6FRC, 6FS0, 6FS1, 6FT7, 6FT8, 6FT9, 6FUM, 6FUN, 6FUO, 6FUP, 6FUQ, 6FUR, 6FVF, 6FVG, 6FWB, 6FXH, 6FZF, 6FZG, 6FZJ, 6FZP, 6FZQ, 6FZR, 6G0O, 6G0P, 6G0Q, 6G0R, 6G0S, 6G24, 6G25, 6G27, 6G29, 6G2B, 6G2C, 6G2E, 6G2F, 6G2O, 6G2V, 6G2X, 6G2Y, 6G2Z, 6G30, 6G5W, 6G5X, 6G6J, 6G6K, 6G6L, 6G6R, 6G98, 6G9U, 6GCY, 6GDY, 6GFA, 6GG1, 6GGA, 6GGB, 6GGC, 6GGD, 6GGE, 6GGF, 6GGN, 6GI6, 6GIN, 6GIP, 6GJW, 6GL8, 6GQE, 6GT3, 6GU2, 6GU6, 6GUC, 6GUE, 6GUH, 6GUK, 6GVA, 6GVX, 6GX6, 6GXB, 6GXE, 6GXK, 6GY5, 6H0W, 6H0X, 6H0Y, 6H0Z, 6H10, 6H11, 6H1D, 6H1E, 6H3K, 6H3Q, 6H46, 6H47, 6H4K, 6H4Z, 6H50, 6H51, 6H52, 6HAX, 6HAY, 6HAZ, 6HBN, 6HBY, 6HCZ, 6HDN, 6HDQ, 6HHP, 6HI3, 6HIA, 6HIE, 6HJ2, 6HKB, 6HKF, 6HKQ, 6HMB, 6HMC, 6HMD, 6HME, 6HMT, 6HMU, 6HN2, 6HN3, 6HNW, 6HNY, 6HOP, 6HOQ, 6HOR, 6HOT, 6HOU, 6HOV, 6HP9, 6HPH, 6HPQ, 6HPT, 6HQU, 6HR2, 6HVH, 6HVI, 6HVJ, 6HXK, 6HXL, 6HXM, 6HYG, 6HYJ, 6HYY, 6I07, 6I0J, 6I0L, 6I0Z, 6I10, 6I11, 6I12, 6I13, 6I14, 6I15, 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6NH3, 6NH4, 6NH5, 6NH6, 6NH7, 6NH8, 6NHB, 6NHC, 6NHF, 6NJA, 6NJZ, 6NK0, 6NK1, 6NK2, 6NKP, 6NKR, 6NKS, 6NKU, 6NKV, 6NKW, 6NKX, 6NKY, 6NKZ, 6NL0, 6NLV, 6NM0, 6NM7, 6NMR, 6NMS, 6NMT, 6NMW, 6NNG, 6NNV, 6NOJ, 6NP9, 6NPZ, 6NRF, 6NRG, 6NRH, 6NRI, 6NRJ, 6NT2, 6NTP, 6NTU, 6NU1, 6NU5, 6NUB, 6NVB, 6NWS, 6NWT, 6O0K, 6O0L, 6O0M, 6O0O, 6O0P, 6O1E, 6O39, 6O3A, 6O4U, 6O4Y, 6O4Z, 6O51, 6O53, 6O5M, 6O6F, 6O6G, 6O89, 6O9B, 6O9C, 6O9X, 6O9Y, 6OA0, 6OA1, 6OA3, 6OAK, 6OAL, 6OB3, 6OCX, 6OD0, 6OIA, 6OIE, 6OIL, 6OIM, 6OKD, 6OLX, 6ONY, 6OPD, 6OQB, 6OQC, 6OQD, 6OQN, 6OSH, 6OSN, 6OSP, 6OSV, 6OTN, 6OWH, 6OWI, 6P05, 6P1D, 6P3D, 6P3P, 6P4V, 6P5S, 6P6D, 6P8W, 6P8X, 6P8Y, 6P8Z, 6PDA, 6PDB, 6PDC, 6PDD, 6PDE, 6PDF, 6PDG, 6PEG, 6PET, 6PF1, 6PG3, 6PG4, 6PG5, 6PG6, 6PG7, 6PG8, 6PG9, 6PGA, 6PGB, 6PGC, 6PGD, 6PGE, 6PGF, 6PGR, 6PGU, 6PGX, 6PJV, 6PKC, 6PLF, 6PPA, 6PQ3, 6PTB, 6PTE, 6PU7, 6PV9, 6PVE, 6PYY, 6PYZ, 6Q0D, 6Q13, 6Q38, 6Q4Q, 6Q6J, 6Q8K, 6QAS, 6QAU, 6QAV, 6QB3, 6QB4, 6QB6, 6QB9, 6QBC, 6QBY, 6QCD, 6QCE, 6QCH, 6QCI, 6QCJ, 6QCN, 6QED, 6QEF, 6QEG, 6QEH, 6QEI, 6QEJ, 6QEY, 6QF9, 6QFC, 6QFQ, 6QGG, 6QGH, 6QGJ, 6QGK, 6QGV, 6QPL, 6QTJ, 6QUU, 6QUV, 6QUW, 6QUX, 6QVG, 6QVL, 6QXJ, 6QYK, 6QYL, 6QYO, 6QYP, 6QYQ, 6QZ5, 6QZ6, 6QZ7, 6QZ8, 6QZB, 6QZH, 6R2L, 6R3E, 6R3S, 6R9H, 6RB1, 6RBC, 6RBI, 6RCB, 6RCF, 6RCM, 6RFE, 6RFF, 6RFI, 6RLC, 6RLW, 6RNU, 6ROL, 6ROY, 6RQ4, 6RTI, 6RWJ, 6RZ6, 6RZ7, 6S1X, 6S4B, 6S55, 6S56, 6S57, 6S6K, 6S70, 6S71, 6S74, 6S77, 6S79, 6S7A, 6S7C, 6S7F, 6S7H, 6S8L, 6S8V, 6SA2, 6SA3, 6SAH, 6SAJ, 6SB8, 6SBO, 6SCM, 6SD9, 6SDC, 6SDD, 6SDE, 6SEQ, 6SER, 6SF3, 6SFI, 6SFJ, 6SFK, 6SFR, 6SG4, 6SGD, 6SGI, 6SGK, 6SHH, 6SHI, 6SHZ, 6SI0, 6SI1, 6SI2, 6SI3, 6SI4, 6SJU, 6SK9, 6SLG, 6SM8, 6SMB, 6SPW, 6SPX, 6SQC, 6ST3, 6SWN, 6SWQ, 6SZM, 6T1I, 6T1J, 6T1L, 6T1M, 6T1N, 6T1O, 6T41, 6T6R, 6T7U, 6T9Z, 6TD4, 6TE6, 6TEL, 6TEN, 6TFU, 6TFV, 6TFW, 6TFY, 6TFZ, 6TG0, 6TG1, 6THW, 6THX, 6THZ, 6TI8, 6TKP, 6TMO, 6TMP, 6TMQ, 6TN0, 6TN2, 6TN4, 6TN5, 6TNC, 6TOF, 6TOG, 6TOH, 6TOI, 6TOJ, 6TOK, 6TOL, 6TOM, 6TON, 6TOO, 6TRN, 6TVE, 6TVG, 6TWA, 6TX0, 6TX2, 6TXF, 6U0A, 6U15, 6U16, 6U17, 6U1U, 6U4Q, 6U4T, 6U65, 6U67, 6U6V, 6U73, 6U8Z, 6UBW, 6UCS, 6UD2, 6UDI, 6UDT, 6UDU, 6UDV, 6UDX, 6UDY, 6UEL, 6UFX, 6UGN, 6UGO, 6UGP, 6UGQ, 6UGR, 6UGZ, 6UH0, 6UJO, 6UKM, 6UKU, 6UKV, 6UKW, 6UKX, 6UKY, 6UKZ, 6UL0, 6ULI, 6ULK, 6ULM, 6ULN, 6UMT, 6UMU, 6UMV, 6UNT, 6URE, 6URJ, 6URK, 6URL, 6URN, 6URQ, 6URR, 6URZ, 6US0, 6US1, 6US7, 6USB, 6USD, 6USI, 6USX, 6USZ, 6UT0, 6UYA, 6UZF, 6UZT, 6UZU, 6V0Q, 6V0S, 6V0U, 6V0X, 6V14, 6V16, 6V17, 6V1B, 6V1D, 6V1E, 6V1F, 6V1H, 6V1K, 6V1L, 6V1U, 6V3W, 6V52, 6V5N, 6V5P, 6V66, 6V6K, 6V6O, 6V74, 6V7C, 6V7D, 6V7E, 6V7F, 6V7Y, 6V87, 6V89, 6V8A, 6V8K, 6V8N, 6V8T, 6V90, 6V9C, 6VBH, 6VC9, 6VEI, 6VFZ, 6VGH, 6VGO, 6VHG, 6VHI, 6VHN, 6VIG, 6VKG, 6VKK, 6VMU, 6VND, 6VO4, 6VO7, 6VPF, 6VPK, 6VQN, 6VR1, 6VR5, 6VRN, 6VTC, 6VTH, 6VUA, 6W0Q, 6W2P, 6W3Q, 6W3U, 6W43, 6W4R, 6W4Z, 6W7F, 6W7G, 6W7J, 6W7K, 6W7L, 6WBE, 6WE3, 6WE4, 6WGH, 6WGN, 6WH1, 6WH2, 6WHB, 6WKA, 6WP3, 6WP4, 6WP5, 6WP6, 6WU8, 6WUW, 6WW3, 6WW4, 6WW8, 6X2M, 6X2P, 6X2R, 6X2S, 6X2U, 6X2X, 6X2Y, 6X3N, 6X3O, 6X3P, 6X7B, 6XDL, 6XLW, 6XLX, 6XOG, 6XOH, 6XOI, 6XOZ, 6XP0, 6XP1, 6XP2, 6XP3, 6XPB, 6XPC, 6XU1, 6XUH, 6XUI, 6XUL, 6XUN, 6XVT, 6XVW, 6XXH, 6XXI, 6XXJ, 6XXK, 6XXL, 6XXM, 6XXR, 6Y09, 6Y1J, 6Y4S, 6Y74, 6Y7Q, 6Y8K, 6YAU, 6YB4, 6YB8, 6YB9, 6YBG, 6YBK, 6YBL, 6YG9, 6YHR, 6YKD, 6YLI, 6YQN, 6YQO, 6YQP, 6YVW, 6YVX, 6YVZ, 6YW0, 6YW1, 6YW2, 6YW3, 6YW4, 6YZJ, 6YZL, 6YZM, 6YZO, 6YZP, 6YZQ, 6YZR, 6YZS, 6YZT, 6YZU, 6YZV, 6YZW, 6YZX, 6Z04, 6Z4D, 6Z83, 6Z9B, 6ZAY, 6ZDC, 6ZDK, 6ZDL, 6ZFA, 6ZFN, 6ZFQ, 6ZHC, 6ZJ1, 6ZJ5, 6ZK6, 6ZRV, 7A04, 7A06, 7A1B, 7A1Z, 7A22, 7A2A, 7A2H, 7A49, 7A4B, 7A62, 7A77, 7A78, 7A79, 7A9Y, 7A9Z, 7AA0, 7AA1, 7ACK, 7AD0, 7AD7, 7AH1, 7AH4, 7AHZ, 7AI0, 7AI1, 7AIA, 7AKI, 7AQF, 7AQG, 7ASU, 7ASV, 7AVQ, 7AVX, 7AVY, 7AVZ, 7AW0, 7AW1, 7AW2, 7AW3, 7AW4, 7B3M, 7B7R, 7B94, 7B9L, 7BCM, 7BKG, 7BOS, 7BOT, 7BSJ, 7C04, 7C7F, 7C7G, 7C7H, 7CNA, 7CTP, 7CYZ, 7D3D, 7DHY, 7DHZ, 7JHD, 7JJM, 7JK7, 7JOO, 7JU5, 7JU6, 7JV8, 7JVM, 7JVN, 7JWS, 7JWT, 7JWU, 7JWV, 7JWW, 7JX9, 7K6I, 7K6J, 7K6K, 7K6L, 7K6M, 7K6T, 7K6U, 7K6X, 7K6Z, 7KBS, 7KCA, 7KCD, 7KIA, 7KIE, 7KK2, 7KK3, 7KK4, 7KK5, 7KK6, 7KKM, 7KKN, 7KKO, 7KKP, 7KKQ, 7KWM, 7LSZ, 7LT0, 7NBJ, 7NBQ

| **Table S2.** Static and flexible docking analysis of chemical structures with molecular similarity to PSK and PSP. | | | | | | | | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ligand | Structure | Molecular properties | Docking | Affinity | EL | HB amino acids | Covalent amino acids (pi-alkyl, Pi-Pi) | VW amino acids |
| Adenosine monophosphate | Diagram  Description automatically generated | miLogP:-1.52  TPSA:186.08  Natoms:23  MW:347.22g/mol  nON:12  nOHNH:6  nviolations:2  nrotb:4  volume:263.88 | Estático | -8.2 | -0.35 | ASP36, ASN117, HIS118, HIS243, GLY392, ARG395, ASP506 | PHE417, PHE500 | ASN245, ARG354, ASN390, GLY392, GLY393, THR446 |
| Flexible | -7.0 | -0.3 | HIS118, HIS243 |  | LEU184, SER244, ASN245, GLY392, GLY393, ARG395, THR446, GLY447, PHE500, ASP506 |
| AB680 | A picture containing radar chart  Description automatically generated | miLogP:0.27  TPSA:189.16  Natoms:35  MW:578.81 g/mol  nON:13  nOHNH:5  nviolations:2  nrotb:9  volume:440.10 | Static | -7.3 | -0.2 | GLU180, HIS440, ARG 441, HIS437, ASP506, GLY507 | MET510, HIS437, HIS440 | LYS433, GLN509, ASP513, GLU514 |
| Flexible | -6.7 | -0.19 | LEU184, ASN186 | HIS118, ASN 122, GLY123, SER185, ASN390, GLY393, PHE417, GLY418 | ASP121, PHE500 |
| CVP | Shape, schematic, line chart  Description automatically generated | miLogP:-5.25  TPSA:268.68  Natoms:34  MW:483.27g/mol  nON:16  nOHNH:11  nviolations:3  nrotb:7  volume:352.07 | Static | -7.2 | -0.21 | GLU180, ARG395, ARG441, GLN444, THR446, GLY447, ASP506 |  | HIS118. GLU224, HIS243, SER244, ASN245, ASN390, GLY392, SER445, PHE500 |
| Flexible | -6.8 | -0.2 | TYR 345, ASP347, GLU400, ARG401, VAL542 |  | LYS256, VAL344, SER352, ASN359, ASP399, PRO540, ALA541 |
| 3-beta-Glucosylcellotriose | Diagram  Description automatically generated | miLogP:-5.69  TPSA:347.83  Natoms:45  MW:666.58 g/mol  nON:21  nOHNH:14  nviolations:3  nrotb:10  volume:548.17 | Static | -6.8 | -0.15 | GLU180, ARG441, HIS440, GLN444 |  | GLU224, HIS243, THR446, GLY447, GLY507 |
| Flexible | -6.5 | -0.14 | ASP366, TYR484, GLU543 |  | ASN362, ASN370, GLY454, HIS456, LEU475, TYR531, LYS534, MET535, PRO540, ARG545 |
| Glycogen | Diagram, schematic  Description automatically generated | miLogP:-5.65  TPSA:347.83  Natoms:45  MW:666.58  nON:21  nOHNH:14  nviolations:3  nrotb:10  volume:548.17 | Static | -6.8 | -0.15 | GLU180, ARG441, GLN444 |  | LEU184, GLU224, SER244, HIS437, THR446, ASP506, GLY507 |
| Flexible | -6.9 | -0.15 | GLU180 |  | LEU 184, MET225, HIS243, HIS437, HIS440, ARG441, THR446, GLY447, GLU448, ASP506, GLY507, GLN509 |
| Laminarin 2 | Diagram, schematic  Description automatically generated | miLogP:-4.45  TPSA:189.53  Natoms:23  MW:342.30g/mol  nON:11  nOHNH:8  nviolations:2  nrotb:4  volume:283.93 | Static | -6.7 | -0.29 | HIS243, ASN390, GLY393 |  | ASP36, ASP85, ASN117, HIS118, LEU184, SER244, ASN245, ARG354, GLY392, GLY393, ARG395, PHE417, GLY447, ASP506 |
| Flexible | -6.8 | -0.29 | GLU180 |  | PHE183, LEU184, GLU224, HIS437, HIS440, ARG441, ASP506, GLY507 |
| Laminarin 3 | Diagram  Description automatically generated | miLogP:-5.25  TPSA:268.68  Natoms:34  MW:504.44g/mol  nON:16  nOHNH:11  nviolations:3  nrotb:7  volume:416.05 | Static | -5.8 | -0.17 | GLU224, ARG441, GLN444, THR446 |  | HIS243, SER244, ARG354, SER445, GLY447 |
| Flexible | -7.2 | -0.21 | ARG441, GLY509 |  | PHE 183, LEU184, GLU224, HIS437, HIS440, ARG 441, ASP506, GLY507 |
| Laminarin 4 | Diagram  Description automatically generated with medium confidence | miLogP:-5.92  TPSA:347.83  Natoms:45  MW:638.36 g/mol  nON:21  nOHNH:14  nviolations:3  nrotb:10  volume:462.87 | Static | -6.4 | -0.14 | GLU180, GLN509 |  | PHE183, LEU184, HIS243, HIS437, HIS440, ARG441, THR446, ASP506, GLY507 |
| Flexible | -4.8 | -0.11 | GLU180, ARG441 |  | GLU224, HIS437, GLN444, ASP506, GLY507, GLN509, MET510 |
| Laminarin 6 | Diagram, schematic  Description automatically generated | miLogP:-6.42  TPSA:506.13  Natoms:67  MW:948.52 g/mol  nON:31  nOHNH:20  nviolations:3  nrotb:16  volume:684.46 | Static | -7.2 | -0.11 | ARG354, LYS433, HIS437, HIS440  GLN444, GLY507, ASP513 |  | GLU180, GLU224, SER244, ARG441, SER445, THR446, GLY447, ASP506  GLN509, MET510  GLU514 |
| Flexible | -6.1 | -0.09 | GLN444  ARG468  GLY507 |  | GLU180, GLU224, LYS227, HIS437, HIS440, ARG441, TYR442 |
| Laminarin 7 | Diagram  Description automatically generated | miLogP:-6.60  TPSA:585.29  Natoms:78  MW:1103.61  nON:36  nOHNH:23  nviolations:3  nrotb:19  volume:795.25 | Static | -7.9 | -0.10 | GLU180, LYS433, HIS437, ARG441 |  | HIS118, LEU184, GLU224, SER244, ASN245, GLY352, ARG354, ASN390, ARG395, HIS440, GLN444, SER445, THR446, GLY447,  PHE500, ASP506,  GLY507, GLN509,  MET510, ASP513 |
| Flexible | -5.7 | -0.09 | GLU180, HIS440, ARG441, GLN444, GLY507 |  | GLU224, HIS437, ASP506, GLN509, MET510 |
| Sizofiran | Chart, diagram  Description automatically generated with medium confidence | miLogP:-5.65  TPSA:347.83  Natoms:45  MW:666.58g/mol  nON:21  nOHNH:14  nviolations:3  nrotb:10  volume:548.17 | Static | -6.7 | -0.14 | ARG441, GLN444, ASP506 |  | GLU118, LEU184, GLU224, SER244, HIS437, HIS440, THR446, GLU448, HIS437 |
| Flexible | -6.5 | -0.13 | HIS440, ARG441, GLY502, GLN509 |  | PHE183, HIS437 |
| PSK | Diagram  Description automatically generated | miLogP:-6.13  TPSA:485.91  Natoms:66  MW:931.52  g/mol  nON:30  nOHNH:19  nviolations:3  nrotb:16  volume:673.80 | Static | -6.3 | -0.095 | GLU180, ARG441, GLY507, MET510 |  | PHE183, LEU184, GLU224, HIS243, SER244, HIS37, HIS440, THR446, GLU500 |
| Flexible | -6.8 | -0.1 | GLU180, ARG441, GLN444, GLN509 |  | PHE183, GLU224, HIS437, HIS440, GLY507 |
| Malt triose | Diagram, schematic  Description automatically generated | miLogP:-5.25  TPSA:268.68  Natoms:34  MW:504.44g/mol  nON:16  nOHNH:11  nviolations:3  nrotb:7  volume:416.05 | Static | -6 | -0.18 | GLU180, ARG441, GLN444 |  | PHE183, LEU184, GLU224, HIS243, SER244, HIS37, HIS440, THR446, GLU500 |
| Flexible | -6.5 | -0.19 | GLU180, ARG441, GLN444 |  | GLU224, HIS243, HIS437, ASP506, GLY507 |
| Beta glucan | Diagram, schematic  Description automatically generated | miLogP:-5.25  TPSA:268.68  Natoms:34  MW:504.44 g/mol  nON:16  nOHNH:11  nviolations:3  nrotb:7  volume:416.05 | Static | -5.6 | -0.17 | ARG441, GLN444 |  | GLU180, GLU224, LYS227, HIS243, THR446 |
| Flexible | -7.5 | -0.23 | GLY507 |  | GLU180, HIS243, HIS440, THR446, GLY447, GLN509 |
| CVG | Chart, schematic, line chart  Description automatically generated | miLogP:-2.03  TPSA:99.38  Natoms:13  MW:194.18g/mol  nON:6  nOHNH:4  nviolations:0  nrotb:2  volume:169.34 | Static | -5.5 | -0.42 | ARG354, ARG395, GLY447 |  | HIS38, ASP85, ASN117, HIS118, HIS243, ASN245, GLY392 |
| Flexible | -6.4 | -0.49 | ARG354, GLY392, ASP506 |  | HIS118, LEU184, HIS243, ASN390, GLY393, ARG395, SER445, THR446, GLY447, GLU448, PHE500 |