

Global docking result analysis

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25 VINA docking runs of the ligand object 3 to the receptor object 1 yielded the following results,
sorted by binding energy [more positive energies indicate stronger binding, and negative energies mean no binding]

Run	Bind.energy[kcal/mol]	Dissoc. constant [pM]	Contacting receptor residues
001	000008.0340	00000001291219.0000	A TYR 455 A ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A GLY 616 A TRP 617 A ASP 618 A TYR 619 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A SER 681 A SER 682 A THR 687 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A LYS 798 A TRP 800 A HIS 810 A GLU 811 A PHE 812 A CYS 813 A SER 814 A ARG 836
002	000008.0340	00000001291219.0000	A TYR 455 A ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A GLY 616 A TRP 617 A ASP 618 A TYR 619 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A SER 681 A SER 682 A THR 687 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A LYS 798 A TRP 800 A HIS 810 A GLU 811 A PHE 812 A CYS 813 A SER 814 A ARG 836
003	000007.6100	00000002641168.0000	A HIS 439 A TYR 455 A ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A GLY 616 A TRP 617 A ASP 618 A TYR 619 A LYS 621 A CYS 622 A ASP 623 A THR 687 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A LYS 798 A CYS 799 A TRP 800 A HIS 810 A GLU 811 A CYS 813 A SER 814 A ARG 836
004	000007.6100	00000002641168.0000	A HIS 439 A TYR 455 A ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A GLY 616 A TRP 617 A ASP 618 A TYR 619 A LYS 621 A CYS 622 A ASP 623 A THR 687 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A LYS 798 A CYS 799 A TRP 800 A HIS 810 A GLU 811 A CYS 813 A SER 814 A ARG 836
005	000007.5200	00000003074446.2500	A HIS 439 A ASP 452 A TYR 455 A LYS 545 A ALA 547 A ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A ASP 618 A TYR 619 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A SER 681 A SER 682 A THR 687 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A GLU 811 A SER 814 A ARG 836
006	000007.5200	00000003074446.2500	A HIS 439 A ASP 452 A TYR 455 A LYS 545 A ALA 547 A ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A ASP 618 A TYR 619 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A SER 681 A SER 682 A THR 687 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A GLU 811 A SER 814 A ARG 836
007	000007.5160	00000003095273.0000	A LEU 245 A THR 246 A ARG 249 A LEU 251 A THR 252 A SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A LEU 316 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A ARG 349 A LEU 389 A ASP 390 A LYS 391 A THR 393 A THR 394 A CYS 395 A PHE 396 A SER 397 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A PRO 677
008	000007.5160	00000003095273.0000	A LEU 245 A THR 246 A ARG 249 A LEU 251 A THR 252 A SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A LEU 316 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A ARG 349 A LEU 389 A ASP 390 A LYS 391 A THR 393 A THR 394 A CYS 395 A PHE 396 A SER 397 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A PRO 677

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009 |          000007.5040 | 00000003158603.2500 | A HIS 439 A ASP 452 A TYR 455 A
ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A GLY 616 A
TRP 617 A ASP 618 A TYR 619 A PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A
SER 682 A SER 759 A ASP 760 A ASP 761 A LYS 798 A CYS 799 A TRP 800 A GLU 811 A
PHE 812 A CYS 813 A SER 814 A ARG 836
010 |          000007.5040 | 00000003158603.2500 | A HIS 439 A ASP 452 A TYR 455 A
ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A GLY 616 A
TRP 617 A ASP 618 A TYR 619 A PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A
SER 682 A SER 759 A ASP 760 A ASP 761 A LYS 798 A CYS 799 A TRP 800 A GLU 811 A
PHE 812 A CYS 813 A SER 814 A ARG 836
011 |          000007.5000 | 00000003180000.0000 | A HIS 439 A TYR 455 A ILE 548 A
SER 549 A ALA 550 A ARG 553 A ARG 555 A THR 556 A GLY 616 A TRP 617 A ASP 618 A
TYR 619 A PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A SER 681 A
SER 682 A THR 687 A ASN 691 A LEU 758 A SER 759 A ASP 760 A ASP 761 A ALA 762 A
LYS 798 A TRP 800 A GLU 811 A CYS 813 A SER 814 A ARG 836
012 |          000007.4780 | 00000003300299.2500 | A HIS 439 A ILE 548 A SER 549 A
ALA 550 A LYS 551 A ARG 553 A ARG 555 A TRP 617 A ASP 618 A TYR 619 A PRO 620 A
LYS 621 A CYS 622 A ASP 623 A THR 680 A SER 681 A SER 682 A THR 687 A ALA 688 A
ASN 691 A SER 759 A ASP 760 A ASP 761 A LYS 798 A TRP 800 A GLU 811 A PHE 812 A
CYS 813 A SER 814 A ARG 836
013 |          000007.4430 | 00000003501133.5000 | A HIS 439 A ASP 452 A TYR 455 A
SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A TRP 617 A ASP 618 A
TYR 619 A PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A SER 681 A
SER 682 A THR 687 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A LYS 798 A
CYS 799 A TRP 800 A GLU 811 A CYS 813 A SER 814 A ARG 836
014 |          000007.3800 | 00000003893931.2500 | A HIS 439 A ASP 452 A TYR 455 A
ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A GLY 616 A
TRP 617 A ASP 618 A TYR 619 A PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A
THR 680 A SER 681 A SER 682 A THR 687 A ASN 691 A SER 759 A ASP 760 A ASP 761 A
ALA 762 A TRP 800 A GLU 811 A CYS 813 A SER 814 A ARG 836
015 |          000007.3330 | 00000004215409.0000 | A HIS 439 A ALA 547 A ILE 548 A
SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A ASP 618 A TYR 619 A LYS 621 A
CYS 622 A ASP 623 A THR 680 A SER 682 A THR 687 A ALA 688 A ASN 691 A LEU 758 A
SER 759 A ASP 760 A ASP 761 A LYS 798 A GLU 811 A PHE 812 A CYS 813 A SER 814 A
ARG 836 A ALA 840 A ARG 858
016 |          000007.2520 | 00000004832963.5000 | A HIS 439 A TYR 455 A SER 549 A
ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A ILE 589 A GLY 590 A TRP 617 A
ASP 618 A TYR 619 A PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A
SER 681 A SER 682 A THR 687 A ALA 688 A ASN 691 A LEU 758 A SER 759 A ASP 760 A
ASP 761 A ALA 762 A TRP 800 A GLU 811 A CYS 813 A SER 814 A ARG 836
017 |          000007.2440 | 00000004898663.5000 | A HIS 439 A ASP 452 A TYR 455 A
TYR 456 A MET 542 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A
GLY 616 A TRP 617 A ASP 618 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A
SER 681 A SER 682 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A ALA 762 A
LYS 798 A CYS 799 A TRP 800 A GLU 811 A SER 814 A ARG 836
018 |          000007.2430 | 00000004906938.5000 | A HIS 439 A ASP 452 A TYR 455 A
ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A TRP 617 A
ASP 618 A TYR 619 A PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A ASP 760 A
ASP 761 A ALA 762 A LYS 798 A TRP 800 A HIS 810 A GLU 811 A CYS 813 A SER 814 A
HIS 816 A ASP 833 A ARG 836 A ALA 840 A ARG 858

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