

# 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	000008.2990	00000000825567.0625	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 THR 556 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 GLU 811 A SER 814 A ARG 836
002	000008.2990	00000000825567.0625	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 THR 556 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 GLU 811 A SER 814 A ARG 836
003	000008.1060	00000001143465.8750	A LEU 245 A THR 246 A ARG 249 A ALA 250 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 THR 394 A CYS 395 A PHE 396 A SER 397 A TYR 456 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A PRO 677
004	000008.1060	00000001143465.8750	A LEU 245 A THR 246 A ARG 249 A ALA 250 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 THR 394 A CYS 395 A PHE 396 A SER 397 A TYR 456 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A PRO 677
005	000008.0760	00000001202855.6250	A LEU 172 A THR 246 A LEU 247 A ARG 249 A THR 252 A SER 255 A LEU 261 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A LEU 270 A SER 318 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A PHE 326 A ARG 349 A THR 394 A CYS 395 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A PRO 677
006	000008.0760	00000001202855.6250	A LEU 172 A THR 246 A LEU 247 A ARG 249 A THR 252 A SER 255 A LEU 261 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A LEU 270 A SER 318 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A PHE 326 A ARG 349 A THR 394 A CYS 395 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A PRO 677
007	000007.9860	00000001400181.6250	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 ASP 623 A ARG 624 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 ALA 762 A LYS 798 A TRP 800 A GLU 811 A PHE 812 A CYS 813 A SER 814 A ARG 836
008	000007.9860	00000001400181.6250	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 ASP 623 A ARG 624 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 ALA 762 A LYS 798 A TRP 800 A GLU 811 A PHE 812 A CYS 813 A SER 814 A ARG 836

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009 |          000007.9770 | 00000001421613.2500 | 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 PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A
THR 680 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 813 A SER 814 A ARG 836
010 |          000007.9770 | 00000001421613.2500 | A LEU 172 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
VAL 315 A LEU 316 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A ARG 349 A
GLU 350 A THR 394 A PHE 396 A TYR 456 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A
ASN 628 A PRO 677
011 |          000007.9770 | 00000001421613.2500 | 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 PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A
THR 680 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 813 A SER 814 A ARG 836
012 |          000007.9590 | 00000001465465.6250 | 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 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 682 A ASN 691 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
013 |          000007.9310 | 00000001536384.5000 | 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
SER 318 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A ARG 349 A THR 394 A
CYS 395 A PHE 396 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A VAL 675 A PRO 677
014 |          000007.8770 | 00000001682993.5000 | 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 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 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
HIS 810 A GLU 811 A CYS 813 A SER 814 A ARG 836
015 |          000007.8330 | 00000001812737.2500 | A HIS 439 A TYR 456 A MET 542 A
LYS 545 A ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A
VAL 557 A ALA 558 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 SER 814 A ARG 836
016 |          000007.8230 | 00000001843592.6250 | 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 THR 556 A ASP 618 A TYR 619 A
PRO 620 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 GLU 811 A CYS 813 A SER 814 A
ARG 836 A ALA 840 A ARG 858 A LEU 862
017 |          000007.8140 | 00000001871811.2500 | A TYR 455 A ARG 553 A ARG 555 A
THR 556 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 682 A GLY 683 A ASP 684 A ALA 685 A THR 686 A THR 687 A ALA 688 A
TYR 689 A ASN 691 A LEU 758 A SER 759 A ASP 760 A ASP 761 A GLU 811 A CYS 813 A
SER 814
018 |          000007.7640 | 00000002036631.8750 | A TYR 455 A ASN 496 A ASN 497 A
LYS 500 A LYS 545 A ARG 553 A ALA 554 A ARG 555 A THR 556 A VAL 557 A ALA 558 A
ARG 569 A LEU 576 A LYS 577 A ALA 580 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 682 A GLY 683 A ASP 684 A ALA 685 A
THR 687 A ALA 688 A TYR 689 A ASN 691 A SER 759 A ASP 760
019 |          000007.6880 | 00000002315374.7500 | A HIS 439 A ASP 452 A TYR 455 A

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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 ALA 762 A LYS 798 A
TRP 800 A HIS 810 A GLU 811 A ARG 836
020 |          000007.6860 | 00000002323203.7500 | 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 VAL 557 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 ASP 684 A THR 687 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A
LYS 798 A GLU 811 A SER 814 A ARG 836
021 |          000007.6850 | 00000002327128.2500 | 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
PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A SER 682 A THR 687 A
ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A ALA 762 A LYS 798 A TRP 800 A
GLU 811 A SER 814 A ARG 836
022 |          000007.6810 | 00000002342892.5000 | 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 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 GLU 811 A
PHE 812 A CYS 813 A SER 814 A ARG 836 A ALA 840 A ARG 858
023 |          000007.6700 | 00000002386796.7500 | A LEU 172 A THR 246 A LEU 247 A
ARG 249 A THR 252 A SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A LEU 270 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
ASN 459 A LEU 460 A PRO 461 A THR 462 A PRO 677
024 |          000007.6230 | 00000002583847.7500 | A PRO 169 A LEU 172 A ALA 176 A
ASN 177 A LEU 245 A THR 246 A ARG 249 A ALA 250 A LEU 251 A THR 252 A SER 255 A
HIS 256 A LEU 261 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 THR 394 A CYS 395 A TYR 456 A
ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A PRO 677
025 |          000007.5780 | 00000002787740.5000 | A HIS 439 A ILE 548 A SER 549 A
ALA 550 A LYS 551 A ARG 553 A ALA 554 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 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 CYS 813 A SER 814 A ARG 836

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After clustering the 25 runs, the following 20 distinct complex conformations were found:

[They all differ by at least 5.0 Å heavy atom RMSD after superposing on the receptor]

Clu	Bind.energy[kcal/mol]	Dissoc. constant [pM]	Contacting receptor residues
001	000008.2990	00000000825567.0625	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 THR 556 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 GLU 811 A SER 814 A ARG 836
002	000008.1060	00000001143465.8750	A LEU 245 A THR 246 A ARG 249 A ALA 250 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 THR 394 A

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CYS 395 A PHE 396 A SER 397 A TYR 456 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A
THR 462 A ASN 628 A PRO 677
003 |          000008.0760 | 00000001202855.6250 | A LEU 172 A THR 246 A LEU 247 A
ARG 249 A THR 252 A SER 255 A LEU 261 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A
LEU 270 A SER 318 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A PHE 326 A
ARG 349 A THR 394 A CYS 395 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A
PRO 461 A PRO 677
004 |          000007.9860 | 00000001400181.6250 | 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 ASP 623 A ARG 624 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 ALA 762 A LYS 798 A TRP 800 A
GLU 811 A PHE 812 A CYS 813 A SER 814 A ARG 836
005 |          000007.9770 | 00000001421613.2500 | 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 PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A
THR 680 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 813 A SER 814 A ARG 836
006 |          000007.9770 | 00000001421613.2500 | A LEU 172 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
VAL 315 A LEU 316 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A ARG 349 A
GLU 350 A THR 394 A PHE 396 A TYR 456 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A
ASN 628 A PRO 677
007 |          000007.9590 | 00000001465465.6250 | 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 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 682 A ASN 691 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
008 |          000007.9310 | 00000001536384.5000 | 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
SER 318 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A ARG 349 A THR 394 A
CYS 395 A PHE 396 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A VAL 675 A PRO 677
009 |          000007.8770 | 00000001682993.5000 | 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 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 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
HIS 810 A GLU 811 A CYS 813 A SER 814 A ARG 836
010 |          000007.8330 | 00000001812737.2500 | A HIS 439 A TYR 456 A MET 542 A
LYS 545 A ILE 548 A SER 549 A ALA 550 A LYS 551 A ARG 553 A ARG 555 A THR 556 A
VAL 557 A ALA 558 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 SER 814 A ARG 836
011 |          000007.8230 | 00000001843592.6250 | 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 THR 556 A ASP 618 A TYR 619 A
PRO 620 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 GLU 811 A CYS 813 A SER 814 A
ARG 836 A ALA 840 A ARG 858 A LEU 862
012 |          000007.8140 | 00000001871811.2500 | A TYR 455 A ARG 553 A ARG 555 A
THR 556 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 682 A GLY 683 A ASP 684 A ALA 685 A THR 686 A THR 687 A ALA 688 A
TYR 689 A ASN 691 A LEU 758 A SER 759 A ASP 760 A ASP 761 A GLU 811 A CYS 813 A

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SER 814
013 |          000007.7640 | 00000002036631.8750 | A TYR 455 A ASN 496 A ASN 497 A
LYS 500 A LYS 545 A ARG 553 A ALA 554 A ARG 555 A THR 556 A VAL 557 A ALA 558 A
ARG 569 A LEU 576 A LYS 577 A ALA 580 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 682 A GLY 683 A ASP 684 A ALA 685 A
THR 687 A ALA 688 A TYR 689 A ASN 691 A SER 759 A ASP 760
014 |          000007.6880 | 00000002315374.7500 | A HIS 439 A ASP 452 A TYR 455 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 ALA 762 A LYS 798 A
TRP 800 A HIS 810 A GLU 811 A ARG 836
015 |          000007.6860 | 00000002323203.7500 | 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 VAL 557 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 ASP 684 A THR 687 A ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A
LYS 798 A GLU 811 A SER 814 A ARG 836
016 |          000007.6850 | 00000002327128.2500 | 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
PRO 620 A LYS 621 A CYS 622 A ASP 623 A ARG 624 A THR 680 A SER 682 A THR 687 A
ALA 688 A ASN 691 A SER 759 A ASP 760 A ASP 761 A ALA 762 A LYS 798 A TRP 800 A
GLU 811 A SER 814 A ARG 836
017 |          000007.6810 | 00000002342892.5000 | 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 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 GLU 811 A
PHE 812 A CYS 813 A SER 814 A ARG 836 A ALA 840 A ARG 858
018 |          000007.6700 | 00000002386796.7500 | A LEU 172 A THR 246 A LEU 247 A
ARG 249 A THR 252 A SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A LEU 270 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
ASN 459 A LEU 460 A PRO 461 A THR 462 A PRO 677
019 |          000007.6230 | 00000002583847.7500 | A PRO 169 A LEU 172 A ALA 176 A
ASN 177 A LEU 245 A THR 246 A ARG 249 A ALA 250 A LEU 251 A THR 252 A SER 255 A
HIS 256 A LEU 261 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 THR 394 A CYS 395 A TYR 456 A
ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A PRO 677
020 |          000007.5780 | 00000002787740.5000 | A HIS 439 A ILE 548 A SER 549 A
ALA 550 A LYS 551 A ARG 553 A ALA 554 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 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 CYS 813 A SER 814 A ARG 836

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While the table above lists the best binding energy in each cluster, it is sometimes helpful to also look at the energy spread [average and standard deviation], the dissociation constant has been recalculated from the average binding energy:

Clu	Members	Bind.energy spread [kcal/mol]	Dissoc. constant [pM]
001	001	000008.2990+-000000.0000	00000000825636.6449

002	001	000008.1060+-000000.0000	00000001143559.7756
003	001	000008.0760+-000000.0000	00000001202953.4853
004	001	000007.9860+-000000.0000	00000001400294.6383
005	001	000007.9770+-000000.0000	00000001421727.4388
006	001	000007.9770+-000000.0000	00000001421727.4388
007	001	000007.9590+-000000.0000	00000001465583.3867
008	001	000007.9310+-000000.0000	00000001536507.1764
009	001	000007.8770+-000000.0000	00000001683128.0487
010	001	000007.8330+-000000.0000	00000001812880.3901
011	001	000007.8230+-000000.0000	00000001843738.7028
012	001	000007.8140+-000000.0000	00000001871958.8236
013	001	000007.7640+-000000.0000	00000002036792.0804
014	001	000007.6880+-000000.0000	00000002315553.9788
015	001	000007.6860+-000000.0000	00000002323384.9048
016	001	000007.6850+-000000.0000	00000002327309.3568
017	001	000007.6810+-000000.0000	00000002343073.5656
018	001	000007.6700+-000000.0000	00000002386981.7447
019	001	000007.6230+-000000.0000	00000002584046.3395
020	001	000007.5780+-000000.0000	00000002787953.9314

The results of the 25 runs have been combined in a single scene at  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock.sce

The 20 clusters have been saved as:

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_001.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_002.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_003.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_004.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_005.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_006.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_007.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_008.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_009.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_010.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_011.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_012.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_013.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_014.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_015.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_016.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_017.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_018.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_019.yob  
C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 3\dock\_020.yob