

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	000007.9640	00000001453150.5000	A PRO 169 A ASP 170 A LEU 172 A LEU 245 A THR 246 A ARG 249 A ALA 250 A LEU 251 A THR 252 A ASN 314 A VAL 315 A LEU 316 A SER 318 A THR 319 A PRO 323 A ARG 349 A GLU 350 A THR 394 A CYS 395 A PHE 396 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A PRO 677
002	000007.9640	00000001453150.5000	A PRO 169 A ASP 170 A LEU 172 A LEU 245 A THR 246 A ARG 249 A ALA 250 A LEU 251 A THR 252 A ASN 314 A VAL 315 A LEU 316 A SER 318 A THR 319 A PRO 323 A ARG 349 A GLU 350 A THR 394 A CYS 395 A PHE 396 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A PRO 677
003	000007.9380	00000001518339.3750	A PRO 169 A LEU 245 A THR 246 A ARG 249 A LEU 251 A THR 252 A SER 255 A TYR 265 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 LEU 387 A LEU 388 A LEU 389 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
004	000007.9380	00000001518339.3750	A PRO 169 A LEU 245 A THR 246 A ARG 249 A LEU 251 A THR 252 A SER 255 A TYR 265 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 LEU 387 A LEU 388 A LEU 389 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
005	000007.9020	00000001613456.2500	A PRO 169 A LEU 172 A LEU 245 A THR 246 A ARG 249 A LEU 251 A THR 252 A VAL 315 A LEU 316 A SER 318 A THR 319 A PRO 323 A ARG 349 A GLU 350 A LEU 388 A LEU 389 A ASP 390 A THR 394 A CYS 395 A PHE 396 A SER 397 A ASP 454 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A ASN 628 A VAL 675 A PRO 677
006	000007.9020	00000001613456.2500	A PRO 169 A LEU 172 A LEU 245 A THR 246 A ARG 249 A LEU 251 A THR 252 A VAL 315 A LEU 316 A SER 318 A THR 319 A PRO 323 A ARG 349 A GLU 350 A LEU 388 A LEU 389 A ASP 390 A THR 394 A CYS 395 A PHE 396 A SER 397 A ASP 454 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A ASN 628 A VAL 675 A PRO 677
007	000007.8210	00000001849826.5000	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 ARG 553 A ARG 555 A THR 556 A VAL 557 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 CYS 813 A SER 814 A ARG 836
008	000007.8210	00000001849826.5000	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 ARG 553 A ARG 555 A THR 556 A VAL 557 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 CYS 813 A SER 814 A ARG 836

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009 |          000007.7740 | 00000002002545.7500 | A PRO 169 A LEU 172 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 270 A ASN 314 A VAL 315 A SER 318 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 CYS 395 A PHE 396 A TYR 456 A ARG 457 A
TYR 458 A ASN 459 A LEU 460 A PRO 461 A ASN 628 A VAL 675 A PRO 677
010 |          000007.7740 | 00000002002545.7500 | A PRO 169 A LEU 172 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 270 A ASN 314 A VAL 315 A SER 318 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 CYS 395 A PHE 396 A TYR 456 A ARG 457 A
TYR 458 A ASN 459 A LEU 460 A PRO 461 A ASN 628 A VAL 675 A PRO 677
011 |          000007.7320 | 00000002149655.5000 | A ARG 173 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 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 PHE 396 A TYR 456 A ARG 457 A
PRO 461 A VAL 675 A PRO 677
012 |          000007.6870 | 00000002319286.0000 | 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 ALA 554 A ARG 555 A THR 556 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 CYS 813 A
SER 814 A ARG 836 A ALA 840
013 |          000007.6230 | 00000002583847.7500 | 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 THR 394 A CYS 395 A
PHE 396 A ARG 457 A LEU 460 A PRO 461 A VAL 675 A PRO 677
014 |          000007.4790 | 00000003294733.7500 | A PRO 169 A ASP 170 A LEU 172 A
ARG 173 A THR 246 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 ASN 314 A VAL 315 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 GLU 350 A THR 394 A CYS 395 A PHE 396 A
TYR 456 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A VAL 675 A
PRO 677
015 |          000007.4480 | 00000003471711.2500 | A PRO 169 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 VAL 315 A LEU 316 A
SER 318 A THR 319 A VAL 320 A PRO 323 A ARG 349 A GLU 350 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 ASN 628 A VAL 675 A PRO 677
016 |          000007.4330 | 00000003560727.7500 | A THR 246 A ARG 249 A THR 252 A
SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 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 ARG 457 A LEU 460 A PRO 461 A VAL 675 A PRO 677
017 |          000007.4130 | 00000003682976.5000 | 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 ASN 314 A VAL 315 A
LEU 316 A SER 318 A THR 319 A VAL 320 A PRO 322 A PRO 323 A ARG 349 A GLU 350 A
THR 394 A CYS 395 A PHE 396 A TYR 456 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A
ASN 628 A PRO 677
018 |          000007.4030 | 00000003745666.0000 | 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 270 A LEU 316 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A THR 324 A
ARG 349 A GLU 350 A LEU 389 A ASP 390 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 ASN 628 A VAL 675 A
PRO 677

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019 |          000007.3880 | 00000003841706.5000 | A PRO 169 A ASP 170 A LEU 172 A
ARG 173 A ALA 176 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 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 CYS 395 A PHE 396 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A
ASN 628 A PRO 677 A GLY 678
020 |          000007.3690 | 00000003966901.2500 | A THR 246 A LEU 247 A ARG 249 A
SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A THR 319 A VAL 320 A PHE 321 A
PRO 322 A PRO 323 A ARG 349 A LEU 387 A LEU 388 A LEU 389 A ASP 390 A THR 394 A
CYS 395 A PHE 396 A SER 397 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A ASN 628 A
PRO 677
021 |          000007.3670 | 00000003980314.5000 | A LEU 245 A THR 246 A ARG 249 A
ALA 250 A LEU 251 A THR 252 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A LEU 316 A
THR 319 A PHE 321 A PRO 322 A PRO 323 A ARG 349 A ASP 390 A LYS 391 A THR 393 A
THR 394 A CYS 395 A PHE 396 A SER 397 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A
THR 462 A SER 664 A VAL 675 A LYS 676 A PRO 677
022 |          000007.3130 | 00000004360135.0000 | A LEU 172 A THR 246 A ARG 249 A
SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A THR 319 A VAL 320 A PHE 321 A
PRO 322 A PRO 323 A ARG 349 A LEU 387 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 PRO 677
023 |          000007.2990 | 00000004464389.5000 | A LEU 172 A THR 246 A LEU 247 A
ARG 249 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 THR 324 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 ASN 628 A PRO 677
024 |          000007.2390 | 00000004940178.5000 | A PRO 169 A LEU 172 A ARG 249 A
THR 252 A SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 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 393 A THR 394 A
CYS 395 A PHE 396 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A
VAL 675 A PRO 677
025 |          000007.1960 | 00000005312049.0000 | A LEU 172 A ARG 249 A THR 252 A
SER 255 A TYR 265 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 THR 324 A ARG 349 A THR 394 A CYS 395 A PHE 396 A SER 397 A
ARG 457 A ASN 459 A LEU 460 A PRO 461 A VAL 675 A PRO 677

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After clustering the 25 runs, the following 18 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	000007.9640	00000001453150.5000	A PRO 169 A ASP 170 A LEU 172 A LEU 245 A THR 246 A ARG 249 A ALA 250 A LEU 251 A THR 252 A ASN 314 A VAL 315 A LEU 316 A SER 318 A THR 319 A PRO 323 A ARG 349 A GLU 350 A THR 394 A CYS 395 A PHE 396 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A PRO 677
002	000007.9380	00000001518339.3750	A PRO 169 A LEU 245 A THR 246 A ARG 249 A LEU 251 A THR 252 A SER 255 A TYR 265 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 LEU 387 A LEU 388 A LEU 389 A

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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
003 |          000007.9020 | 00000001613456.2500 | A PRO 169 A LEU 172 A LEU 245 A
THR 246 A ARG 249 A LEU 251 A THR 252 A VAL 315 A LEU 316 A SER 318 A THR 319 A
PRO 323 A ARG 349 A GLU 350 A LEU 388 A LEU 389 A ASP 390 A THR 394 A CYS 395 A
PHE 396 A SER 397 A ASP 454 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A
PRO 461 A ASN 628 A VAL 675 A PRO 677
004 |          000007.8210 | 00000001849826.5000 | 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 ARG 553 A ARG 555 A THR 556 A
VAL 557 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 CYS 813 A SER 814 A
ARG 836
005 |          000007.7740 | 00000002002545.7500 | A PRO 169 A LEU 172 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 270 A ASN 314 A VAL 315 A SER 318 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 CYS 395 A PHE 396 A TYR 456 A ARG 457 A
TYR 458 A ASN 459 A LEU 460 A PRO 461 A ASN 628 A VAL 675 A PRO 677
006 |          000007.7320 | 00000002149655.5000 | A ARG 173 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 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 PHE 396 A TYR 456 A ARG 457 A
PRO 461 A VAL 675 A PRO 677
007 |          000007.6870 | 00000002319286.0000 | 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 ALA 554 A ARG 555 A THR 556 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 CYS 813 A
SER 814 A ARG 836 A ALA 840
008 |          000007.4790 | 00000003294733.7500 | A PRO 169 A ASP 170 A LEU 172 A
ARG 173 A THR 246 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 ASN 314 A VAL 315 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 GLU 350 A THR 394 A CYS 395 A PHE 396 A
TYR 456 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A VAL 675 A
PRO 677
009 |          000007.4330 | 00000003560727.7500 | A THR 246 A ARG 249 A THR 252 A
SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 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 ARG 457 A LEU 460 A PRO 461 A VAL 675 A PRO 677
010 |          000007.4130 | 00000003682976.5000 | 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 ASN 314 A VAL 315 A
LEU 316 A SER 318 A THR 319 A VAL 320 A PRO 322 A PRO 323 A ARG 349 A GLU 350 A
THR 394 A CYS 395 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 |          000007.4030 | 00000003745666.0000 | 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 270 A LEU 316 A THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A THR 324 A
ARG 349 A GLU 350 A LEU 389 A ASP 390 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 ASN 628 A VAL 675 A
PRO 677
012 |          000007.3880 | 00000003841706.5000 | A PRO 169 A ASP 170 A LEU 172 A
ARG 173 A ALA 176 A LEU 245 A THR 246 A ARG 249 A ALA 250 A LEU 251 A THR 252 A

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SER 255 A HIS 256 A LEU 261 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 CYS 395 A PHE 396 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A
ASN 628 A PRO 677 A GLY 678
013 | 000007.3690 | 00000003966901.2500 | A THR 246 A LEU 247 A ARG 249 A
SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A THR 319 A VAL 320 A PHE 321 A
PRO 322 A PRO 323 A ARG 349 A LEU 387 A LEU 388 A LEU 389 A ASP 390 A THR 394 A
CYS 395 A PHE 396 A SER 397 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A ASN 628 A
PRO 677
014 | 000007.3670 | 00000003980314.5000 | A LEU 245 A THR 246 A ARG 249 A
ALA 250 A LEU 251 A THR 252 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A LEU 316 A
THR 319 A PHE 321 A PRO 322 A PRO 323 A ARG 349 A ASP 390 A LYS 391 A THR 393 A
THR 394 A CYS 395 A PHE 396 A SER 397 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A
THR 462 A SER 664 A VAL 675 A LYS 676 A PRO 677
015 | 000007.3130 | 00000004360135.0000 | A LEU 172 A THR 246 A ARG 249 A
SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 A THR 319 A VAL 320 A PHE 321 A
PRO 322 A PRO 323 A ARG 349 A LEU 387 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 PRO 677
016 | 000007.2990 | 00000004464389.5000 | A LEU 172 A THR 246 A LEU 247 A
ARG 249 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 THR 324 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 ASN 628 A PRO 677
017 | 000007.2390 | 00000004940178.5000 | A PRO 169 A LEU 172 A ARG 249 A
THR 252 A SER 255 A TYR 265 A ILE 266 A LYS 267 A TRP 268 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 393 A THR 394 A
CYS 395 A PHE 396 A TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A
VAL 675 A PRO 677
018 | 000007.1960 | 00000005312049.0000 | A LEU 172 A ARG 249 A THR 252 A
SER 255 A TYR 265 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 THR 324 A ARG 349 A THR 394 A CYS 395 A PHE 396 A SER 397 A
ARG 457 A ASN 459 A LEU 460 A PRO 461 A VAL 675 A PRO 677

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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	000007.9640+-000000.0000	00000001453267.0365
002	002	000007.7805+-000000.1575	00000001980851.5873
003	002	000007.6750+-000000.2270	00000002366923.1745
004	001	000007.8210+-000000.0000	00000001849972.5172
005	001	000007.7740+-000000.0000	00000002002702.6691
006	001	000007.7320+-000000.0000	00000002149824.0431
007	001	000007.6870+-000000.0000	00000002319467.0703
008	001	000007.4790+-000000.0000	00000003294982.4334
009	001	000007.4330+-000000.0000	00000003560994.8972
010	001	000007.4130+-000000.0000	00000003683252.0893

011		001		000007.4030+-000000.0000		00000003745947.3147
012		001		000007.3880+-000000.0000		00000003841993.6870
013		001		000007.3690+-000000.0000		00000003967197.1861
014		001		000007.3670+-000000.0000		00000003980610.5678
015		001		000007.3130+-000000.0000		00000004360455.9799
016		001		000007.2990+-000000.0000		00000004464720.5971
017		001		000007.2390+-000000.0000		00000004940541.6339
018		001		000007.1960+-000000.0000		00000005312434.7039

The results of the 25 runs have been combined in a single scene at

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock.sce

The 18 clusters have been saved as:

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_001.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_002.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_003.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_004.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_005.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_006.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_007.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_008.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_009.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_010.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_011.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_012.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_013.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_014.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_015.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_016.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_017.yob

C:\Users\mr.laptop\Desktop\New KS-AGU in cavity 2\dock_018.yob