

# 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	000009.1970	00000000181346.6875	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 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 LEU 389 A ASP 390 A LYS 391 A THR 393 A THR 394 A CYS 395 A PHE 396 A SER 397 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A VAL 675 A PRO 677
002	000009.1970	00000000181346.6875	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 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 LEU 389 A ASP 390 A LYS 391 A THR 393 A THR 394 A CYS 395 A PHE 396 A SER 397 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A VAL 675 A PRO 677
003	000008.9850	00000000259362.7969	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 LEU 316 A THR 319 A PRO 323 A ARG 349 A LEU 388 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 ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A VAL 675 A PRO 677
004	000008.9850	00000000259362.7969	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 LEU 316 A THR 319 A PRO 323 A ARG 349 A LEU 388 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 ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A VAL 675 A PRO 677
005	000008.9490	00000000275610.6563	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 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 THR 462 A ASN 628 A PRO 677
006	000008.9490	00000000275610.6563	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 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 THR 462 A ASN 628 A PRO 677
007	000008.7920	00000000359234.9375	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 LEU 316 A THR 319 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 PRO 677
008	000008.7920	00000000359234.9375	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 LEU 316 A THR 319 A PHE 321 A PRO 322 A PRO 323 A

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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 PRO 677
009 |          000008.7090 | 00000000413255.2188 | 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 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
010 |          000008.7090 | 00000000413255.2188 | A THR 246 A ARG 249 A THR 252 A
SER 255 A TYR 265 A TRP 268 A SER 318 A THR 319 A VAL 320 A PHE 321 A PRO 322 A
PRO 323 A ARG 349 A LEU 388 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 LYS 676 A PRO 677 A GLY 678
011 |          000008.7090 | 00000000413255.2188 | 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 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
012 |          000008.6030 | 00000000494216.6563 | 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 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 TYR 458 A ASN 459 A LEU 460 A
PRO 461 A THR 462 A VAL 675 A PRO 677
013 |          000008.5950 | 00000000500935.0938 | 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 TYR 456 A ARG 457 A ASN 459 A LEU 460 A PRO 461 A VAL 675 A PRO 677
014 |          000008.4860 | 00000000602115.1250 | A ALA 176 A ASN 177 A GLY 179 A
GLU 180 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 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 ASN 459 A
LEU 460 A PRO 461 A VAL 675 A PRO 677
015 |          000008.4590 | 00000000630188.9375 | 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 THR 324 A ARG 349 A
LEU 388 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 VAL 675 A
PRO 677
016 |          000008.4060 | 00000000689160.3750 | 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 270 A
VAL 315 A LEU 316 A SER 318 A THR 319 A PHE 321 A PRO 322 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
TYR 456 A ARG 457 A TYR 458 A ASN 459 A LEU 460 A PRO 461 A ASN 628 A PRO 677
017 |          000008.3590 | 00000000746056.5625 | A LEU 172 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 SER 318 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 VAL 675 A PRO 677
018 |          000008.3550 | 00000000751110.4375 | 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 LEU 316 A
THR 319 A VAL 320 A PHE 321 A PRO 322 A PRO 323 A THR 324 A ARG 349 A LEU 389 A

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ASP 390 A LYS 391 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 VAL 675 A LYS 676 A PRO 677
019 |          000008.3500 | 00000000757475.9375 | 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 TRP 268 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 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 ASN 628 A PRO 677
020 |          000008.3330 | 00000000779524.9375 | 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 VAL 315 A SER 318 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 LYS 391 A THR 394 A CYS 395 A PHE 396 A ARG 457 A ASN 459 A LEU 460 A
PRO 461 A ASN 628 A PRO 677
021 |          000008.3270 | 00000000787459.1875 | A LEU 172 A ARG 173 A ALA 176 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
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
022 |          000008.2530 | 00000000892217.6250 | A GLU 136 A LYS 160 A ASP 161 A
TYR 163 A ASP 164 A VAL 166 A GLU 167 A ASP 452 A TYR 455 A ARG 457 A TYR 458 A
LYS 551 A ARG 553 A ALA 554 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 682 A ASN 691 A
ASP 760 A ASP 761 A PHE 793 A SER 795 A ALA 797 A LYS 798
023 |          000008.2240 | 00000000936975.1250 | A PHE 165 A PRO 169 A LEU 172 A
THR 246 A ARG 249 A THR 252 A SER 255 A TYR 265 A ILE 266 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 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 VAL 675 A PRO 677
024 |          000008.2040 | 00000000969143.8750 | 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 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 LEU 387 A LEU 389 A ASP 390 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 PRO 677
025 |          000008.1520 | 00000001058046.5000 | 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 THR 324 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 TYR 456 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 15 distinct complex conformations were found:

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

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Clu |Bind.energy[kcal/mol]|Dissoc. constant [pM]| Contacting receptor residues
-----+-----+-----+-----
001 |          000009.1970 | 00000000181346.6875 | 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
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 LEU 389 A ASP 390 A LYS 391 A THR 393 A THR 394 A
CYS 395 A PHE 396 A SER 397 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A
VAL 675 A PRO 677

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002 | 000008.9850 | 00000000259362.7969 | 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 LEU 316 A THR 319 A PRO 323 A  
ARG 349 A LEU 388 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 ARG 457 A ASN 459 A LEU 460 A PRO 461 A THR 462 A ASN 628 A  
VAL 675 A PRO 677  
003 | 000008.9490 | 00000000275610.6563 | 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 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 THR 462 A  
ASN 628 A PRO 677