Description of the intermolecular contacts between HER2 extracellular domain and Trastuzumab Fab.

[+] No. of intermolecular contacts: 76

[+] No. of charged-charged contacts: 6

[+] No. of charged-polar contacts: 8

[+] No. of charged-apolar contacts: 21

[+] No. of polar-polar contacts: 1

[+] No. of apolar-polar contacts: 9

[+] No. of apolar-apolar contacts: 31

[+] Percentage of apolar NIS residues: 38.72

[+] Percentage of charged NIS residues: 20.43

[++] Predicted binding affinity (kcal.mol-1): -10.4

[++] Predicted dissociation constant (M) at 25.0˚C: 2.3e-08

Listing of residue-residue interactions. Chain A corresponds to HER2 extracellular domain. Chain B corresponds to trastuzumab Fab.

MET 589 A TYR 671 B

GLU 598 A TYR 714 B

GLU 303 A GLN 849 B

TYR 588 A TYR 671 B

PHE 573 A TRP 935 B

PRO 572 A HIS 713 B

ILE 591 A PHE 675 B

ALA 559 A ARG 895 B

GLU 303 A GLY 851 B

LYS 583 A PHE 940 B

PRO 603 A PHE 675 B

PRO 590 A SER 672 B

PHE 573 A TYR 941 B

LYS 569 A TYR 714 B

LYS 583 A GLY 939 B

PRO 571 A ALA 654 B

ASP 596 A ASN 652 B

PRO 557 A ASN 891 B

PRO 572 A ARG 886 B

MET 589 A PHE 675 B

TYR 588 A PHE 675 B

GLU 558 A ARG 886 B

GLU 558 A THR 894 B

PRO 571 A THR 715 B

LEU 586 A PHE 940 B

PRO 603 A SER 672 B

PHE 573 A ARG 886 B

GLU 303 A PRO 850 B

ASP 570 A GLY 939 B

TYR 588 A LEU 676 B

PRO 590 A TYR 671 B

PRO 557 A TYR 893 B

ASP 570 A TYR 941 B

PRO 603 A THR 653 B

PRO 571 A TYR 714 B

PRO 584 A PHE 940 B

PRO 584 A TYR 671 B

ASP 560 A ARG 895 B

ALA 535 A ASP 898 B

ASP 560 A THR 716 B

ALA 535 A LYS 901 B

PRO 572 A THR 716 B

GLU 558 A TYR 888 B

PRO 571 A HIS 713 B

ALA 600 A TYR 714 B

GLN 602 A THR 653 B

PRO 572 A TRP 935 B

PHE 573 A TYR 869 B

PRO 590 A PHE 675 B

GLN 561 A ARG 895 B

ASN 534 A ASP 898 B

LEU 586 A SER 678 B

ASP 304 A GLY 851 B

GLU 558 A TYR 869 B

LYS 583 A ASP 938 B

PRO 584 A GLY 939 B

PRO 557 A TYR 869 B

GLY 556 A TYR 893 B

ASN 534 A LYS 901 B

PRO 572 A THR 715 B

GLU 598 A ASP 650 B

ASP 560 A ARG 886 B

LEU 586 A TYR 677 B

GLU 303 A GLY 852 B

PRO 572 A TYR 714 B

LEU 586 A TYR 671 B

TYR 532 A ARG 895 B

CYS 601 A THR 653 B

PRO 572 A TYR 941 B

PRO 571 A TYR 941 B

ALA 302 A GLY 851 B

GLU 598 A ASN 652 B

GLU 558 A ARG 895 B

PHE 555 A TYR 893 B

LEU 586 A LEU 676 B

GLU 558 A TYR 893 B