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

[+] No. of intermolecular contacts: 80

[+] No. of charged-charged contacts: 3

[+] No. of charged-polar contacts: 12

[+] No. of charged-apolar contacts: 25

[+] No. of polar-polar contacts: 5

[+] No. of apolar-polar contacts: 22

[+] No. of apolar-apolar contacts: 13

[+] Percentage of apolar NIS residues: 38.54

[+] Percentage of charged NIS residues: 20.41

[++] Predicted binding affinity (kcal.mol-1): -12.7

[++] Predicted dissociation constant (M) at 25.0˚C: 4.7e-10

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

VAL 286 A ASP 867 B

THR 268 A THR 866 B

VAL 286 A THR 866 B

LEU 295 A TYR 868 B

VAL 286 A ASN 890 B

THR 268 A ARG 910 B

HIS 245 A VAL 908 B

LEU 244 A ARG 910 B

LYS 311 A SER 939 B

PRO 294 A TYR 868 B

HIS 296 A TYR 671 B

LEU 244 A SER 907 B

VAL 286 A ASN 888 B

VAL 286 A SER 891 B

LYS 311 A GLY 937 B

LEU 295 A ARG 934 B

THR 290 A ASP 867 B

SER 313 A TYR 675 B

THR 284 A ASP 867 B

LYS 311 A TYR 941 B

HIS 296 A LEU 936 B

LYS 128 A SER 911 B

LYS 314 A ARG 676 B

LYS 314 A TYR 675 B

PRO 315 A TYR 675 B

PHE 257 A SER 894 B

LEU 244 A ASP 909 B

GLY 287 A ASN 888 B

LYS 311 A PRO 938 B

SER 288 A ASN 890 B

LEU 244 A VAL 908 B

PHE 257 A TYR 716 B

PHE 269 A ARG 910 B

HIS 245 A ASN 890 B

THR 284 A THR 866 B

ASP 285 A ASN 888 B

VAL 286 A THR 869 B

PRO 247 A SER 891 B

PHE 257 A LYS 901 B

PHE 236 A SER 911 B

GLY 270 A ARG 910 B

TYR 252 A ILE 895 B

HIS 245 A PRO 889 B

VAL 286 A TYR 868 B

PRO 315 A ARG 676 B

ASP 285 A PRO 938 B

HIS 245 A GLY 892 B

PHE 257 A TYR 896 B

THR 254 A LYS 901 B

PRO 294 A ASP 867 B

LYS 314 A TYR 671 B

GLY 287 A THR 866 B

SER 288 A THR 866 B

LYS 311 A LEU 936 B

HIS 245 A SER 891 B

SER 313 A TYR 671 B

CYS 289 A ASP 867 B

ASN 297 A PRO 938 B

SER 272 A ARG 910 B

CYS 246 A ASN 890 B

HIS 296 A GLY 937 B

PRO 315 A THR 678 B

PRO 315 A TYR 671 B

CYS 246 A SER 891 B

HIS 296 A SER 939 B

LEU 234 A SER 911 B

CYS 312 A TYR 671 B

ALA 248 A SER 891 B

ASN 297 A GLY 937 B

CYS 246 A ARG 910 B

HIS 245 A ASP 909 B

SER 288 A ASP 867 B

PHE 236 A ARG 910 B

ASP 255 A LYS 901 B

PRO 315 A TYR 677 B

THR 268 A ASN 890 B

LEU 244 A ASN 890 B

GLY 287 A ASN 890 B

VAL 286 A PRO 889 B

PHE 257 A ILE 895 B