

Supplementary table S2. The interactions between 2Rs15d and HER2 domain I. Also see Figure S2. Distances only given in case of hydrogen bonds or electrostatic interactions.

2Rs15d			HER2 domain I		Interaction (distance)
Residue	Group	FR/CDR	Residue	Group	
Cys32	side chain	CDR1	Asn177	backbone	Van der Waals
Cys32	side chain	CDR1	Gln178	backbone	Van der Waals
Cys32	side chain	CDR1	Leu179	backbone	Van der Waals
Cys32	side chain	CDR1	Ala180	backbone	Van der Waals
Cys32	backbone CO	CDR1	Ala180	backbone NH	hydrogen bond (2.88 Å)
Cys32	side chain	CDR1	Leu181	backbone	Van der Waals
Cys32	backbone CO	CDR1	Leu181	backbone NH	hydrogen bond (3.81 Å)
Gly33	side chain	CDR1	Gln178	backbone	Van der Waals
Gly33	backbone NH	CDR1	Gln178	backbone CO	hydrogen bond (3.43 Å)
Gly33	side chain	CDR1	Leu181	side chain	Van der Waals
Met34	backbone	FR	Leu181	side chain	Van der Waals
Tyr37	side chain OH	FR	Tyr112	side chain OH	hydrogen bond (2.82 Å)
Tyr37	side chain	FR	Leu181	side chain	hydrophobic
Tyr37	side chain	FR	Leu183	side chain	hydrophobic
Glu44	side chain	FR	Arg157	side chain	electrostatic (4.23 Å)
Arg45	backbone CO	FR	Gln156	side chain NH2	hydrogen bond (2.96 Å)
Arg45	side chain	FR	Leu183	side chain	hydrophobic
Leu47	side chain	FR	Asn111	side chain	Van der Waals
Leu47	side chain	FR	Tyr112	side chain	Van der Waals
Arg50	side chain	FR	Asp110	backbone CO	hydrogen bond (2.68 Å)
Arg50	side chain	FR	Asn111	side chain CO	hydrogen bond (2.53 Å)
Arg50	side chain	FR	Leu179	side chain	Van der Waals
Gly53	side chain	CDR2	Gln178	side chain	Van der Waals
Gly53	backbone NH	CDR2	Gln178	backbone CO	hydrogen bond (2.82 Å)
Asp54	side chain	CDR2	Gln178	side chain	Van der Waals

2Rs15d			HER2 domain I		Interaction (distance)
Asp54	backbone NH	CDR2	Gln178	side chain CO	hydrogen bond (3.38 Å)
Trp58	side chain	FR	Asp110	side chain	hydrogen bond (2.91 Å)
Ala96	side chain	CDR3	Leu181	side chain	hydrophobic
Val97	backbone	CDR3	Leu181	side chain	Van der Waals
Cys98	side chain	CDR3	Leu181	side chain	Van der Waals
Leu101	side chain	CDR3	Lys170	backbone	Van der Waals
Leu101	side chain	CDR3	Phe173	side chain	hydrophobic
Leu101	side chain	CDR3	Lys153	backbone	Van der Waals
Leu101	side chain	CDR3	His174	backbone	Van der Waals
Leu101	side chain	CDR3	Asn177	side chain	Van der Waals
Leu101	side chain	CDR3	Ala180	side chain	hydrophobic
Leu101	side chain	CDR3	Arg217	side chain	Van der Waals
Glu102	side chain	CDR3	Lys170	side chain	electrostatic (3.62 Å)
Thr103	side chain	CDR3	Thr182	backbone NH	hydrogen bond (3.10 Å)
Thr103	side chain	CDR3	Leu183	backbone CO	hydrogen bond (3.78 Å)
Trp105	side chain	FR	Leu183	side chain	hydrophobic