

Supplementary table S1. X-ray crystallographic data collection and refinement statistics

	HER2-2Rs15d
Data collection statistics	
Wavelength (Å)	0.9999
Resolution range (Å)	47.794 - 2.246 (2.326 - 2.246)
Space group	oP: P2 ₁ 2 ₁ 2 ₁
a, b, c (Å)	66.52, 113.52, 137.43
α, β, γ (°)	90, 90, 90
Mosaicity (°)	0.091
Total number of measured reflections	162919 (15517)
Unique reflections	49524 (4790)
Multiplicity	3.3 (3.2)
Completeness (%)	98.10 (96.6)
<I/σ(I)>	9.65 (1.70)
Wilson B-factor (Å ²)	39.53
R _{meas} (%)	10.31 (70.91)
CC _{1/2} (%)	99.5 (66.4)
A.U. contains	one HER2-2Rs15d complex
Refinement statistics	
CC*	0.999 (0.893)
CC _{work}	0.941 (0.841)
CC _{free}	0.936 (0.764)
R _{work} (%)	18.48 (25.68)
R _{free} (%)	22.01 (29.39)
Number of non-hydrogen atoms	5581
macromolecules	5157
ligands	54
Protein residues	673

	HER2-2Rs15d
RMS bond lengths (Å)	0.007
RMS bond angles (°)	0.99
Ramachandran favored (%)	97.0
Ramachandran allowed (%)	3.5
Ramachandran outliers (%)	0.0
Rotamer outliers (%)	1.2
Clashscore	4.23
Average B-factor (Å ²)	49.20
macromolecules	48.95
ligands	81.35
solvent	48.02
Number of TLS groups	10
PDB ID	5MY6