

Supplementary Table 2 Data collection and refinement statistics (molecular replacement)

	T4L- β 1AR/ Carazolol	T4L- β 1AR/ Nb6B9/ BI-167107	T4L- β 1AR/ Nb6B/ Norepinephrine	T4L- β 1AR/ Nb6B9/ Epinephrine
Data collection				
Space group	P1	C121	C121	C121
Cell dimensions				
a, b, c (Å)	52.1, 52.8, 142.8	378.0, 66.2, 47.9	376.8, 66.0, 47.8	378.0, 66.2, 47.9
α, β, γ (°)	92.1, 90.7, 116.7	90.0, 93.9, 90.0	90.0, 93.5, 90.0	90.0, 93.9, 90.0
Resolution (Å)	50 - 2.5 (2.6 -2.5)	50 - 2.6 (2.7-2.6)	50 - 2.7 (2.8-2.7)	50- 3.13 (3.244 - 3.132)
R_{sym} or R_{merge}	0.384 (1.446)	0.327 (0.951)	0.404 (1.428)	0.345 (1.339)
$I / \sigma I$	9.18 (1.44)	4.66 (0.90)	10.32 (0.99)	5.59 (1.37)
Completeness (%)	100 (87.6)	96.7 (85.0)	100 (99.9)	96.8 (58.3)
Redundancy	33.3 (7.0)	6.64 (2.33)	41.6 (9.16)	11.4 (7.6)
CC1/2(%)	99.7 (48.2)	99.1 (45.1)	99.5 (51.8)	98.2 (50.6)
Refinement				
Resolution (Å)	20-2.5	20-2.6	20-2.7	20-3.1
No. reflections (test set)	46851 (2418)	35258 (1994)	32439 (1989)	20331 (1746)
$R_{\text{work}} / R_{\text{free}}$	0.2267 / 0.2637	0.247/0.275	0.235/0.262	0.239/0.245
No. atoms				
Protein	7012	4463	4433	4424
Ligand	44	27	12	13
Others (Lipids, ions, water)	321	179	133	89
B -factors (Å ²)				
Receptor	90.29	86.02	70.41	81.32
T4L	44.66	55.83	41.99	53.00
Nb 6B9	no	117.79	105.49	118.61
Ligand	87.64	78.44	51.99	66.38
Others (Lipids, ions, water)	62.75	83.14	73.56	89.89
R.m.s. deviations				
Bond lengths (Å)	0.006	0.008	0.004	0.005
Bond angles (°)	0.72	1.04	0.70	0.63
Ramachandran statistics				
Favored regions (%)	97.67	98.75	98.76	98.93
Allowed regions (%)	2.33	1.25	1.24	1.07
Outliers (%)	0.00	0.00	0.00	0.00

*Values in parentheses are for highest-resolution shell.

Supplementary information, Table. S2| Data collection and refinement statistics (molecular replacement)

The data collection and refinement statistics of T4L- β_1 AR/carazolol, T4L- β_1 AR/BI-167107/Nb6B9,

T4L- β_1 AR/norepinephrine/Nb6B9 and T4L- β_1 AR/epinephrine/Nb6B9.