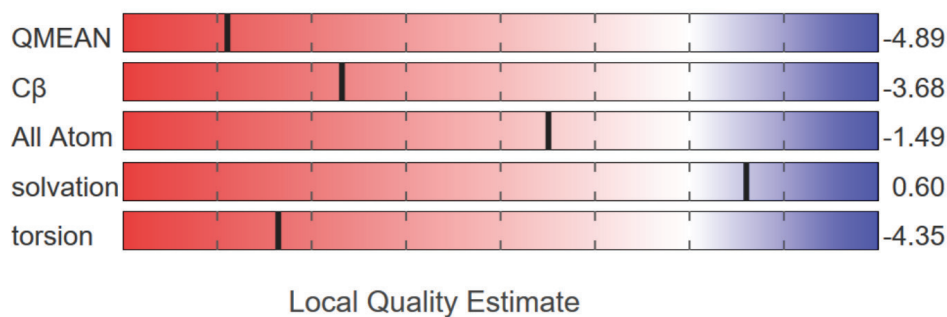
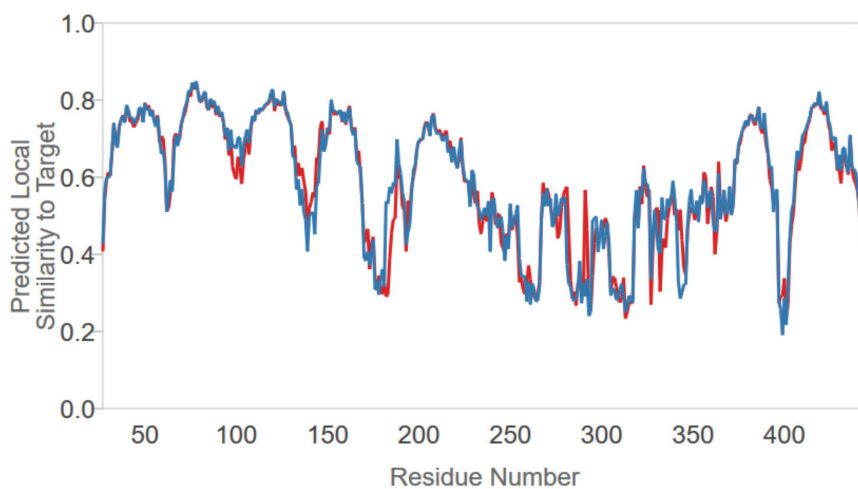


**FIG. S1.** Ramachandran plot of the selected model generated by SWISS-MODEL.



**FIG. S2.** Quality estimate of the homology model.



**FIG. S3.** Predicted Local Similarity to target for the homology model.

TABLE S1. The top 50 filtered templates generated by SWISS-MODEL

Template	Seq Identity	QSQE	Resolution	Seq Similarity	Coverage	Description
5uen.1.B	23.50	0.44	3.20 Å	0.31	0.85	Adenosine receptor A1, Soluble cytochrome b562, Adenosine receptor A1
5uen.1.A	23.50	0.43	3.20 Å	0.31	0.85	Adenosine receptor A1, Soluble cytochrome b562, Adenosine receptor A1
5v54.1.A	32.11	0.16	3.90 Å	0.35	0.85	5-hydroxytryptamine receptor 1B, OB-1 fused 5-HT1b receptor, 5-hydroxytryptamine receptor 1B
5v54.1.B	32.11	0.15	3.90 Å	0.35	0.85	5-hydroxytryptamine receptor 1B, OB-1 fused 5-HT1b receptor, 5-hydroxytryptamine receptor 1B
4iaq.1.A	31.95	0.15	2.80 Å	0.35	0.86	Chimera protein of human 5-hydroxytryptamine receptor 1B and <i>E. Coli</i> soluble cytochrome b562
4iar.1.A	32.20		2.70 Å	0.36	0.85	Chimera protein of human 5-hydroxytryptamine receptor 1B and <i>E. Coli</i> soluble cytochrome b562
4u15.2.A	23.66		2.80 Å	0.32	0.87	Muscarinic acetylcholine receptor M3, Lysozyme, Muscarinic acetylcholine receptor M3
5zhp.1.A	23.16		3.10 Å	0.32	0.87	Muscarinic acetylcholine receptor M3, Endolysin, Endolysin, Muscarinic acetylcholine receptor M3
5zhp.2.A	23.16		3.10 Å	0.32	0.87	Muscarinic acetylcholine receptor M3, Endolysin, Endolysin, Muscarinic acetylcholine receptor M3
4u15.1.A	23.66		2.80 Å	0.32	0.87	Muscarinic acetylcholine receptor M3, Lysozyme, Muscarinic acetylcholine receptor M3
5wiu.1.A	29.61		1.96 Å	0.34	0.86	D(4) dopamine receptor, soluble cytochrome b562 chimera
5tgz.1.A	19.11		2.80 Å	0.28	0.90	Cannabinoid receptor 1, Flavodoxin, Cannabinoid receptor 1
5dsg.2.A	21.72		2.60 Å	0.31	0.88	Muscarinic acetylcholine receptor M4, Endolysin, Endolysin, Muscarinic acetylcholine receptor M4
5dsg.1.A	21.72		2.60 Å	0.31	0.88	Muscarinic acetylcholine receptor M4, Endolysin, Endolysin, Muscarinic acetylcholine receptor M4
5tvn.1.A	27.44		2.90 Å	0.33	0.84	Chimera protein of human 5-hydroxytryptamine receptor 2B and <i>E. Coli</i> soluble cytochrome b562
5zkq.1.B	17.22	0.04	2.90 Å	0.28	0.88	Platelet-activating factor receptor, Endolysin, Endolysin, Platelet-activating factor receptor
6bqg.1.A	29.37		3.00 Å	0.34	0.84	5-hydroxytryptamine receptor 2C, Soluble cytochrome b562
5tud.1.A	26.12		3.00 Å	0.33	0.84	5-hydroxytryptamine receptor 2B, Soluble cytochrome b562 chimera
6drz.1.A	26.77		3.10 Å	0.33	0.85	5HT2B receptor, BRIL chimera
5yc8.1.A	22.40		2.50 Å	0.32	0.85	Muscarinic acetylcholine receptor M2, Redesigned apo-cytochrome b562, Muscarinic acetylcholine receptor M2
4ib4.1.A	26.51		2.70 Å	0.33	0.85	Chimera protein of human 5-hydroxytryptamine receptor 2B and <i>E. Coli</i> soluble cytochrome b562
5zkb.1.A	22.40		2.95 Å	0.32	0.85	Muscarinic acetylcholine receptor M2, Apo-cytochrome b562, Muscarinic acetylcholine receptor M2
6dry.1.A	25.65		2.92 Å	0.32	0.85	5HT2B receptor, BRIL chimera
5mzj.1.A	24.22		2.00 Å	0.31	0.85	Adenosine receptor A2a, Soluble cytochrome b562, Adenosine receptor A2a
6a93.1.A	29.17		3.00 Å	0.34	0.80	5-hydroxytryptamine receptor 2A, Soluble cytochrome b562
4nc3.1.A	26.51		2.80 Å	0.33	0.85	Chimera protein of human 5-hydroxytryptamine receptor 2B and <i>E. Coli</i> soluble cytochrome b562
5iu7.1.A	24.22		1.90 Å	0.31	0.85	Adenosine receptor A2a, Soluble cytochrome b562, Adenosine receptor A2a
5zk8.1.A	23.44		3.00 Å	0.33	0.85	Muscarinic acetylcholine receptor M2, Redesigned apo-cytochrome b562, Muscarinic acetylcholine receptor M2
6drx.1.A	26.65		3.10 Å	0.33	0.84	5HT2B receptor, BRIL chimera
5uig.1.A	23.70		3.50 Å	0.31	0.85	Adenosine receptor A2a, Soluble cytochrome b562, Adenosine receptor A2a
6aqf.1.A	23.24		2.51 Å	0.31	0.85	Adenosine receptor A2a, Soluble cytochrome b562, Adenosine receptor A2a
6mh8.1.A	24.21		4.20 Å	0.31	0.84	Adenosine receptor A2a, Soluble cytochrome b562 chimeric construct
6bqh.1.A	29.37		2.70 Å	0.34	0.84	5-hydroxytryptamine receptor 2C, Soluble cytochrome b562

TABLE S1. Continued

Template	Seq Identity	QSQE	Resolution	Seq Similarity	Coverage	Description
5jtb.1.A	24.21		2.80 Å	0.31	0.84	Adenosine receptor A2a, Soluble cytochrome b562, Adenosine receptor A2a
6a93.2.A	29.17		3.00 Å	0.34	0.80	5-hydroxytryptamine receptor 2A, Soluble cytochrome b562
5gli.1.A	16.00		2.50 Å	0.28	0.89	Endothelin Receptor Subtype-B
6j21.1.A	18.30		3.20 Å	0.30	0.86	Substance-P receptor, Endolysin
6j20.1.A	17.99		2.70 Å	0.30	0.86	Substance-P receptor, Endolysin
5xpr.1.A	16.46		3.60 Å	0.28	0.89	Endothelin B receptor, Endolysin, Endothelin B receptor
5nj6.1.A	18.35		4.00 Å	0.30	0.84	Proteinase-activated receptor 2, Soluble cytochrome b562, Proteinase-activated receptor 2
5nnd.1.A	18.04		2.80 Å	0.30	0.84	Lysozyme, Proteinase-activated receptor 2, Soluble cytochrome b562, Proteinase-activated receptor 2
4pxz.1.A	18.65		2.50 Å	0.29	0.86	P2Y purinoceptor 12, Soluble cytochrome b562
4py0.1.A	18.65		3.10 Å	0.29	0.86	P2Y purinoceptor 12, Soluble cytochrome b562
4z34.1.A	17.21		3.00 Å	0.29	0.81	Lysophosphatidic acid receptor 1, Soluble cytochrome b562
4z35.1.A	17.21		2.90 Å	0.29	0.81	Lysophosphatidic acid receptor 1, Soluble cytochrome b562
6g79.1.D	36.15		NA	0.38	0.76	5-hydroxytryptamine receptor 1B
4ntj.1.A	18.65		2.62 Å	0.29	0.86	P2Y purinoceptor 12, Soluble cytochrome b562, P2Y purinoceptor 12
5xjm.1.A	17.55		3.20 Å	0.29	0.84	Type-2 angiotensin II receptor, Soluble cytochrome b562, Type-2 angiotensin II receptor
6do1.1.A	20.00		2.90 Å	0.31	0.83	Type-1 angiotensin II receptor, Soluble cytochrome b562 BRIL fusion protein
5zkq.1.A	17.22		2.90 Å	0.28	0.88	Platelet-activating factor receptor, Endolysin, Endolysin, Platelet-activating factor receptor