Electronic supplementary information

Computational insights into the binding mechanism of antagonists with Neuropeptide B/W Receptor 1

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Supplementary Figures

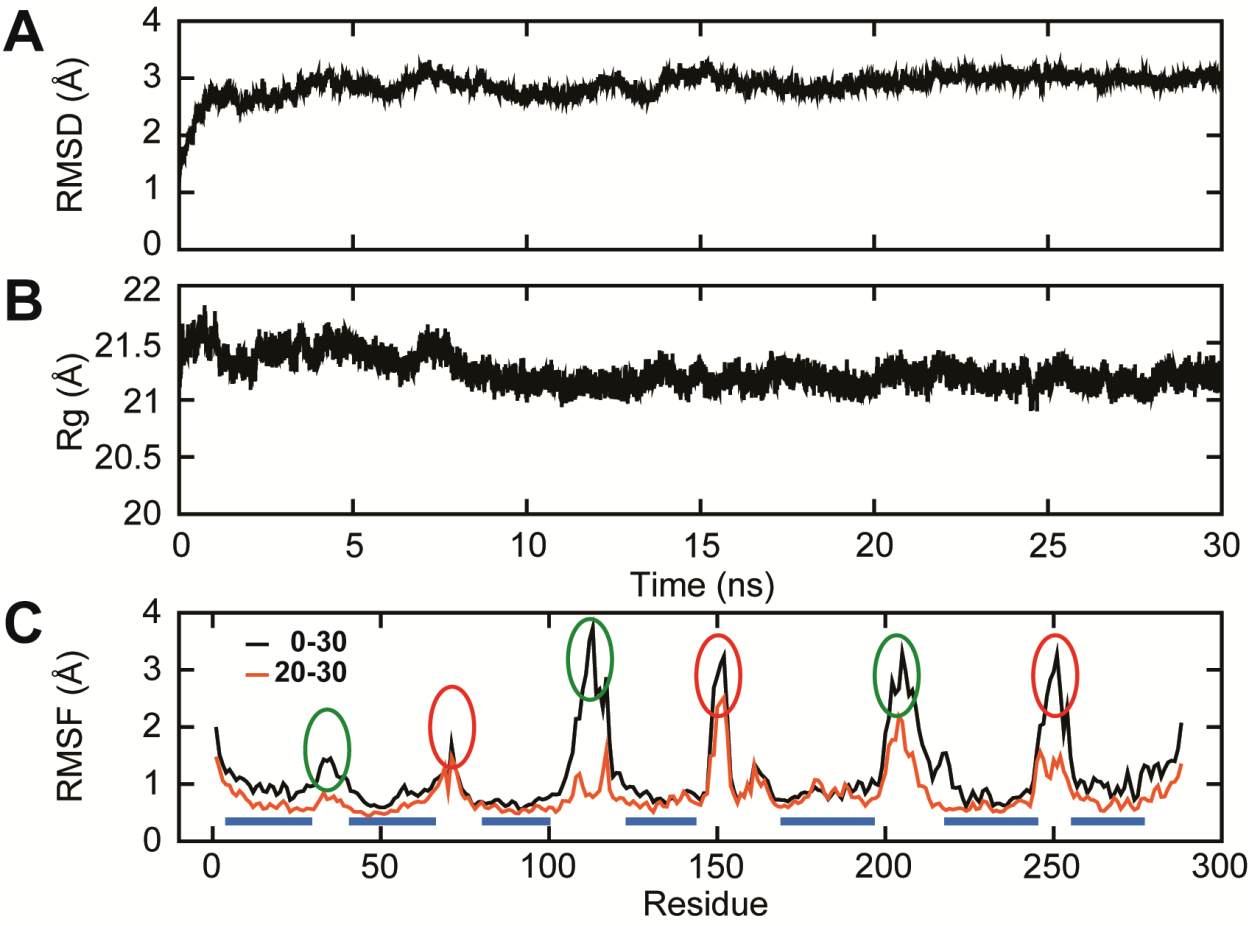

Fig. S1

Analysis of the stability parameters of the modeled NPBWR1 as a function of 30-ns MD simulation time. (a) RMSD as a function of time, (b) Rg as a function of time and (c) RMSF as a function of residue number. The RMSF was measured throughout (black) and between 20 and 30-ns (orange) MD trajectories. TM helices are indicated with blue bars at the bottom of the curves, ECL and ICL regions are marked with green and red circles, respectively.

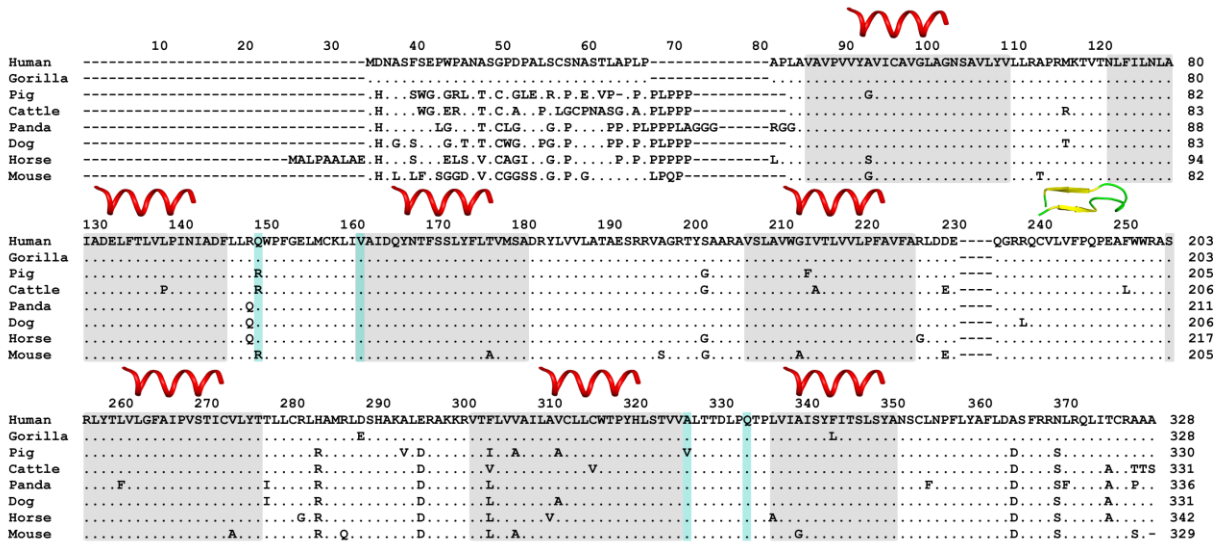

Fig. S2

Multiple sequence alignment of NPBWR1 sequences from eight mammals showing residue differences throughout the sequences. The 7TM helical domains are indicated by a helix at the top of grey colored boxes. The ECL2 between residues 178 and 202 is indicated by a β-hairpin structure at the top. Identical residues are shown as dots, and gaps are represented by dashes. The alignment was constructed with Clustal Omega tool using the reference sequences obtained from NCBI. The alignment was visualized through GeneDoc program [Nicholas, K.B., Nicholas H.B. Jr., and Deerfield, D.W. II. 1997 GeneDoc: Analysis and Visualization of Genetic Variation, EMBNEW.NEWS 4:14].

Supplementary Tables

Table S1

Comparative structure validation scores of NPBWR1 and its template, NOFQ receptor (4EA3)

Servers		NPBWR1	4EA3 (template)
Procheck	Most favored regions (%)	91.40	92.30
	Additionally allowed Regions (%)	7.50	7.30
	Generously allowed Regions (%)	0.40	0.00
	Disallowed regions (%)	0.80	0.40
	G-factor	0.09	0.34
Verify3D	Averaged 3D-1D Score > 0.2 (%)	57.79	52.33
ERRAT	Overall Quality (%)	97.13	93.46
ProSA	Z-Score	-3.87	-2.99
ProQ	LG score	2.46	2.88
	MaxSub	0.18	0.23
MolProbity	Cβ deviations >0.25Å	0	0
	Residues with bad bonds (%)	0.00	0.00
	Residues with bad angles (%)	0.00	0.00

Table S2

The various energy scores (kcal mol^{-1}) obtained for NPBWR1-antagonist complexes through Autodock

Conformations	Ligand Efficiency	Intermol. Energy	vdWhbdesolv energy	Electrostatic energy	Unbound Energy	Binding energy
1z	-0.33	-9.42	-9.20	-0.22	-0.34	-8.23
9h	-0.27	-9.31	-9.25	-0.05	-0.96	-8.11
9i	-0.23	-11.58	-10.32	-1.97	-1.97	-8.81