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SUPPLEMENTARY ONLINE DATA

Complex between α-bungarotoxin and an α7 nicotinic receptor ligand-binding domain chimaera

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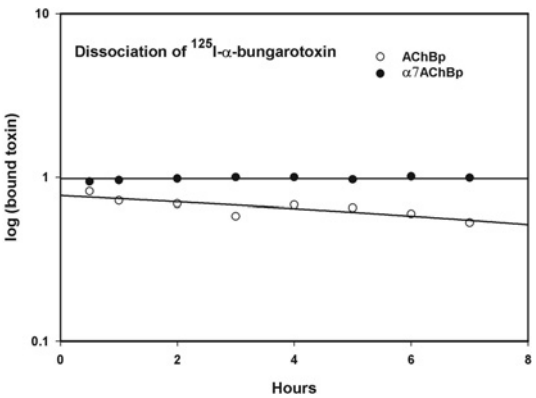

Figure S1 Dissociation of ^{125}I-labelled α-btx from the α7/AChBP chimaera and AChBP

Dissociation of ^{125}I-labelled α-btx bound to either the α7/AChBP chimaera or AChBP bound to an anti-FLAG M2 agarose affinity gel as described in the Experimental section of the main text.

Table S1 Inter-residue contacts between α-btx and the α7/AChBP chimaera

Inter-residue contacts were calculated using CNS with a 4.5 Å distance cut-off.

(a) Interacting residue pairs between α-btx and the α7/AChBP chimaera principal subunit

α7/AChBP principal subunit	α-btx
Tyr^{91}	Phe^{32}
Tyr^{91}	Arg^{36}
Trp^{145}	Phe^{32}
Arg^{150}	Ser^{9}
Arg^{150}	Pro^{10}
Glu^{181}	Ser^{9}
Arg^{182}	Asp^{30}
Arg^{182}	Val^{39}
Phe^{183}	Thr6
Phe^{183}	Ser^{9}
Phe^{183}	Ile^{11}
Phe^{183}	Val^{40}
Tyr^{184}	Asp^{30}
Tyr^{184}	Phe^{32}
Tyr^{184}	Arg^{36}
Tyr^{184}	Val^{39}
Glu^{185}	Met^{27}
Glu^{185}	Lys^{38}
Glu^{185}	Val^{40}
Glu^{185}	Pro^{69}
Cys^{186}	Lys^{70}
Lys^{188}	Ile^{11}
Lys^{188}	His^{68}
Lys^{188}	Lys^{70}
Lys^{188}	Gln^{71}
Pro^{190}	Ser^{9}
Tyr^{191}	Arg^{36}

(b) Interacting residue pairs between α-btx and the α7/AChBP chimaera complementary subunit

α7/AChBP complementary subunit	α-btx
Ser^{32}	Ser^{34}
Ser^{34}	Ser^{34}
Leu^{36}	Val^{31}
Trp^{53}	Val^{31}
Trp^{53}	Phe^{32}
Gln^{55}	Ser^{35}
Gln^{114}	Ser^{35}
Leu^{116}	Ser^{34}
Leu^{116}	Ser^{35}
Asp^{160}	Cys^{29}
Asp^{160}	Ser^{34}

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The structural co-ordinates reported will appear in the PDB under accession code 4HQP.

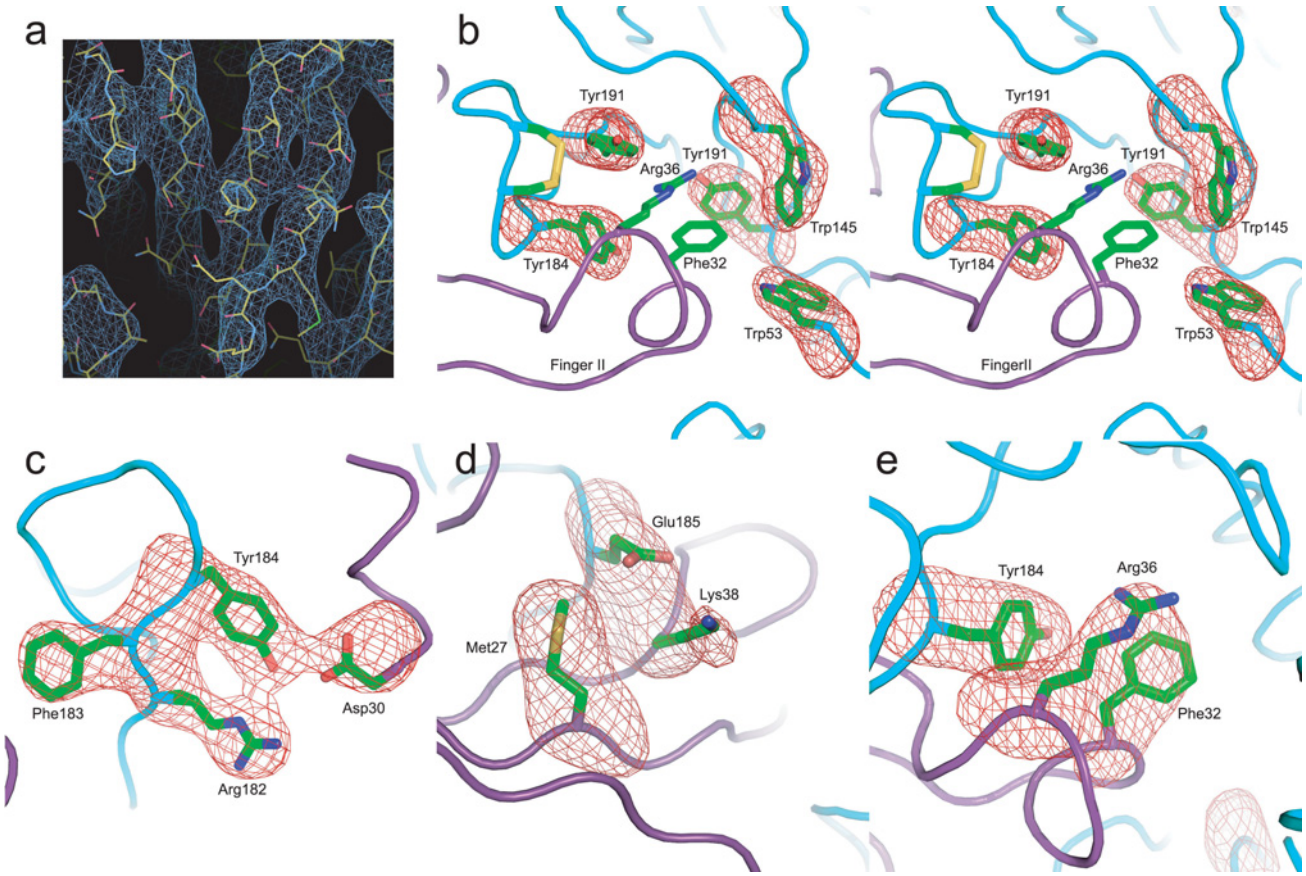

Figure S2 Representative regions of the α7/AChBP chimaera–α-btx structure showing well-defined electron density

(**a**) Part of the $2F_o - F_c$ electron density map. (**b**) Stereo view of the simulated annealing omit map calculated for the ligand-binding site residues contoured at the 4.0 σ level. (**c**) Simulated annealing omit map calculated for Arg^{182}, Phe^{183} and Tyr^{184} from the α7/AChBP chimaera and Asp^{30} from α-btx contoured at the 4.0 σ level. (**d**) Simulated annealing omit map calculated for Glu^{185} from the α_7/AChBP chimaera and Met^{27} and Lys^{38} from α-btx contoured at the 4.0 σ level. (**e**) Simulated annealing omit map calculated for Tyr^{184} from the α7/AChBP chimaera and Phe^{32} and Arg^{36} from α-btx contoured at the 4.0 σ level.

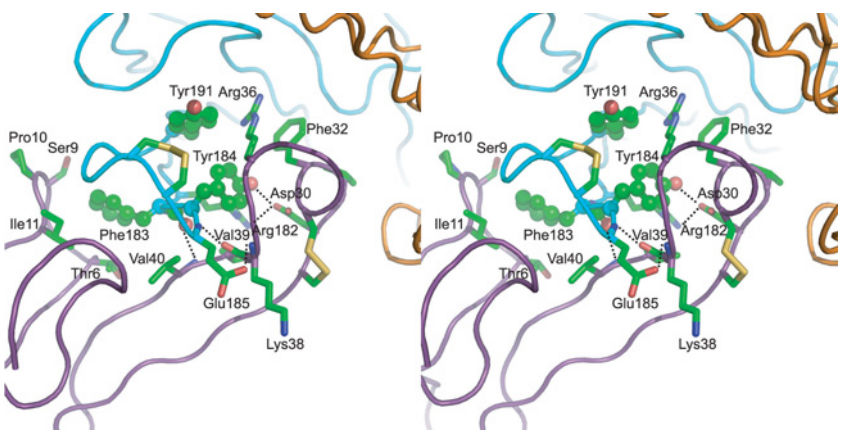

Figure S3 Stereo view of the interaction network surrounding loop C (cyan)

α-btx is in purple, the principal subunit in cyan and the complementary subunit in orange. Residues Phe^{183}, Tyr^{184} and Tyr^{191} are shown as spheres, and hydrogen bonds as dotted lines.

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