

Table S1: Highest probability paths for each residue in the NQN mutation site (D91, E177, D178) and ketamine binding site (N152, D153, D154, F174, L176, K183)

	β1-β2 Loop	Pre-TM1
Subunit B to subunit B		
D91	V90, V89, D88, A87, D86, S107, A108, R109, T36, A34, K33 , T244, E243, N239, I236, I233	N/A
D178	E177, L176, Y23, N152, V155, F156 , P113, L114, E35, A34, K33 , T244, E243, N239, I236, I233	E177, L176, Y23, N152, V155, F156, T158, G159, Q193, Y194, F195, S196, N200 , E243, N239, I236, I233
E177	L176, Y23, N152, V155, F156 , P113, L114, E35, A34, K33 , T244, E243, N239, I236, I233	L176, Y23, N152, V155, F156, T158, G159, Q193, Y194, F195, S196, N200 , E243, N239, I236, I233
N152	V155, F156, L157, L30, D31, K33 , T244, E243, N239, I236, I233	N/A
D153	D154, F156, L157, L30, D31, K33 , T244, E243, N239, I236, I233	N/A
D154	F156, L157, L30, D31, K33 , T244, E243, N239, I236, I233	N/A
F174	N173, A172, K183, Y129, H127, L126, F37, T36, A34, K33 , T244, E243, N239, I236, I233	A175, L176, Y23, N152, V155, F156, T158, G159, Q193, Y194, F195, S196, N200 , E243, N239, I236, I233
L176	Y23, N152, V155, F156 , P113, L114, E35, A34, K33 , T244, E243, N239, I236, I233	Y23, N152, V155, F156, T158, G159, Q193, Y194, F195, S196, N200 , E243, N239, I236, I233
K183	Y129, H127, L126, F37, T36, A34, K33 , T244, E243, N239, I236, I233	N/A
Subunit B to subunit A		
D91	V90, V89, D88, A87, D86, R85, A84, N83, E82, Y28, S29, L30, D31, K33, T244, E243, N239, I236, I233	N/A
D178	E177, L176, Y23, L24, I25, E26, C27, Y28, S29, L30, D31, K33 , T244, E243, N239, I236, I233	N/A
E177	L176, Y23, L24, I25, E26, C27, Y28, S29, L30, D31, K33 , T244, E243, N239, I236, I233	N/A
N152	V155, F156, L157, L30, D31, K33 , P247, K248, N245, T244, E243, N239, I236, I233	N/A
D153	D154, F156, L157, L30, D31, K33 , P247, K248, N245, T244, E243, N239, I236, I233	N/A
D154	F156, L157, L30, D31, K33 , P247, K248, N245, T244, E243, N239, I236, I233	N/A
F174	A175, L176, Y23, L24, I25, E26, C27, Y28, S29, L30, D31, K33 , T244, E243, N239, I236, I233	N/A
L176	Y23, L24, I25, E26, C27, Y28, S29, L30, D31, K33 , T244, E243, N239, I236, I233	N/A
K183	Y129, N80, V81, E82, Y28, S29, L30, D31, K33, T244, E243, N239, I236, I233	N/A
Subunit B to subunit C		
D91	V90, V89, D88, R105, V79, N80, V110, F37, T36, E35, A34, K33, T244, E243,	N/A

	N239, I236, I233	
D178	E177, L176, Y23, N152, V155, F156, P113, L114, E35, A34, K33, T244, E243, N239, F238, I236, I233	R179, R133, V132, I131, L130 Y129, H127, T125, Q124, S123, D122, F121, Y194, F195, S196, N200, E243, N239, I236, I233
E177	L176, Y23, N152, V155, F156, P113, L114, E35, A34, K33, T244, E243, N239, F238, I236, I233	L176, Y23, N152, V155, F156, T158, G159, Q193, Y194, F195, S196, N200, E243, N239, F238, I236, I233
N152	V155, F156, T158, P113, L114, E35, A34, K33, T244, E243, N239, I236, I233	V155, F156, T158, G159, Q193, Y194, F195, S196, N200, E243, N239, I236, I233
D153	D154, F156, T158, P113, L114, E35, A34, K33, T244, E243, N239, I236, I233	D154, F156, T158, G159, Q193, Y194, F195, S196, N200, E243, N239, I236, I233
D154	F156, T158, P113, L114, E35, A34, K33, T244, E243, N239, I236, I233	F156, T158, G159, Q193, Y194, F195, S196, N200, E243, N239, I236, I233
F174	N/A	N173, A172, P171, K170, V168, A167, T166, F165, S164, E163, I162, D161, Q193, Y194, F195, S196, N200, E243, N239, I236, I233
L176	Y23, N152, V155, F156, P113, L114, E35, A34, K33, T244, E243, N239, F238, I236, I233	Y23, N152, V155, F156, T158, G159, Q193, Y194, F195, S196, N200, E243, N239, F238, I236, I233
K183	N/A	Y129, H127, T125, Q124, S123, D122, F121, Y194, F195, S196, N200, E243, N239, I236, I233

*Residues colored black, red, and green belong to subunits B, A, and C, respectively.

*Residues in the β 1- β 2 loop or pre-TM1 are highlighted in bold