

S1 Table. Parameters for homology modeling in YASARA.

| Parameter | Value |
|-------------------|-------|
| PsiBLASTs | 1 |
| EValue Max | 0.5 |
| Templates Total | 5 |
| Templates SameSeq | 1 |
| OligoState | 4 |
| Alignments | 5 |
| LoopSamples | 50 |
| TermExtensions | 90 |
| Speed | Slow |