SMC method for protein segment construction

1: $x_0^{(j)} = \emptyset, j = 1, 2, \ldots, N$
2: **for** i from 1 to $l - 3$ **do**
3:     **for** j from 1 to N **do**
4:         Construct list $L_i^{(j)}$ of possible pairs (ϕ', ψ') for amino acid i
5:         **for** n from 1 to 100 **do**
6:             Propagate $x_{i-1}^{(j)} \to x_i^{(j,n)}$ as follows:
7:             Draw one (ϕ_i, ψ_i) pair from $L_i^{(j)}$ and $\omega_i \sim p(\omega_i)$, and sample up to n_s side chain positions for χ_i.
8:             **if** $i = 1$ **then**
9:                 Let $\{s_{i,j,n}^{(k)}\}_{k=1}^{N_s}$ contain the n_s positions for χ_1
10:             **else**
11:                 Propagate $\{s_{i-1,j,n}^{(k)}\}_{k=1}^{N_s} \to \{s_{i,j,n}^{(k)}\}_{k=1}^{N_s}$ using embedded side chain filter: set $\{s_{i,j,n}^{(k)}\}_{k=1}^{N_s}$ to be the N_s vectors of $\chi_{1:i}$ with the lowest energies among the $N_s \times n_s$ combinations of $\chi_{1:i-1}$ with χ_i.
12:             **end if**
13:         **end for**
14:     **end for**
15:     Sample N particles from $\{x_i^{(j,1)}, \ldots, x_i^{(j,100)}\}_{j=1}^N$ to be $x_i^{(1)}, \ldots, x_i^{(N)}$
16: **end for**
17: Do final processing (including analytical closure for last three amino acid positions) and output conformations.