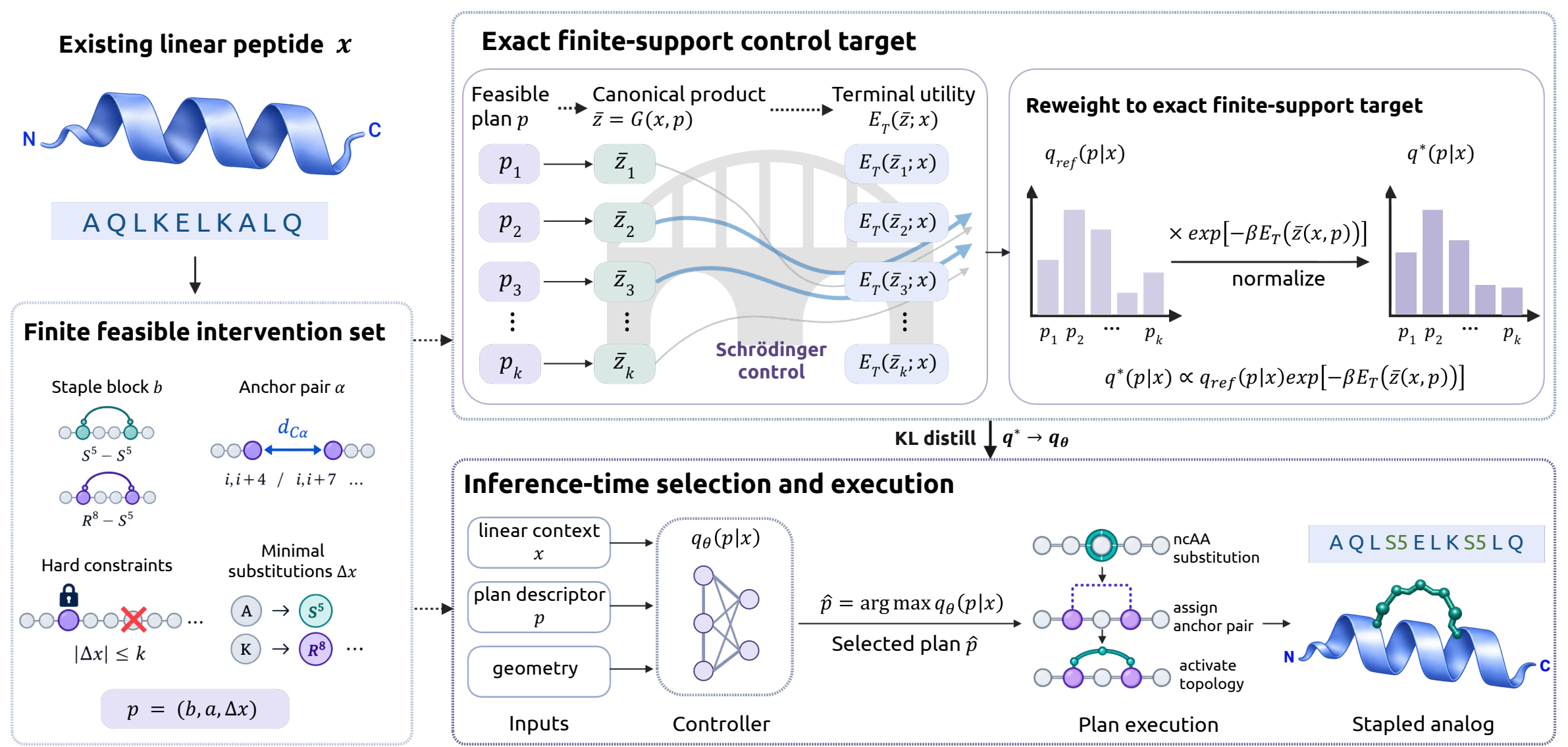

Existing linear peptide x
N
C
A Q L K E L K A L Q
Finite feasible intervention set
Staple block b
$S^5 - S^5$
$R^8 - S^5$
Anchor pair α
$d_{C\alpha}$
$i,i+4$ / $i,i+7$ ...
Hard constraints
$|\Delta x| \le k$
Minimal substitutions Δx
A → S^5
K → R^8
$p = (b, a, \Delta x)$
Exact finite-support control target
Feasible plan p
Canonical product $\bar{z} = G(x,p)$
Terminal utility $E_T(\bar{z};x)$
p_1 p_2 p_3 p_k
$\bar{z}_1$ $\bar{z}_2$ $\bar{z}_3$ $\bar{z}_k$
$E_T(\bar{z}_1;x)$ $E_T(\bar{z}_2;x)$ $E_T(\bar{z}_3;x)$ $E_T(\bar{z}_k;x)$
Schrödinger control
Reweight to exact finite-support target
$q_{ref}(p|x)$
$\times\, exp[-\beta E_T(\bar{z}(x,p))]$
normalize
$q^*(p|x)$
$q^*(p|x) \propto q_{ref}(p|x) exp[-\beta E_T(\bar{z}(x,p))]$
KL distill $q^* \to q_\theta$
Inference-time selection and execution
linear context x
plan descriptor p
geometry
Inputs
$q_\theta(p|x)$
Controller
$\hat{p} = \arg\max q_\theta(p|x)$
Selected plan $\hat{p}$
ncAA substitution
assign anchor pair
activate topology
Plan execution
A Q L S5 E L K S5 L Q
N
C
Stapled analog