

AcrIIA4 Anti-CRISPR Protein – 5vw1.pdb

AcrIIA4 model to be judged has a purple/light blue/dark blue/white backbone.

What is Displayed	How it is Displayed	Why it is Important
N Terminus	Blue or Green Endcap	Amino terminus – beginning of the protein chain
C Terminus	Red or Pink Endcap	Carboxyl terminus – end of the protein chain
Beta Pleated Sheets	White painted backbone	Secondary structures with hydrogen bonding between parallel peptides
Alpha Helices	Light blue painted backbone	Secondary structures with hydrogen bonding between amine groups and carboxyl groups, with 3.6 residues per turn and a separation of 1.5 Å
3_{10} Helix	Dark blue colored backbone	Secondary structures like alpha helices, with 3 residues per turn and a separation of 2.0 Å
Lys18	Amino acid sidechain	Prevents entrance of non-complimentary DNA in RuvC active site
Ser20, Thr22, Asp23, Asn25, Ser26	LEGO bricks	Prevents Cutting of non-target DNA by blocking RuvC active site
Asp14, Asn36	Amino acid sidechain	Interacts with Topo to prevent PAM recognition

Ala38, Asn39, Glu40, Tyr67	Sidechains made from black beads	Prevents PAM nucleotide stabilization and recognition; interacts with CTD
RuvC Domain of CRISPR Cas9 (residues 1-60, 755-785, and 960-1003)	Light blue alpha-carbon backbone	AcrIIA4 binds to the RuvC domain of the CRISPR Cas9 Protein to prevent cleavage of DNA non-complimentary strand.
Topo Domain of CRISPR Cas9 (residues 1102-1144)	Orange alpha-carbon backbone	AcrIIA4 binds to the Topo domain to prevent PAM recognition by the Cas9 protein.
CTD Domain of CRISPR Cas9 (residues 1200-1338)	White alpha-carbon backbone	AcrIIA4 binds to the CTD domain to prevent PAM recognition by the Cas9 protein.
Important CRISPR sidechains	Toothpick halves	AcrIIA4 sidechains interact with these sidechains in the Cas9 protein to inhibit its function in various ways.