AcrIIA4 Anti-CRISPR Protein – 5vw1.pdb S. Brunswick HS A (Team 38)

AcrIIA4 model to be judged has an orange/silver/white/dark blue backbone.

What is Displayed	How it is Displayed	Why it is Important
N Terminus	Blue Endcap	Amino terminus – beginning of the protein chain
C Terminus	Red Endcap	Carboxyl terminus – end of the protein chain
Beta Pleated Sheets	Silver painted backbone	Secondary structures with hydrogen bonding between parallel peptides
Alpha Helices	White 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, Asp23	Amino acid sidechain	Prevents entrance of non-complimentary DNA in RuvC active site
Ser20	Sidechain made from black beads	Prevents cutting of non-complimentary strand by occupying RuvC active site
Asn25, Ser26	Amino Acid Sidechain Model	Prevents Cutting of non-target DNA by blocking RuvC active site
Asp14, Asn36	Paperclips	Interacts with Topo to prevent PAM recognition
Asn39, Asp69, Glu70	3D Printed Sidechain	Prevents PAM nucleotide stabilization and recognition; interacts with CTD

Ala38, Tyr67	Amino Acid Sidechain Model	Interacts with CTD to prevent PAM recognition
Asp37, Glu40	Red and White Pushpin	Prevents PAM recognition through inhibition of CTD
RuvC Domain of CRISPR Cas9 (residues 960-1021)	Yellow 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 1102-1149)	Red 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)	Light blue alpha-carbon backbone	AcrIIA4 binds to the CTD domain to prevent PAM recognition by the Cas9 protein.
sgRNA Nucleotides 37-82	Dark blue mini-toober with a green 5' cap and a pink 3' cap	Cas9 must first form a complex with sgRNA for AcrIIA4 to bind to the Cas9 protein.
Important CRISPR sidechains	Unpainted toothpick halves	AcrIIA4 sidechains interact with these sidechains in the Cas9 protein to inhibit its function in various ways.

*Full-size toothpicks are for support only