This PyMOL command selects the SOS1-derived α-helical region (residues 929–944) that interacts with KRAS, providing a structural starting point for designing peptide inhibitors targeting the KRAS–SOS1 interface.

# Fetch the HRAS–SOS1 complex

fetch 1nvu, async=0

bg\_color white

remove hetatm

# Select SOS1 peptide (residues 929–944) in chain S

select sos1\_peptide, chain S and resi 929-944

# Display the SOS1 peptide as a cartoon and color it

show cartoon, sos1\_peptide

color orange, sos1\_peptide

# Select and show HRAS (chain R)

select kras, chain R

show cartoon, kras

color cyan, kras

# Zoom on the SOS1 peptide region

zoom sos1\_peptide

This PyMOL command setup visualizes the β-hairpin motif from the epidermal growth factor receptor (EGFR) dimer structure (PDB: 1IVO), highlighting the dimerization arm residues 246–253 (sequence **YNPTTYQM**) from chain A in yellow. These residues form a β-hairpin structure responsible for asymmetric dimerization of EGFR, which is overexpressed in cancer. The visualization displays chain B as a semi-transparent surface to provide spatial context, illustrating how disruption of this β-hairpin-mediated interface could potentially inactivate the kinase and serve as a strategy for therapeutic inhibition.

fetch 1IVO, async=0

remove not polymer

bg\_color white

remove hetatm

# Extract chain B as a separate object

create EGFR\_chainB, chain B

# Hide everything first

hide everything

# Show chain A as cartoon

show cartoon, chain A

color magenta, chain A

# Show chain B as transparent surface

show surface, EGFR\_chainB

color gray60, EGFR\_chainB

set transparency, 0.5, EGFR\_chainB

# Highlight beta-hairpin peptide on chain A (residues 246–253)

select beta\_hairpin, chain A and resi 246-253

show sticks, beta\_hairpin

color yellow, beta\_hairpin

# Set display and rendering options

bg\_color white

set stick\_radius, 0.25

set cartoon\_highlight\_color, yellow, chain A

set ray\_opaque\_background, off

zoom beta\_hairpin

ray 1200,900

This PyMOL command setup highlights the two potential interaction sites of Nac1 involved in homodimerization, selecting and displaying residues 12–24 and 44–60 from chain A as distinct α-helical or disordered peptide segments, while showing chain B of the dimer as a semi-transparent surface to provide structural context for analyzing and optimizing peptide-mediated interactions.

# Fetch the Nac1 dimer

fetch 3ga1, async=0

bg\_color white

remove hetatm

# Extract chain B as a separate object

extract nac1\_chainB\_obj, chain B

# Select first Nac1 peptide (residues 12–24) in chain A

select nac1\_peptide1, chain A and resi 12-24

show cartoon, nac1\_peptide1

color yellow, nac1\_peptide1

# Select second Nac1 peptide (residues 44–60) in chain A

select nac1\_peptide2, chain A and resi 44-60

show cartoon, nac1\_peptide2

color magenta, nac1\_peptide2

# Show extracted chain B as a transparent surface

show surface, nac1\_chainB\_obj

color cyan, nac1\_chainB\_obj

set transparency, 0.5, nac1\_chainB\_obj

# Zoom to focus on both peptides

zoom nac1\_peptide1 or nac1\_peptide2