

# Characterisation of protein kinase CK2 $\alpha$ mutants related to Okur-Chung Neurodevelopmental Syndrome

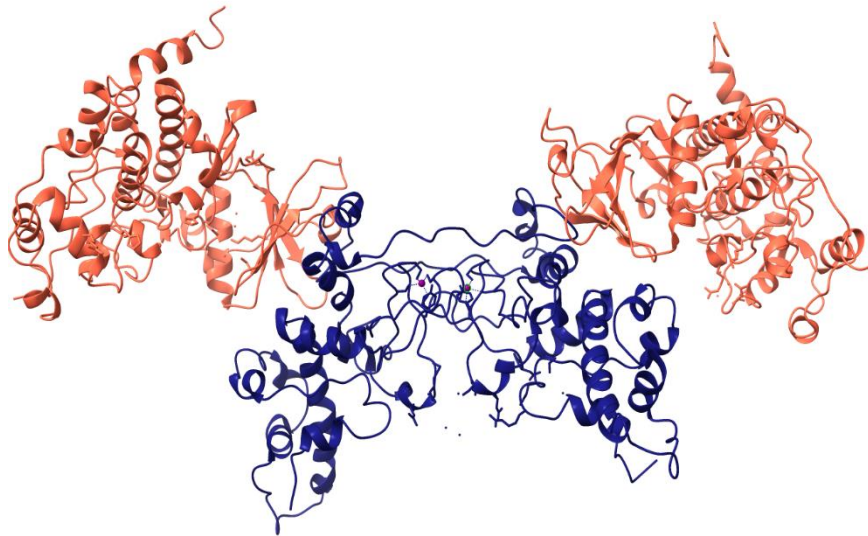


Figure 1: Holoenzyme structure of Protein Kinase 2. Two CK $\alpha$  chains are depicted in salmon. Two CK $\beta$  chains are depicted in midnight blue. The coordinated Zinc atoms are colored in purple. Made with ChimeraX [10]. File source is from Protein Data Bank under the Code of 1JWH, published by Niefind et. al. (2001) [11].

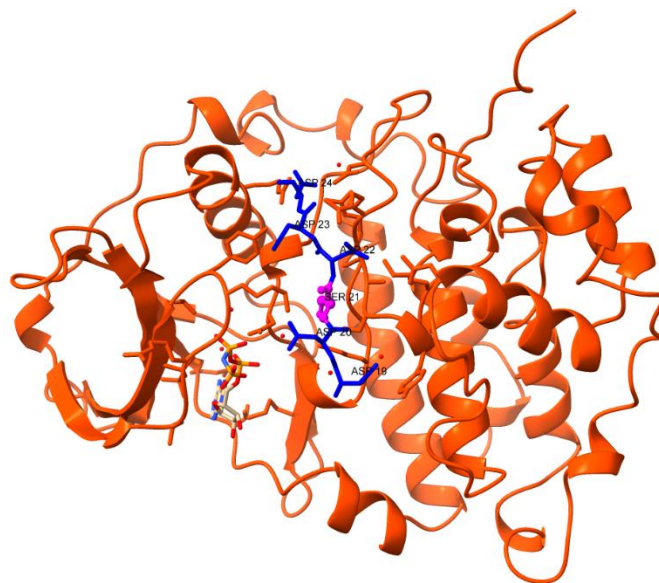


Figure 2: 3D structure of the catalytic subunit CK2 $\alpha$ . In blue: chain A, in red: chain B. Modelled substrate peptide is colored in blue, with the phosphorylated serine colored in magenta. Made available by Niefind et. al. (2003). PDB code: 2PVR [12].

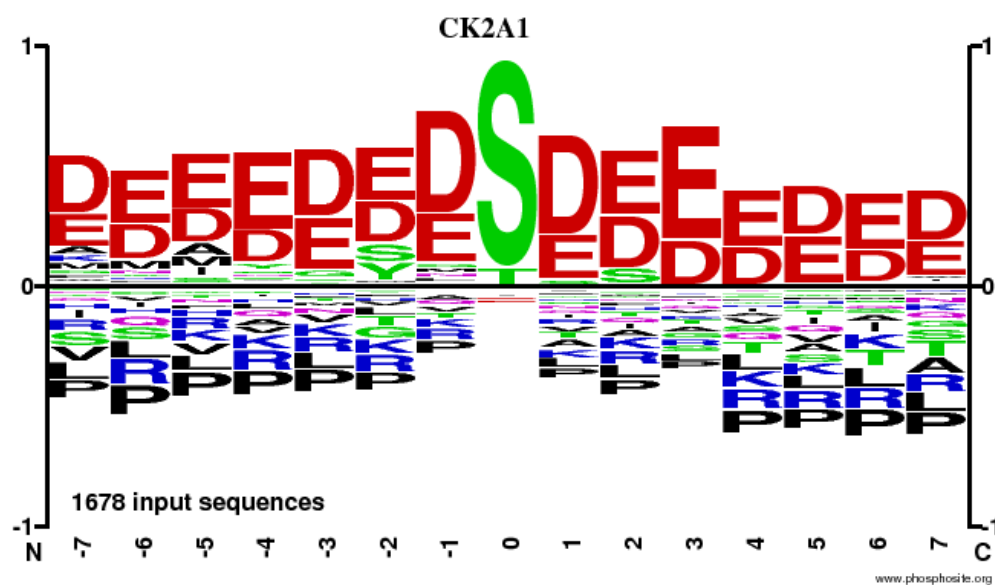


Figure 3: Protein sequence logo describing favored amino acid in the substrate sequence of substrates of protein CK2 $\alpha$ . Entry: human CSNK2A1 on phosphosites.org.

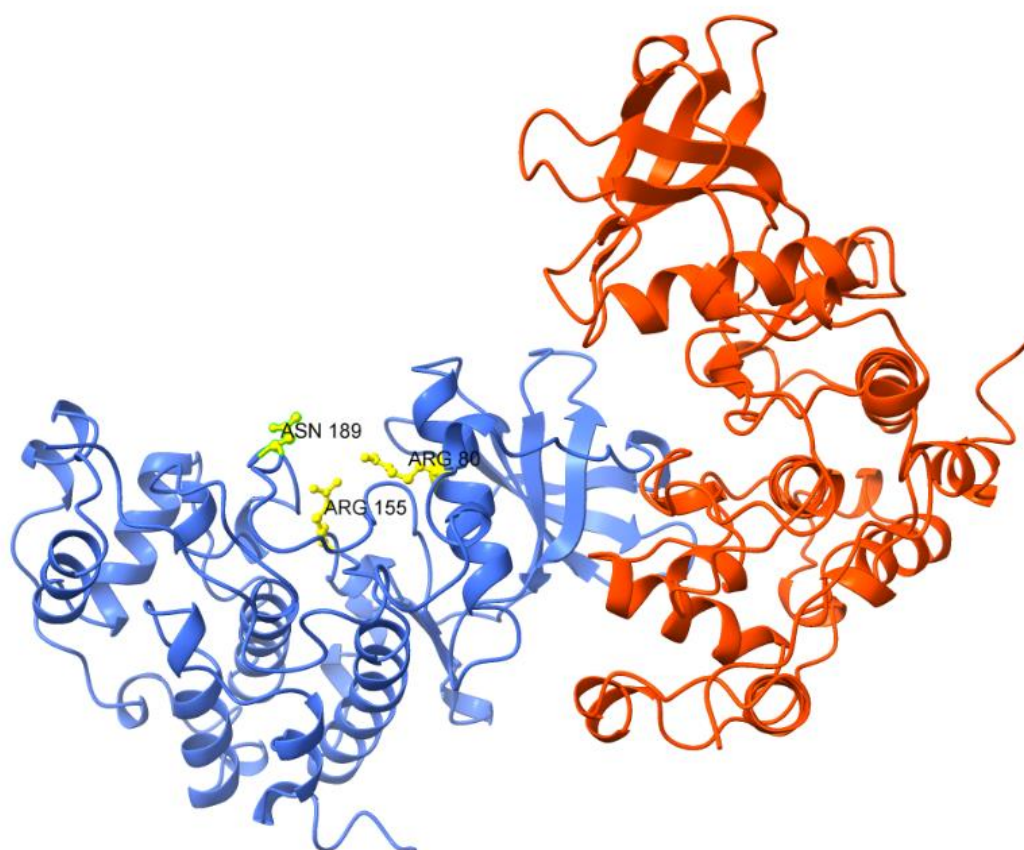


Figure 4: The coordination of Arginine80 and two other amino acids (Asn189 & Arg155) in the 3D structure of CK2 $\alpha$ . This position resembles the p+3 substrate binding region. Refined model provided by Christian Werner. In yellow and labelled: R80, R155, N189. Edited with ChimeraX [10].

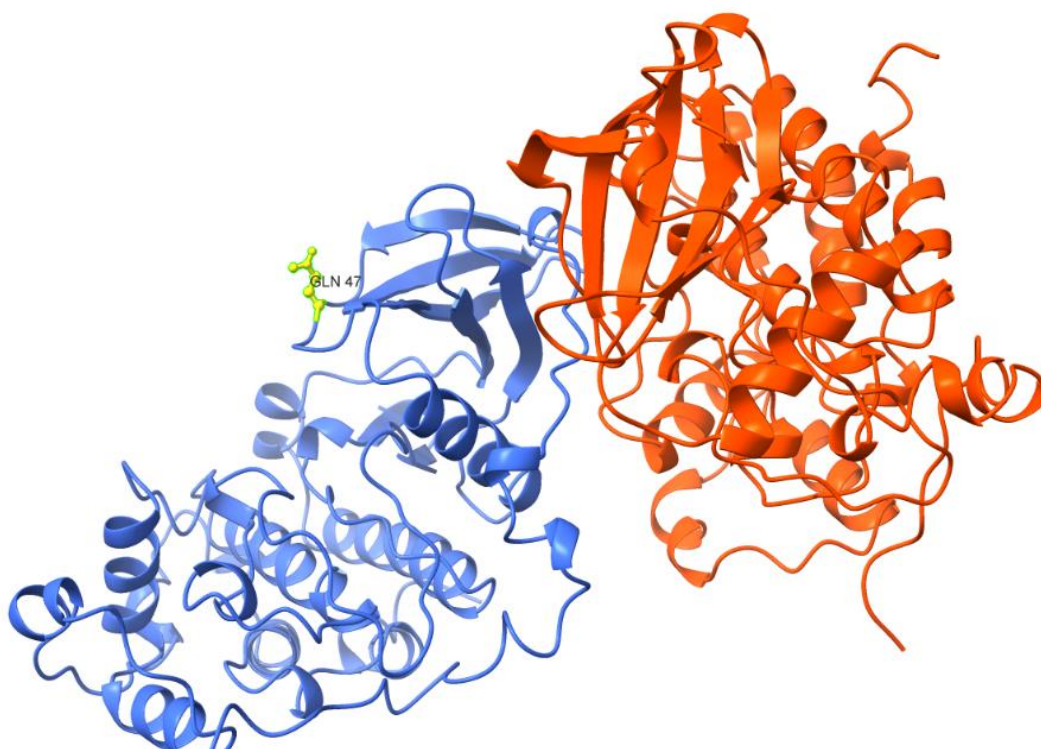


Figure 5: R47Q position in CK2 $\alpha$ , located at the ATP/GTP loop. Refined model provided by Christian Werner. In yellow and labelled: mutation with arginine replaced by a glutamine. Edited by ChimeraX [10]



Figure 6: 0.5 mg/mL CK2 $\alpha$  R80H full-length crystallized with mother liquid of 0.2 M lithium sulphate, 25% w/v PEG 3350, 0.1 M Bis-TRIS/HCl, pH 6.5 in ratio from 2:1. The reservoir was filled with a saturated PEG 3350 solution. One needle-like crystal is visible.

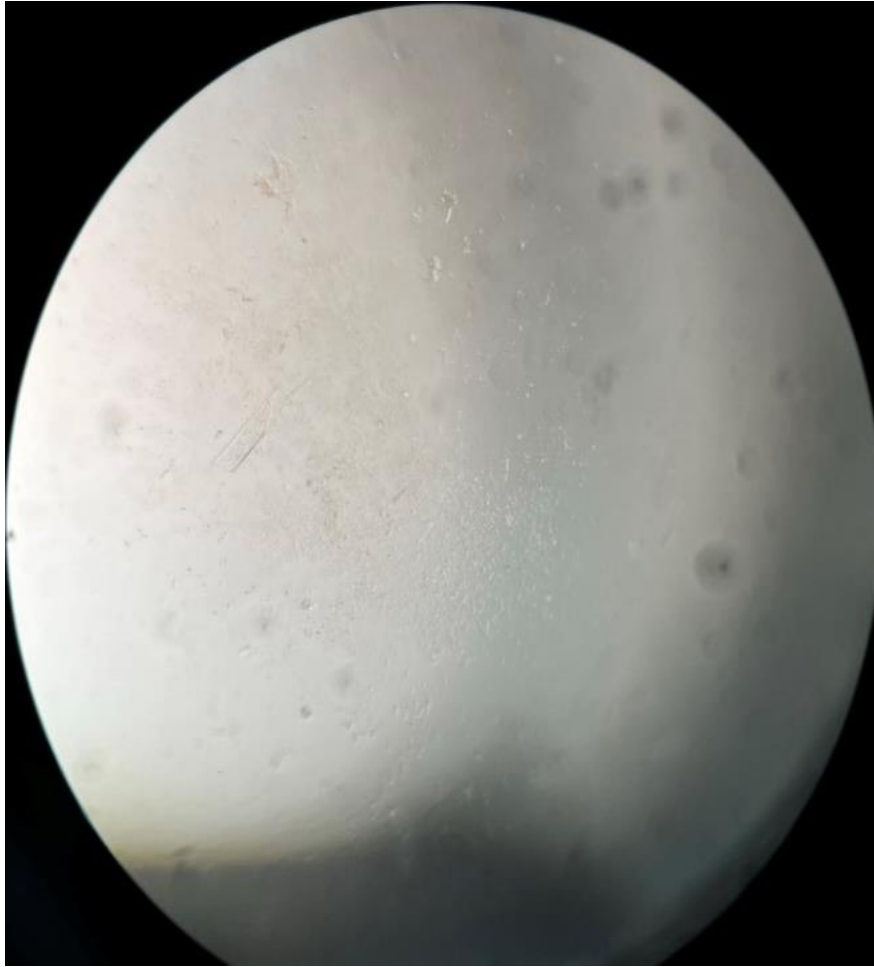


Figure 7: 0.5 mg/mL CK2α R80H full-length crystallized with mother liquid of 0.2 M lithium sulphate, 25% w/v PEG 3350, 0.1 M Bis-TRIS/HCl, pH 6.5 in ratio from 2:1. The reservoir was filled with a saturated PEG 3350 solution. One razor blade-shaped crystal is visible.

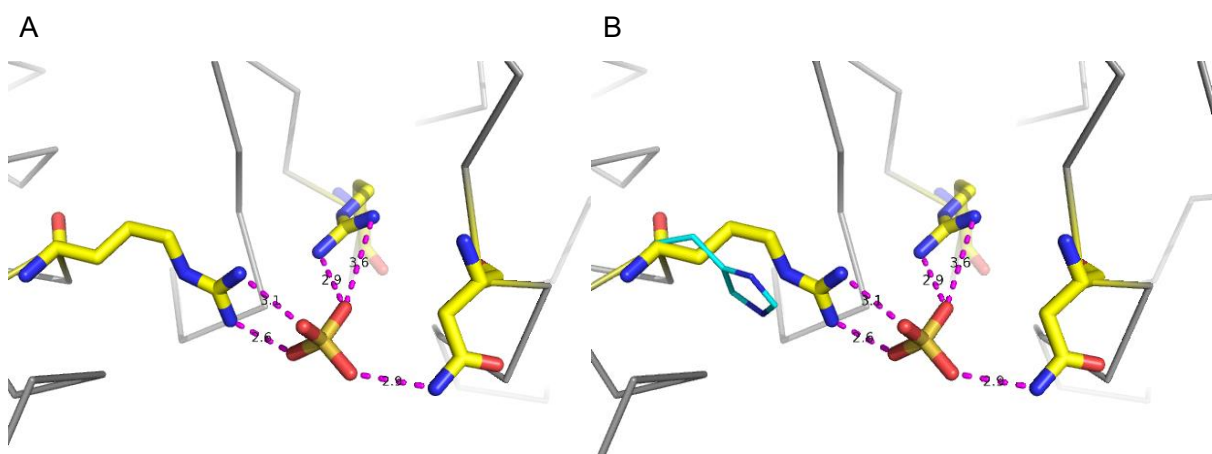


Figure 8: Predicted substitute model of the 3D structure for variant CK2α1-335 R80H, with the Arginine80 side chain presented in the left side of the figures. A) Wildtype structure of the protein. The Arg80 coordinates the p+3 substrate recognition position together with Arg155 and Asn189. B) Arg80 overlapped with the modelled histidine side chain marked in bright blue. Data provided by Christian Werner. Edited by PyMol [27]