

Structural and Functional Consequences of Three Cancer-Associated Mutations in the Oncogenic Phosphatase Shp2

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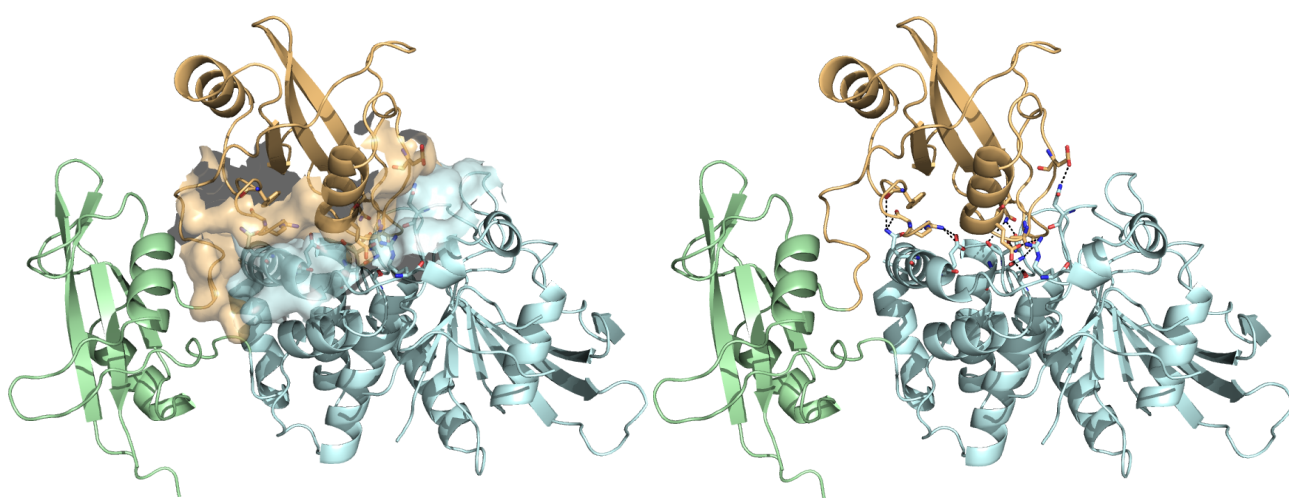
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SUPPLEMENTARY INFORMATION



Hydrogen Bonds

GLN256 (NE2) : ARG4 (O)
GLN256 (NE2) : PHE7 (O)
GLN510 (NE2) : GLY60 (O)
ASN281 (ND2) : GLU69 (OE1)
GLN506 (NE2) : ALA72 (O)
SER502 (HG) : GLU76 (OE2)
GLN256 (OE1) : ARG4 (HE)
GLN506 (O) : ASN58 (ND2)
GLN506 (OE1) : ASN58 (ND2)

Salt Bridge Interactions

ARG265 (NH2) : GLU76 (OE1)
GLU258 (OE2) : ARG4 (NH1)
GLU258 (OE1) : ARG4 (NH1)

Supplemental Figure 1. The buried surface area between N-SH2 and PTP domains involves 70 residues (32 from N-SH2 and 38 from PTP) and covers 1176 Å². There are 9 hydrogen bond and 3 salt bridge contributions to this interface. PDB: 2SHP and QtPISA¹ were used for this analysis.

References

- [1] Krissinel, E., and Henrick, K. (2007) Inference of macromolecular assemblies from crystalline state, *J Mol Biol* 372, 774-797.