

Modelling the activation pathways in full length Src kinase

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Tab.1S

SH2-KD (Closed Apo)	SH3-KD (Closed Apo)	SH3-Linker (Closed Apo)
155R 526Q	95R 287N	95R 252T
160R 365D	95R 289T	95R 255L
160R 397N	117D 318R	118W 253Q
179T 527Y	—	135N 251Q
200K 528Q	—	91D 249K
217R 531E	—	117D 253Q
157E 321K	—	115E 257K
201H 527Y	—	—
237L 532N	—	—

Hydrogen bonds (HB) in c-Src domains, for the Closed Apo conformation. HB among the residues of SH2 and KD domains (column 1), of SH3 and KD domains (column 2), and of SH3 and linker domains (column 3) are reported.

Tab.2S

SH2-KD (Open)	SH3-KD (Open)	SH3-Linker (Open)
—	11R 221E	11R 168T
—	32G 247E	12T 174D

—	13E 228N	14T 173K
—	13E 231K	34W 169Q
—	—	51N 167Q
—	—	52Y 166P
—	—	7D 165K
—	—	51N 168T
—	—	31E 173K

Hydrogen bonds (HB) among c-Src domains, for the Open conformation. No HB among the residues of SH2 and KD domains have been identified (column 1). HB among the residues of SH3 and KD domains (column 2), and of SH3 and linker domains (column 3) are reported.

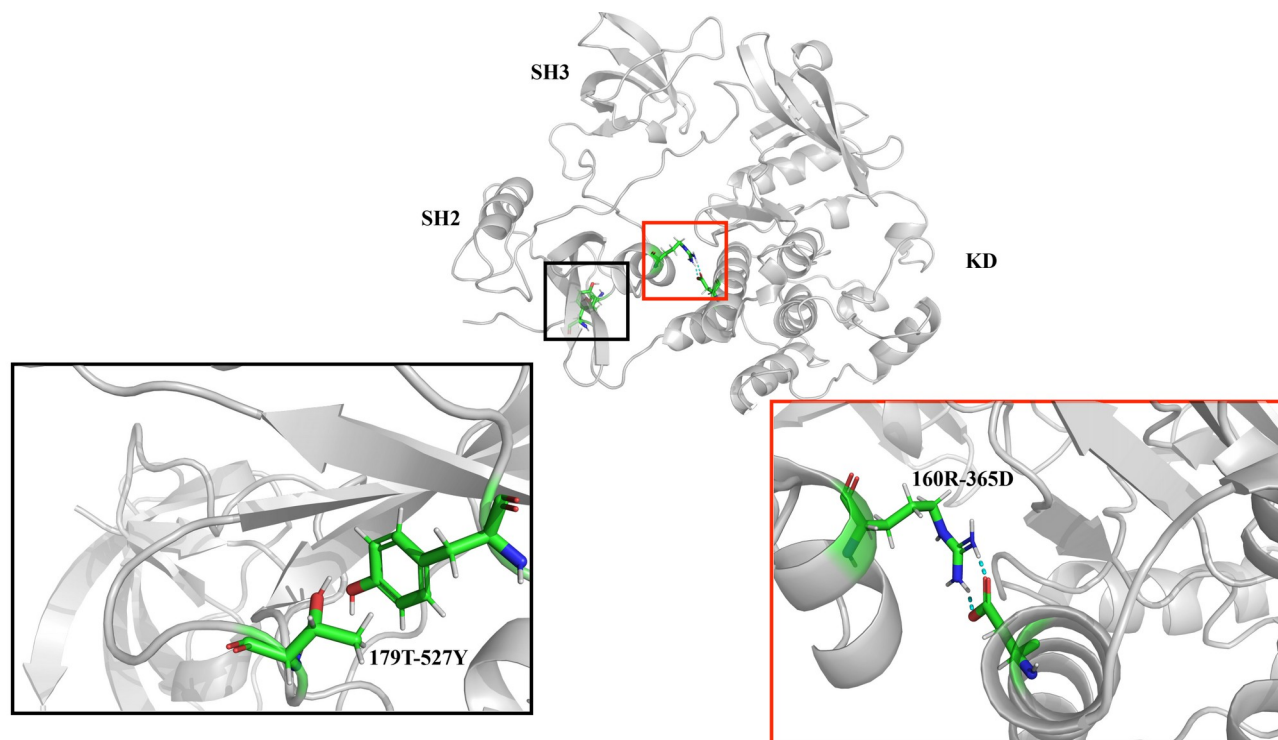


Fig. 1S HB between the residues **179T-527Y** (black box) and **160R-365D** (red box) stabilizing c-Src in close conformation. The residues **179T** and **160R** belong to SH2 domain, the residues **527Y** and **365D** belong to KD domain.

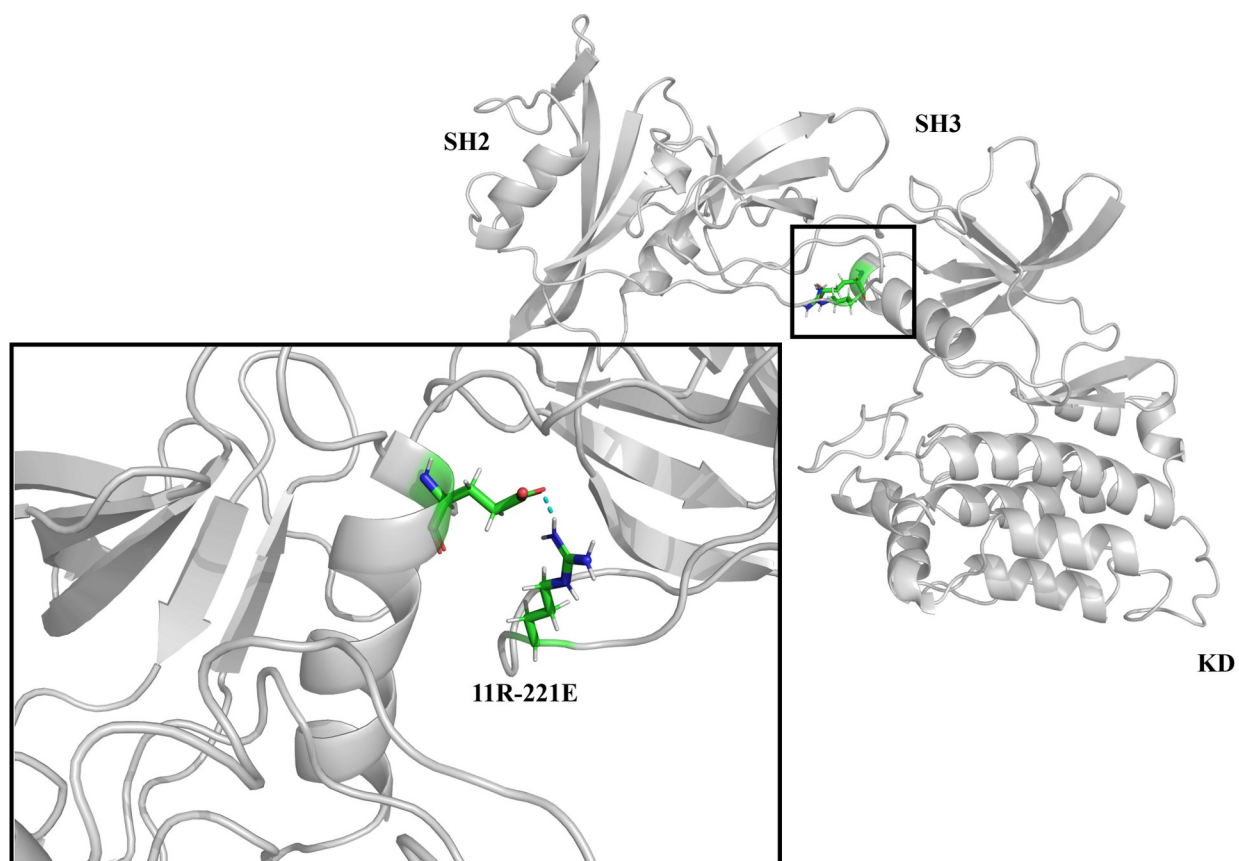


Fig. 2S HB between the residues **11R-221E** belonging, respectively, to SH3 and KD domains for c-Src in Open conformation.

