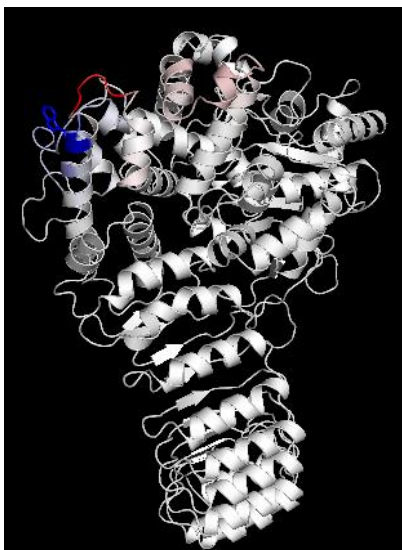


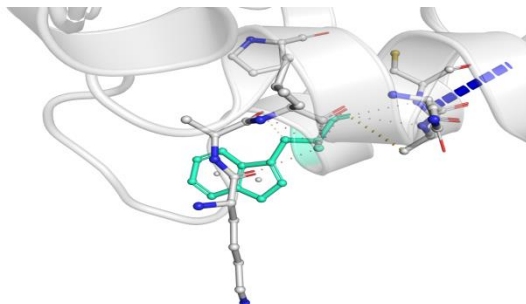
Supplementary Figure S3. The changes in the vibrational entropy and interatomic interactions upon mutations in the LRR domain of nod2. (A) Amino acids colored according to the vibrational entropy change upon mutation. BLUE represents a rigidification of the structure and RED a gain in flexibility. Images are provided y Dynamut. (B) Interatomic interactions. Residues are presented by light-green sticks among their surrounding residues involving in different interactions. Images are provided y Dynamut.

A

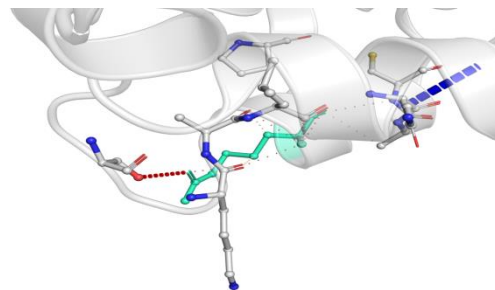
R702W



B

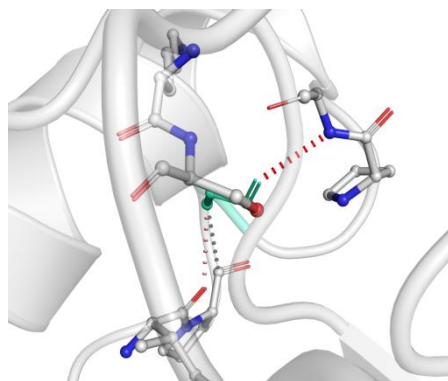
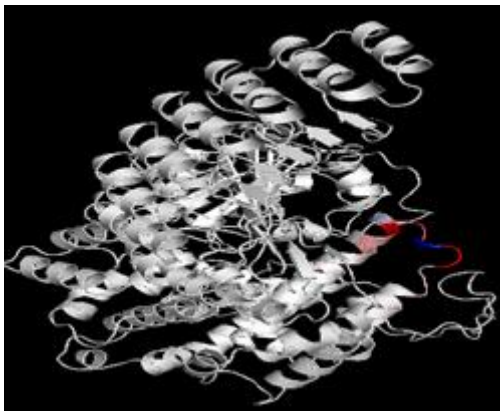


Interatomic reactions of the
mutant residue

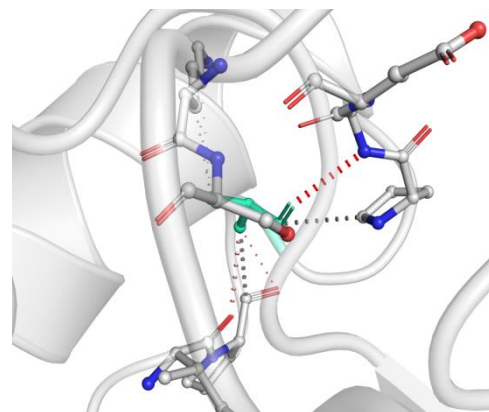


Interatomic reactions of the
wild residue

A725G

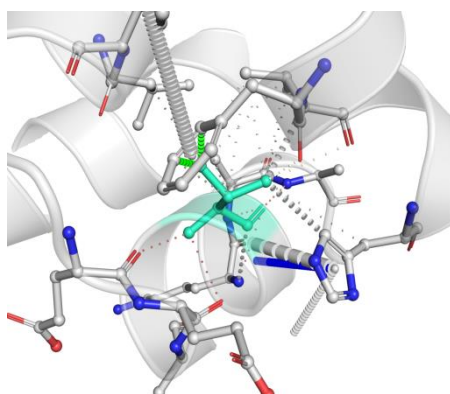
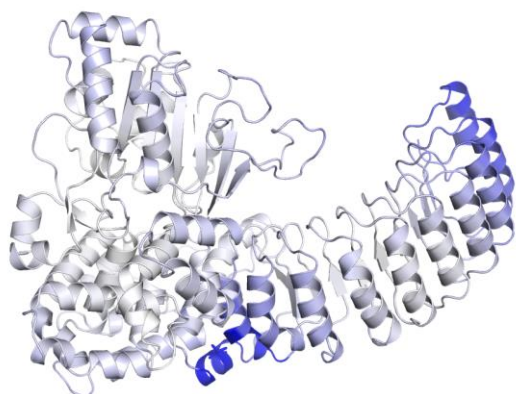


Interatomic reactions of the
mutant residue

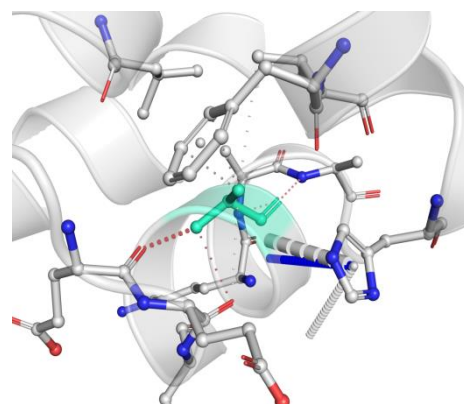


Interatomic reactions of the wild
residue

A755V

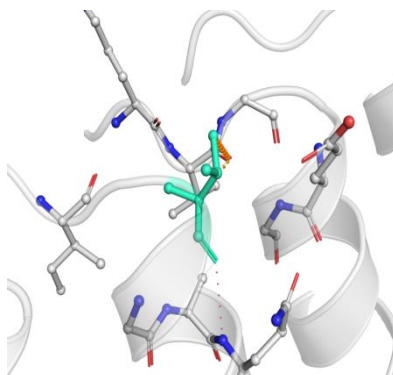
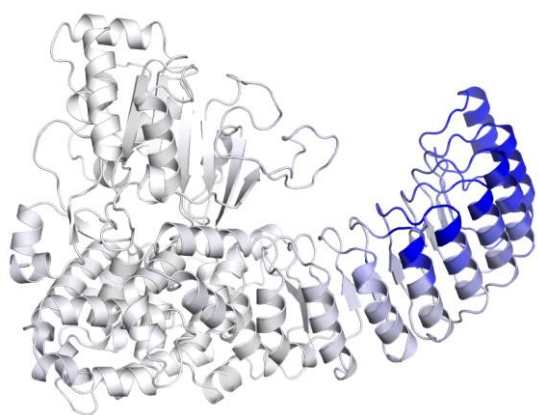


Interatomic reactions of the mutant residue

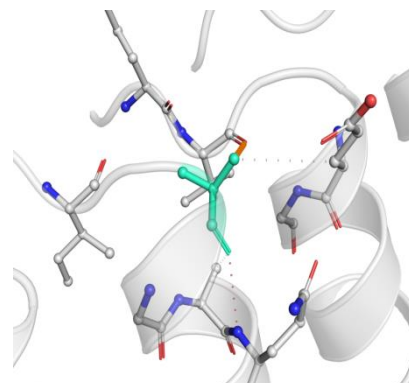


Interatomic reactions of the wild residue

A885T

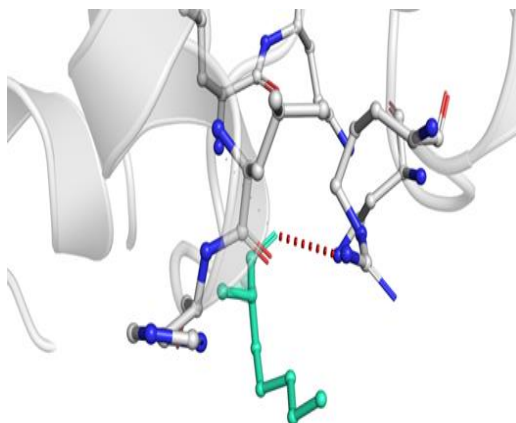
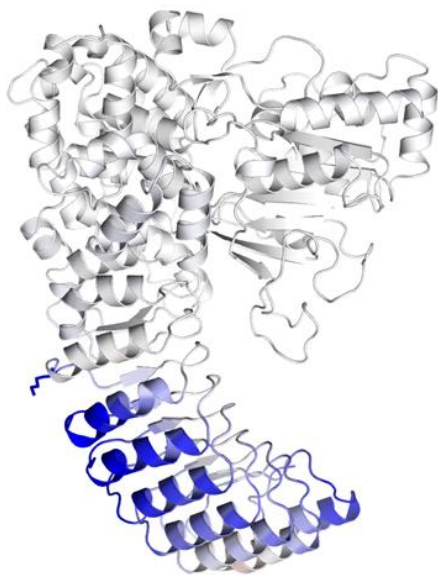


Interatomic reactions of the mutant residue

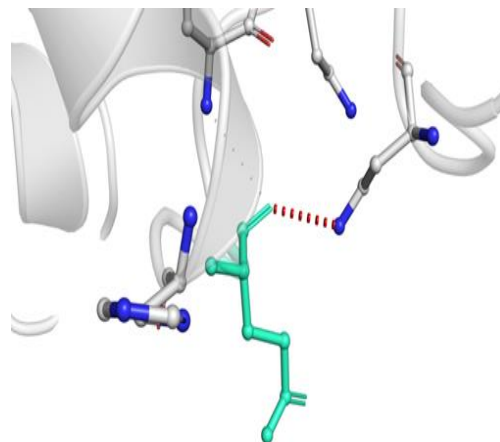


Interatomic reactions of the wild residue

G843K

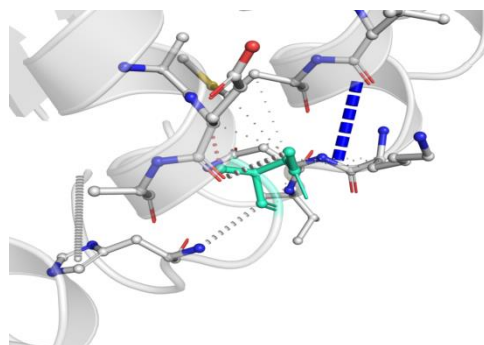


Interatomic reactions of the mutant residue

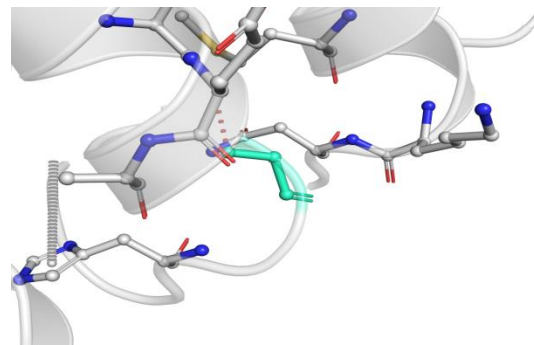


Interatomic reactions of the wild residue

G924D

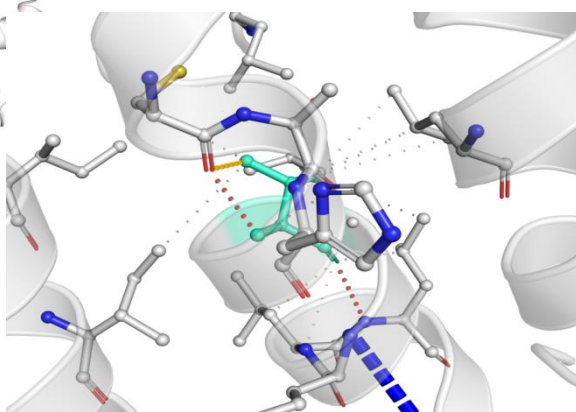
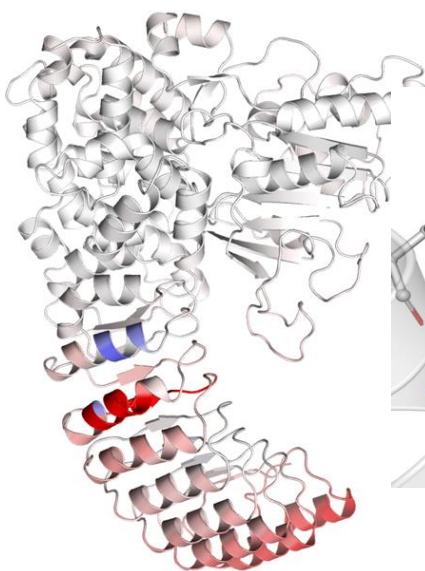


Interatomic reactions of the mutant residue

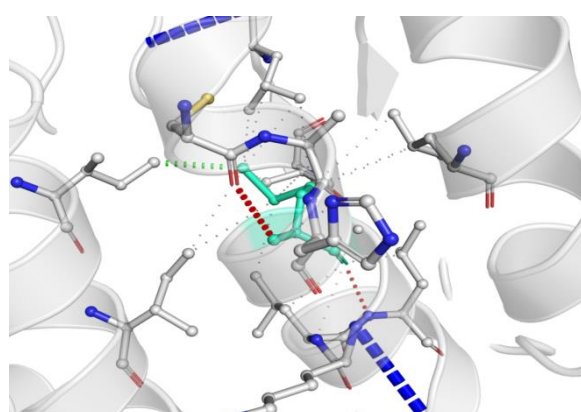


Interatomic reactions of the wild residue

M863V

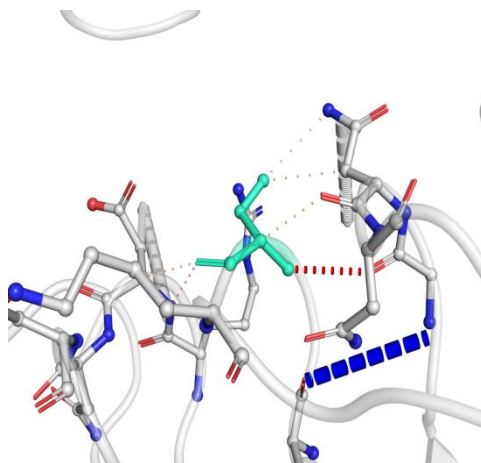
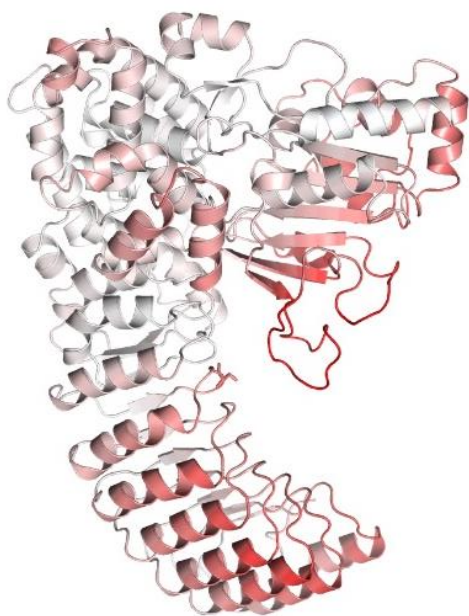


Interatomic reactions of the mutant residue

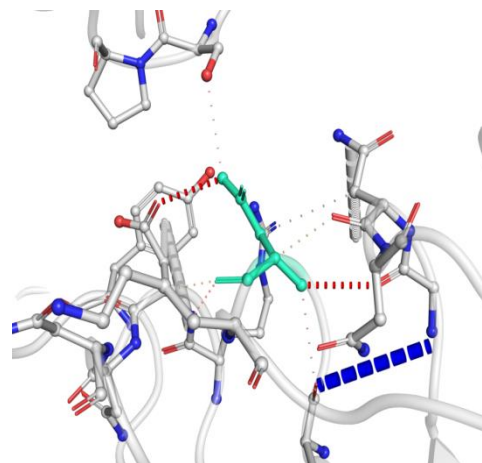


Interatomic reactions of the wild residue

N852S

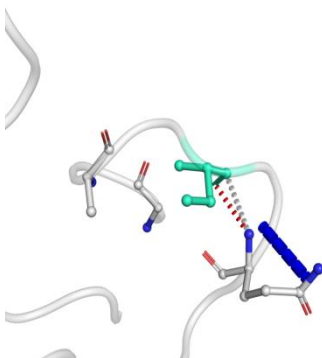
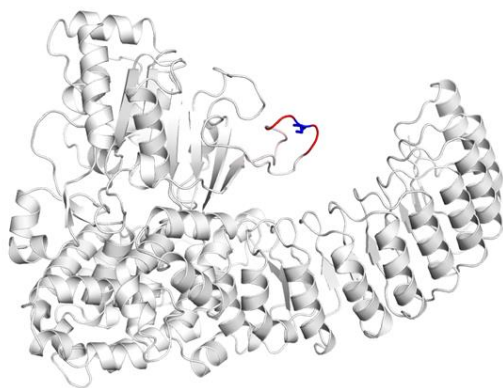


Interatomic reactions of the mutant residue

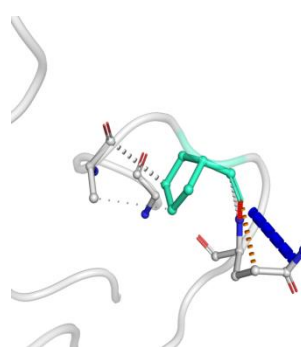


Interatomic reactions of the wild residue

P268S

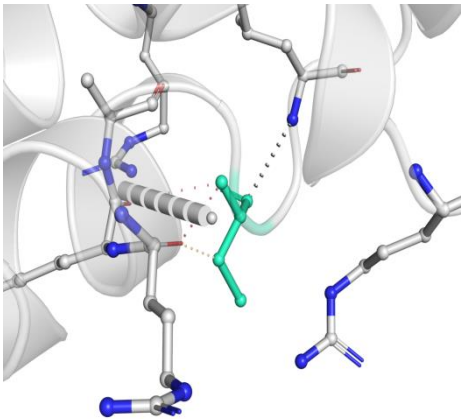
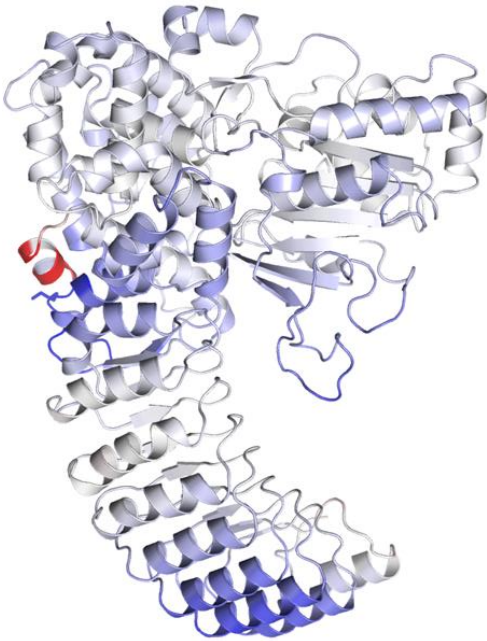


Interatomic reactions of the mutant residue

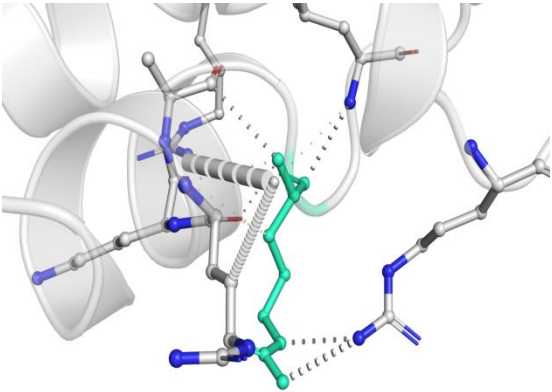


Interatomic reactions of the wild residue

R760C

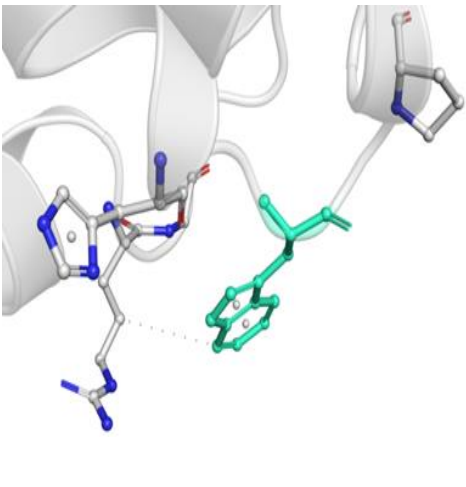
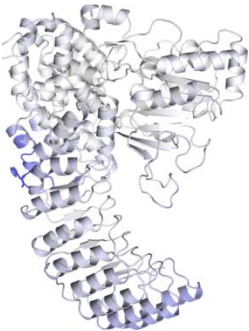


Interatomic reactions of the mutant residue

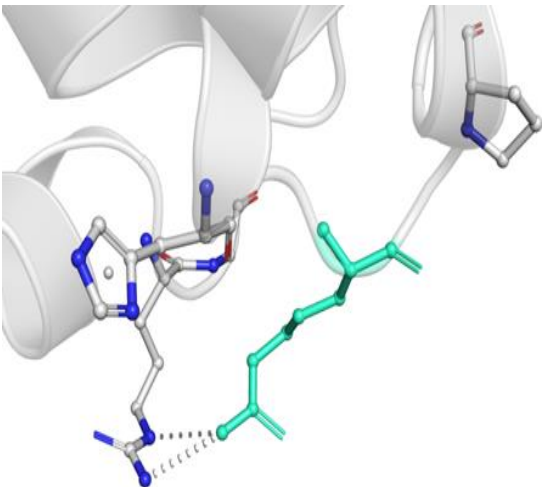


Interatomic reactions of the wild residue

R790w)

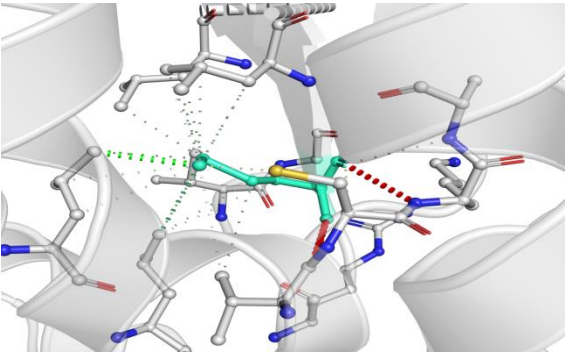
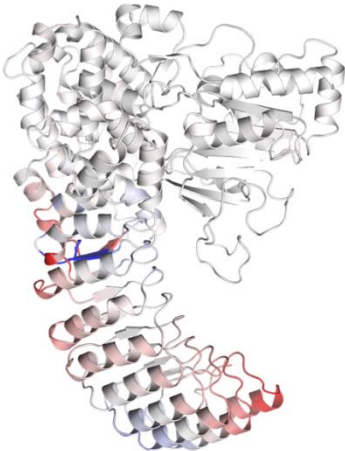


Interatomic reactions of the mutant

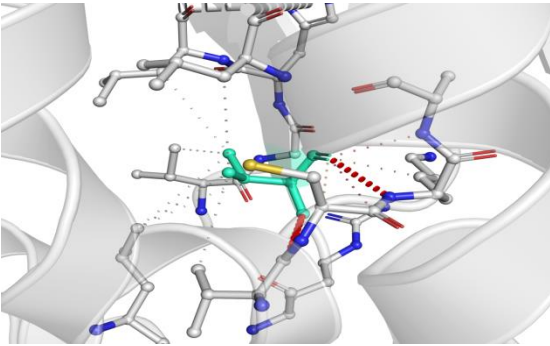


Interatomic reactions of the wild residue

V793M

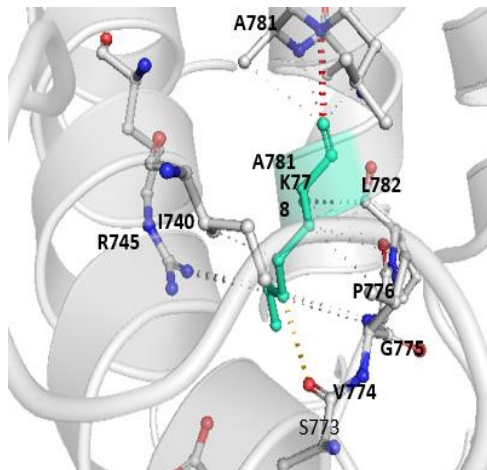
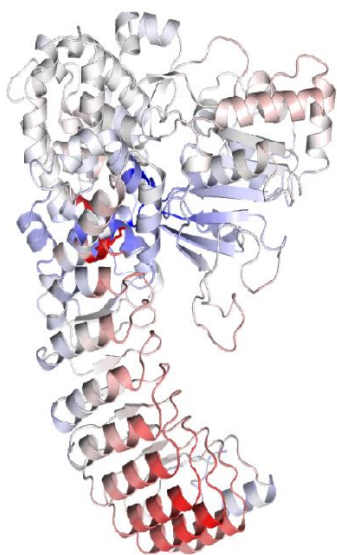


Interatomic reactions of the mutant residue

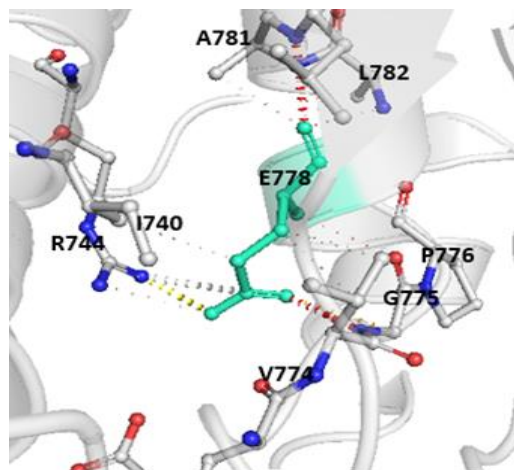


Interatomic reactions of the wild residue

E778k

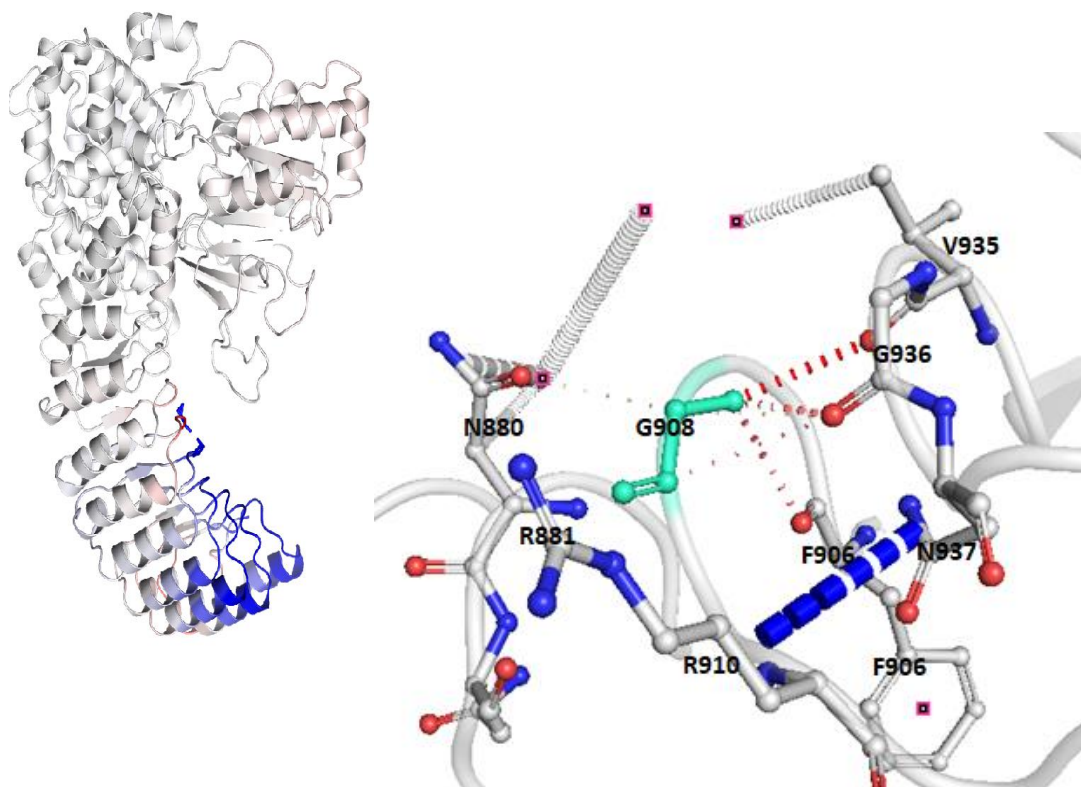


Interatomic reactions of the mutant residue

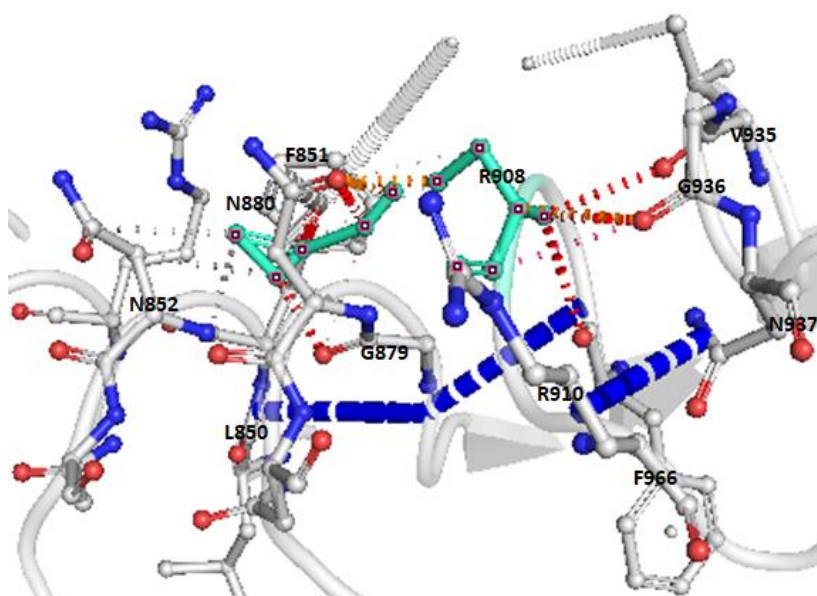


Interatomic reactions of the wild residue

G908R



Interatomic reactions of the mutant residue



Interatomic reactions of the wild residue

Color definition for contacts ▲

Bond Type	Color
Hydrogen bonds	Red
Water mediated hydrogen bonds	Red
Weak hydrogen bonds	Orange
Water mediated weak hydrogen bonds	Orange
Halogen bonds	Blue
Ionic interactions	Yellow
Metal complex interactions	Purple
Aromatic contacts	Cyan
Hydrophobic contacts	Dark Green
Carbonyl contacts	Magenta