

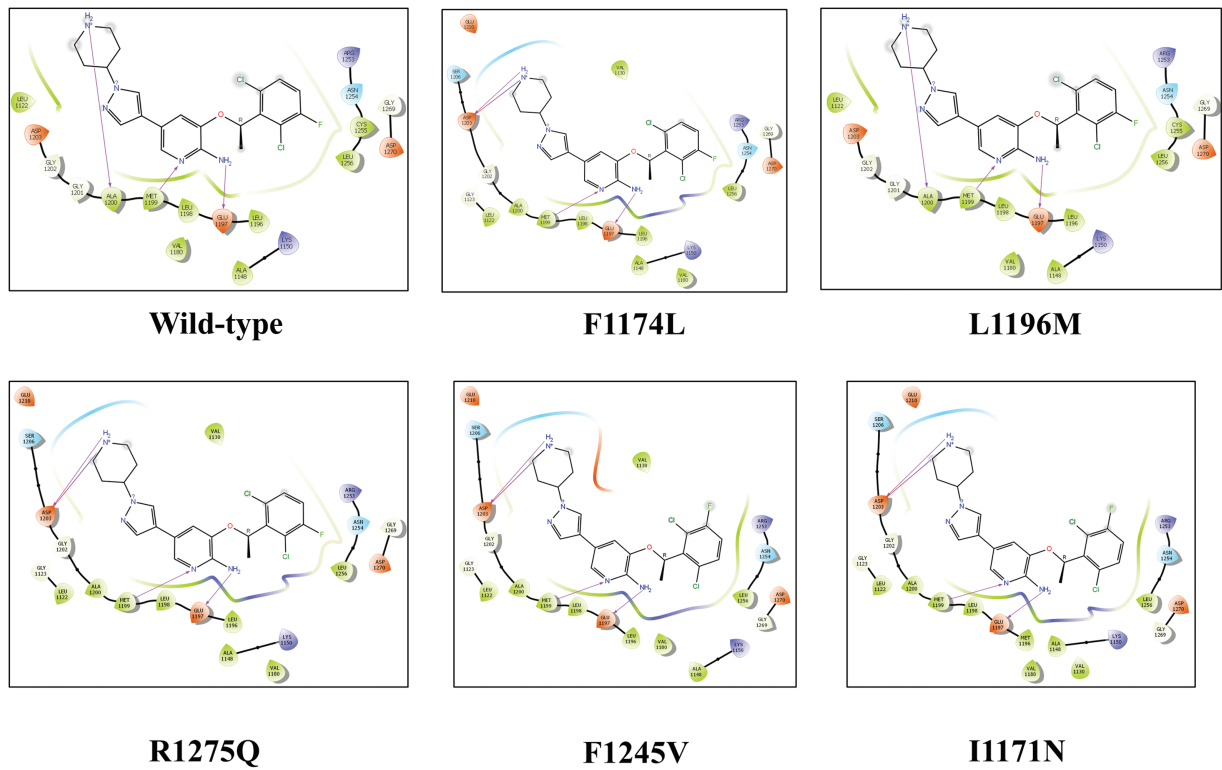
**Suppl. Table 1** Computational predictions for the screening of deleterious SNPs using various tools

Missense SNP	PolyPhen-2	SIFT	Predict SNP	PANTHER	PhD-SNP	SNAP	MetaLR
I1171N	Probably damaging	Deleterious	Deleterious	Probably damaging	Neutral	Deleterious	Damaging
F1174L	Probably damaging	Deleterious	Neutral	Probably damaging	Neutral	Deleterious	Tolerated
F1174V	Probably damaging	Deleterious	Deleterious	Probably damaging	Deleterious	Neutral	Damaging
F1174C	Probably damaging	Deleterious	Deleterious	Probably damaging	Deleterious	Neutral	Damaging
L1196M	Probably damaging	Deleterious	Neutral	Probably damaging	Neutral	Neutral	Damaging
F1245V	Probably damaging	Deleterious	Deleterious	Probably damaging	Deleterious	Deleterious	Damaging
F1245C	Probably damaging	Deleterious	Deleterious	Probably damaging	Deleterious	Neutral	Damaging
R1275Q	Probably damaging	Deleterious	Deleterious	Probably damaging	Deleterious	Deleterious	Damaging
R1275L	Probably damaging	Deleterious	Deleterious	Probably damaging	Deleterious	Deleterious	Damaging

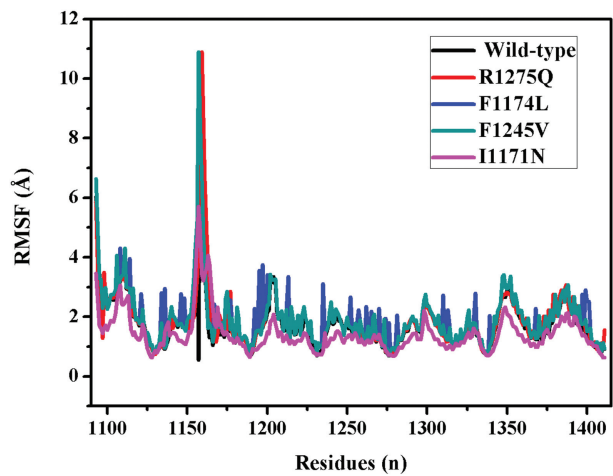
Abbreviation: SNP, single-nucleotide polymorphism.

**Suppl. Table 2** Docking scores of wild-type and other mutant structures with crizotinib drug molecule

Protein structures	Binding energy (kcal/mol)	Amino acid involved in interactions
Wild-type	-5.896	Ala1200, Glu1197, Met1199
I1171N	-7.436	Asp1203, Glu1197, Met1199
F1174L	-9.593	Asp1203, Glu1197, Met1199
F1174V	-9.587	Asp1203, Glu1197, Met1199
F1174C	-9.502	Asp1203, Glu1197, Met1199
L1196M	-5.917	Ala1200, Glu1197, Met1199
F1245V	-9.702	Asp1203, Glu1197, Met1199
F1245C	-9.458	Asp1203, Glu1197, Met1199
R1275Q	-9.988	Asp1203, Glu1197, Met1199
R1275L	-9.943	Asp1203, Glu1197, Met1199



Suppl. Fig. 1 Two-dimensional interaction diagram of the crizotinib in different wild and mutant structures of anaplastic lymphoma kinase (ALK) protein.



Suppl. Fig. 2 Root mean square fluctuation (RMSF) plot of the all-mutant complex with wild-type obtained from molecular dynamics (MD) simulation study.