

Fig. 5a: GTP-bound WT NRAS per-residue distance histograms to residue 61. Per-residue distance distributions were calculated between heavy atoms of residue 61 and those of 9 chosen residues which frequently interact with Q61 across all simulations. Histograms represent the percentage of frames in which a specific minimum distance was observed. Each plot corresponds to one of the 9 residues: residues 10, 16, 37, 58, 59, 60, 62, 63, and 68.

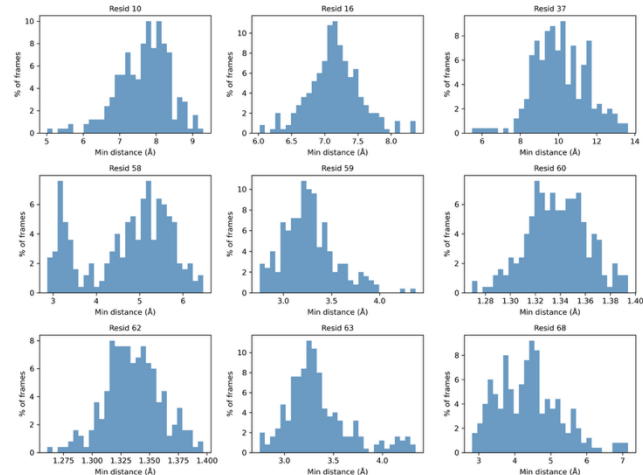


Fig. 5b: Overlapping GTP-bound WT NRAS per-residue distance histograms to residue 61. This histogram displays the same data as Fig. 5a but shows the histograms of all residues overlapping on one plot.

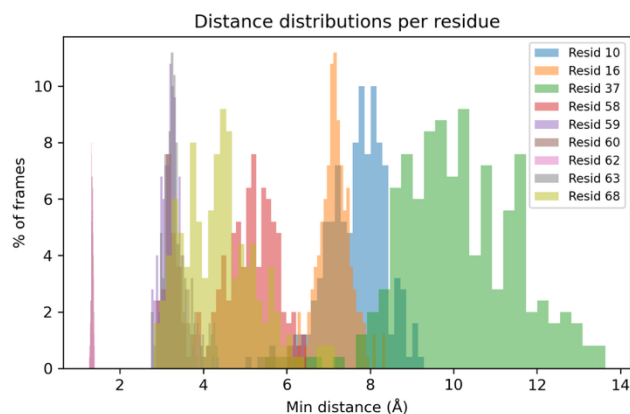


Fig. 6a: GTP-bound Q61R mutant NRAS per-residue distance histograms to residue 61. Per-residue distance distributions were calculated between residue 61 and each of 9 chosen residues which frequently interact with R61 across all simulations. Histograms represent the percentage of frames in which a specific minimum distance was observed. Each plot corresponds to one of the 9 residues: residues 10, 16, 37, 58, 59, 60, 62, 63, and 68.

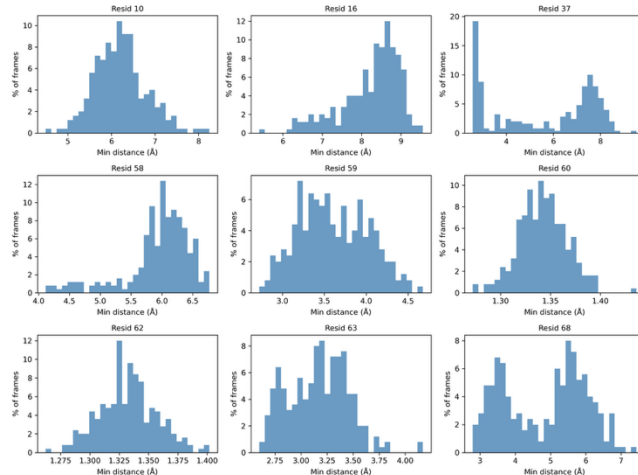


Fig. 6b: Overlapping GTP-bound Q61R mutant NRAS per-residue distance histograms to residue 61. This histogram displays the same data as Fig. 6a but shows the histograms of all residues overlapping on one plot.

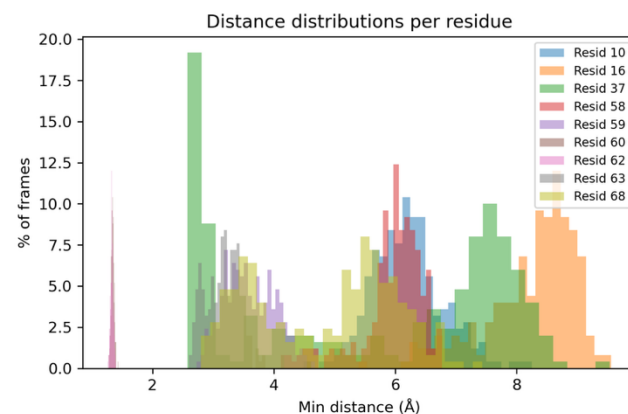


Fig. 7: Paired bar graph comparing mean minimum distances from residue 61 for WT and Q61R mutant. The mean values are the calculated means of each of the histograms shown in Fig. 5a and 6a.

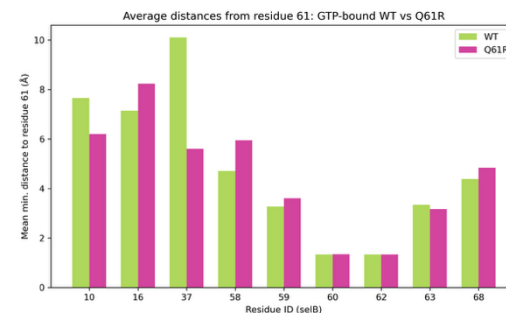


Fig. 8: Top: Processed PDB structure of GTP-bound WT, with residue Q61 in blue. Bottom: Processed PDB structure of GTP-bound Q61R, with residue R61 in blue. Residues that were on average closer to residue 61 in WT (Fig. 7) are shown in green, and residues that were on average closer to residue 61 in Q61R are shown in pink.

