

1 **Dynamics of the personalities of PCSK9 on missense variants**
2 **(rs505151 and rs562556) from elderly cohort studies in Brazil**

3 Vitor Galvão Lopes¹, Victor Fernandes de Oliveira¹, Livia Mendonça Munhoz Dati¹, Michel
4 Satya Naslavsky², Glaucio Monteiro Ferreira^{1†} and Mario Hiroyuki Hirata^{1†}

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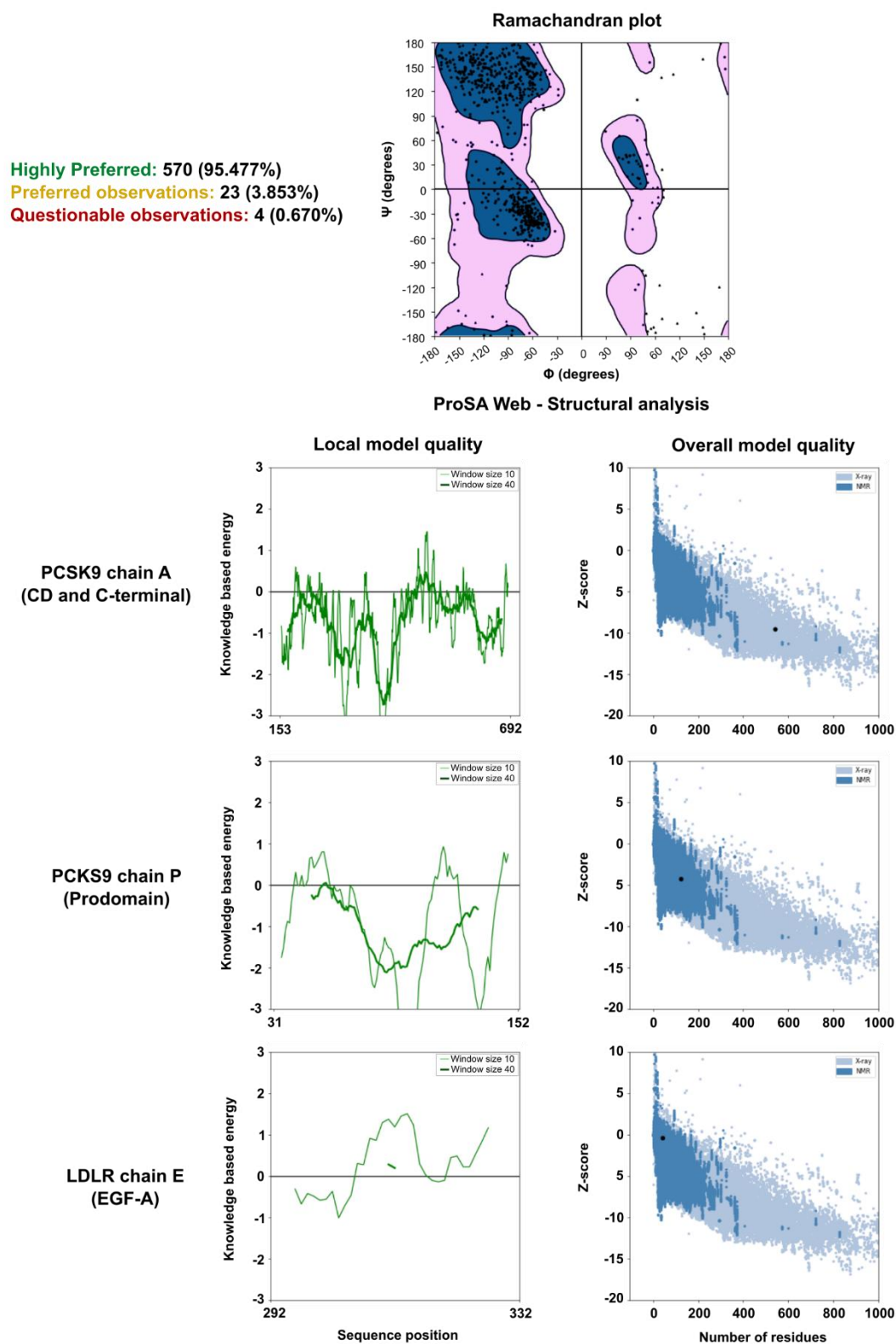
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22 **Supplementary material**

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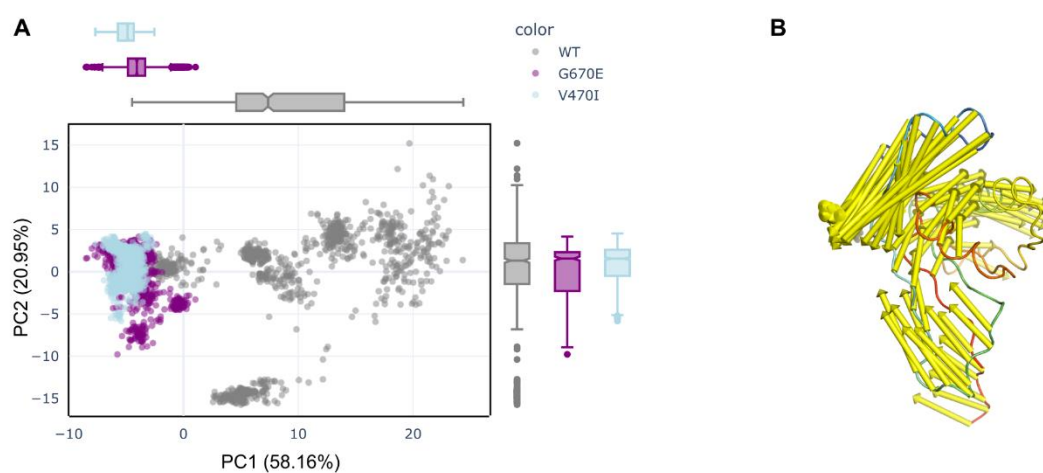
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25 **Figure S1:** Tridimensional structure model assessment through Ramachandran Plot and ProsaWeb

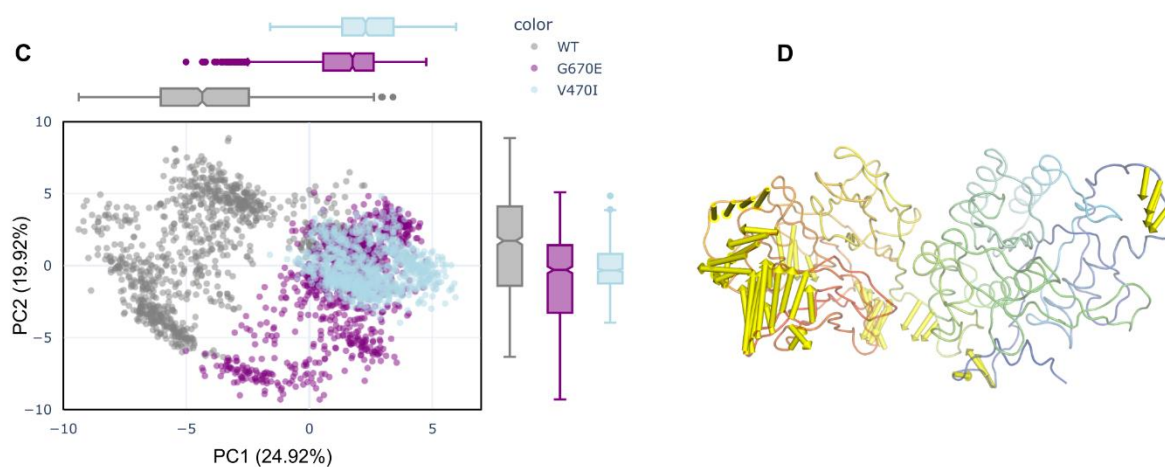
26 analysis for each chain (local quality and overall model quality). The Ramachandran plot shows the

27 torsional dihedral angles along with the backbone structure. The local model quality trendline
 28 represents the average energy of the i^{th} residue + 9 residues (Window size 10) and the i^{th} residue + 39
 29 residues (Window size 40). The overall model quality demonstrates the reconstructed model as a black
 30 dot among all the determined experimentally protein structures (dark blue (NMR) and light blue (X-
 31 ray)).
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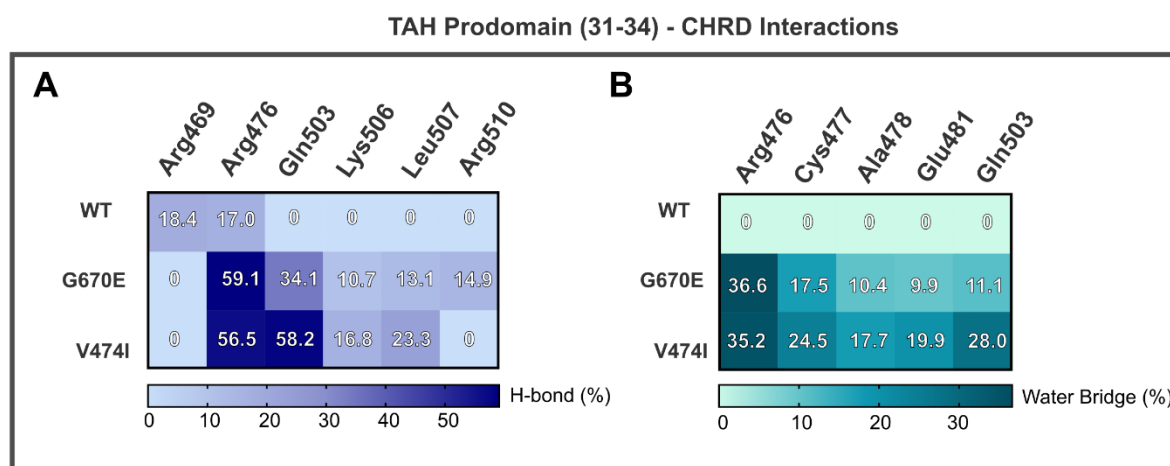
Prodomain: 2D PCA and modevector



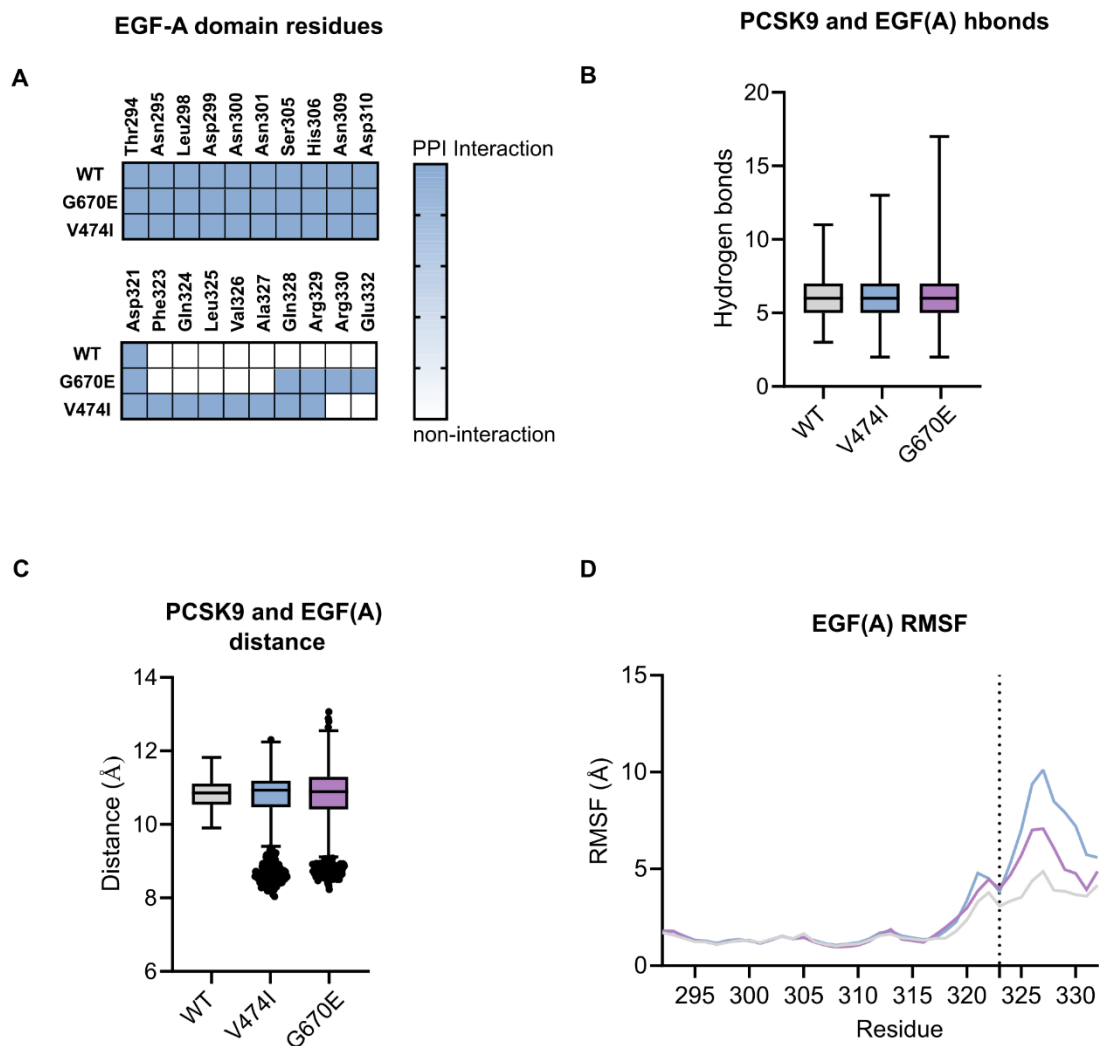
Catalytic and CHR domains: 2D PCA and modevector



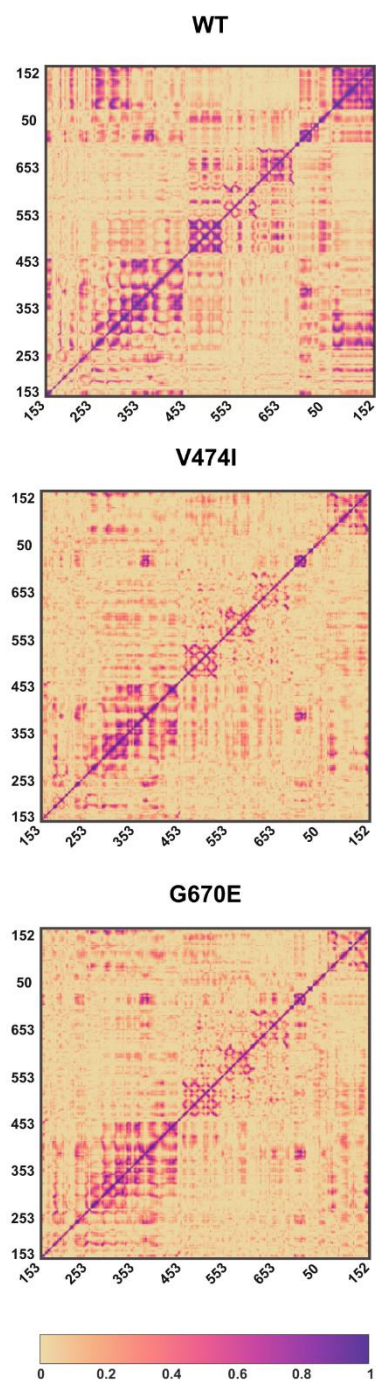
35 **Figure S2:** The Principal Component Analysis data per domain generated by Gromacs 2022
 36 (gmx_covar & gmx_anaieg). The 2D plots of PC1 and PC2 are prodomain (A) and catalytic & CHR
 37 domains (C). The modevectors (yellow arrows) represent the total collective motion along all
 38 simulations on the prodomain (B) and catalytic & CHR (D).
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 41 **Figure S3:** Interaction data of interdomain TAH Prodomain (31-34) – CHR D among simulations. The
 42 bonding prevalence (ratio of interacting frames by the total frames) of (A) hydrogen bonding and (B)
 43 water-bridge for CHR D residues.
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 47 **Figure S4:** Interaction and flexibility behavior between PCSK9 and EGF(A). (A) Residues from
 48 EGF(A) that interact with PCSK9, blue indicate interaction and white indicates non-interaction. (B)
 49 Hydrogen bond count between PCSK9 and EGF(A) (C) Distance of PCSK9 interaction surface and
 50 EGF(A) residues calculated by the center of mass. (D) Root Mean Square Fluctuation for EGF(A)
 51 residues. The vertical dotted line marks the residues of the N-terminal (323-332) that interacted only in
 52 the variant simulations.
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Figure S5: Full Perturbation Response Scanning (PRS) matrix for WT and variants simulations

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